LA-UR- 10-02414

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Title: Materials Capability Review
Los Alamos National Laboratory
May 3-6, 2010

Author(s): Antoinette Taylor

Intended for: Materials Capability Review
May 3-6, 2010

Los Alamos
NATIONAL LABORATORY
EST. 1943

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Form 836 (7/06)

Materials Capability Review

Los Alamos National Laboratory
May 3-6, 2010

LA-UR-10-xxx

On the cover: Micrograph of a plutonium alloy containing 0.6% (by weight) gallium cooled to -150°C that went through a partial martensitic transformation from delta to the alpha prime phase. The alpha prime platelets (white) formed in the leaner gallium regions and along crystallographic orientations.

Contents

2010 Materials Capability Review Committee

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Tab 1

Los Alamos NATIONAL LABORATORY EST. 1943

Agenda

Materials Capability Review
Los Alamos National Laboratory
Oppenheimer Study Center, Jemez Room

May 3-6, 2010

University House
TA-3, Bldg. 443

Monday Evening, May 3, 2010 (evening session by invitation only) *heavy snacks for 30*

6:00 Opening Session – Committee Gathering – Issue Badges *Jean get names to Evan* *Paper name tents*

6:30 Director's Welcome .... Ike Richardson
Deputy Laboratory Director

6:45 Introductions/Agenda .... Susan Seestrom
Associate Director, Experimental Physical Sciences

7:00 Committee Charge .... Terry Wallace
Principal Associate Director, Science, Technology & Engineering

7:15 Executive Session .... Gary Was
Committee Chair

J. Robert Oppenheimer Study Center
TA-3, Bldg. 207, Cochiti Room

Tuesday May 4, 2010

7:00 Meet visitors in lobby of Buffalo Thunder .... Evan Sanchez
Protocol Planner, Protocol Office

7:05 Bus leaves hotel .... Taxi Service

7:45 Name Badges and Coffee *Continental Breakfast for Committee; Coffee for everyone*

8:00 Logistics .... ADEPS Staff
Experimental Physical Sciences Directorate

8:10 Welcome .... Susan Seestrom
Associate Director, Experimental Physical Sciences

Purpose:
Institutional Host(s): Susan Seestrom, ADEPS 505-665-4454 Classification Level: Unclassified/SRD Sigma 1-10 Page 1
Technical Host(s): Antoinette Taylor, MPA 505-665-1131 Dress: Business/Business Causal
Protocol POC: Evan Sanchez 505-667-5223 Revised: April 6, 2010, 2010 (jme)
Catering: ARAMARK, 7-4628, 695-9503
LANL Update: 505-667-6622 or 1-877-723-4101: Provides information about changes in the Laboratory schedule (i.e., closings or delays) Protocol Office will adhere to all weather delays/closings

Los Alamos NATIONAL LABORATORY EST. 1943

Agenda

8:20 Materials Overview .... Antoinette (Toni) Taylor
Division Leader, Materials Physics & Applications

8:50 Materials Strategy .... Wendy Cieslak
Division Leader, Materials Science & Technology

9:20 MaRIE Update .... John Sarrao
Program Director, Office of Science & MaRIE

9:50 Break

10:05 **Actinide** Overview .... Gordon Jarvinen
Acting Director of Seaborg Institute(ADSMS)

10:10 Plutonium Science and Research Strategy .... David Clark
Capture Manager for Pu, Institutes

10:40 LDRD-DR Review: First Principles Predictive Capabilities for Transuranic Materials: Mott Insulators to Correlated Metals .... Richard Martin
Scientist, Physics and Chemistry of Materials (T-1)

11:40 LDRD-DR Discussion with Taylor, Sarrao, Cieslak, and Priedhorsky – ***Priedhorsky on travel; asked for sub***

11:55 Committee Photo

12:00 Working Lunch with Early Career Staff and Postdocs (*by invitation only*)
Toni springing for pizza lunch; order salads/desserts from Aramark; drinks for everyone provided; take extra plates and forks

1:00 Actinide Poster Presentations and Session .... Various Staff

2:30 **Materials Dynamics** Overview .... Anna Zurek
Group Leader, Structure/Property Relations (MST-8)

2:35 An Overview of Experiments to Evaluate Dynamic Materials Properties ... Rick Martineau
Program Manager, Dynamic Materials (ADW)

2:55 Damage Evolution under Dynamic Conditions: Experimentation and Modeling .... John Bingert
Team Leader, Structure/Property Relations (MST-8)

3:15 Proton Radiography: Studying Dynamic Properties of Shock-Loaded Materials And High Explosives .... Andy Saunders

Purpose:
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Classification Level: Unclassified/SRD Sigma 1-10
Dress: Business/Business Causal
Revised: April 6, 2010, 2010 (jme)

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Los Alamos NATIONAL LABORATORY EST. 1943

Agenda

Team Leader, Subatomic Physics (P-25)

3:35 Break

3:50 Materials Dynamics Poster Presentations and Session .... Various Staff

5:15 Executive Session (closed session)..Gary Was
Committee Chair

5:45 Drive Committee to Dinner at Buffalo Thunder

6:15 Hosted working Dinner *(by invitation only)*
Panel Discussion of Materials Strategy
Evan will arrange and have tables like last year; reception at 6:30; dinner at 6:45; panel at 7:10ish

Wednesday May 5, 2010

7:00 Meet visitors in lobby of Buffalo Thunder.. Evan Sanchez
Protocol Planner, Protocol Office

7:05 Bus leaves hotel .... Taxi Service

8:00 Executive Session (closed session)...Gary Was
Committee Chair

Continental Breakfast for Committee; Coffee for everyone

8:15 Overview of **Global Security** .... William Rees, Jr.
Principal Associate Director, Global Security

Requested talk from Anne Menefee

8:45 Materials in Global Security ....Dan Thoma
Director, Materials Design Institute

8:50 Nuclear Detection Materials.. Ed McKigney
Scientist, Safeguards Science & Technology (N-1)

9:10 Active Terahertz Metamaterials for Global Security .... John O'Hara
Scientist, Center for Integrated Nanotechnologist (MPA-CINT)

9:30 Global Security Poster Presentations and Session .... Various Staff

11:20 Working Lunch with Customers (*by invitation only*)
Should we have our people pay for lunch or bring their own? Drinks for everyone

Purpose:
Institutional Host(s): Susan Seestrom, ADEPS 505-665-4454
Technical Host(s): Antoinette Taylor, MPA 505-665-1131
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Los Alamos NATIONAL LABORATORY EST. 1943

Agenda

Jean invited externals already but no one can come; Jean to invite internals soon

12:30 **Electronic & Photonic Materials** Research Overview ....Darryl Smith
Scientist, Physics of Condensed Matter & Complex Systems (T-4)

12:45 Imaging Electron Spin Transport in Semiconductor Spintronic Devices....... Scott Crooker
Scientist, Condensed Matter & Magnet Science (MPA-CMMS)

1:10 Casimir Interactions...Diego Dalvit
Scientist, Physics of Condensed Matter & Complex Systems (T-4)

1:35 Photonic & Electronic Materials Poster Presentations and Session .... Various Staff

3:00 Walk/Bus to Tour *half the go to tour first, then poster session – swap with other half; put all uncleared in tour first so they can return to Study Center after*

3:15 Tour of Electron Microscopy Laboratory... Wendy Cieslak
Division Leader, Materials Science & Technology

Evan getting Sigma Schienberg room

4:00 Classified Poster Session .... Various Staff

5:00 Walk/Bus to Study Center

5:15 Executive Session (closed session)...Gary Was
Committee Chair

6:45 Drive visitors to Dinner at Gabriel's (no host), then Buffalo Thunder .... Taxi Service

Thursday, May 6, 2010

Continental Breakfast for Committee; Coffee for everyone
Should we try to block some parking spots near CINT for them?

8:00 Committee Members arrive at LANL at **TA-3-1420 (Wijiji Conference Room)**

8:15 **Emergent Phenomena – CINT Overview**.. David Morris
Co-Director and Group Leader, Center for Integrated Nanotechnologist (MPA-CINT)

8:35 Novel Functional Semiconductor Nanocrystal Quantum Dots and Nanowires
For Applications Involving Energy Conversion...............................Jennifer Hollingsworth
Scientist, Physical Chemistry & Applied Spectroscopy (C-PCS)

9:05 Nanoscale Features in Graphene .... Alexander Balatsky

Purpose:

Institutional Host(s):	Susan Seestrom, ADEPS 505-665-4454	Classification Level: Unclassified/SRD Sigma 1-10	Page 4
Technical Host(s):	Antoinette Taylor, MPA 505-665-1131	Dress: Business/Business Causal	
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Agenda

Scientist, Physics of Condensed Matter & Complex Systems (T-4)

9:25 Emergent Phenomena - CINT Poster Presentations and Session .... Various Staff
And Tour of CINT Facility

Box lunches
Jean reserved the MSL Meeting Place for this

11:15 Executive Session (closed session)..Gary Was
Committee Chair

12:15 Lunch (closed session)... Ike Richardson
Deputy Laboratory Director

Jean reserved the MSL Aud for this

1:00 Out Brief...Gary Was
Committee Chair

2:00 Committee Departs

Purpose:

Institutional Host(s):	Susan Seestrom, ADEPS 505-665-4454	Classification Level:	Unclassified/SRD Sigma 1-10	Page 5
Technical Host(s):	Antoinette Taylor, MPA 505-665-1131	Dress:	Business/Business Causal	
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CHARTER
For the 2010 Los Alamos National Laboratory Materials Capability Review Committee

The 2010 "Capability Review" process at LANL significantly differs from the Division reviews of prior years. The Capabilities being reviewed (some 4-8 per year) are deliberately chosen to be crosscutting over the Laboratory, and therefore will include not only several experimental, theoretical and simulation disciplines, but also contributions from multiple line organizations. This approach is consistent with the new Laboratory organizational structure, focusing on agile and integrated capabilities applied to present national security missions, and also nurtured to be available for rapid application to future missions.

The overall intent is that the Committee **assess** the quality of the science, engineering, and technology identified in the agenda, and **advise** the LANS Board of Governors and Laboratory management.

Specifically, the Committees will:

- Assess the quality of science, technology and engineering within the Capability in the areas defined in the agenda. Identify issues to develop or enhance the core competencies within this capability.

- Evaluate the integration of this capability across the Laboratory organizations that are listed in the agenda in terms of joint programs, projects, proposals, and/ or publications. Describe the integration of this capability in the wider scientific community using the recognition as a leader within the community, ability to set research agendas, and attraction and retention of staff.

- Assess the quality and relevance of this capability's science, technology and engineering contributions to current and emerging Laboratory programs, including Nuclear Weapons, Threat Reduction/Homeland Security, and Energy Security.

- Advise the Laboratory Director/Principal Associate Director for Science, Technology and Engineering on the health of the Capability including the current and future (5 year) science, technology and engineering staff needs, mix of research and development activities, program opportunities, environment for conducting science, technology and engineering.

The specific charge for the Materials Capability Review is to assess the Los Alamos Laboratory Directed Research and Development project titled, "First Principles Predictive Capabilities for Transuranic Materials: Mott Insulators to Correlated Metals " using the criteria performance, quality, and relevance for the current status of the project. The committee is requested to provide advice on future direction of the project.

Ver. 2010.02
October 20, 2009

Instructions for the Los Alamos National Laboratory Fiscal Year 2010 Capability Reviews

Introduction

Los Alamos National Laboratory (LANL) uses external peer review to measure and continuously improve the quality of its science, technology and engineering (STE). LANL uses capability reviews to assess the STE quality and institutional integration and to advise Laboratory Management on the current and future health of the STE. Capability reviews address the STE integration that LANL uses to meet mission requirements. STE capabilities are define to cut across directorates providing a more holistic view of the STE quality, integration to achieve mission requirements, and mission relevance. The scope of these capabilities necessitate that there will be significant overlap in technical areas covered by capability reviews (e.g., materials research and weapons science and engineering). In addition, LANL staff may be reviewed in different capability reviews because of their varied assignments and expertise. LANL plans to perform a complete review of the Laboratory's STE capabilities (hence staff) in a three-year cycle. The principal product of an external review is a report that includes the review committee's assessments, commendations, and recommendations for STE.

The Capability Review Committees serve a dual role of providing assessment of the Laboratory's technical contributions and integration towards its missions and providing advice to Laboratory Management. The assessments and advice are documented in reports prepared by the Capability Review Committees that are delivered to the Director and to the Principal Associate Director for Science, Technology and Engineering (PADSTE). Laboratory Management will use this report for STE assessment and planning. The report is also provided to the Department of Energy (DOE) as part of LANL's Annual Performance Plan and to the Los Alamos National Security (LANS) LLC's Science and Technology Committee (STC) as part of its responsibilities to the LANS Board of Governors.

LANL has defined fifteen STE capabilities. Table 1 lists the seven STE capabilities that LANL Management (Director, PADSTE, technical Associate Directors) have identified for review in Fiscal Year (FY) 2010. The FY 2010 capability reviews must be **completed by June 30, 2010** to allow sufficient time for the reports and results to be incorporated into the 2010 STE evaluations by the Department of Energy National Nuclear Security Agency and the LANS LLC STC for the LANS Board of Governors.

These instructions identify responsibilities and provide guidance to those organizing, participating in and performing capability reviews at LANL in FY 2010. These instructions have been refined based on experiences with capability reviews from 2007 - 2009. Any questions or comments on these instructions should be directed to the Program Manager for the LANL Science and Technology Base Programs Peer Review and Metrics Office at stbprm-admin@lanl.gov or 505-667-7824.

Ver. 2010.02
October 20, 2009

Table 1. FY 2010 LANL science, technology and engineering capability reviews, organizing associate director (AD), and Los Alamos National Security, LLC Science and Technology Committee point-of-contact (STC POC).

Capability	Organizing AD	STC POC/co-POC
Chemical Sciences	ADCLES	Bercaw/Navrotsky
Computational Physics and Applied Math	ADTSC	Karin/Long
Earth and Space Sciences	ADCLES	Beckwith/Vogt
Electrodynamics and Accelerators	ADEPS	Falcone/Vogt
Materials Research	ADEPS	Navrotsky/Bercaw
Nuclear and Particle Physics, Astrophysics and Cosmology	ADTSC	Rosner/Vogt
Weapons Science	ADW	Peddicord/Vogt

Ver. 2010.02
October 20, 2009

Roles and Responsibilities

LANL Director/PADSTE

1. Determines capabilities to be reviewed and review schedule.
2. Appoints an Organizing AD (OAD) for each capability review.
3. Works with the OAD to create a specific charge for each capability review.
4. Participates in Capability Review Committee member selection as needed.
5. In conjunction with the STC Chair approves the Capability Review Chair and members.
6. Invites the Capability Review Chair and members.
7. Hosts the Capability Review Chairs meeting before the review cycle starts.
8. Provides the charge to the Capability Review.
9. Attends executive session at closeout.
10. Ensures report is delivered by requested deadline.
11. Provides the Capability Review report to the STC Chair for distribution to the STC.
12. Addresses the Capability Review recommendations through the PADSTE Management Review Board assigning actions and resources. The PADSTE will determine if the actions are tracked through the LANL performance tracking system.
13. Incorporates review recommendations and issues into LANL STE planning and assigns actions.
14. Provides summary response for all capability reviews to Capability Review Committee Chairs and to the STC Chair.

LANS, LLC STC Chair (STC Chair)

1. Appoints STC members to serve as the point-of-contact (POC) and co-point-of-contact (co-POC) for each Capability Review Committee.
2. In conjunction with the LANL Director/PADSTE, approves the Capability Review Committee Chair and members.
3. The STC Chair and/or the Vice Chair may attend any Capability Review meeting as observers. Up to 2 STC members (including Chair and Vice Chair, as coordinated through the STC Chair) may attend a Capability Review meeting as observers. Observers may participate in discussions and attend all sessions, but may not participate in drafting the report.

LANS, LLC STC Point of Contact (POC) / co-Point of Contact (co-POC)

1. Working with the Organizing AD (OAD), compiles a list of potential Capability Review Committee members based on input from the Laboratory, University of California (UC), and STC members. (UC Office of the President (UCOP) collects input from UC, including from the Academic Senate). At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The POC does not count for either of these requirements.

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2. Working with the OAD, prioritizes the list of potential Capability Review Committee Chairs and members. The list is given to the PADSTE and the STC Chair for approval.
3. The POC or OAD, as appropriate, contacts the recommended Capability Review Chair to ask if the person will serve; the PADSTE officially invites the Chair.
4. Reviews the prioritized Capability Review Committee membership candidate list with the selected Capability Review Chair and OAD; the STC Chair and PADSTE are notified of any changes.
5. Works with the Capability Review Committee Chair and OAD to identify potential dates for the Capability Review meeting.
6. With dates in hand, the POC, OAD, or Capability Review Committee Chair, as appropriate, contacts the proposed Capability Review Committee members regarding their willingness to serve until approximately 9 members, including the Chair, are enlisted. At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The Capability Review organizing team (i.e., OAD, Capability Review Committee Chair, and POC) maintains contact during this step and consults if issues arise.
7. Participates in developing the Capability Review meeting agenda with the OAD and Capability Review Committee Chair.
8. Attends the Capability Review Chairs meeting hosted by the PADSTE before the review cycle starts.
9. Attends the Capability Review meeting as an ex-officio member, participates as a full member, including attendance at executive sessions, but does not participate in drafting the report.

LANL Organizing Associate Director (OAD)

1. Coordinates with LANL Director/PADSTE and with ADs who contribute to the capability to develop the Capability Review scope.
2. Works with the POC to prioritize the list of potential Capability Review Committee Chairs and members. The list is given to the PADSTE and the STC Chair for approval.
3. The OAD or POC, as appropriate, contacts the recommended Capability Review Committee Chair to ask if the person will serve; the PADSTE officially invites the Chair.
4. Reviews the prioritized Capability Review Committee membership candidate list with the selected Capability Review Committee chair and POC; the STC Chair and PADSTE are notified of any changes.
5. Works with the Capability Review Committee Chair and POC to identify potential dates for the Capability Review meeting.
6. With dates in hand, the OAD, POC, or Capability Review Committee Chair, as appropriate, contacts the proposed Capability Review Committee members regarding their willingness to serve until approximately 9 members, including the Chair, are enlisted. At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The Capability Review organizing team (i.e., OAD,

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Capability Review Committee Chair, and POC) maintains contact during this step and consults if issues arise.

7. Participates in developing the review agenda with the POC and Capability Review Committee Chair.
8. Identifies Los Alamos Laboratory Directed Research and Development (LDRD) project to be reviewed for the current year. The LANL LDRD Office can assist in project identification.
9. Attends the Capability Review Chairs meeting hosted by the PADSTE before the review cycle starts.
10. Compiles and sends background information to the Capability Review Committee before the review.
11. Provides logistics for the Capability Review meeting, including meeting rooms, necessary security for classified sessions, etc.
12. Works with the Capability Review Committee Chair to maintain review agenda and schedule.
13. Provides additional information requested by the Capability Review Committee.
14. Addresses Capability Review recommendations assigned by Director/PADSTE.

Capability Review Committee Chairperson

1. Reviews the prioritized Capability Review Committee membership candidate list with the selected OAD and POC; the STC Chair and PADSTE are notified of any changes.
2. Works with the organizing AD and POC to identify potential dates for the Capability Review meeting.
3. With dates in hand, the OAD, POC, or Capability Review Committee Chair, as appropriate, contacts the proposed Capability Review Committee members regarding their willingness to serve until approximately 9 members, including the Chair, are enlisted. At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The Capability Review organizing team (i.e., OAD, Capability Review Committee Chair, and POC) maintains contact during this step and consults if issues arise.
4. Participates in developing the Capability Review meeting agenda with the POC and OAD. The Chair ensures sufficient executive time in the agenda for committee discussions.
5. Attends a meeting of the Capability Review Committee Chairs hosted by the PADSTE before the review cycle starts.
6. Distributes information about the meeting to Capability Review Committee members as necessary.
7. Presides over the review by keeping to the agenda, managing deliberations of the Capability Review Committee, and assigning tasks to Capability Review Committee members as appropriate.
8. Prepares and leads executive out-brief to the Director/PADSTE.
9. Provides Capability Review report to the LANL Director/PADSTE within 30 days of the review.

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Capability Review Committee Members

1. Attend review and complete tasks assigned by Capability Review Committee Chair.
2. Provide unbiased and objective evaluation of the topics within the capability being assessed.
3. Provide written material to Capability Review Committee Chair with sufficient time to meet schedule.

Assessment

The evaluation of designated topics must address the following two criteria:

1) Comparison to peers -- State how the work compares to similar or related work conducted by others.
2) Sustainability -- State the extent to which the reviewed activities strengthen or weaken LANL capabilities. How does the activity/contribution build core competencies or other resources that contribute to the vitality of the capability and the long-term vigor of the Laboratory and its ability to meet the needs of the nation?

Laboratory Directed Research and Development Assessments for FY 2010 Capability Reviews

The Director/PADSTE will charge each Capability Review Committee to assess a single Laboratory Directed Research and Development (LDRD) project related to the capability. Many of the LDRD projects will be in their first year so the Capability Review Committee will be able to provide guidance on both the STE and the programmatic development of the project.

The Capability Review Committee is requested to prepare a one-half to one page assessment of the LDRD project that will be included in the Capability Review report and in the LDRD Annual Report to the DOE. The selected LDRD project will be included in the agenda as a presentation, and the Capability Review Committee will be asked to assess the project using the following criteria:

1. Performance: Is the project making good progress against its first year milestones? Has the PI assembled the appropriate team, collaborators, and facilities? Is the project plan re-assessed on a regular basis, in the light of new opportunities and unanticipated difficulties, to maximize the project's impact at the end of 3 years?
2. Quality: Are the initial S&T results of high quality compared to national and international peers? If the project is past its first year, then are project participants publishing in the archival literature and prestigious conferences?
3. Relevance: How do the project goals relate to the strategic directions of the Laboratory? Have the PI and program development mentor (PDM) developed a

transition plan, mapping out the project's future S&T direction after the LDRD funding concludes? Have the first steps of the transition plan been taken?

The Capability Review Committee's advice on future directions for the project is requested.

Briefing management

At the end of it's meeting, the Capability Review Committee will brief its findings to LANL Management. Attendance at this briefing, other than senior management (Director/PADSTE), remains at the discretion of the Capability Review Committee Chair and the Director/PADSTE. The out-brief should provide executive style highlights of the assessments and advice for the capability. The Capability Review Committee should prioritize its assessment and advice for the out-briefing (and the report). Specifically, the Capability Review Committee should deliberate in its executive session to identify and prepare for presentation:

1) 3 to 7 most notable contributions observed in the review, and
2) 3 to 7 most important "actionable" recommendations.

Each of these components of the out-briefing should be presented in order of decreasing importance or significance (highest, next to highest, etc.). The rationale behind prioritization is to engage the wisdom and experience of the Capability Review Committee to identify the true pinnacles and the most significant challenges. It is the distinctiveness of the greatest achievements and the magnitude of the greatest challenges that characterize the excellence of an organization/program.

By prioritizing a limited number of items, Capability Review Committees are able to focus their feedback and enable meaningful follow up by LANL Management. A template containing recommended content for the out-briefing can be found in the Appendix of this document.

Preparing the Capability Review report

The Capability Review Committee must submit its assessment and advice via written report. The final copy is due to the Program Manager in the Science and Technology Based Programs Peer Review and Metrics Office within 30 working days of the end of the Capability Review meeting. The Capability Review Committee Chair is responsible for delegating writing assignments, coordinating inputs, editing the final document, and submitting it.

A suggested report template can be found in the Appendix of this document. The template includes abstracts of the areas to be assessed and headings delineating the areas in which specific advice has been requested. The assessment of the LDRD project can follow the same format, but the three criteria (performance, quality, and relevance) that were identified in these instructions need to be addressed.

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October 20, 2009

Appendix

Capability Review Out-Brief Template

Acknowledgement and Recognition
- Opening remarks
- Feedback on execution of review

Assessment of Topics in the Agenda
- Comparison to peers, mission/program relevance, integration
- Assessment of LDRD project

Prioritized Conclusions
- Top 3 to 7 Capability Review Committee "actionable" recommendations
- Top 3 to 7 most notable science, technology and engineering contributions

Special topics
- Any needs for additional information or meetings
- Topics of enduring interest beyond the annual review cycle (e.g. from prior reviews)
- Improvements in capability review process

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Capability Review Committee Report Template

Title
Table of Contents
Executive Summary
Introduction
Assessment

- Review Elements *(directly from agenda)*
- Review element 1
  - Scope of the review
    - *Can use pre-written element description (single 50-300 word abstract written by LANL contributor summarizing goal of contribution and key results)*
  - Analysis (*in terms of one or more of these 4 facets)*
    - Approach
    - Implementation
    - Results
    - Impact of work
  - Assessment
    - Comparison to peers
    - Sustainability
- Review element 2
- Review element n
- Review of LDRD project
  - Performance
  - Quality
  - Relevance
  - Capability Review Committee's advice on future directions for the project

Prioritized Conclusions

- Top 3 to 7 most notable science, technology and/or engineering contributions (or other high performance indicators)
- Top 3 to 7 Capability Review Committee "actionable" recommendations

Acknowledgements
Appendices

- Capability Review Committee Meeting Agenda
- Roster of Capability Review Committee Members
- Additional inputs or documents used in assessment by Capability Review Committee

Tab 2

Materials at LANL

A.J. Taylor (MPA-DO)

The scientific and technical area of materials has been a foundational capability at Los Alamos National Laboratory since the Laboratory's inception. The materials capability currently encompasses a wide array of technical disciplines, research topics, organizations and sponsors. Central to the Laboratory's materials capability is the vision of intentional control of functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material. Achieving this goal requires a program of synthesis, fabrication, characterization, and theory and modeling across a wide range of materials relevant to current and anticipated missions of the Laboratory. This materials program enables innovative research and development at the boundaries of chemistry, physics, theory and materials science that translates fundamental discovery to materials production in strategic areas such as actinide science.

In this presentation, we will first describe the structure of the current Materials Capability Review. Next, we will present an overview of materials work supported by a variety of the Laboratory's sponsors. Included in this discussion will be the materials science base inspired by our national user facilities: the Lujan Center, the Center for Integrated Nanotechnologies and the National High Magnetic Field Laboratory. Finally, we will describe our benchmarking efforts to critically review the materials capability at LANL.

Materials at LANL

Materials Capability Review 2010

Toni Taylor
Division Leader
Materials Physics and Applications

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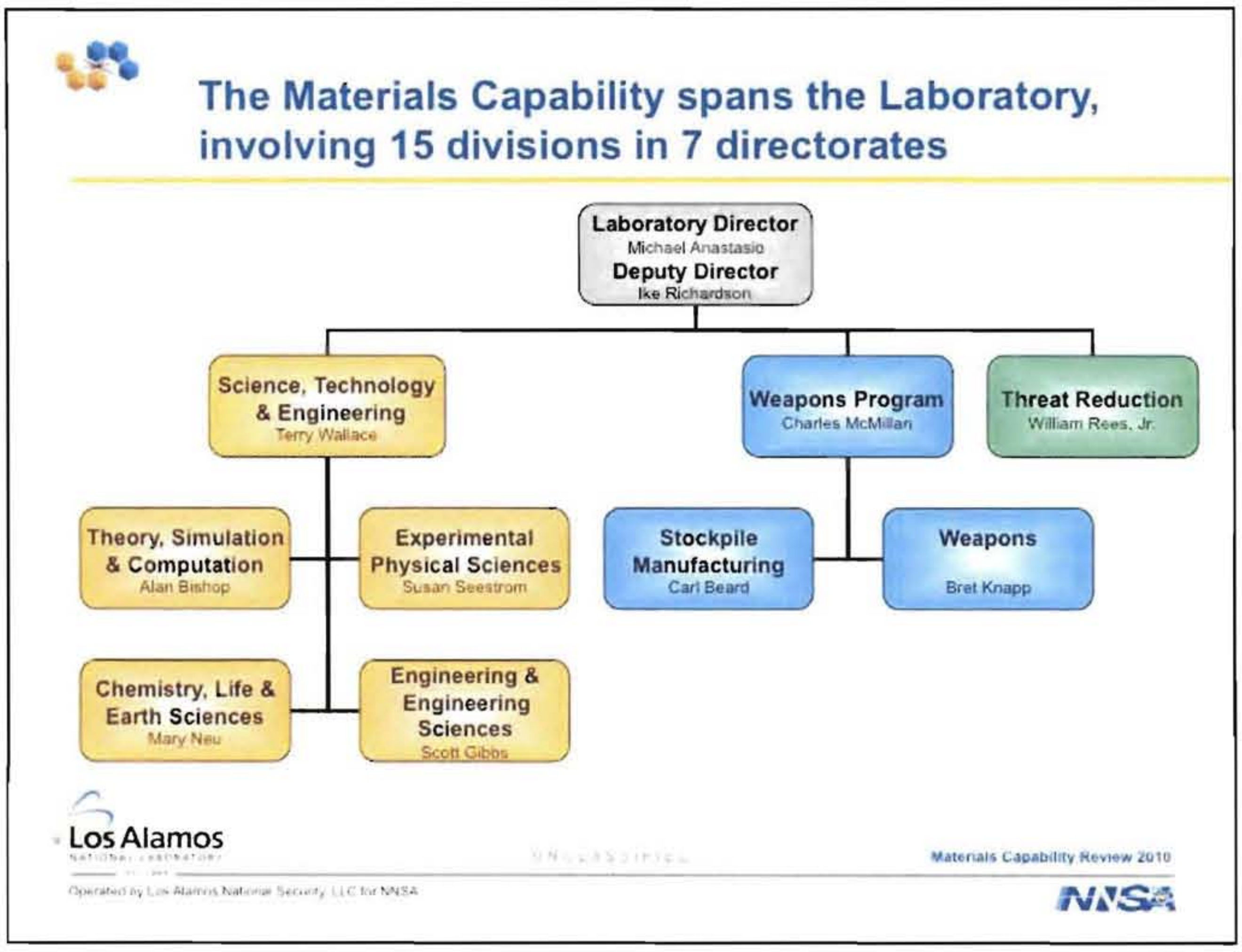
Materials have been important at LANL since the Manhattan Project!


The Materials Capability spans the Laboratory, involving 15 divisions in 7 directorates
Laboratory Director
Michael Anastasio
Deputy Director
Ike Richardson
Science, Technology & Engineering
Terry Wallace
Weapons Program
Charles McMillan
Threat Reduction
William Rees, Jr.
Theory, Simulation & Computation
Alan Bishop
Experimental Physical Sciences
Susan Seestrom
Stockpile Manufacturing
Carl Beard
Weapons
Bret Knapp
Chemistry, Life & Earth Sciences
Mary Neu
Engineering & Engineering Sciences
Scott Gibbs
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NNSA


The Materials Strategy advances LANL Vision and Missions, which in return advance our Capability
Applications
Nuclear Deterrence
Global Threat Reduction
Energy Security
Premier National Security Science Laboratory
Solutions
Controlled Functionality
Emergent Phenomena
Extreme Environments
Defects and Interfaces
Science
VISTAS
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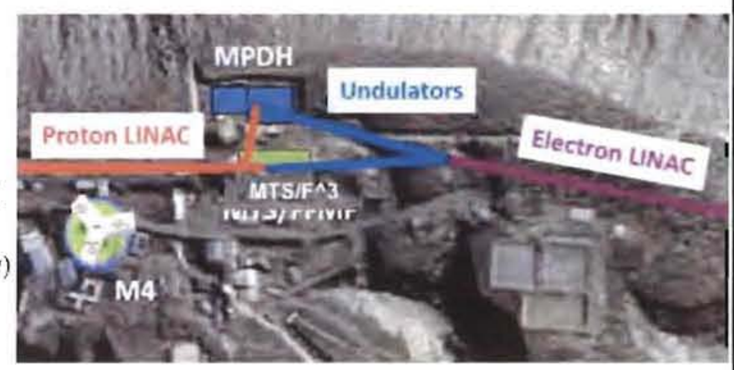
MaRIE will provide the first comprehensive set of co-located tools to realize transformational advances in materials performance in extremes

MaRIE will enable the transition from "observation" to "control"

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging
(MPDH: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities
(F^3: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure
(M4: Making, Measuring & Modeling Materials Facility)



MaRIE will provide unprecedented international user resources

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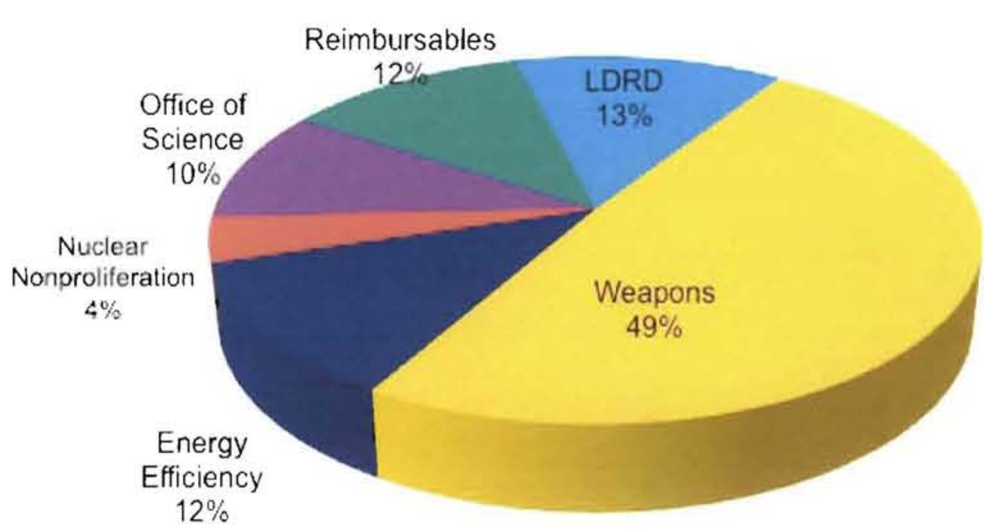
Materials R&D at LANL is funded by numerous sponsors



Materials @ LANL is a $320M Enterprise

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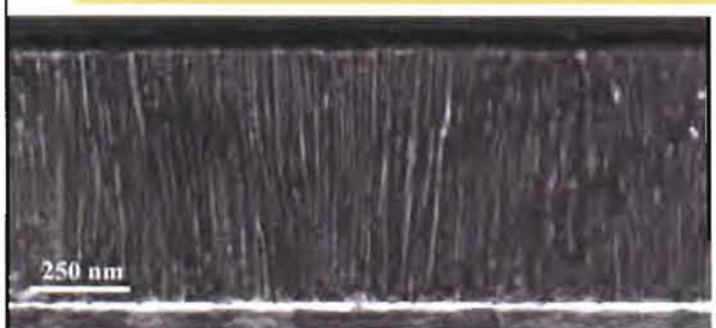
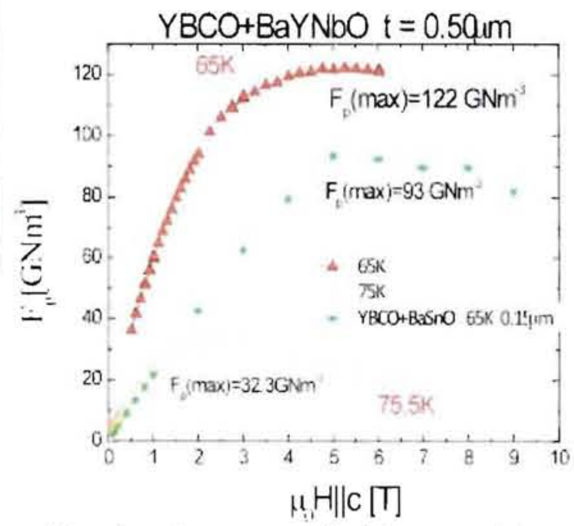
Applied Energy: Record flux pinning force in YBaCuO films with engineered defect structures controlled by growth dynamics



Very high density of BaYNbO nanorods extend nearly through a 0.7 μm thick YBCO film

- $J_c(76K, 1T) > 2\ MA/cm^2$
- $F_{pmax}(76K) = 32.3\ GN/m^3$



Pinning force vs. field normal to the film with optimized BaYNbO nanorods

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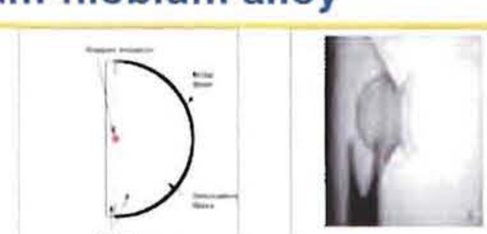
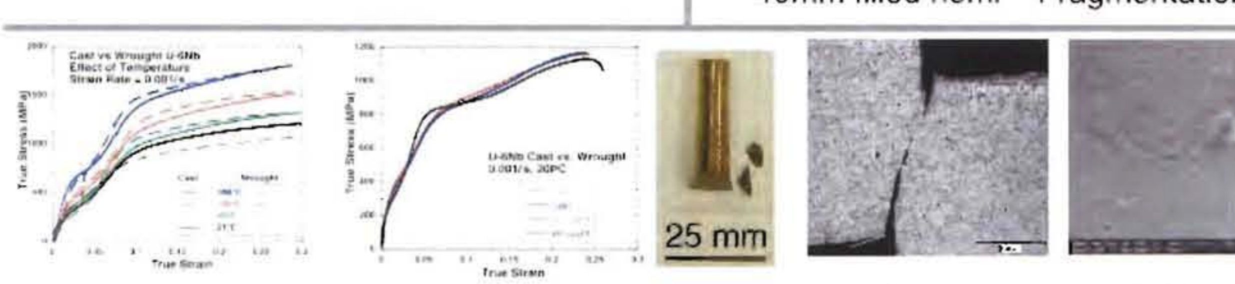
Nuclear Weapons: Comparison of wrought versus cast processing of a uranium-niobium alloy

Wrought Direct Cast



40mm filled hemi Fragmentation



e.g. Compression Tension Taylor Optical SEM ....

Cast material exhibits mechanical behavior identical to wrought but is more resistant to shear localization

Grain size may create material behavior differences in the Taylor rod tests

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Our greatest assets are our people!

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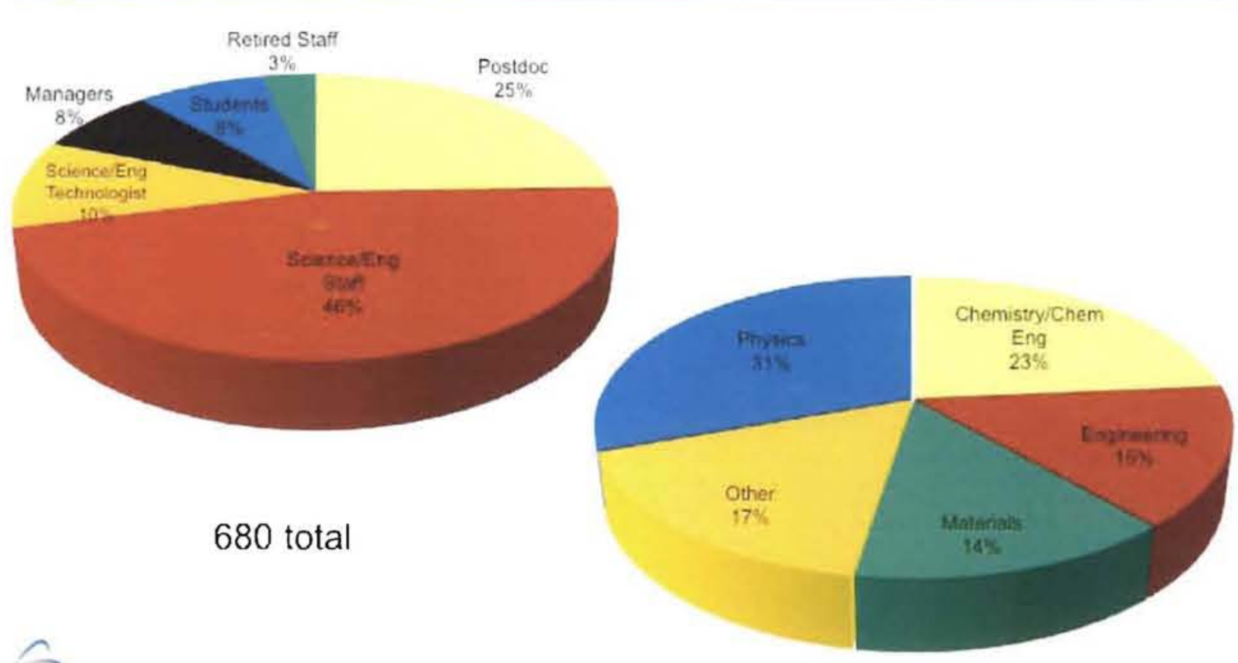
Materials staff demographics in 2010 exhibit diversity in position and discipline



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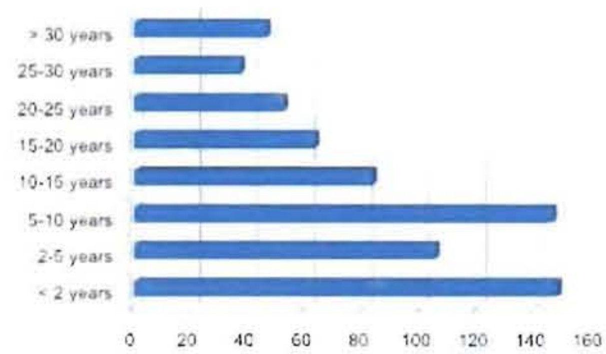
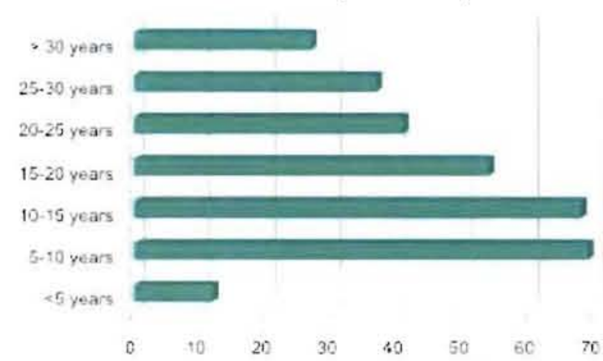
Materials staff demographics 2010—distribution by years of experience exhibits a reasonable trend





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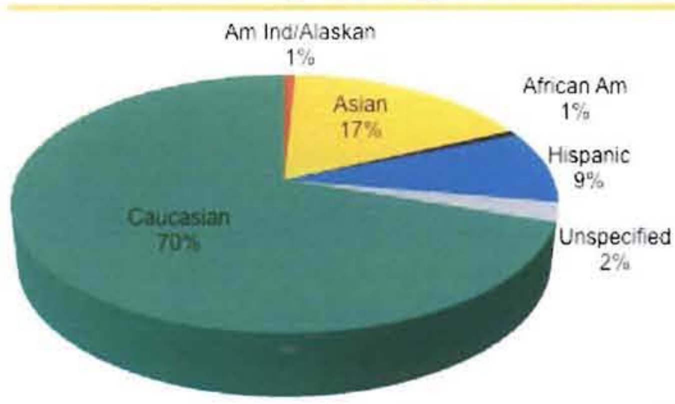
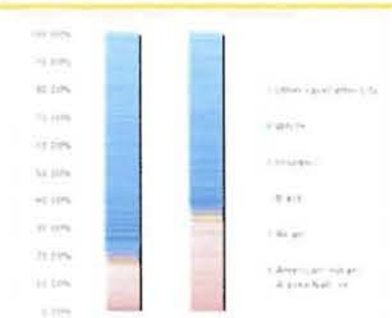
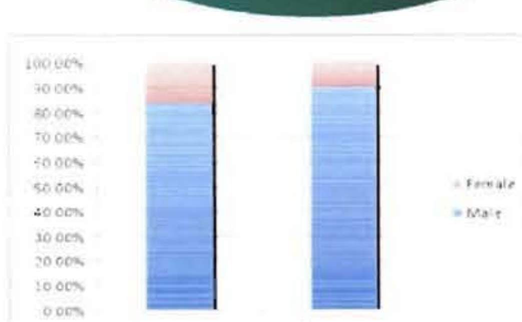
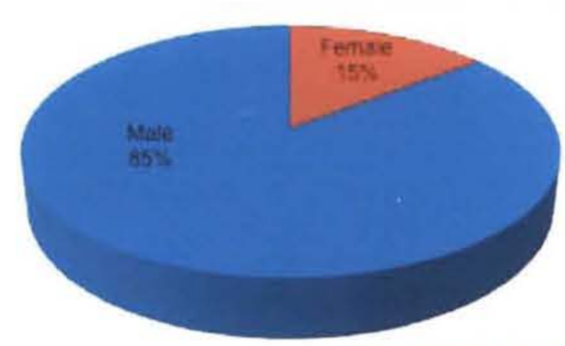
Materials staff demographics 2010—distribution by ethnicity and gender needs improvement









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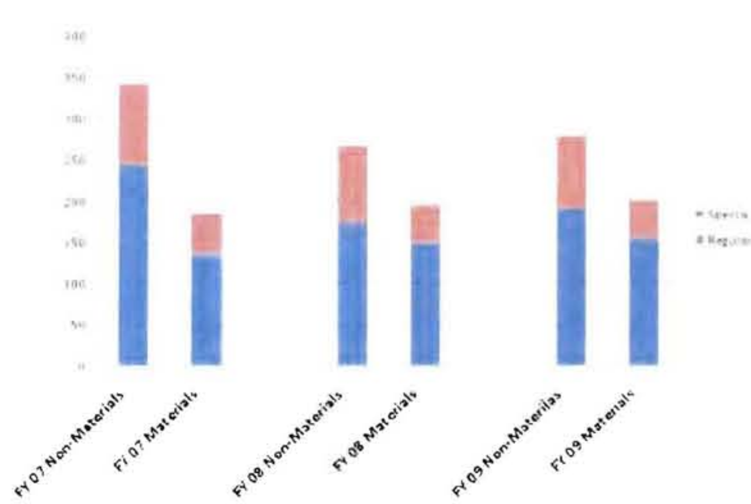
Our strong postdoc population is an important avenue for recruitment in Materials @ LANL

Population of postdoctoral researchers



Materials Postdoc conversions

Year	#	%
2007	7	23
2008	12	27
2009	14	33

LANL Postdoc conversions

Year	#	%
2007	19	22
2008	25	25
2009	24	27

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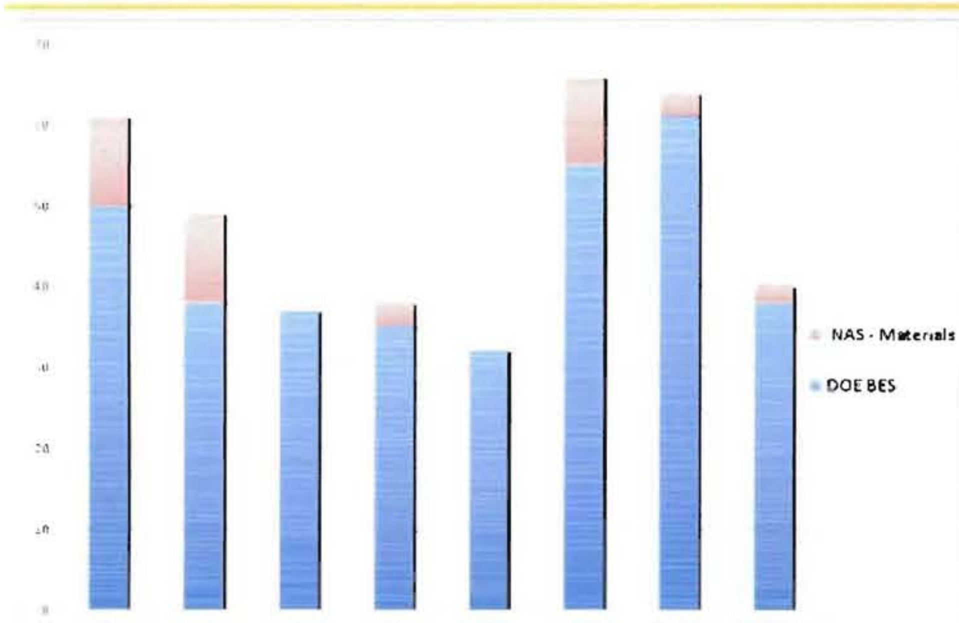
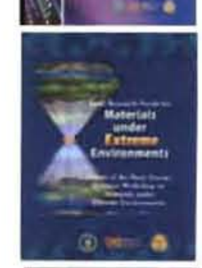
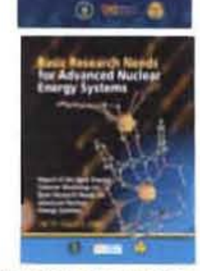
LANL staff demonstrate leadership through service on national materials panels







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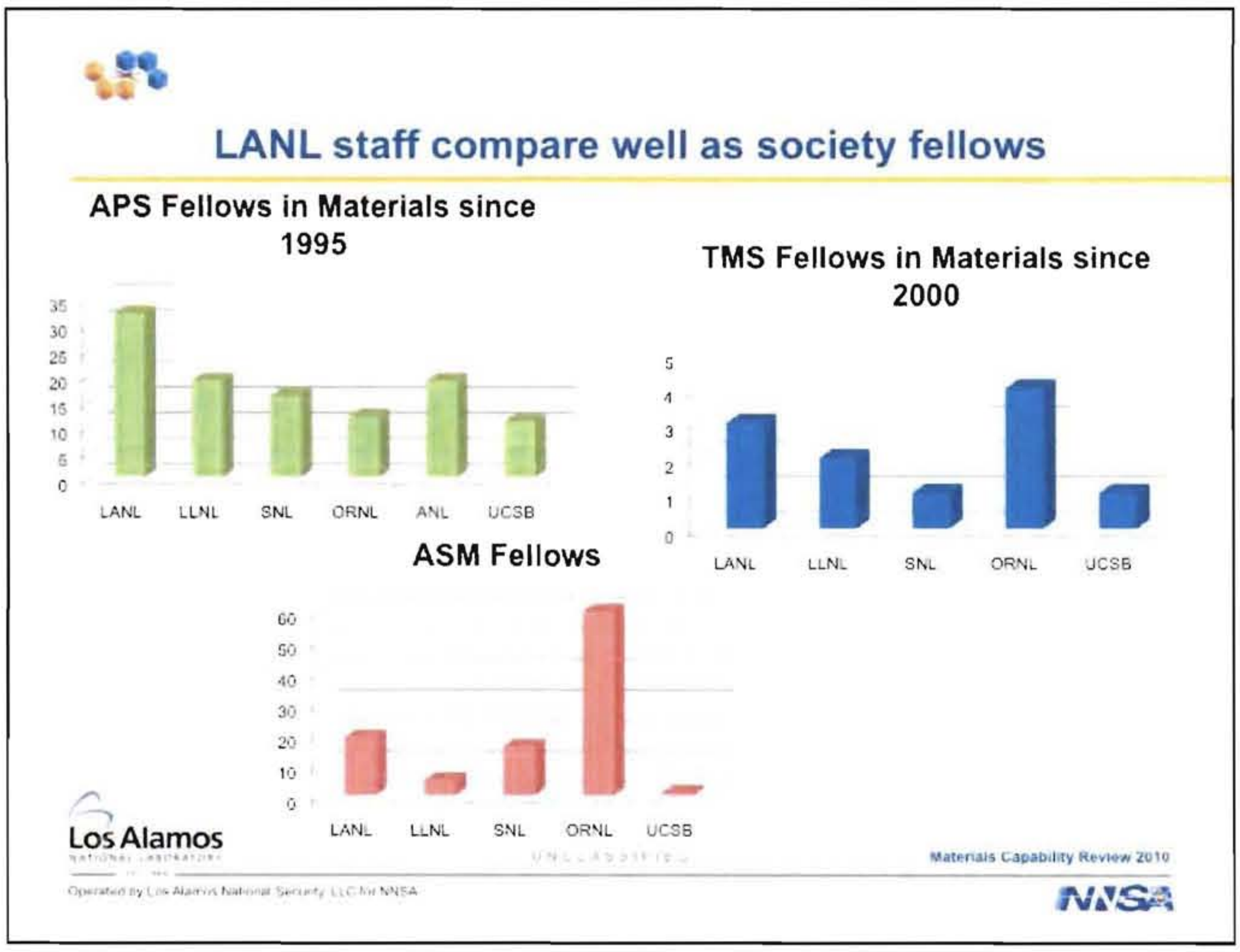
LANL staff compare well as society fellows
APS Fellows in Materials since 1995
35
30
25
20
15
10
5
0
LANL
LLNL
SNL
ORNL
ANL
UCSB
TMS Fellows in Materials since 2000
5
4
3
2
1
0
LANL
LLNL
SNL
ORNL
UCSB
ASM Fellows
60
50
40
30
20
10
0
LANL
LLNL
SNL
ORNL
UCSB
Los Alamos
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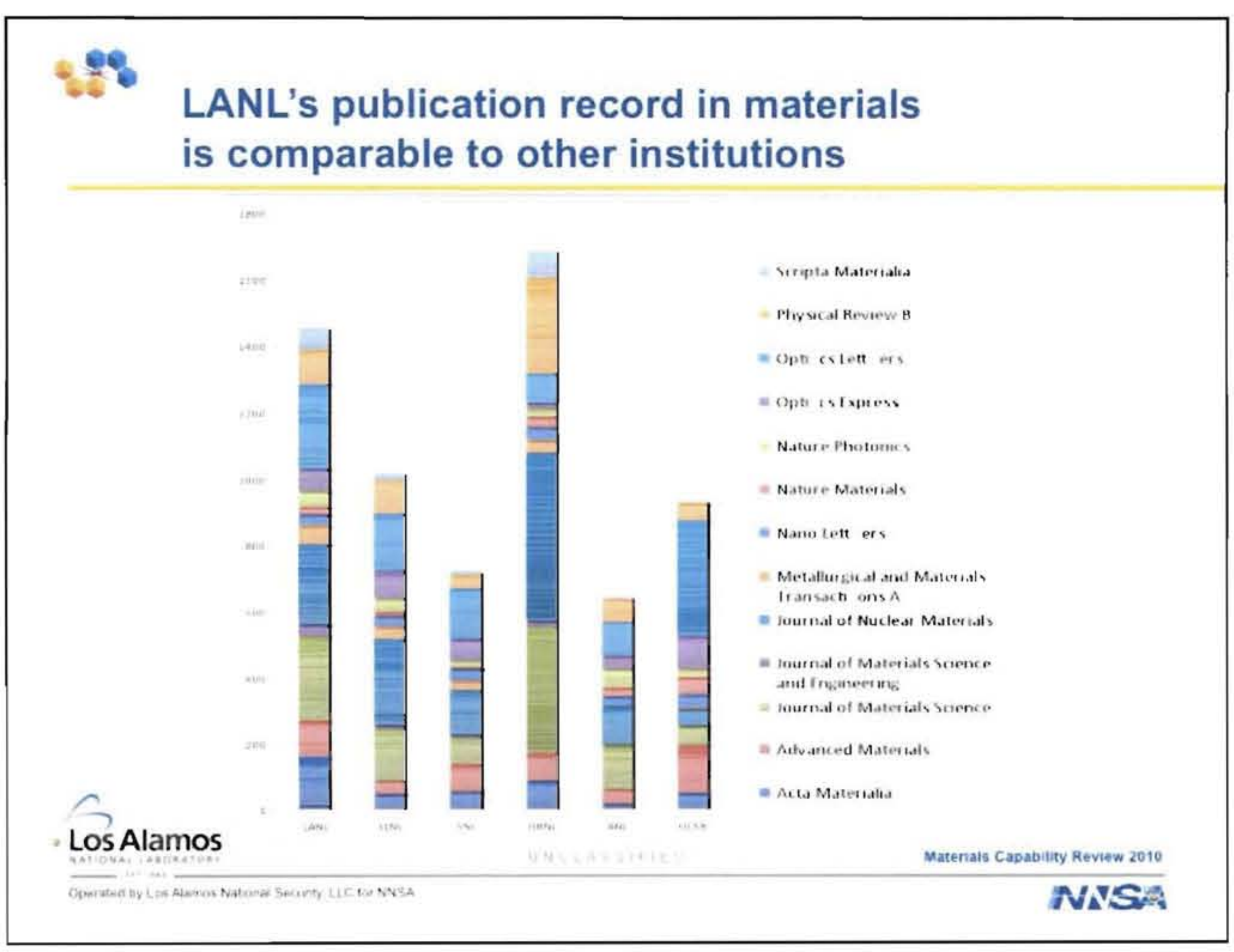
LANL's publication record in materials is comparable to other institutions
Scripta Materialia
Physical Review B
Optics Letters
Optics Express
Nature Photonics
Nature Materials
Nano Letters
Metallurgical and Materials Transactions A
Journal of Nuclear Materials
Journal of Materials Science and Engineering
Journal of Materials Science
Advanced Materials
Acta Materialia
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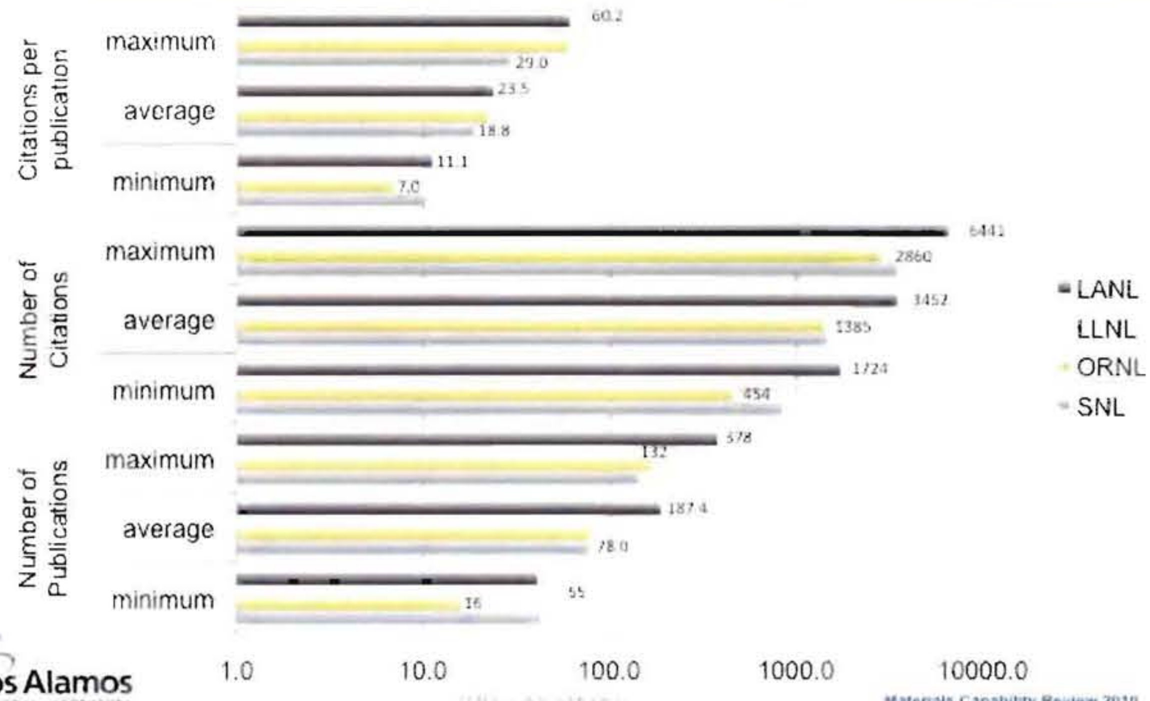
LANL's top publishers also compare favorably to other institutions



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Our Leadership Development Initiative prepares our future leaders

- Yearly program in EPS to develop future scientific leaders at LANL
- Spans 4 divisions in EPS; majority are from materials capability
- Includes mentoring, coaching, intensive leadership institute, communications class
- Class projects on networking and funding for early careers scientists
- 9 graduates from 2009-2010
- New 2010-2011 class with 14 participants

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Four materials-centric LANL institutes/centers provide outreach to the academic community

Institute for Multiscale Materials Studies (IMMS) with UCSB

- Techniques, simulations & collaborations to bridge the length and time scales for enhanced materials understanding with a strong emphasis on soft materials: complex structural response

Materials Design Institute (MDI) with UC Davis focuses on

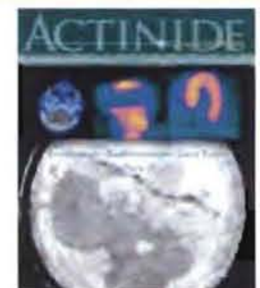
- 3D microscopy and visualization for data processing; Multi-functional materials; Materials synthesis and crystal growth; Dynamic behavior of materials

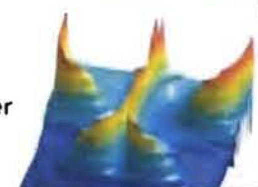
Seaborg Institute (LANL branch) with other UC campuses

- Chemical, physical, nuclear, and metallurgical properties of the lighter actinide elements, with a special emphasis on plutonium: a national center for the education and training in transactinium science

Center for Nonlinear Studies (CNLS)

- Research in nonlinear and complex systems phenomena, including nonlinear excitations in materials, soft condensed matter, granular materials, colloids.



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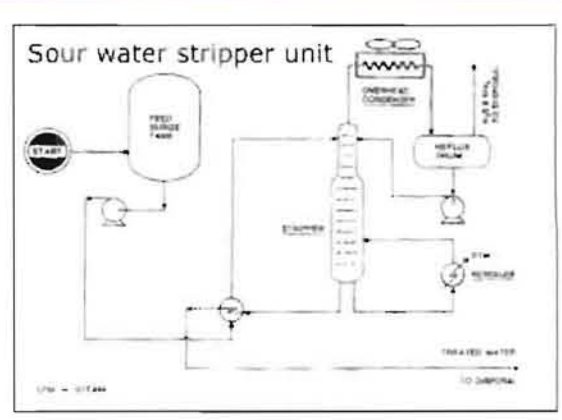
Outreach to industry: Atomistic modeling to understand refinery corrosion in collaboration with Chevron

Chevron

- Nascent program to apply LANL expertise in interfacial molecular dynamics and atomistic models coupled with innovations in surface and electrochemical characterization to problems in corrosion control relevant to Chevron Upstream and Global Manufacturing processes. (300K, 2009-2010)
- Pilot Study: Develop interfacial models to advance our understanding of the influence of cyanides on corrosion and wet H2S cracking in Hydroprocessing, FCC, Coker, Amine and Waste Water Treatment plants.
- Move Chevron beyond empirical based guidelines for corrosion and materials lifetime management towards a policy based on a stronger fundamental understanding of the materials-environment interactions.



Atomistic Models of Surface Processes, Surface Characterization

Predicted corrosion states under sour water conditions.

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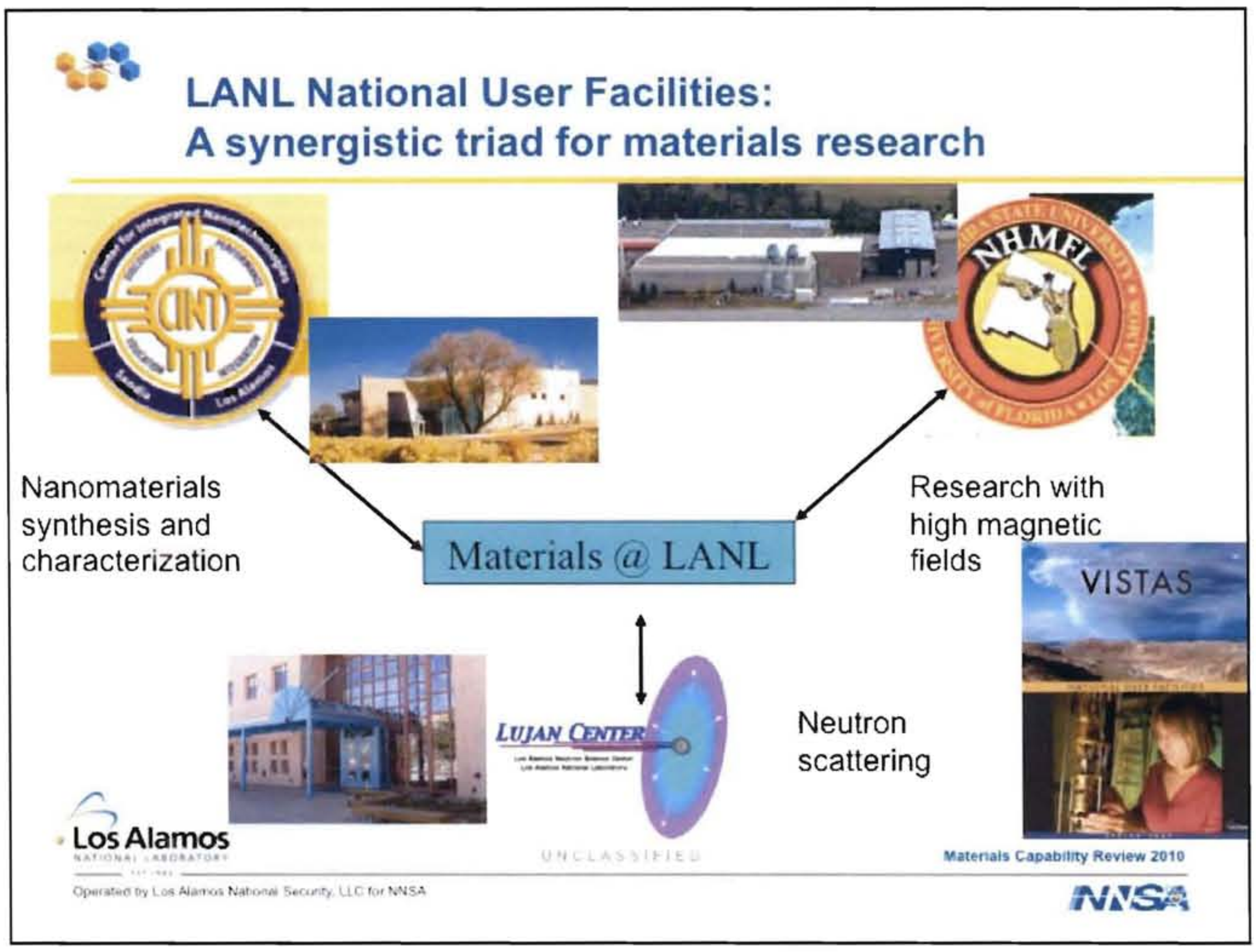
CD Taylor, RS Lillard (LANL), A O'Connor, G Butler (Chevron)

NNSA


LANL National User Facilities:
A synergistic triad for materials research
Nanomaterials synthesis and characterization
Materials @ LANL
Research with high magnetic fields
NHMFL
VISTAS
LUJAN CENTER
Neutron scattering
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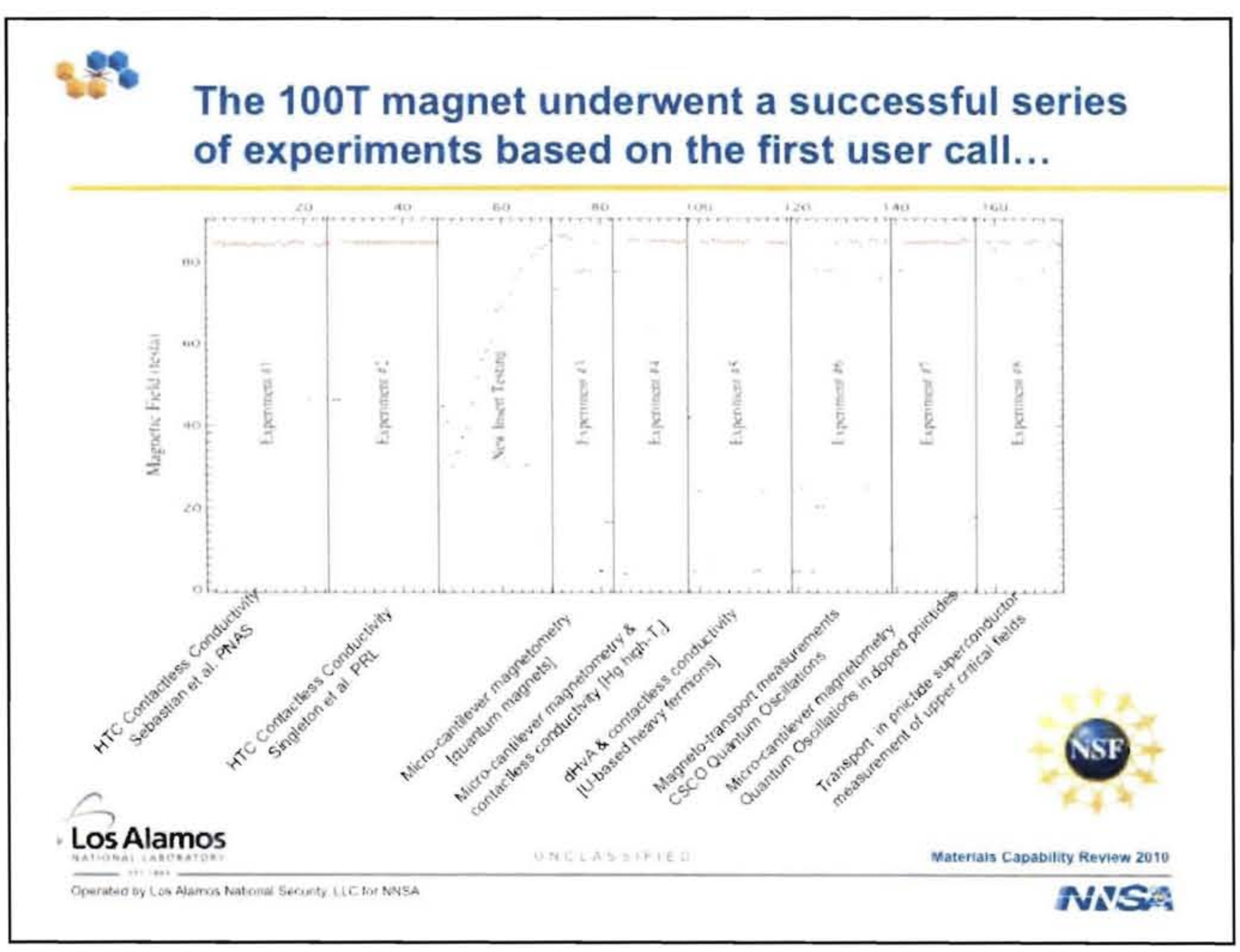
The 100T magnet underwent a successful series of experiments based on the first user call…
Magnetic Field (tesla)
HTC Contactless Conductivity Sebastian et al. PNAS
HTC Contactless Conductivity Singleton et al. PRL
Micro-cantilever magnetometry [quantum magnets]
Micro-cantilever magnetometry & contactless conductivity [Hg high-Tc]
dHvA & contactless conductivity [U-based heavy fermions]
Magneto-transport measurements CSCO Quantum Oscillations
Micro-cantilever magnetometry Quantum Oscillations in doped pnictides
Transport in pnictide superconductor measurement of upper critical fields
NSF
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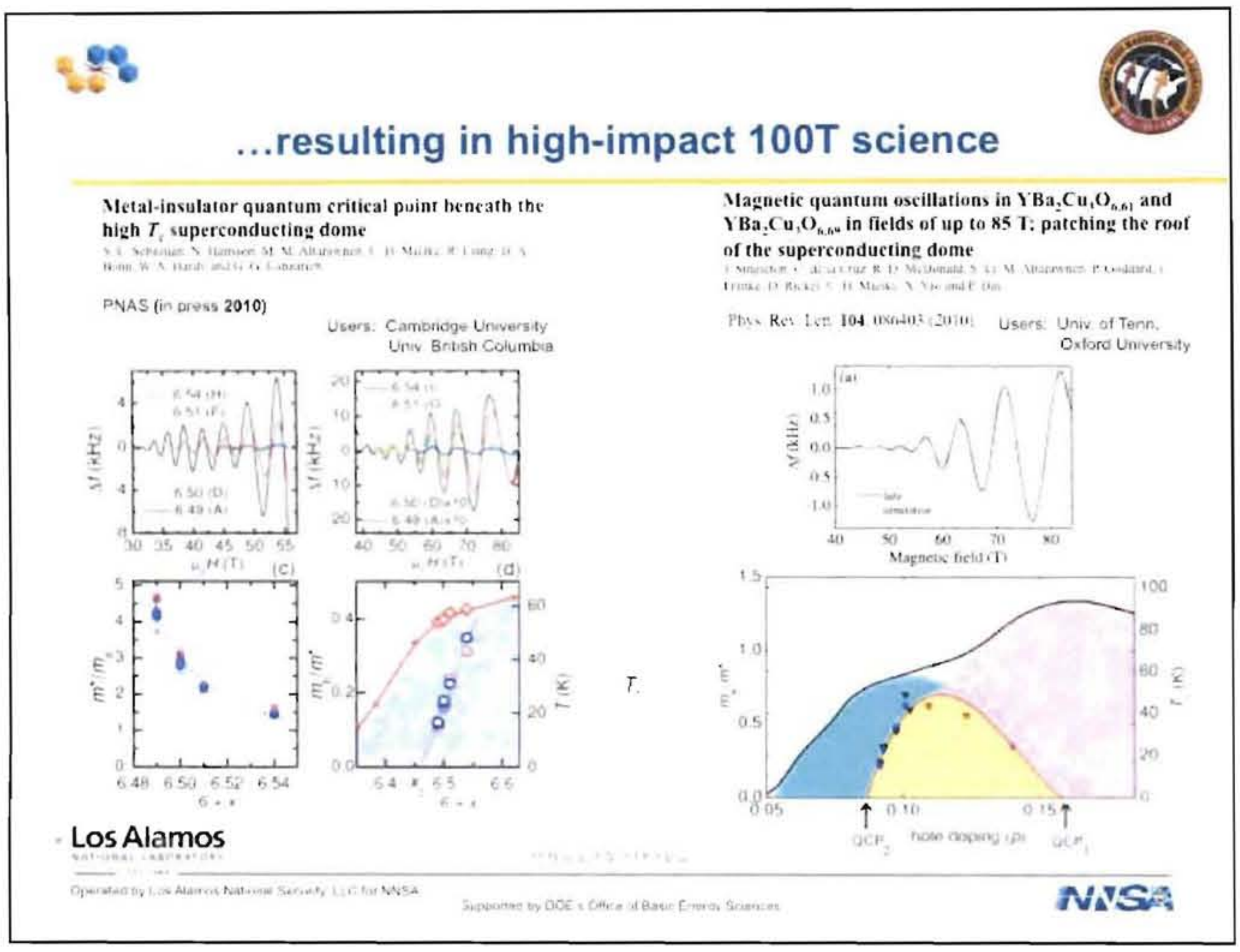

...resulting in high-impact 100T science
Metal-insulator quantum critical point beneath the high T_c superconducting dome
PNAS (in press 2010)
Users: Cambridge University
Univ. British Columbia
Magnetic quantum oscillations in $YBa_2Cu_3O_{6.61}$ and $YBa_2Cu_3O_{6.69}$ in fields of up to 85 T: patching the roof of the superconducting dome
Phys. Rev. Lett. 104 086403 (2010)
Users: Univ. of Tenn.
Oxford University
Magnetic field (T)
hole doping (p)
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Supported by DOE's Office of Basic Energy Sciences
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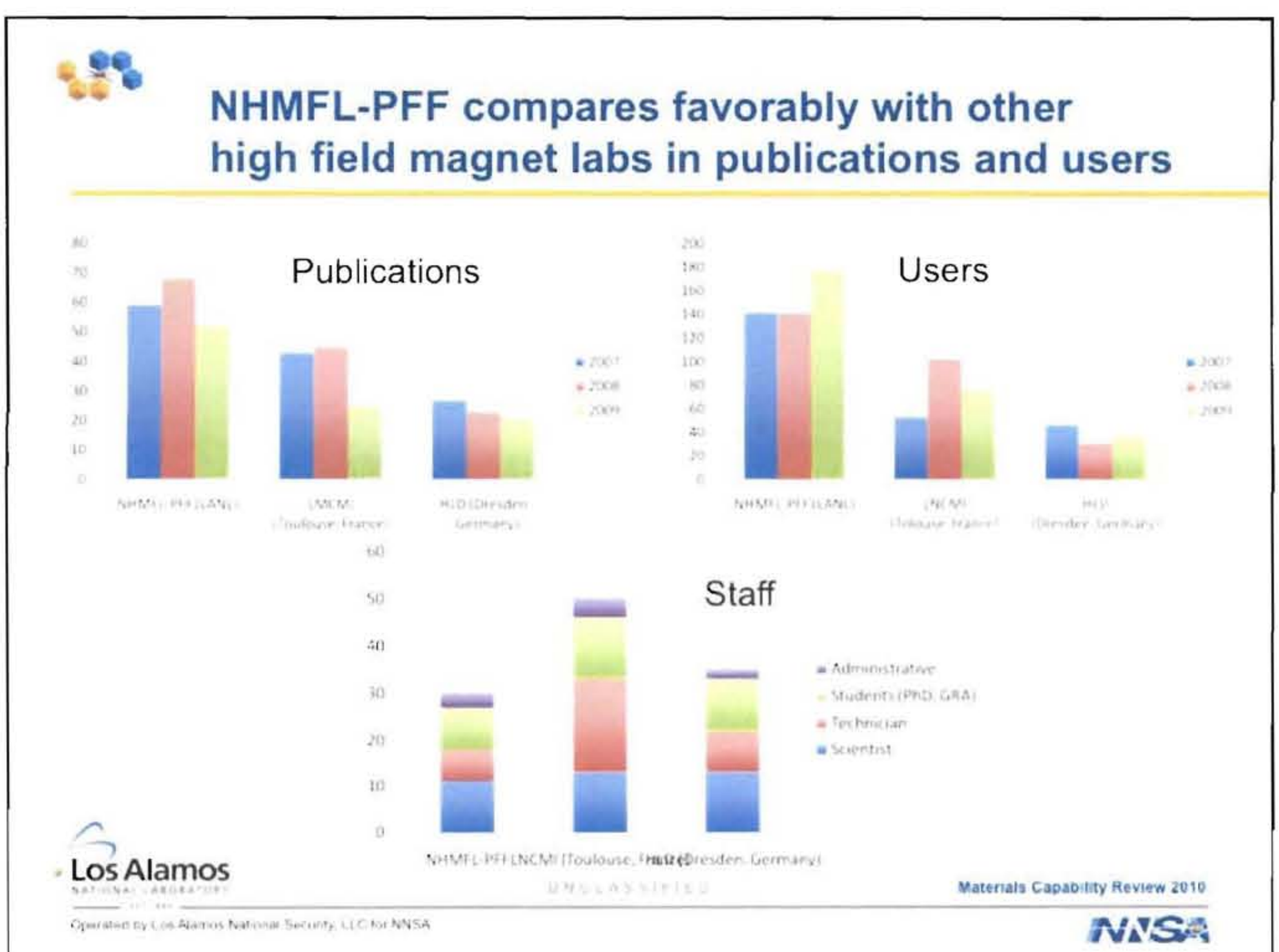

NHMFL-PFF compares favorably with other high field magnet labs in publications and users
Publications
Users
Staff
Administrative
Students (PhD, GRA)
Technician
Scientist
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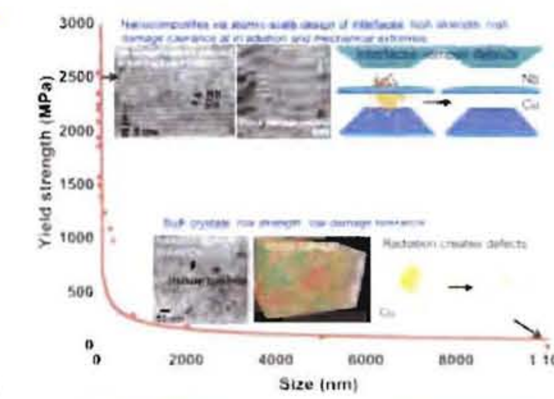
Our user facilities played a key role in LANL's new Energy Frontier Research Centers

Center for Materials at Irradiation and Mechanical Extremes (CMIME)
(LLNL, UIUC, MIT)

Center for Advanced Solar Photophysics
(NREL, Rice, UC...)



Partner roles in EFRCs

- **Science of Precision Multifunctional Nanostructures for Electrical Energy Storage** Univ of Maryland
- **EFRC for Solid State Lighting Science** Sandia
- **Photosynthetic Antenna Research Center** Washington Univ
- **Center on Materials for Energy Efficient Applications** UCSB
- **Center for Energy Frontier Research in Extreme Environments** Carnegie Institution of Washington

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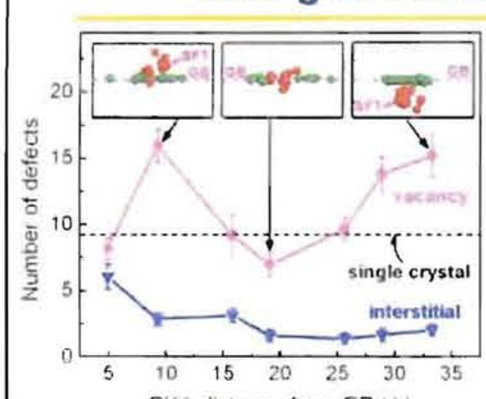
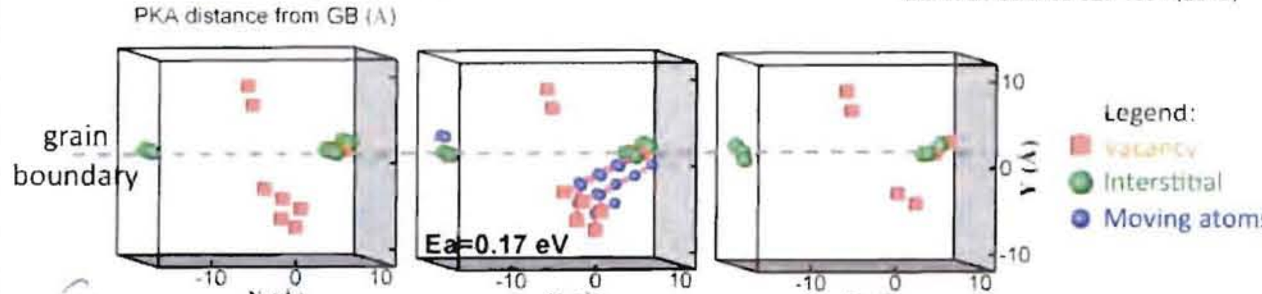
Efficient annihilation of radiation-induced defects near grain boundaries



The combination of interstitial emission and defect diffusion towards grain boundaries explains why nanocrystalline materials, such as oxide dispersion strengthened steels, with high fractions of grain boundaries have better radiation tolerance than their polycrystalline counterparts.

Bai et al. *Science* **327** 1631 (2010)



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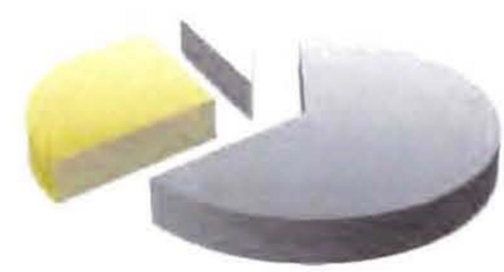
LDRD
CMIME
NNSA

The Materials Capability has a significant footprint in the LDRD portfolio at LANL

LANL Total LDRD

	%	$M
DR	58.9	73.6
ER	34.7	43.4
PRD	6.4	8.0
Total	100	125.0

Materials LDRD



	%	$M
DR	36.4	26.8
ER	28.2	12.2
PRD	39.0	3.1
Total	37.6	47.0

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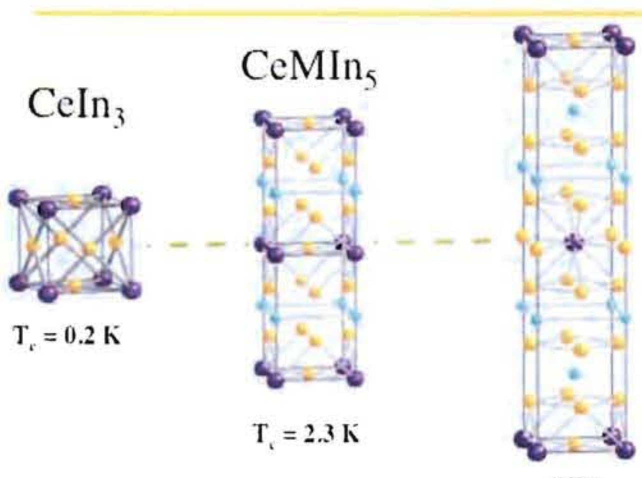
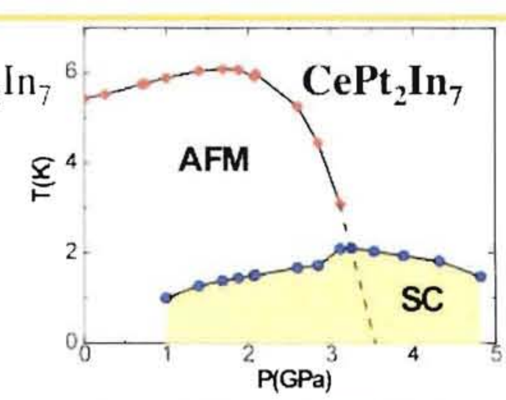
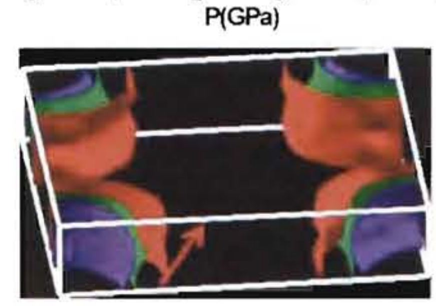
Design principles discover new superconductor





Reducing Dimensionality

Additional spacer layer creates a quasi 2-d material which was correctly anticipated to be superconducting



Fermi surface is quasi 2-D

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Most major recommendations from the 2009 Materials Capability Review are being addressed

- Improve the self-assessment of the Materials Capability at LANL with bench-marking.
- Materials Strategy: Broaden the engagement of people and programs. Frame the strategy within the broad national context. Use to develop a strategy for innovative materials research in the face of decreasing weapons funding.
- MaRIE: vastly more understandable this year with better differentiation of the LANL strengths. Need to build support from the other Labs (Sandia and LLNL and non-DP Labs,) and industry.
- Materials for Energy: define and articulate theme areas, formulate and disseminate your strategic vision and its connection to the Lab mission.
- Actinides: Replace Pu Manufacturing with Pu Readiness. Actinide materials should be reviewed yearly.
- Develop a hiring strategy to populate the competencies that are considered sub-critical and to ensure that you compete successfully for the best people, especially in the experimental arena.
- Address issues of overwhelming bureaucracy, clumsy handling of foreign nationals and inadequate infrastructure.

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Themes presented in prior Materials Capability Reviews were based on materials competencies

Concept: All competencies will be reviewed on a three year cycle with strong connections made with programs

MATERIALS UNDER EXTREME CONDITIONS	DESIGNED MATERIALS	MATERIALS, THEORY, MODELS, SIMULATION	TOOLS/ FACILITIES	SPECIFIC MATERIALS CLASSES
Materials Dynamics	TR Requirements	Multi-time/ length scale modeling	*LANSCE*	Actinide Materials
High Pressure	Energy Security Requirements	*Mechanical Behavior*	CINT	*Nanomaterials*
High Magnetic Field	Manufactured NW Components	Micro-structural evolution, Alloy phase Stability and Physical Properties	NHMFL	Polymers Bio-materials
Irradiation Matter Interactions, corrosion	*Synthesis*	Condensed Matter Physics	EML, IBML, Scanning Probe Microscopy..	HE

2007
2008
2009

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We are organizing future Materials Capability Reviews based on the Materials Strategy

	FY-10	FY-11	FY-12
Overview	• Materials Overview • Materials Strategy • MaRIE update	Materials at LANL MaRIE Overview	Materials at LANL
Emergent phenomena	CINT/Nanoscience	Soft matter/ Polymers	Condensed Matter Physics/NHMFL
Defects and Interfaces	Electronic/ Photonic Materials	Actinides (Nuclear Energy focus)	Surface science/ corrosion
Extreme Environments	Materials Dynamics	Radiation Environments/ IBML	HE/High Pressure
Programmatic Element	Materials for Global Security	Energy Security	NW-- Actinides
Critical Issues	Actinide Overview • Pu strategy • Actinide DR review	LANSCE	PF4/CMRR

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2010 Materials Capability Review

- **Materials Vision**
  - Materials Strategy: Wendy Cieslak
  - MaRIE update: John Sarrao
- **Emergent Phenomena: CINT/Nanoscience**
  - Lead: David Morris, CINT Co-Director, with tour of CINT and new Electron Microscopy Laboratory
- **Defects and Interfaces: Electronic/Photonic Materials**
  - Lead: Darryl Smith
- **Extreme Environments: Material Dynamics**
  - Lead: Anna Zurek with programmatic overview by Rick Martineau, C2 Program Manager
- **Programmatic Element: Materials for Global Security**
  - Lead: Dan Thoma with programmatic overview by Will Rees, PAD-GS
- **Critical Issues: Actinide Materials**
  - Lead: Gordon Jarvinen, Director, LANL Seaborg Institute
  - Pu strategy: David Clarke
  - 1st year LDRD-DR review: "First Principles Predictive Capabilities for Transuranic Materials: Mott Insulators to Correlated Metals," Rich Martin

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Your feedback on the performance of the Materials Capability is requested

- **Scientific Leadership as Evidenced by:**
  - Leadership in an International technical community
  - Publication of highly cited research results
  - Flux of innovative ideas and proposals
  - Hiring and training of next generation's leaders
- **Programmatic Impact**
- **Sustaining a *Cross-Laboratory* Materials Community**
- **Vision for the Materials Capability as it underpins our Mission**
  - Progress on LANL's Materials Strategy – enroute to MaRIE

We value the committee's feedback on LANL materials capability structure and strategic vision.

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Materials for the Future

W. Cieslak (MST-DO)

One year ago, we presented the initial vision, mission and theme areas for Los Alamos National Laboratory's materials for the future strategy. This year, we will update progress on further defining the strategy and initiating implementation planning. The strategy was released in the Spring 2010 issue of the *Experimental Physical Science Vistas* publication (please see www.lanl.gov/orgs/adeps/VISTAS). Early stages of implementation have focused on completing an analysis of strengths, weaknesses, opportunities and threats working with scientists, engineers and program managers across the laboratory. The goal is to provide actionable recommendations to nurture the forward-looking scientific base of our materials capability.

Materials for the Future

Materials Capability Review 2010

Wendy R. Cieslak
Division Leader
Materials Science & Technology

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Materials at Los Alamos

Key Actions and Timeline - 2010

- VISTAs publication of Materials Strategy
- SWOT brainstorming with broad representation across LANL materials
- Consolidate SWOT working with Guiding Coalition
- Launch metrics effort to validate strengths and weaknesses
- Dialogue with LANL programs to validate opportunities and threats
- Town Halls to further socialize and seek input
- Define a focused set of 3-5 priority Goals for Materials
- Seek feedback at Materials Capability Review in May
- Refine and prioritize actions to achieve Goals (implementation plan)

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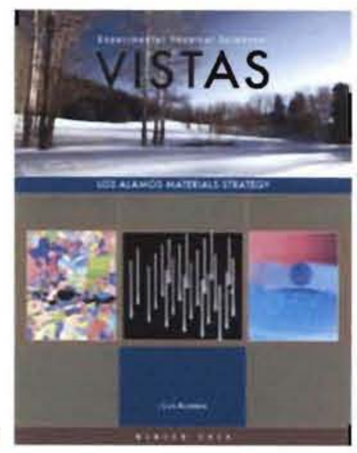
LANL Materials Pillar: Vision, Mission & Strategy

VISION

Controlled Functionality



MISSION

We pursue the discovery science and engineering required to establish design principles, synthesis pathways and manufacturing processes for advanced materials to control functionality relevant to ensuring the U.S. nuclear deterrent, reducing global threats, and solving emerging national challenges.

STRATEGY

We predict and control functionality through forefront science and engineering across three themes:

- **Defects and Interfaces**
- **Extreme Environments**
- **Emergent Phenomena**

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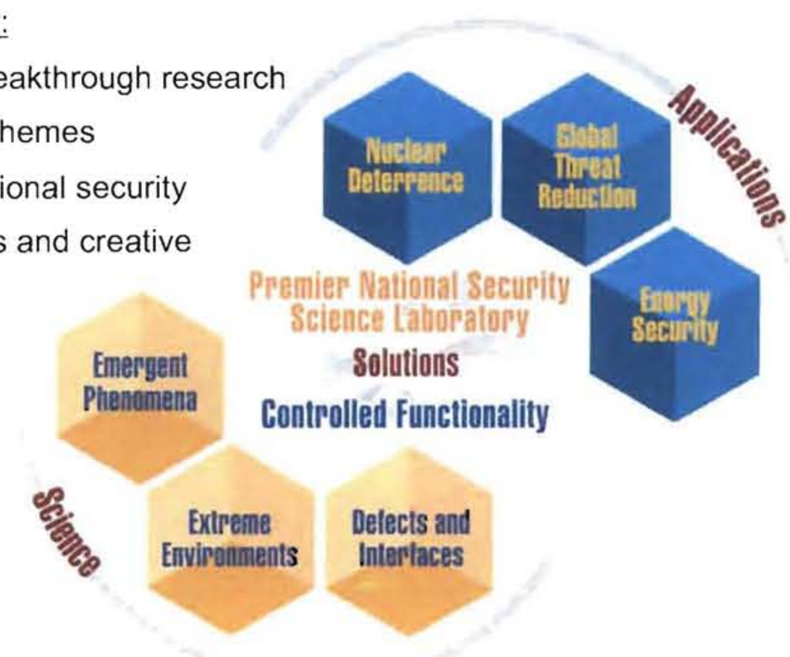
The Materials Strategy advances LANL Vision and Missions, which in return advance our Capability

We are differentiated by:

- Outstanding quality, breakthrough research
- Integration across the themes
- Science relevant to national security
- People who are curious and creative



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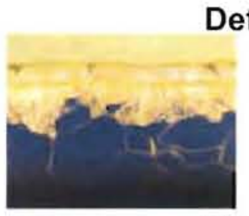
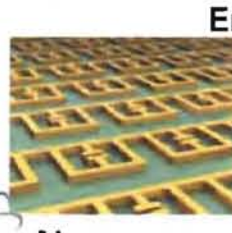
LANL Materials will be differentiated through forefront science that crosscuts three themes



Defects and Interfaces – the mechanistic understanding and control of inhomogeneities, across all appropriate length and time scales, that govern materials functionality

Extreme Environments – the underlying principles enabling the understanding of the interactions of materials with extreme conditions in order to create 1) environmentally tolerant properties and 2) the ability to exploit extreme environments to tune materials functionality



Emergent Phenomena – the science required to discover and understand complex and collective forms of matter that exhibit novel properties and respond in new ways to environmental conditions, enabling the creation of materials with innate functionality

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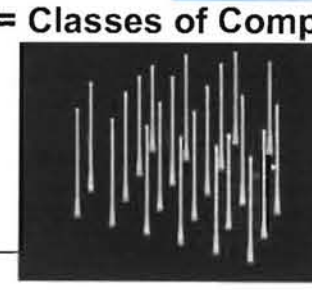
Theme Areas break into Constituent Classes that define the scope of our research

- **Defects and Interfaces = Classes of Functionality**
  - Mechanical/Structural
  - Chemical/Compatibility
  - Electronic/Photonic
- **Extreme Environments = Classes of Environments**
  - Radiation
  - Thermomechanical
  - Electromagnetic Fields
  - Chemical/Electrochemical
- **Emergent Phenomena = Classes of Competing Interactions**
  - Intrinsic
  - Extrinsic
  - Adaptive Response



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Materials at Los Alamos

SWOT Analysis is a good tool for revealing key advantages and gaps

Strengths

- *Internal focus*: What do we have that is world-class and/or differentiating, and why?
- Include institutional strengths that could be brought to bear on materials

Opportunities

- *External focus*: What do the nation and our sponsors need?

Weaknesses

- *Internal focus*: What internal deficiencies compromise our strengths?
- Identify gaps such as where we don't have a critical mass of people

What are potential Solutions?

Threats

- *External focus*: What might keep us from taking advantage of opportunities?
- Think about competitors

What are potential Solutions?

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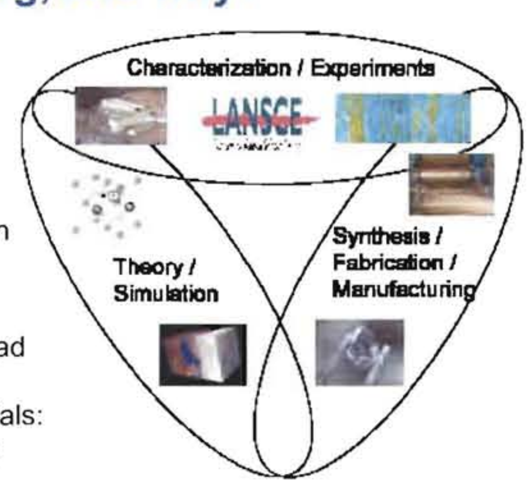
Materials at Los Alamos

Strengths: What do we have that is world-class or differentiating, and why?



- **It's the people!**
  - Depth of expertise, especially recognized for discovery science
  - Creativity and curiosity
  - Interdisciplinary ideation across vast breadth
  - Integration of theory, modeling and simulation with experiment and over materials lifetime
- **Unique world-class facilities**
  - National User Facilities: LANSCE (Lujan, pRad and WNR on path to MaRIE), NHMFL, CINT
  - Leadership in actinide and radioactive materials: Soup-to-nuts from design through delivery at TA-55, CMR, Sigma and IPF
  - Energetic materials synthesis and diagnostics
  - Multiscale capabilities at extremes: e.g., dynamic materials testing from laser flyers to gas guns to DARHT and U1a
  - Computation (capability and capacity and speed) among best in world
- **Ability to do classified and OUO research**

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Weaknesses: What internal deficiencies compromise our strengths?

- **Program development, execution and management**
  - Need institutional coordination and consistency, discipline, mid-scale efforts, agility
  - We try to do it all, but one size does not fit all sponsors
  - Not always deliver what's needed on time and for a reasonable cost
- **Transition from lab into national solutions has been challenging**
  - When the PI also has applications knowledge, the program takes off
  - Time horizon of our research vs. the agencies' needs is a severe disconnect
  - STE organizations must weigh if "job shop" requests might lead to R&D
- **Risk aversion = escalating requirements, costs and time**
  - Even the simplest things can seem impossible to accomplish or take resources way out of proportion to the impact
  - Rush to implement compliance when not fully thought out
- **We try to do everything, results in "death by salami"**
  - Need deliberate invest/divest decisions regarding technical weaknesses
- **Aging and dispersed capabilities**
  - People, equipment and disciplines are isolated
  - Our facilities are becoming an embarrassment
  - Expertise spread really thin. The deep thinking is what suffers first.

Opportunities: What do the nation and our sponsors want?

- **We exist in a set of competitor labs and each of us bring different strengths to our sponsors**
  - Know where we're good and focus in those areas
  - Be proactive in working as "one lab" to capitalize upon our strengths
  - Encourage external partnering and collaboration – think strategically about who to partner with for certain things (eg. top 5) and where we choose not to partner
- **Build explicit linkages to customers**
  - Materials-enabled solutions
  - Develop an agile infrastructure (program and line) to translate science into application.
  - For basic research, need to articulate the notion of how it might be useful
  - Can do better in Tech transfer – LANL is highest winner of RD100
- **Need to understand limits of existing materials and develop new materials**
  - Overcome the "leap of faith" from materials starting condition to performance in extreme environments, develop predictive capability from science basis
  - Establish areas for LANL leadership in Materials (next slide)

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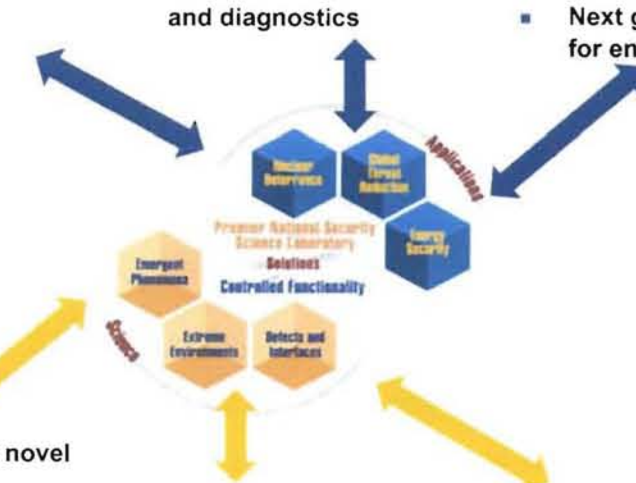
Areas of leadership for LANL Materials (preliminary)

- Actinides
- Materials under thermomechanical extremes
- Materials attribution
- Sensors and detectors – materials and diagnostics
- Fuels, targets and structural materials for fission/fusion
- Next generation conductors for energy transmission



- Materials having novel functionality
- Multifunctional materials
- Creating and diagnosing extreme conditions
- Designer materials optimized for specific needs

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Threats: What might keep us from taking advantage of opportunities?

- **We are a broad-based national security science laboratory and yet still an NNSA lab**
  - Shift of NNSA budget away from fundamental science and associated infrastructure
  - Becoming overly committed on large-scale milestones "death march"
  - Lack of (inter)-national policy for all things nuclear had kept things in stasis
  - Weapons uplift will tend to slow our momentum with other programs
  - NNSA gets between lab and other customers
  - Other DOE programs compete mission across all labs
  - Buying incremental product rather than integrated leadership
  - *At what point can we no longer provide the transformational leadership?*
- **Short term view of majority of sponsors toward capability and infrastructure maintenance**
- **Limited set of sponsors willing to support foundational discovery science**
- **Most of materials is small-scale science, and small scale science is hard to sell**
- **Competition for programs, especially from labs, universities and defense contractors**
- **Competition for people, especially from labs, universities and industry broadly**

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Solutions:
Actions we might take to mitigate weaknesses or threats and capitalize on strengths or opportunities

- **Foster our scientific and technical leaders for the future**
  - Serious human capital planning: Recruit, retain and reinvest
  - Key hires for the institution with associated funding (probably not a single type of funding)
  - PostDoc program is great, need conscious planning for the next 5-10 years of the career
  - Establish mechanisms to sustain careers around rapidly evolving science and annual funding
  - Teach them how to connect into programs – synthesis of basic-to-applied within individuals as much as possible, and across a given group
  - Re-establish mobility to move up, down and around within the lab
- **Align program "pull" and science "push"**
  - Balance long term/short term needs and strategies
  - Improve communications program-to-scientists, consider a seminar series
  - Connect LDRD and PD strengths and successes with opportunities with sponsors
  - Get technical line managers back to Washington to meet with sponsors
  - Incentivize DLs and GLs to integrate capabilities, team to get new programs, share facilities
- **Integrated plan for facility and equipment development relevant to materials**
  - Anticipate MaRIE and invest in its development
  - Define that core that makes us differentiating to the competition and must be state-of-the-art
- **Articulate and permeate the Strategy. Make the strategy real. Communicate well throughout the laboratory. Connect the words to the actions.**

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Our Strategy has had a demonstrable effect on LDRD research categories

- **The LDRD DR Grand Challenge in *Materials: Discovery Science to Strategic Applications***
  - Controlled Functionality through discovery and application of fundamental materials properties and materials synthesis processing and fabrication techniques, from the atomic level, through nano- to microscopic scales, to bulk material
  - Cultivation of the transformational science of materials, that encompasses new understanding and novel materials that enable radical new technologies to meet our future mission needs
  - Explicitly calls out the three theme areas of our strategy
- **The ER Call for FY2011 includes two Materials categories**
  - Defects and Interfaces in Materials
  - Emergent Phenomena in Materials Functionality

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Existing LDRD-DR Projects in Materials map across all three strategic theme areas

FY08-10
- EE: Hot Spot Physics and Chemistry in Energetic Materials Initiation
- DI: Design, Synthesis, and Theory of Molecular Scintillators
- EP: Carrier Multiplication in Nanoscale Semiconductors for High-Efficiency, Generation-III Photovoltaics
- EP: Ultrafast Nanoscale XUV Photoelectron Spectroscopy
- EE: Advanced Fuel Forms with Microstructures Tailored to Induce Fission Product Separation During Service

FY09-11
- DI/EE: Enhanced Radiation Damage Resistance via Manipulation of the Properties of Nanoscale Materials
- EP: Predictive Design of Noble Metal Nanoclusters
- EP: Understanding Anisotropy to Develop Superconductors by Design
- EE: Spatial-temporal frontiers of atomistic simulations in the petaflop computational world

FY10-12
- DI: Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage Evolution
- EP: Understanding and Controlling Complex States Emerging from Frustration
- EP: First Principles Predictive Capabilities for Transuranic Materials: Mott Insulators to Correlated Metals
- EP: Understanding, Exploiting, and Controlling Competing Interactions in Complex Oxides

LDRD-DR Materials proposals for FY11-13 continue to round out our strategic themes

•EP: A National Program for the Fundamental Understanding of the 5f Electrons of Plutonium - Eric D. Bauer

•DI: Hydrogen Effects in Delta-Stabilized Pu Alloys: Fundamental Thermodynamics and Interactions at Reduced Dimensionality - Daniel S. Schwartz

•EE: First Reactions: Simple Molecule Chemistry Behind the Shock Front - Dana Dattelbaum

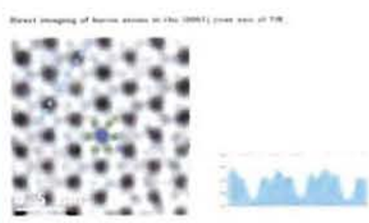
•EE: Tunable explosive materials with on demand performance - Robert J. Scharff

•DI: Innovative and validated sub-micron to mesoscale modeling of the evolution of interface structure and properties under extreme strains - Irene J. Beyerlein

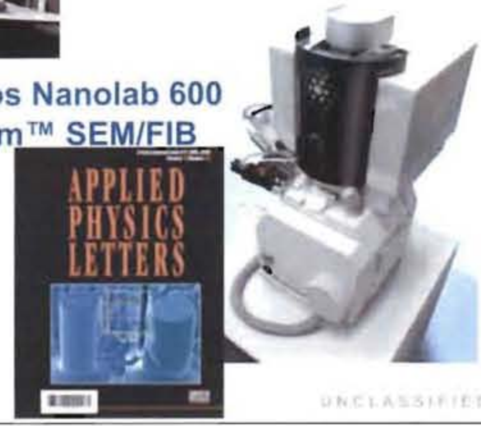
•EE: Characterization of Radiation Effects in Refractory Alloys using the Isotope Production Facility at LANSCE – Yongqiang Wang

We are actively stewarding our Electron Microscopy capabilities

FEI Titan 80-300™ S/TEM



FEI Helios Nanolab 600 DualBeam™ SEM/FIB



- Two new state-of-the-art instruments will enable us to meet critical needs of current (EFRC, LDRD, GNEP, WP, CINT, WFO) and future (path-to-MaRIE) programs
- We have chartered a LANL-wide Electron Microscopy Steering Committee (EMSC)
- The EMSC hosted an in-reach workshop in January 2010 that generated substantive technical and tactical dialogue
- Electron microscopy facilities at LANL are widespread. The Electron Microscopy Laboratory (EML) includes six instruments in the Materials Science Complex and four adjunct in the Sigma Building. In addition, there are over 10 known non-EML SEM's at LANL that are individually owned and operated. The EMSC is taking a role to coordinate the facilities and communicate our capabilities.
- Electron microscopy at LANL is undergoing a leap forward in capabilities, collaborative management, and visibility

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Next Steps

- **Define a focused set of 3-5 priority goals for Materials For each:**
  - Articulate attributes of desired end state
  - Establish tactics that we can implement in next 2 years
  - Recommend actions to ADs and above
  - Vet with programs and partner with them to achieve

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Guiding Coalition Membership

- Wendy Cieslak and Jack Shlachter, MST
- Toni Taylor and David Watkins, MPA
- Gene Peterson, C (Alternate: Basil Swanson)
- Stephen Lee, CCS (Alternate: Frank Alexander)
- Jay Dallman, DE (Alternate: Mike Stevens)
- Dave Funk, HX
- Kurt Schoenberg, LANSCE (Alternate: Alex Lacerda)
- Doug Fulton, P (Alternate: Cris Barnes)
- Tony Redondo, T (Alternate: John Wills, Mark Schraad)
- John Sarrao, SC and MaRIE
- Nan Sauer, Institutes (Alternate: Dan Thoma, Ed Kober)
- Mike Bernardin, XTD (Alternate: Steve Sterbenz)
- Mark Chadwick, XCP (Jon Boettger)

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MaRIE Update

J.L. Sarrao (SPO-SC)

Matter-Radiation Interactions in Extremes (MaRIE) is LANL's signature facility concept for providing transformational materials solutions for today's and tomorrow's national security needs. In this presentation, we'll discuss the why, what, and how of MaRIE, including progress on facility definition since last year's Materials Capability Review, and provide an update on MaRIE's current planning activities. These planning activities include a roadmap of needed capabilities for achieving process aware materials performance and coordination with LANL's institutional materials strategy.

MaRIE Update

John Sarrao

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Objectives

- Current Definition: The Why/What/How of MaRIE
  - You've heard about MaRIE in past years
  - Is the story better?
- MaRIE FY10 Status & Plans
  - Defining a path to CD-0; LANSCE-R and beyond
  - Are we making progress on a credible plan?
- Your Advice/feedback
  - How can you help (advocacy and promoting partnerships)?
  - Last Year:
    - " vastly more understandable this year with better differentiation of the LANL strengths. **Need to build support from the other Labs (Sandia and LLNL and non-DP Labs,) and industry.** "

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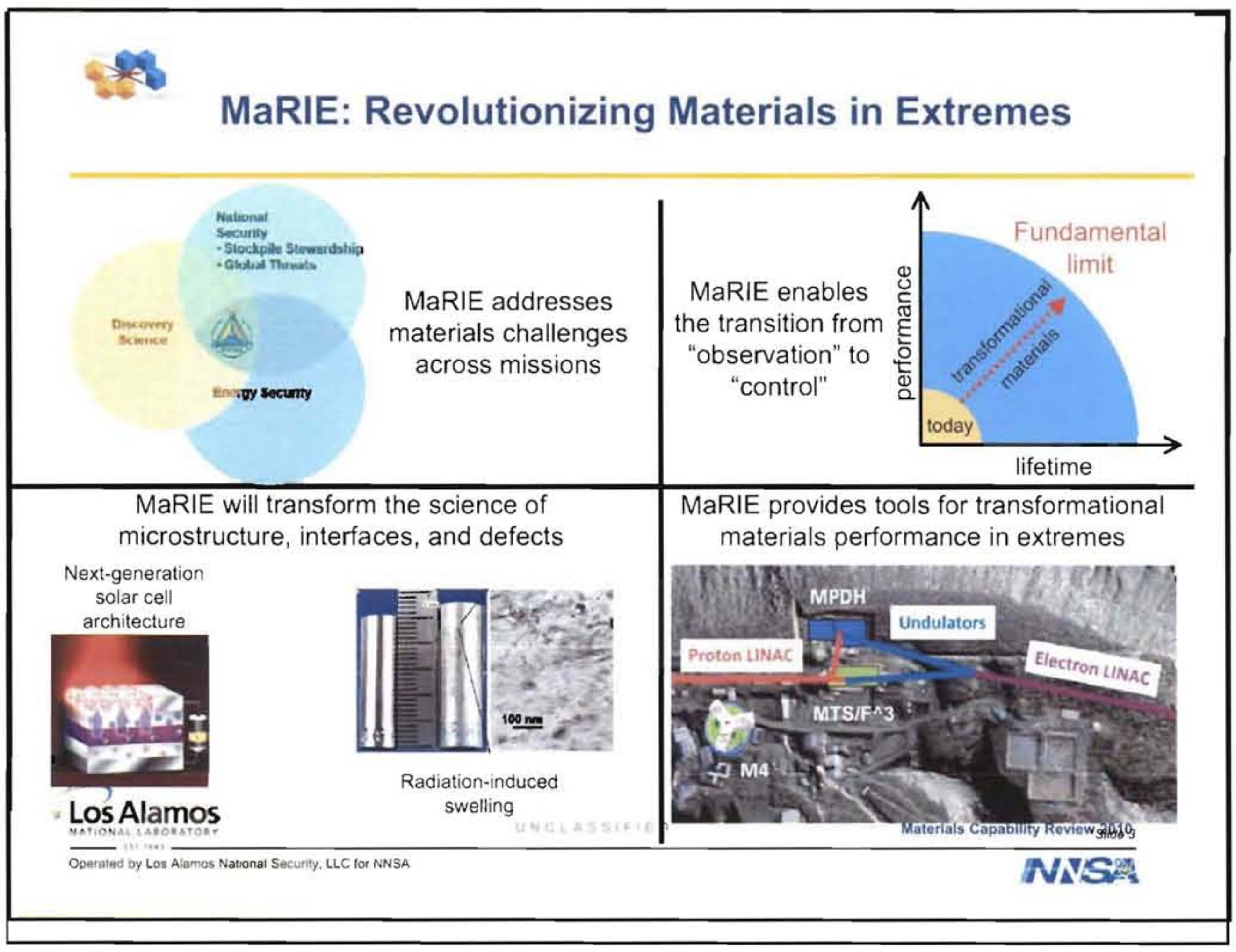
MaRIE: Revolutionizing Materials in Extremes
National Security
• Stockpile Stewardship
• Global Threats
Discovery Science
Energy Security
MaRIE addresses materials challenges across missions
MaRIE enables the transition from "observation" to "control"
Fundamental limit
performance
transformational materials
today
lifetime
MaRIE will transform the science of microstructure, interfaces, and defects
Next-generation solar cell architecture
100 nm
Radiation-induced swelling
MaRIE provides tools for transformational materials performance in extremes
MPDH
Undulators
Proton LINAC
Electron LINAC
MTS/F^3
M4
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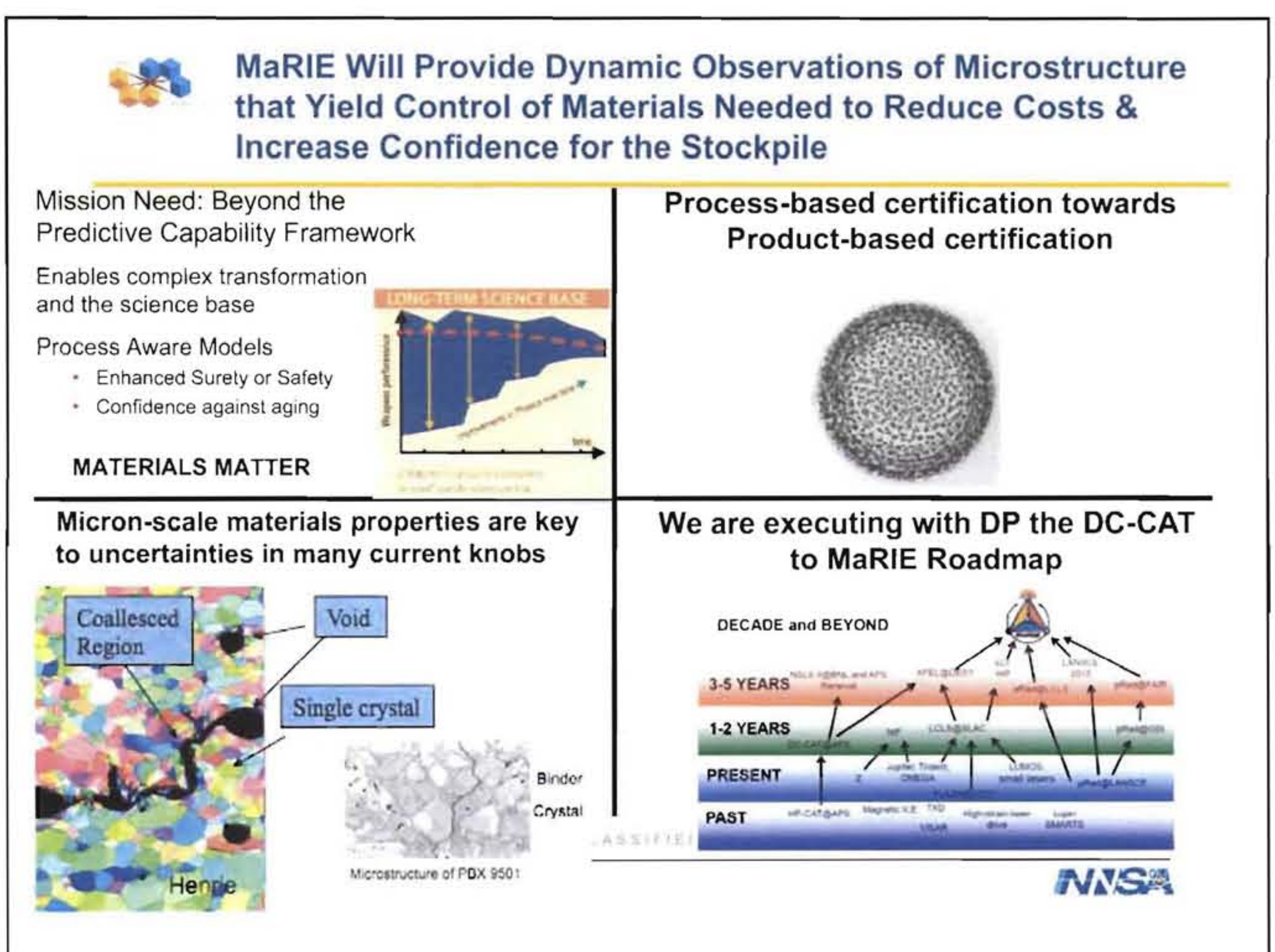
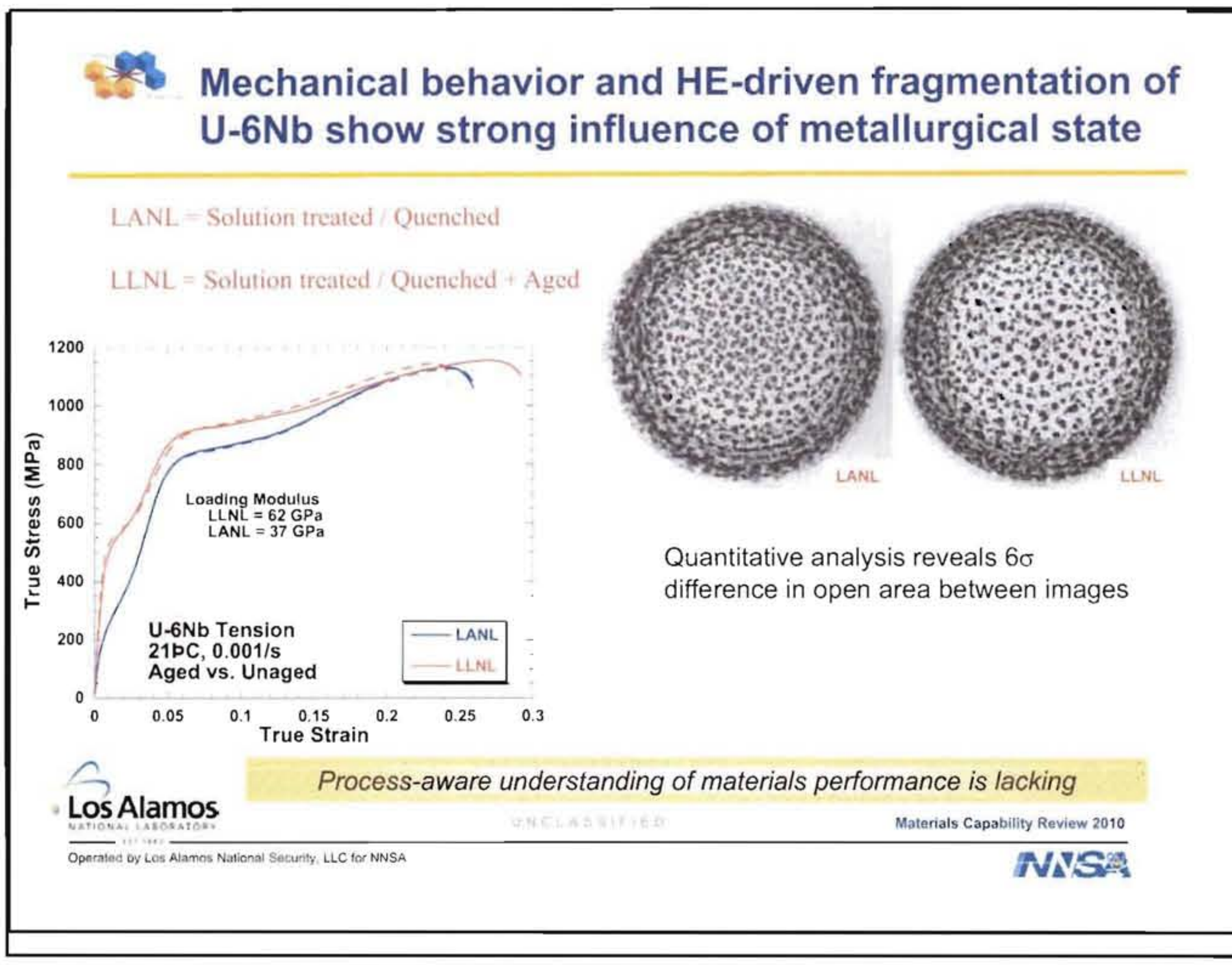

MaRIE Will Provide Dynamic Observations of Microstructure that Yield Control of Materials Needed to Reduce Costs & Increase Confidence for the Stockpile
Mission Need: Beyond the Predictive Capability Framework
Enables complex transformation and the science base
Process Aware Models
• Enhanced Surety or Safety
• Confidence against aging
MATERIALS MATTER
LONG-TERM SCIENCE BASE
Process-based certification towards Product-based certification
Micron-scale materials properties are key to uncertainties in many current knobs
Coallesced Region
Void
Single crystal
Binder
Crystal
Henpie
Microstructure of PBX 9501
We are executing with DP the DC-CAT to MaRIE Roadmap
DECADE and BEYOND
3-5 YEARS
1-2 YEARS
PRESENT
PAST
NNSA


Mechanical behavior and HE-driven fragmentation of U-6Nb show strong influence of metallurgical state
LANL = Solution treated / Quenched
LLNL = Solution treated / Quenched + Aged
True Stress (MPa)
True Strain
Loading Modulus
LLNL = 62 GPa
LANL = 37 GPa
U-6Nb Tension
21ÞC, 0.001/s
Aged vs. Unaged
LANL
LLNL
Quantitative analysis reveals 6σ difference in open area between images
Process-aware understanding of materials performance is lacking
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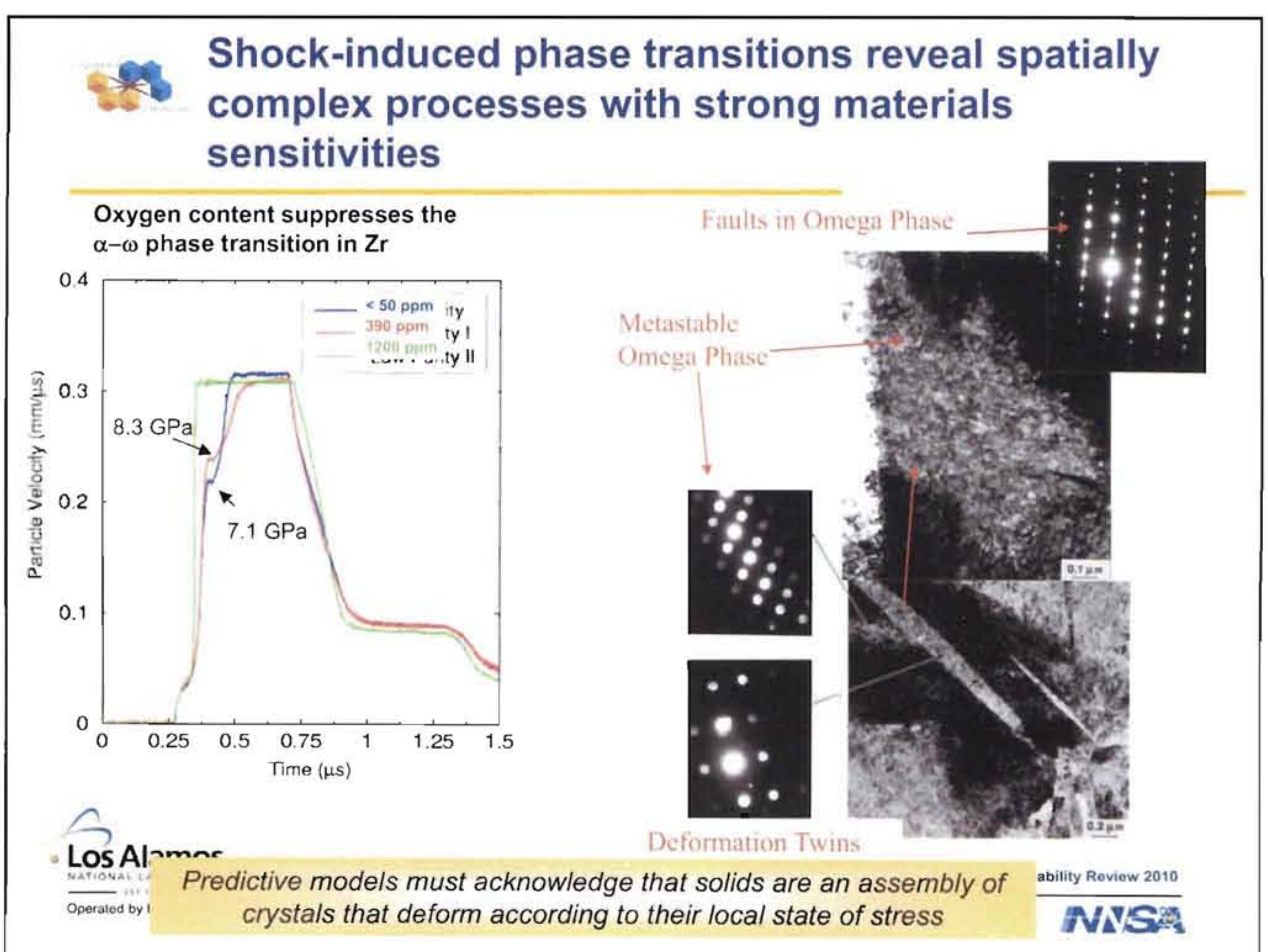
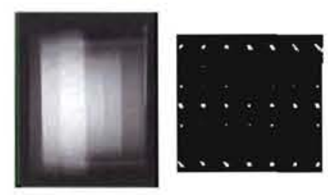

Shock-induced phase transitions reveal spatially complex processes with strong materials sensitivities
Oxygen content suppresses the α–ω phase transition in Zr
Particle Velocity (mm/μs)
Time (μs)
< 50 ppm
390 ppm
1200 ppm
8.3 GPa
7.1 GPa
Faults in Omega Phase
Metastable Omega Phase
Deformation Twins
Los Alamos
Predictive models must acknowledge that solids are an assembly of crystals that deform according to their local state of stress
NNSA

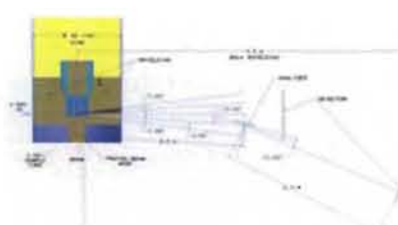
MaRIE : What does success look like?

- **Predicting materials performance, including failure, in extremes of pressure and strain for multi-phase materials**
- **Developing radiation resistant structural materials and fuels by design**
- **Exploiting complex materials and architectures for next generation electronics**



Simultaneous diffraction & dynamic density imaging

Defect manipulation in multiphase materials



In situ characterization in extreme environments

In-situ, transient measurements on real materials in extremes

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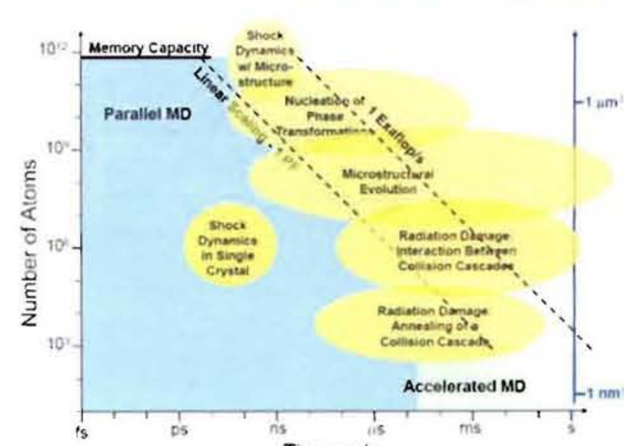
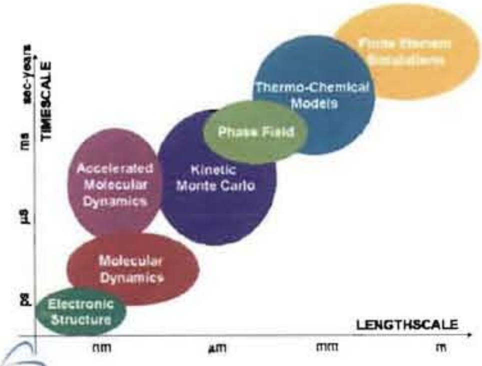
Experimental tools with unprecedented resolution are needed to validate and test the limits of modeling and simulation

One of the greatest challenges in multi-scale modeling is the physically-based treatment of defects and interfaces





Anticipated advances in petaflop/s and exaflop/s computing – with advanced models - put us on the verge of accessing new phenomena on the micron scale

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MaRIE provides the first comprehensive set of co-located tools to realize transformational advances in materials performance in extremes

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

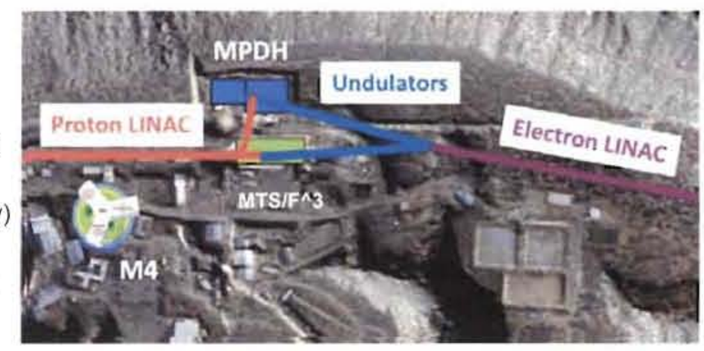
(MPDH: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(F^3: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(M4: Making, Measuring & Modeling Materials Facility)



MaRIE will provide unprecedented international user resources

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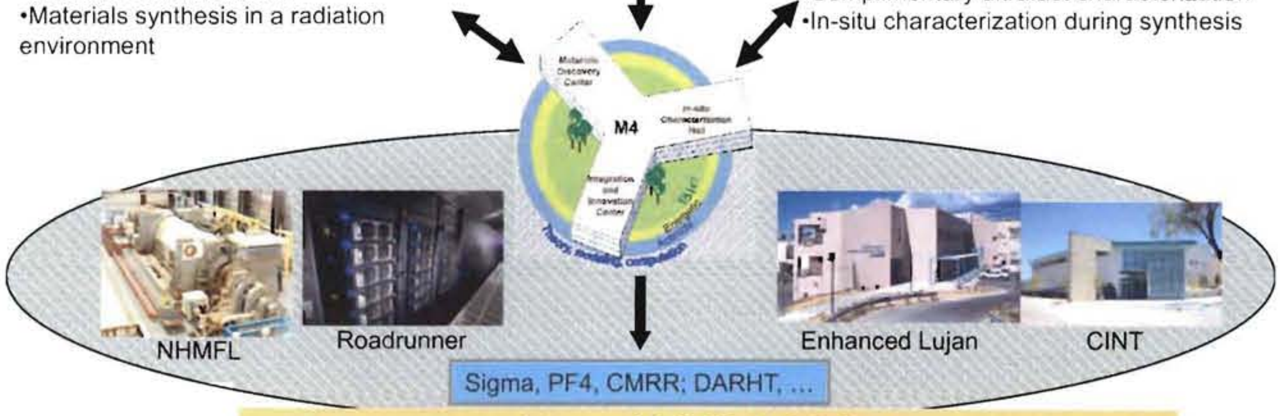
MaRIE: Integration is key – integrated facility capabilities and gateway to broader LANL

Portal to the External User Community

F^3
- Pre and post irradiation characterization
- Radiation hard materials
- Materials synthesis in a radiation environment

MPDH
- Samples with controlled microstructure
- Complimentary ultrafast characterization
- In-situ characterization during synthesis



Integrated Solid State Solutions
- Materials with process-aware controlled microstructure
- New radiation hard materials (self healing materials)
- Next generation photovoltaics/Advanced radiation detectors

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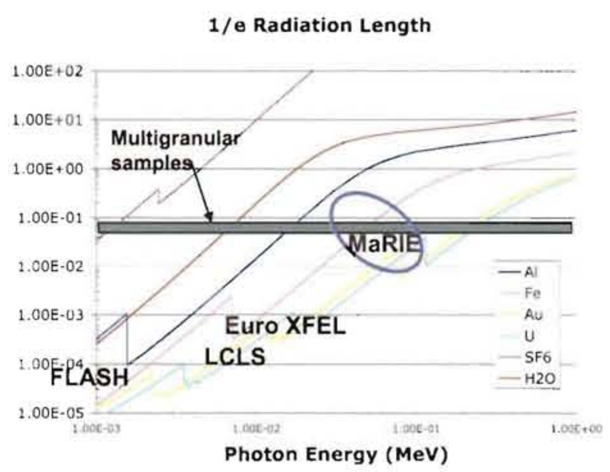
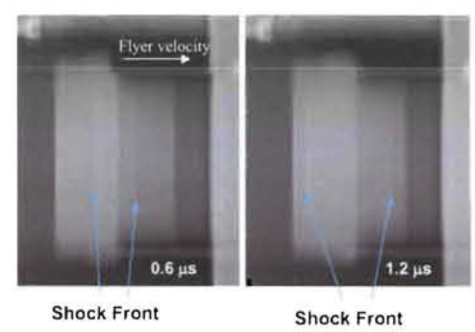
Through Multi-Probe Diagnostic Hall, MaRIE provides unique scattering and imaging capabilities to bridge the micron gap in extreme environments

A high-energy-photon (50-115 keV) XFEL allows multigranular sample penetration and multipulse dynamics without significant sample perturbation





pRad absolute Density:
$\rho = 3.07 \pm 0.03$ g/cm^3 (1.1%)

Meanwhile, proton microscopy can provide absolute density and velocities through the sample volume

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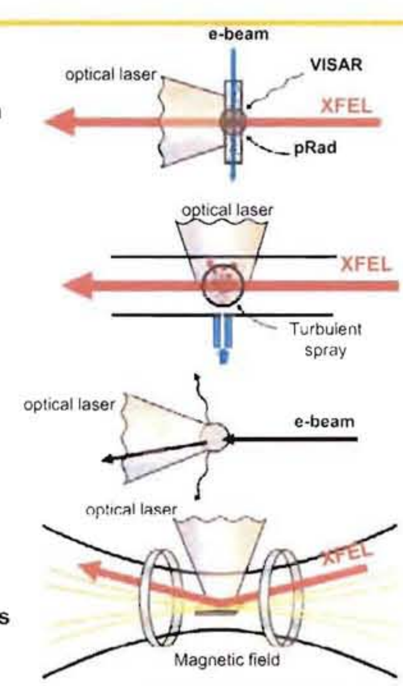
Frontier experiments identify performance gaps that form the basis of MaRIE's functional requirements

- **Meso-scale Material Dynamics**
  - Response of multi-granular material to dynamic deformation
  - Evolution of radiation-damage cascade
  - Micron-scale insights towards predicting high explosives
  - Includes key earth science materials
- **Multi-scale Fluid Dynamics**
  - Measure 3D multi-scale mean flow and turbulence
  - Variable material turbulent flows for diverse applications
  - Ability to measure *all* relevant scales for validation
- **Extreme Field Interactions with Matter**
  - Light intensities >10^{24}W/cm^2
  - 10–200 MeV gamma-ray nuclear physics
- **Emergent Phenomena in Complex Materials**
  - Ultrafast (10–100 fs) measurements in Extreme Environments



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Facility Definition Process

Science-driven Requirements Lead to Integrated Facility Needs Fulfilled by MaRIE

User Driven Science → (Material Needs) → Functional Requirements → (Alternatives Analyses) → Performance Gaps → (Preferred Alternative & Roadmap) → Facility Concept

Decadal Challenges Report (01/10)

MaRIE 1st Expts (03/10)

MaRIE Technical Alternatives (06/10)

MaRIE Pre-Conceptual Definition (06/10)

Radiation Extremes
- Thermal Transport
- Phase Stability
- Strength & Structural Integrity
- Corrosion
- Swelling

Control of Complex Materials & Processes
- Superconductivity
- High Explosives
- Energy Conversion & Storage
- Radiation Extremes

ironments
- reme p, T, strain rat
- h-flux fast n irradiat
- ecial nuclear & haza
- terials
- ctronic state excitati
- B extremes

surements
- Microstructure
  - Crystallography, composition, phase, defect density
- Imaging
  - Density, ejecta, particles, strain, cracks, corrosion layers, & interface control
- Phys & Chem properties

Synthesis with Characterization
- Ability to predict new mat'ls
- Defect/interface control

$^{2}s^{-1}$ fast n w/ relevant m, trans- n, He & H ion

keV coherent, x-ray source

c charged imaging

Intense ion source for isochoric heating of solid matter to 10-100 eV

Extremely short optical photon pulses for pumping & probing

Synthesis capability
- Single crystal growth
- Metastable phases
- Flexible fabrication & processing
- 10-nm control of 2D & 3D structures

MaR existing $B investments at LANSCE with the addition of the:
- XFEL
- Multiprobe Diagnostic Hall
- Fission-Fusion Materials Facility
- Making, Measuring, & Modeling Material Facility

Slide 13

We are actively engaging the scientific community through research needs workshops

Decadal Challenges for Predicting and Controlling Materials Performance in Extremes

December 6-10, 2009 • Santa Fe, New Mexico

- **Jan 20-22, 2009** — **"Research Frontiers and Capability Gaps for Controlling and Designing Functional Materials**
- **July 29-31, 2009** — **"Structural Materials Under Extreme Conditions"**
- **Sept 21-23, 2009** — **"Opportunities for Studies of Activated Samples at National User Facilities"**
- **Sept 23-25, 2009** — **"21 st Century Needs in Compression Science"**

"...purpose is to identify the scientific challenges and research directions to achieve predictive materials performance in extreme environments...the workshop will focus specifically on needed capabilities and tools to seize this opportunity...Outcomes will be documented in a publicly available workshop report..."

External Workshop Leadership: Todd Allen, Steve Zinkle; Paul Follansbee, George Crabtree; Roger Falcone, Bob Cauble, Rus Hemley, Malcolm McMahon; Tony Rollett, Tomas Diaz de la Rubia, Richard Lesar

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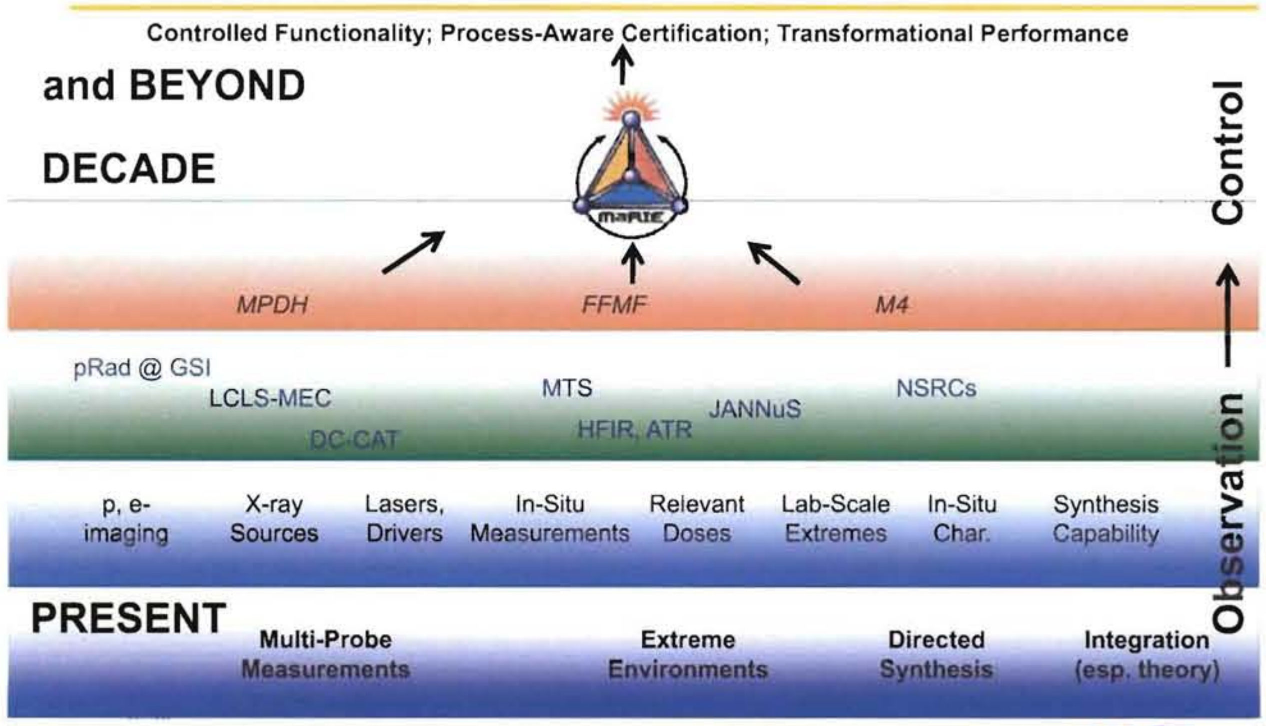
We have developed a Roadmap that identifies capabilities on the road to MaRIE and partnering opportunities



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Consistent with our roadmap, we are fostering strategic partnerships

- National Laboratories
  - -LLNL & SNL: nuclear weapons
  - -ORNL & INL: nuclear energy
  - -ANL & LBNL & SLAC, and FNAL: photon and proton accelerator development
  - -SRNL, PPPL, BNL, PNNL, JLAB: ongoing outreach
  - -Ames, NREL, NETL: initial interactions
- Universities
  - -Key partners in community outreach/first experiments teams
    - -typically not stewards of large-scale facilities
- Industry
  - -Focus on consortia advocacy
    - -pillar specific; lead with F^3

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LANSCE remains a key step on the road to MaRIE AND an important institutional priority

- **LANSCE-R reached CD-1, Oct. 2009**
- **President's FY11 Budget request put LANSCE-R on the "to be terminated" list**
- **Actions being pursued:**
  - Convert existing project funding to operating/maintenance funding
  - Support ongoing operational funding to allow responsible stewardship/future reliability of LANSCE
  - Communicate importance of continuing LANSCE operations to weapons program within NNSA and to DOE (SC, NE)
  - Champion importance of experimental capabilities for materials in extremes for current and future weapons program needs

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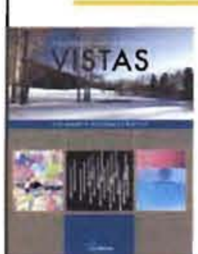
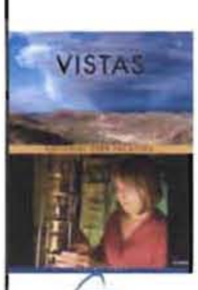
Following our materials strategy, we are doing MaRIE science now





Current and *pending* MaRIE-relevant LDRD-DR investments

Kurt Sickafus	Advanced Fuel Forms with Microstructures Tailored to Naturally Induce Fission Product Separation During Service
Dana Dattelbaum	Hot Spot Physics and Chemistry in Energetic Materials Initiation
Rico Del Sesto	Design, Synthesis, and Theory of Molecular Scintillators
George Rodriguez	Ultrafast Nanoscale XUV Photoelectron Spectroscopy
Mike Nastasi	Enhance Radiation Damage Resistance via Manipulation of the Properties of Nanoscale Materials
Jen Martinez	Predictive Design of Noble Metal Nanoclusters
Filip Ronning	Understanding Anisotropy to Develop Superconductors by Design
Tim Germann	Spatial-temporal frontiers of atomistic simulations in the petaflop computational world
Darcie Dennis-Koller	Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage Evolution
Ivar Martin	Understanding and Controlling Complex States Emerging from Frustration
Quanxi Jia	Understanding, Exploiting, and Controlling Competing Interactions in Complex Oxides
Chris Stanek	*Radioparagenesis: Robust Nuclear Waste Form Design and Novel Materials Discovery*
Dana Dattelbaum	*First Reactions: Simple Molecule Chemistry Behind the Shock Front*
Robert Scharff	*Tunable explosive materials with on demand performance*
Irene Beyerlein	*Innovative and validated sub-micron to meso-scale modeling of the evolution of interface structure and properties under extreme strains*
Yongqiang Wang	*Characterization of Radiation Effects in Refractory Alloys using the Isotope Production Facility at LANSCE*
Bruce Carlsten	*Exploiting Hamiltonian Properties of Beams to Revolutionize X-Ray Free-Electron Laser Architectures*

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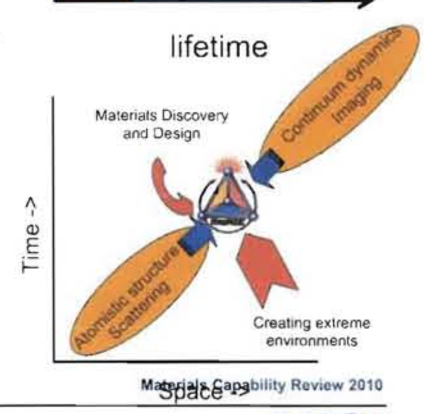
MaRIE will be the first capability with unique co-located tools necessary to realize transformational advances in materials performance in extremes

- **"The micron frontier" is key to solving transformational materials grand challenges**
- **MaRIE will provide unique capabilities**
  - Accessing materials irradiation/damage extremes
  - Simultaneous *in situ* imaging & scattering measurements
  - Accelerating materials discovery and solutions through control of defects and interfaces
- **MaRIE provides unprecedented international user resources for the transition from observation to control**
- **Facility definition being driven by community-validated performance gaps & functional requirements**
- **LANSCE is essential for MaRIE's success**



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Tab 3

Actinide Science Overview

G. Jarvinen (ADSMS)

Knowledge of the actinide elements has been critical to the mission of Los Alamos National Laboratory since the beginning, and remains so today. Under the National Nuclear Security Administration's Programmatic Environmental Impact Statement for Complex Transformation, the Laboratory has been designated the Center of Excellence for Plutonium Science. The first talk in this session will provide an update on the effort at LANL to develop a plutonium science and research strategy for the next decade. The second talk and the poster session will provide examples of ongoing research efforts in actinide materials science relevant to all the major mission areas at the Laboratory. These examples include recent experimental and theoretical efforts to understand the bonding in actinide materials and molecular complexes; to study oxidation and hydriding reactions of actinide metals; to investigate new nuclear fuel structures and their behavior under irradiation; and to prepare improved nuclear waste forms.

Plutonium Science and Research Strategy

D.L. Clark (INST-OFF)

The plutonium science and research strategy session defines research needs and opportunities for plutonium research and development efforts that share a common underpinning of the Laboratory's missions in nuclear deterrence, global threat reduction, and energy security. The strategy details areas of science that must be strengthened to preserve capability, retain staff, and enable work on high national security priorities. The strategy emphasizes fundamental understanding of materials, actinide science, and radiation-materials interactions, all coupled to predictive science that integrates theory, simulation, modeling, and complex experimentation.

Plutonium Science and Research Strategy

David Clark
National Security Science Education Center
Institutes Office (INST-OFF)
Plutonium Strategy Leader

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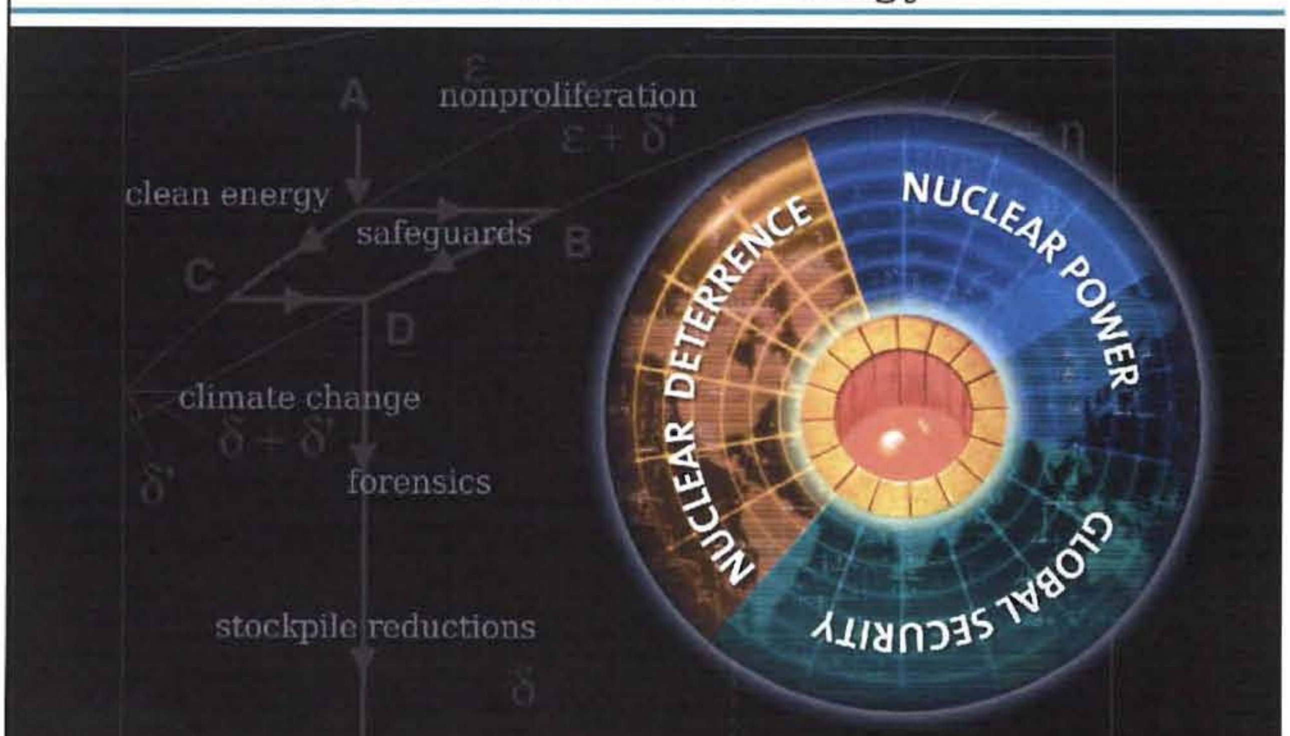
plutonium
science and research strategy



Slide 3

The Nexus of Plutonium

Plutonium: the nexus of significant issues facing society over the next century

Nuclear Deterrence. Reduce the size of nuclear arsenals while ensuring that nuclear weapons are safe and reliable without nuclear testing.

Sustainable Nuclear Energy. A growing worldwide consensus that nuclear power can reduce greenhouse gases while increasing domestic power generation.

Reduce Global Nuclear Threats. Promote international security by preventing the spread of nuclear weapons, securing nuclear materials against theft and diversion.

These interlocking issues define the future challenges in plutonium science, and form the basis for this plutonium science strategy

"Guaranteeing our stockpile ... allows us to pursue deep nuclear reductions without compromising our security"

"We must harness the power of nuclear energy on behalf of our efforts to combat climate change, and to advance peace opportunity for all people".

"Proliferation of nuclear weapons has become an overarching strategic problem for the contemporary world"

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Slide 4

The Plutonium Challenge

- > 2200 MT throughout the world, grows by 75 MT/yr through ingrowth in nuclear reactors
  - Spent nuclear fuels
  - Nuclear weapon's components
  - Legacy materials
  - Wastes
- As a nation, we are irreversibly invested in plutonium into any foreseeable future.
- There is a continuing obligation to understand and manage this material responsibly in all applications.

- Because of the complexity of plutonium, a complete understanding of plutonium science needed to address national needs is still lacking, while much of the knowledge base rests with aging and retiring scientists.

We must develop a deeper science-based understanding of plutonium behavior than we ever had when testing was possible.

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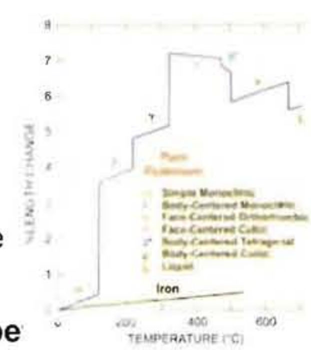
Slide 5

Working with plutonium is complex and difficult

Pu science is complex

- The 5f electron story
- There is no fully satisfactory theory for Pu
- The most complex element



There is little Pu science left in programs

- We have not mounted a Pu science program commensurate with the challenges of the CTBT and a smaller stockpile

Faster computers and better design work increase the gap be what we know about Pu and what we should know

The work is difficult

- Radioactivity and toxicity handling
- Regulatory environment has a strangling effect
- Cost of facilities squeeze out science
- Secrecy limits talent and peer review
- Some critical skills are endangered

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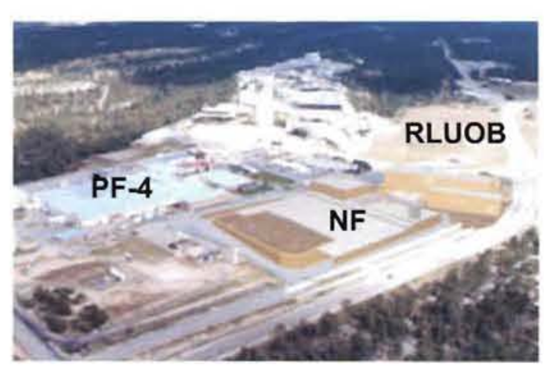
Slide 6

Vision for the Plutonium Center of Excellence

Los Alamos serves a key role as a consolidated Center of Excellence for Pu activities against this national obligation



As a Center of Excellence we must:

- maintain a collection of world-class leaders promoting internal and external collaborations.
- provide expert assistance in the event of a national security issue involving plutonium
- provide guidance for investment decisions on new capabilities and projects involving plutonium
- maintain a central repository and clearinghouse for publications and historical materials on plutonium science and engineering
- promote publication and training opportunities for the next generation of plutonium scientists and engineers, so as to provide meaningful and challenging work.

We must develop a fundamental scientific understanding of plutonium – one that can be more readily preserved and taught to future generations.

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Slide 7

Our Strategy is Built upon Three Goals

- Our strategy is framed around three goals and fourteen supporting objectives that address the Laboratory's enduring roles in plutonium science and the technical, programmatic, and funding relationships between them.

Rejuvenate, strengthen and integrate plutonium and actinide science as required by national security programmatic needs.

•Pu & actinide materials research in fundamental physics, chemistry, modeling and simulation in support of Laboratory missions – *8 objectives*

Recapitalize our scientific infrastructure and capabilities.

•Re-establish key functions and core capabilities in plutonium and actinide research, and ensure historical data are mined and captured for the future – *4 objectives*

Increase workforce strength.

•Ensure that plutonium and actinide science, technology, and engineering are sustainable and desirable fields of study in support of the retention of a world-class workforce – *2 objectives*

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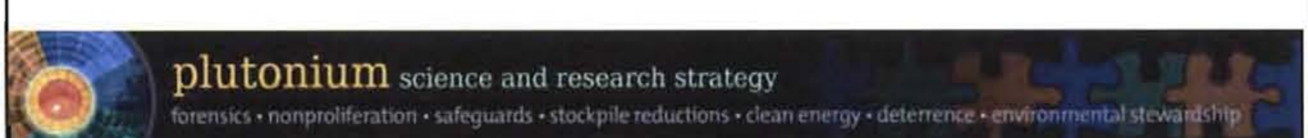
Slide 8



Goal 1: Rejuvenate, strengthen and integrate plutonium and actinide science as required by national security programmatic needs.

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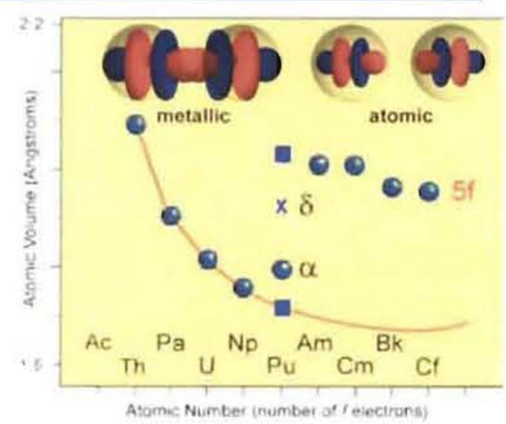
Slide 9

Objective 1: Plutonium Electronic Structure

Improve our understanding of the electronic structure of plutonium and light actinides.



Strategies

- ***Pure Pu***. Develop improved theories to better describe the effects of correlation on the electronic structure and bonding properties
- ***Pu & Actinide Compounds***. The properties of Pu cannot be understood in isolation from a more general theory of its alloys and compounds and other actinide materials
- ***Pu Alloys & Aging***. Develop an electronic structure model for alloys and aged Pu since alloys are used in weapons and in energy applications
- ***Pu Surfaces, Interfaces, Thin Films, & Defects***. Reduced dimensionality usually enhances electronic correlation effects, and yet must be well understood in order to model many materials properties and effects of processing
- ***Pu Molecules***. Investigate the basic electronic structure considerations underpinning bonding and covalency in actinide/ligand interactions

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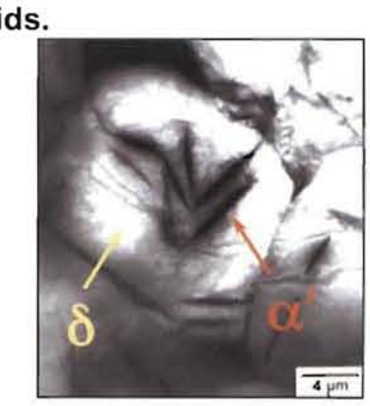
Slide 10

Objective 2: Thermodynamic and Thermal Properties

Improve our understanding of thermodynamic and thermal properties in plutonium and actinide alloys, compounds, and colloids.

Thermal and thermodynamic properties of Pu alloys and compounds are important to the understanding of Pu behavior in all applications.



Strategies

- Investigate structural phase stability, thermal expansion, elastic moduli, heat capacity, thermal conductivity, and the role of impurities in phase stability.
- Many fundamental thermal and thermodynamic properties of plutonium alloys and compounds, essential properties for all applications, remain unknown and must be targeted.
- Determine the effect of radiolysis and radiation damage on structural phases and their relationship to extreme environments.

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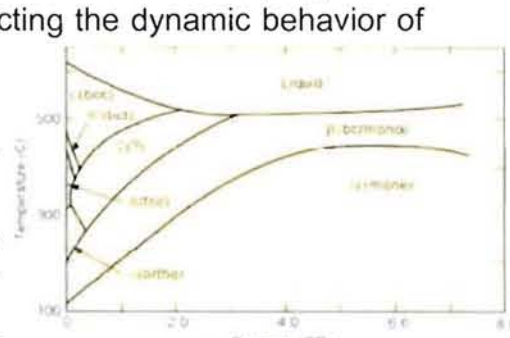
Slide 11

Objective 3 - Dynamic Pu Behavior

Achieve a fundamental understanding of the dynamic behavior of plutonium across pressure, temperature, time, and phase space.

Integrate theory, experiments, modeling, and simulations to develop age- and process-aware multi-phase EOS models for predicting the dynamic behavior of pure and alloyed Pu.



Strategies

- ***Equation of state (EOS).*** On-and-off Hugoniot Multi-phase EOS models as a function of P and T.
- ***Strength and Damage.*** Multi-phase strength, damage, and spall models as a function of strain rate, T, P, impulse shape, and length-scale.
- ***Ejecta.*** Multi-phase ejecta models as a function of drive, pressure, temperature, and environment.
- ***Interfacial Dynamics.*** Multi-phase interfacial dynamics models as a function of V, P, T, and interface conditions.
- ***Surrogates and Scaling.*** Use of surrogate materials and scaled experiments that isolate various dynamic behavior phenomena related to Pu.

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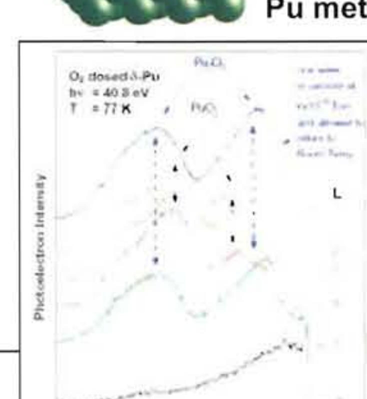
Objective 4 – Pu Surface Science

Improve our understanding of plutonium surfaces and interfaces.

Because plutonium is very reactive, its surfaces are easily affected dramatically and potentially catastrophically. Plutonium surface reactions are not sufficiently well understood to provide the predictive capabilities necessary for supporting nuclear weapons and energy applications.

Strategies

- ***Surface phase relationships.*** For corrosion reactions, the bulk phase diagram likely has little relevance to thin films of oxide in contact with metal. Thus, diffusion of electrons, oxide anions, and impurities (Ga, Am) are clearly important for understanding corrosion
- ***The science of reduced dimensionality.*** The role of impurities and defects on surface reactions at the solid-liquid and solid-gas interface. Of great importance for understanding of surface reactions of Pu in long-term storage, in corrosion of spent nuclear fuels and nuclear weapons



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Slide 13

Objective 5 – Advanced Chemical Separations

Develop advanced chemical separations for weapon's plutonium purification, advanced nuclear energy systems, nuclear forensics, and environmental management.

Strategies

Fundamental knowledge of bonding in fluid phases could revolutionize our capabilities to design more selective extraction systems.

New process & separations chemistry for new metal preparation processes with a smaller facility footprint, reduced waste generation, and a domestic supply of Am.

New separations processes for nuclear fuel cycles using alkaline solutions, ionic liquids or soft donor ligands to minimize proliferation risks, and allow for Pu burning to reduce inventories.

New ultra micro-scale radiochemical separations processes for plutonium and other actinides for nuclear forensics applications

Pilot demonstration for processing Challenging Material. Nearly 13 MT of excess Pu exist with significant chloride impurities can be processed using a chloride process developed for recycle of weapon's plutonium from molten salt operations.

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Slide 14

Objective 6 – Nuclear Energy Systems

Develop innovative nuclear energy systems.

Providing science and technology to help change a decades-old industrial paradigm, create viable, safe, long-term options for waste management, and develop technology and architectures that further strengthen the nonproliferation regime.

Nuclear Fuels and Materials for higher power operation, higher burnup, minimization of proliferation risks, and provide new options for waste management strategies.

Modeling and Simulation multiscale, multidimensional and predictive models for nuclear fuels, materials, separations, safeguards, fuel casting, balance of plant.

Materials Management and Control MPC&A technologies, international frameworks for nonproliferation and security, and the development of risk assessment tools and methods

Used Fuel and Waste Management actinide and environmental science to develop new waste forms and repository concepts

Innovative Reactor Designs such as pairing Th/Pu fuel with fast reactor technology to reduce Pu inventories for proliferation risk reduction.

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Slide 15

Objective 7 – Detection and Analysis

Expand our capabilities in detection and analysis of nuclear and radiological materials. This technical basis will define the approach to next generation safeguards, forensics, and treaty verification.

Strategies

- ***Improve the fidelity of nuclear data*** and enhance theory and modeling capability in fundamental nuclear processes involving Pu.
- ***Next generation nuclear material characterization***. Signatures from single particles to bulk quantities; advanced laboratory & field based NDA and DA technologies for next generation safeguards and treaty verification.
- ***Signature definition, analysis, and interpretation***: Establish the technical basis to model the evolution of "signatures" and devise methods for exploiting those signatures to gain knowledge.
- ***Nuclear detection challenges***. Stand-off detection, detection of shielded SNM, reducing "false positives" by increasing our focus on the integration of science, engineering and information management.

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Objective 8 – Plutonium Environmental Behavior

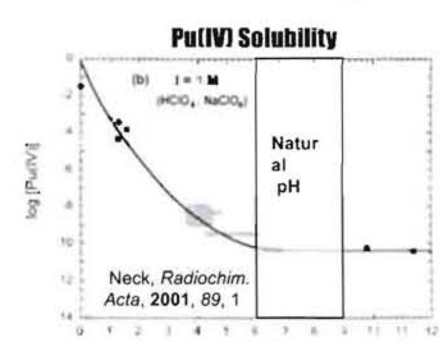
Improve our understanding of plutonium environmental behavior to ensure proper environmental stewardship of nuclear materials. Pu environmental behavior is an essential element of legacy cleanup, site selection and licensing new repository concepts.

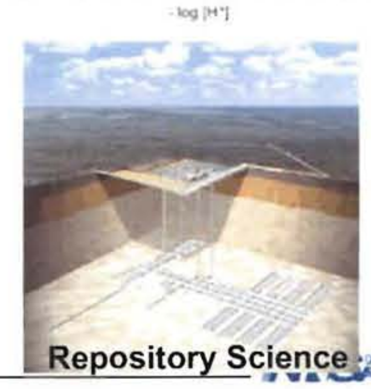
Strategies

Develop the fundamental knowledge of the chemical and physical processes of plutonium in natural systems. LANL is a unique test bed for study of plutonium behavior in natural environments.

Enhance the basis for nuclear energy production. Growth of nuclear power is coupled to waste management. New understanding of Pu behavior in geologic media is needed.

Plutonium corrosion and colloid formation has been implicated in Pu transport around the world. The mechanisms of formation, reactive behavior, and their physical properties remain inadequately studied and understood.





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Slide 17

Goal 2: Recapitalize the scientific infrastructure and unique capabilities for plutonium science, technology, and engineering.

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Slide 18

Objective 9 – Plutonium priority in LDRD

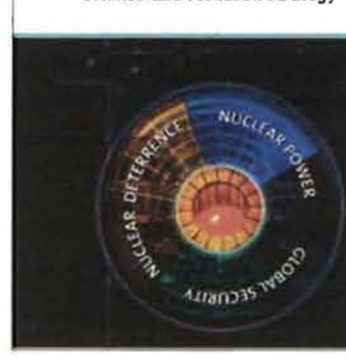
Re-establish an institutional priority for plutonium science in the Laboratory Directed Research and Development (LDRD) program. Driven by and consistent with the importance of plutonium to the national security mission of the NNSA Laboratories, establish an LDRD priority and define grand challenges for plutonium and actinide science.

Lifetime extension, nuclear energy, nuclear forensics, nuclear waste management, and re -manufacturing of plutonium pits represent serious technical challenges in the chemistry, physics and materials science of plutonium. Strengthening fundamental actinide science and engineering in a range of areas from molecular solution chemistry to materials science will be necessary to support these plutonium science missions.

Strategies

Engage actinide experts to define Grand Challenges and institutional priorities in plutonium science. Involve the scientific community as a whole to capture support from LDRD and other sponsors

plutonium
science and research strategy



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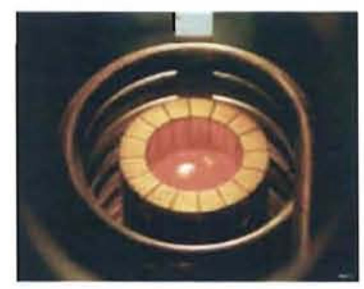
Slide 19

Objective 10 – Restore Scientific Infrastructure

Develop an integrated strategy to strengthen and restore plutonium scientific infrastructure. Maintain state-of-the-art infrastructure that provides research opportunities for world-class studies in plutonium science.

Strategies



Develop an instrumentation strategy to provide and maintain state-of-the-art instrumentation for world-class studies in plutonium science, to attract/retain future workers, and defines a recognizable endpoint with LANL distinguishable as a Plutonium Center of Excellence.

Establish a capability for research-quality alpha phase plutonium that is an essential starting point for a large number of experiments for many programs. Establish new capabilities for chill-casting, post-cast thermal or pressure processing, levitation zone refining, and levitation vacuum distillation.

Develop/establish a large single crystal capability for plutonium science. The ability to routinely prepare useful single crystals is essential for many studies. Investigate the feasibility of using strain-annealing and other crystal growth techniques for preparation of single crystals of plutonium alloys.

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Objective 11 – Special isotopes for small-scale R&D

Establish a small-scale plutonium research and development effort using Pu-242 and other scarce and unique materials and isotopes. Meaningful quantities of Pu-242 metal and alloys can be utilized in radiological facilities which function under lower security and lower hazard levels.

Strategies

- ***High purity alpha-phase Pu***. Develop new approaches to purify, process, and manage small lot samples of alpha phase plutonium metal. This will form the basis of a recycle/recovery/reuse program of Pu-242 metal for R&D studies.
- ***Isotope enrichment to increase stocks for R&D***. Re-establish isotope separation techniques to enrich the Pu-242 content to support a small-scale R&D effort.
- ***Explore use of Pu-244***. As a stretch goal, there are 65 Mark-18A targets containing Pu-244 in storage at SRS that represents ~90% of the world's inventory. Chemical and isotope separation could make these unique isotopes available as a national resource.

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Objective 12 – Pu Digital Library

Consolidate classified publication databases and provide a user friendly classified library, based on the LANL Unclassified Library archiving and search infrastructure. Building on the current isolated searchable databases (including classified databases) throughout the Laboratory (X, SMS, RFETS), utilize the preservation architecture to develop a classified plutonium digital library.

Strategies

Initiate a major archiving effort, resulting in a digital library on plutonium within nuclear weapons knowledge and information management program. This effort is tailored after an architectural design capturing nuclear test history and knowledge.

•Create demonstration system with 15,000 UCNI documents (Rocky Flats) on the unclassified Research Library network

•Deploy a "Research Library in the Red" system on the classified ESN (already underway – NNSA funded)

•Prioritize physical document collections for digitization

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plutonium science and research strategy

forensics • nonproliferation • safeguards • stockpile reductions • clean energy • deterrence • environmental stewardship

Goal 3: Increase workforce strength

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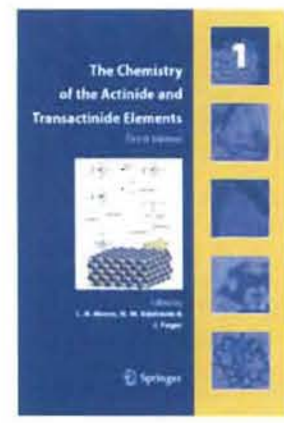
Objective 13: Promote Technical Work

Promote Technical Work, Accomplishments and Collaboration which Enhance LANLs External Visibility and Stature in Plutonium and Actinide Science.

Strategies include



- **Establish an annual Pu Science and Engineering Award**
- **Establish a Prestigious Visiting Scholar Position**
- **Maintain monthly Plutonium Working Group**
- **Foster the enhancement and preparation of foundational texts** in Pu/actinide science in critical areas such as nuclear non -proliferation, Pu or actinide chemistry and material science, etc.
- **Promote participation in national and international conferences** and enhance staff engagement in conference or workshop organizing committees and national review panels aligned with plutonium
- Track LANL publications and reports in plutonium and actinide
- **Continue sponsoring *Plutonium Futures – The Science* International Conference**

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Objective 14 – Promote education and training

Promote education and training for the future plutonium and actinide research and development workforce. Ensure the continued excellence of the Pu and actinide research workforce by training, recruiting and retention.

Strategies include

- **Establish a substantive (6-12 Mo) plutonium-focused science training school** to educate new staff or students on all aspects of the plutonium mission and establish mentor relationships.
- **Enhance plutonium-focused technical series** including workshops, tutorials, short courses and lectures,
- **Increase university interactions** through Seaborg/Institutes Office and promote strong collaborations with leading universities.
- **Identify funding opportunities for pipeline educational programs** (undergraduate to postdoctoral fellow) aligned with the LANL Plutonium Center of Excellence.
- **Increase the number of Postdoctoral Fellows** in Pu /actinide science, broaden the awareness of Seaborg postdoctoral fellowships program through outreach.

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Path Forward

We identify the following ***priority areas*** for investment that have the highest potential for immediate impact in a specific research or technology area.

- **Establishing an institutional priority for plutonium science** within our internal institutional investment program – Laboratory Directed Research and Development (LDRD).
- **Enabling small-scale plutonium research using plutonium-242**. Small-scale experiments with this isotope can be conducted in non-nuclear facilities to reduce the operational difficulties of working with plutonium, and enhance our academic interactions.
- **Consolidating publication databases**. Major archiving efforts have already been established, and we have captured tens of thousands of important reports from production sites such as Rocky Flats. We will develop a user friendly classified library, based on the LANL Unclassified Library archiving and search infrastructure.

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Progress has been made

A number of activities which are essential to this strategy have already been initiated, and significant progress has been made towards achieving our strategic goals:

An NNSA Plutonium Enterprise Strategy has been initiated to assure that plutonium facilities and technical base are sustained.

CMRR Radiological Laboratory/Utility Office Building (RLUOB) is nearly complete, and will provide essential radiological laboratory space for small-scale research on Pu, classrooms and simulations laboratories central to our strategy.

CMRR Nuclear Facility will replace aging facilities while better protecting the health and safety of workers, the public, and the environment.

Branches of the Glenn T. Seaborg Institute have been established to integrate research programs, promote external visibility, and promote education and training of students, visiting scientists, and faculty in actinide science.

A National Security Education Center with partner universities has been established to enhance recruitment and retention at the Laboratory.

The "Plutonium Futures – The Science" International Conference has been established to facilitate international dialogue on plutonium science.

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Our plutonium strategy will ensure we lead this important science for the nation

Foster support for a "Plutonium Center of Excellence"

- Reinvigorate Pu science and engineering
- Reestablish Pu science as a sustainable and desirable field of study
- Work with programs to insure greater investment in Pu science as a key component of sustainability
- Need greater emphasis on Pu science in LDRD process
- Success and priority for actinide science
- Manufacturing and actinide R&D share a symbiotic relationship at TA-55
- Provide intellectually stimulating work while sustaining core capabilities
- Reduce operational difficulties of working with Plutonium

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LDRD-DR Review: First Principles Predictive Capabilities for Transuranic Materials: Mott Insulators to Metals

R. Martin (T-1); J. Joyce (MPA-CMMS); A. Burrell, T. McCleskey, B. Scott (MPA-MC); S. Conradson (MST-8), S. Kozimor (C-IIAC); T. Durakiewicz (MPA-CMMS); E. Batista (T-1)

A first principles predictive capability for strongly correlated materials has long been problematic and is one of the grand challenges of electronic structure. Strong correlations manifest themselves in two closely related classes of materials: Mott insulators and correlated metals, both of which figure prominently in aspects of the LANL mission ranging from energy security to the weapons program. Over the past decade, significant progress has been made on the Mott insulator front by members of our team. The correlated metal regime remains a problem, and it is that void we address here. A serious effort to confront this problem requires a close integration and communication between theory and experiment. It demands single-crystal quality, well-characterized samples, experiments specifically chosen to probe the most basic and revealing aspects of electronic structure, and innovative new approaches from theory. Crucial elements have emerged in the past year placing this high bar within reach for materials containing transuranic elements central to the Laboratory mission. Unique capabilities at LANL now admit synthesis and characterization of single-crystal quality transuranic (hot) thin films, and very recent conceptual breakthroughs in theory suggest a practical path forward for the correlated metallic phase. Success in this project would remove the principal remaining roadblock standing in the way of a predictive capability for materials that rivals that available now for molecular systems and would significantly impact the fields of quantum chemistry, materials science, and condensed matter physics.

First Principles Predictive Capabilities for Transuranic Materials: Mott insulators to metals

LDRD/DR: October 1, 2009

Eve Bauer, A. K. Burrell, Quanxi Jia, M. McCleskey, B. L. Scott

Tomasz Durakiewicz, Kevin Graham, John Joyce
Steve Conradson, Patrick Kennedy, Stosh Kozimor

Enrique Batista, **Richard L. Martin,** Jianmin Tao, Tony Rappe (CSU)
Jason Ellis, Miguel Morales, Takeshi Tsuchimochi, Gustavo Scuseria (Rice)
Alberto Ambrosetti, Shi Guo, Kevin Rasch, Lubos Mitas (NCSU)

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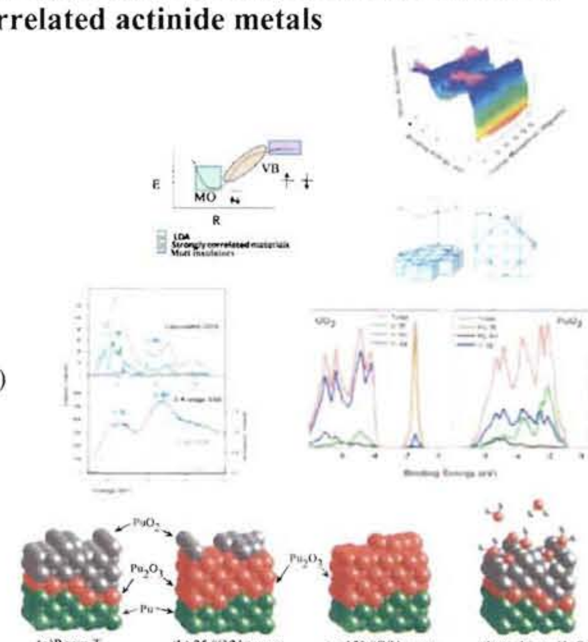
What do we want to do and why?

We wish to develop a first principles predictive tool to describe the electronic structure and behaviour of strongly correlated actinide metals

Why do this?
- none now exists: 'f-electron grand challenge'
- actinide materials at core of LANL mission
  - Pu Center of Excellence
- general tool needed
  - threat reduction (scintillators)
  - environmental contexts ($PuO_{2.25}$)
  - nuclear fuel cycles (UC, UN, UO_2),
  - weapons contexts (PuO_2, Pu_2O_3, δ-Pu)
  - radiation resistant materials

Why now?
- transuranic capability in PAD
- transuranic capability in ARPES
- transuranic capability in XAS
- conceptual breakthroughs in theory

Why us?
- capabilities unique to LANL



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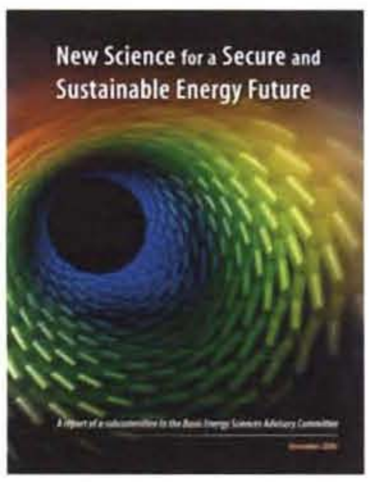
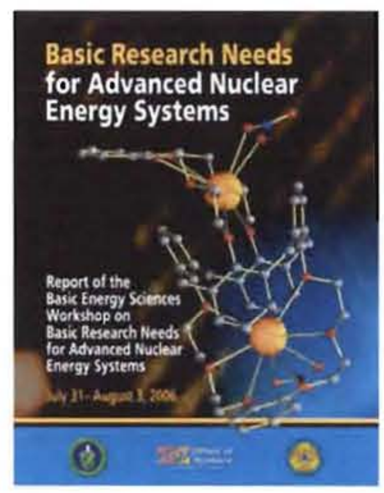
Significance



"The scientific challenge is to develop a well-formulated and predictive **first-principle theory** for relativisitic correlated *f*-electron materials and complexes" (p. 88, ANES)



"It will take 'dream teams' of highly educated talent, equipped with forefront tools, and focused on the most pressing challenges to increase the rate of discovery. To make progress most rapidly, these teams must work to close gaps between needs and **capabilities in synthesis, measurement, theory, and computation**" (New Science for a Secure and Sustainable Energy Future).

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The problem

Bristol (1937) : electrical conduction mechanisms

deBoer and Verwey : conductivity data
NiO, CoO, MnO, Fe_2O_3, Mn_2O_3, Mn_3O_4, Co_3O_4
all insulators – very surprising!
in ionic picture, all have partially filled d bands,
Bloch-Wilson band theory implies they should be metals

they suggested that when the barrier for tunneling between sites is large, there may be a critical range in which conductivity varies rapidly as a function of the barrier height

Wilson : noted the similarity with the sharp energy levels of the 4f electrons in rare earth compounds;

Peierls: suggested the Coulomb interaction between electrons caused them to localize on the cation sites, implying a drastic breakdown of band theory

Mott: chaired the conference, summarized these remarks for the published proceedings

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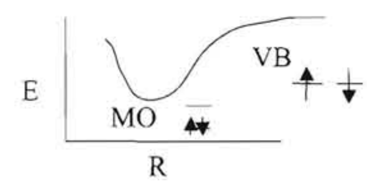
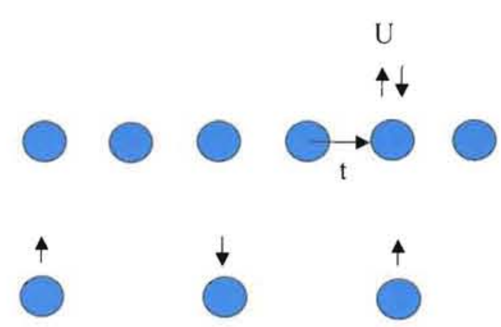
Mott insulators



Mott (1949); Hubbard (1955)
on-site electron–electron repulsion

molecular orbital vs. valence bond limit:
competition between delocalization and Coulomb repulsion
hopping (t) vs. on-site U

H_n



t/U large;
delocalized (metal)

t/U small;
localized (insulator)
Gap ~ U

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Mott insulators and conventional DFT

	Δ_{LDA}	Δ_{exp}	m_{LDA}	m_{exp}
$CaCuO_2$ (d^9)	0.0	1.5	0.0	0.65
CuO(d^9)	0.0	1.4	0.0	0.65
NiO(d^8)	0.2	4.0,4.3	1.0	1.7,1.9
CoO(d^7)	0.0	2.4	2.3	3.4,3.8
FeO(d^6)	0.0	2.4	2.3	3.3
MnO(d^5)	0.8	3.6-3.8	4.4	4.6,4.8
La_2CuO_4(d^9)	0.0	2.0	0.0	0.5
$LaTiO_3$(d^1)	0.0	0.2	0.0	--
UO_2(f^2)	0.0	2.0	0.0	1.7

LDA: yields metals as opposed to insulators;
when it supports a gap it's usually too small
same holds for GGA, meta-GGA

Alternatives:
SIC Perdew and Zunger, PRB **23**, 58(1981).
LDA+U Anisomov, et al., PRB **44**, 943(1991).
GWA Hybertsen and Louie, PRL **55**, 1418 (1985).

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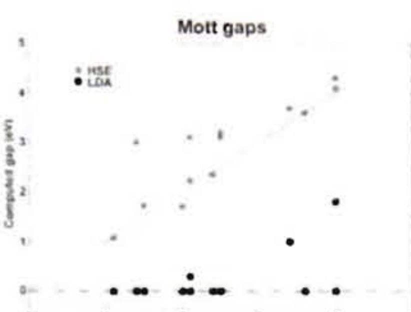
Progress and problems with density functional theory (DFT)

Hybrid DFT: Becke (1993)
4th generation functional
includes component of full, nonlocal HF exchange

PBE0, HSE:

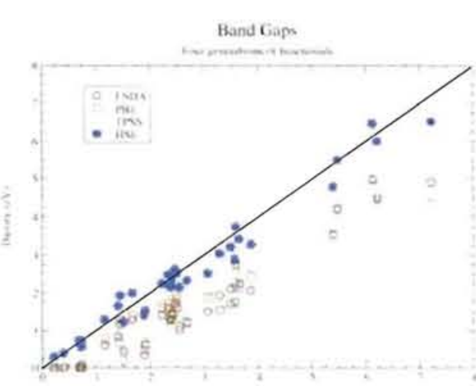
$$E_{xc} = [\, 1/4\, E_x^{HF} + 3/4\, E_x^{PBE}] + E_c^{PBE}$$

revolutionized molecular quantum chemistry
solids: improved gaps, lattice constants, magnetic properties, densities-of-states, optical spectra, dielectric constants



L. E. Roy, R. L. Martin, and G.E. Scuseria (2008):

MnO, FeO, CoO, NiO, CuO $CaCuO_2$, La_2CuO_4, $LaCrO_3$, $LaMnO_3$, $LaFeO_3$, $CeBr_3$, Ce_2O_3, UO_2.



Heyd, Peralta, Scuseria, and Martin, JCP **123**, 174101 (2005).

SC-40 bandgaps(eV)

	LSDA	PBE	TPSS	HSE
Mean absolute error:	1.136	1.127	0.977	0.263

hybrid DFT suggests UO_2 quite ionic; PuO_2 covalent
appears to have problems with correlated metals;
I-M in MnO; PES of UPt_3, UN

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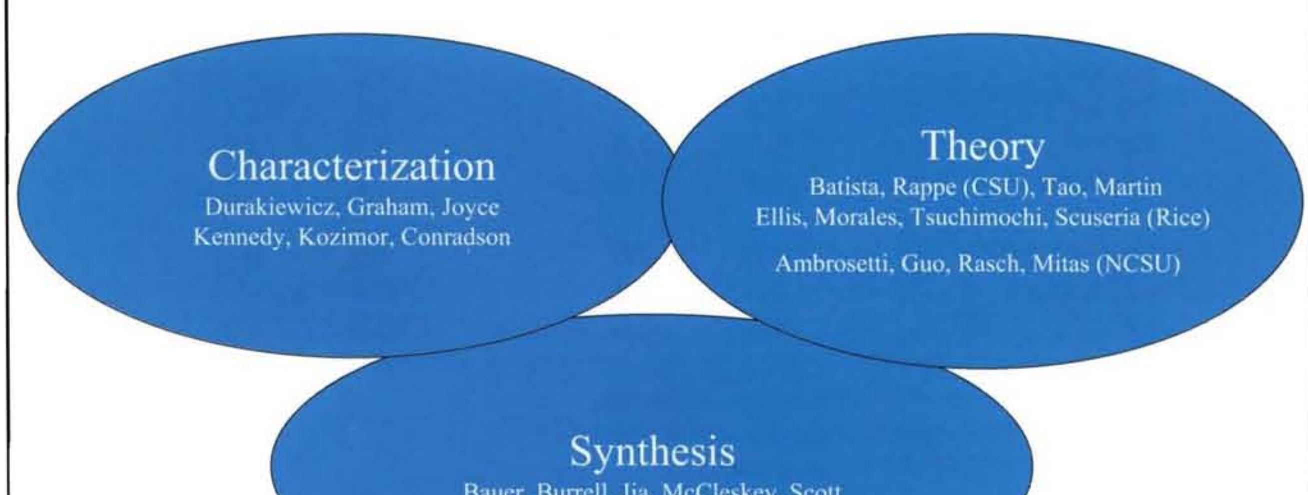
The team

We propose to synthesize and characterize AnC, AnN, AnO_2 (An=U, Np,Pu) thin films, a series which spans correlated metals -> Mott insulator, and to develop a fifth generation "functional" capable of treating the correlated metal



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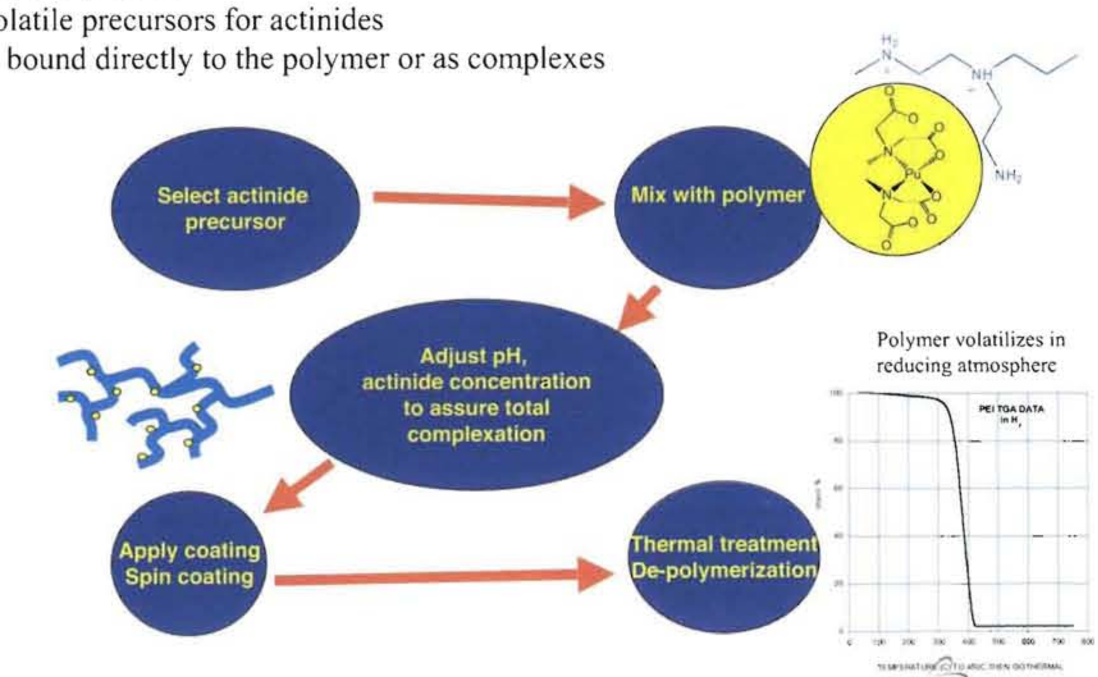
Polymer Assisted Deposition (PAD)

Eve Bauer, Tony Burrell, Quanxi Jia, Mark McCleskey

- Water-based process
- Non-volatile precursors for actinides
- Metals bound directly to the polymer or as complexes



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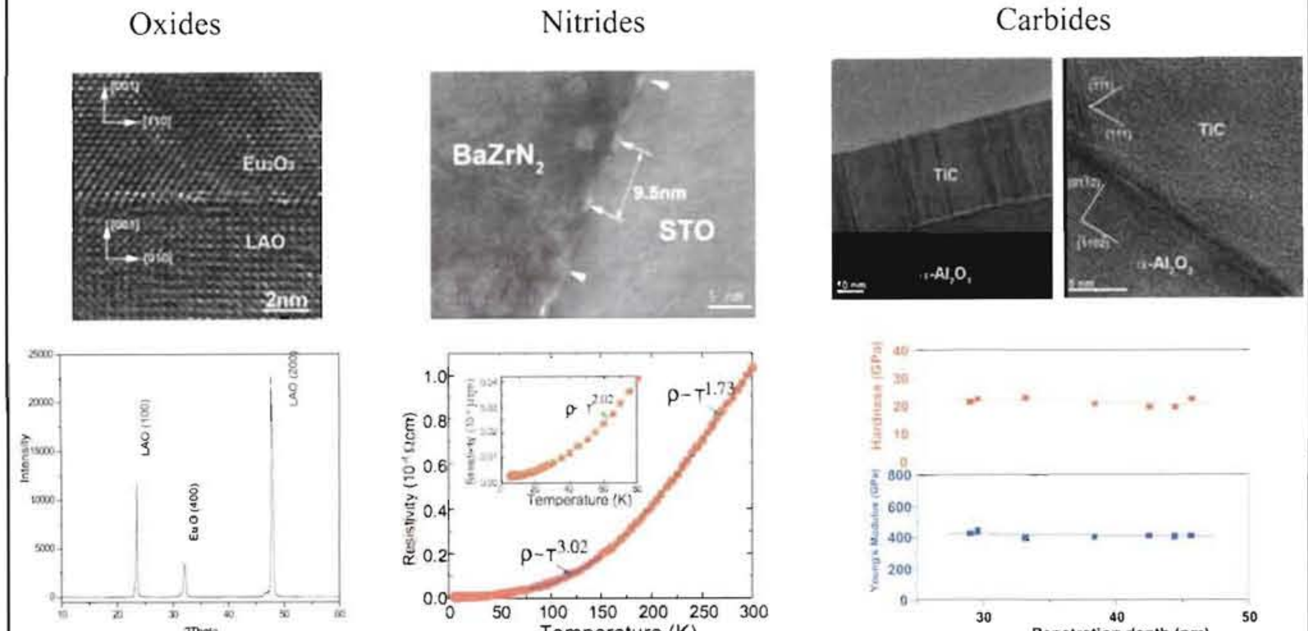
Epitaxial Films by PAD

Versatile solution route with control of stoichiometry

Oxides Nitrides Carbides



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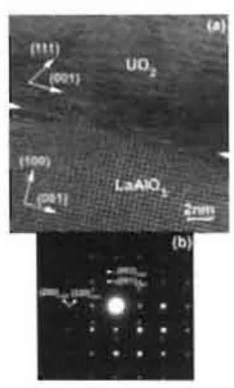
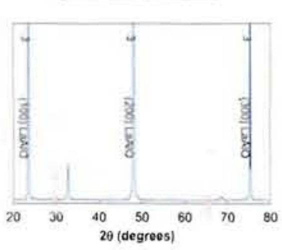
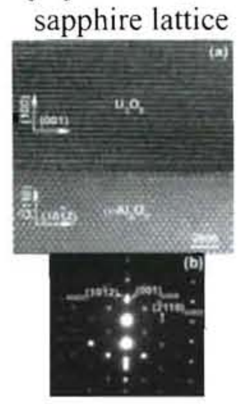
Control of Valence State

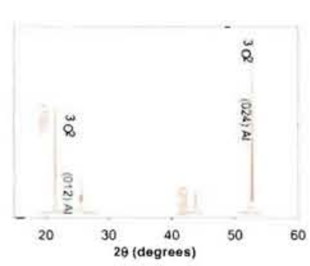
UO_2 on LAO lattice



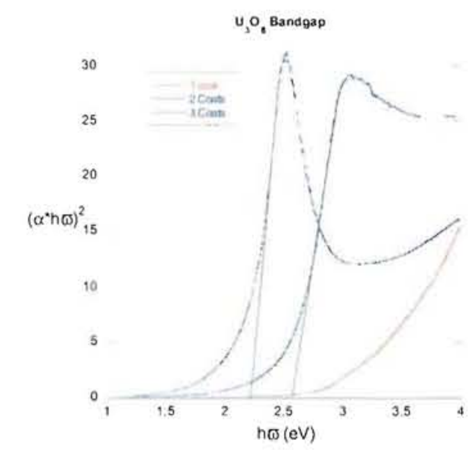


U_3O_8 on hexagonal sapphire lattice





First single crystal quality samples of U_3O_8 allow for measurement of band gap



2 coats 2.55 eV
3 coats 2.21 eV
Thy (HSE): Δ = 2.2eV

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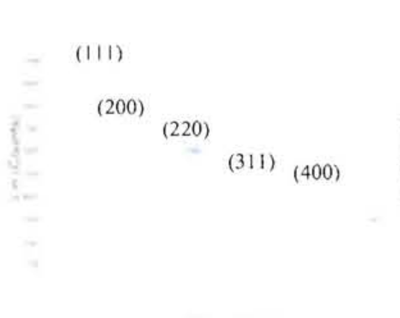
Substrate Influence on Epitaxy of NpO_2 Films

Buffer layers deposited by PAD can help

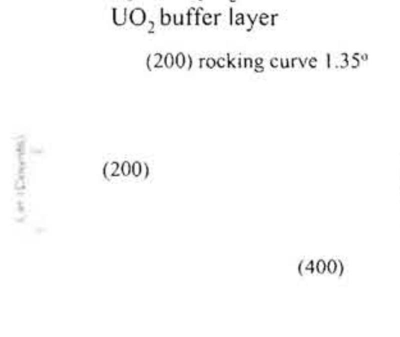
Lattice match and surface termination are important

Best films obtained on YSZ

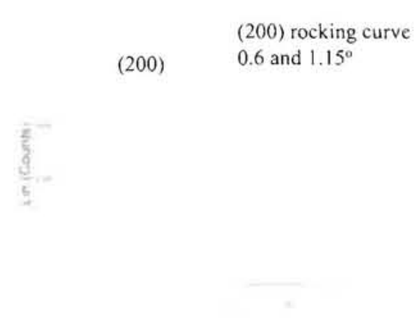
Polycrystalline NpO_2 on LAO



Aligned NpO_2 on LAO with UO_2 buffer layer



Aligned NpO_2 on YSZ



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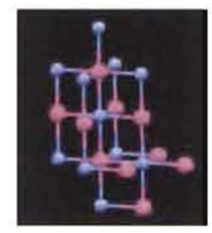
Approach to Nitrides

UN_2 obtained on LAO, N appears to come from EDTA

UN_2 on LAO (400)



UN_2

U_2N_3

UN

	Lattice
UN_2	5.30
UN	4.89
LAO (45°)	5.37
YSZ	5.13

Can UN_2 -> UN in the thin films?

Typically as one heats UN_2 -> U_2N_3 -> UN

UN_2 and UN lattices are both cubic

contraction of the unit cell

nitrogen moves from O_h to T_d sites

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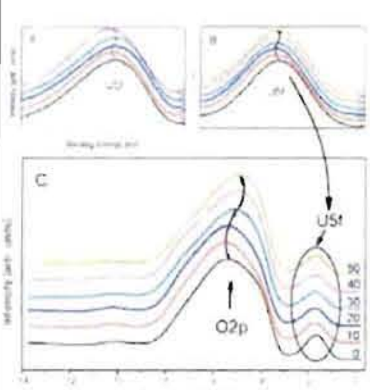
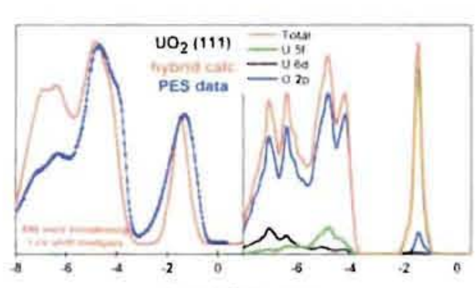
Photoemission

Tomasz Durakiewicz, John Joyce

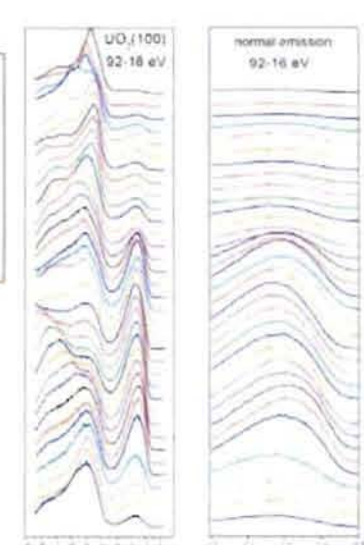


A.K. Burrell, *et al., Adv. Mater.*, ***19**, 3559–3563 (2007)*



L.E. Roy, *et. al*, J. of Computational Chemistry **29**, 2288(2008)

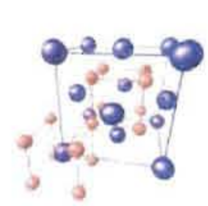
Hybrid DFT in excellent agreement with experiment



J.J. Joyce, *et. al,* Mat. Res. Soc. Symp. Proc. **986**, 35–40 (2007).

UO_2 single crystal ARPES equivalent to PAD sample

ionic solid;
small, but measureable dispersion



$R_{U-U} = 3.87A$

resonant PES:
peak near E_F : *f* character
normal emission => probing bulk

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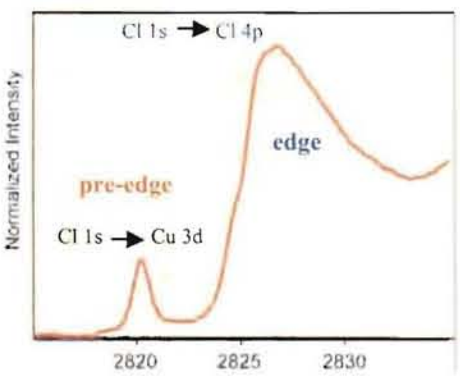
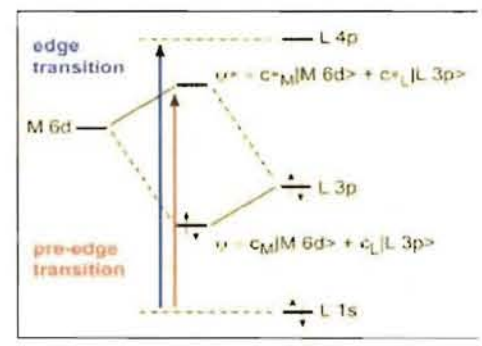
X-ray absorption measurements

Steve Conradson, Stosh Kozimor

Ligand K-edge XAS is a well-defined, quantitative probe of covalency in M-L bond

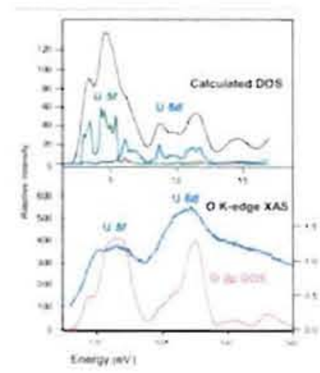


Cl K-edge XAS: $CuCl_4^{2-}$



$\sigma_{1s,\psi^*} \sim |< Cl_{1s} | r | \psi^* >|^2 \sim c_L^{*2} |< Cl_{1s} | r | Cl_{3p} >|^2$

Good agreement for UO_2
-- will provide details of bonding interactions in AnC, AnN, AnO_2



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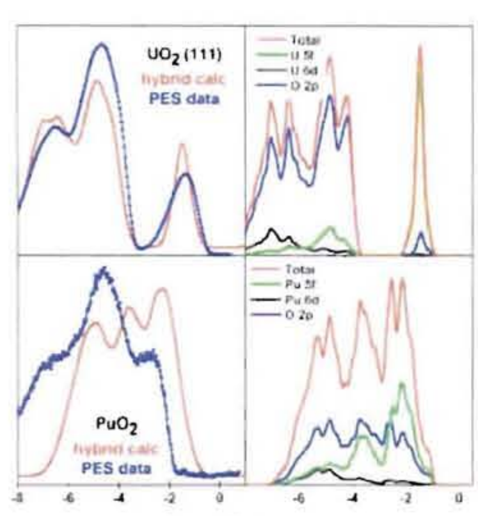
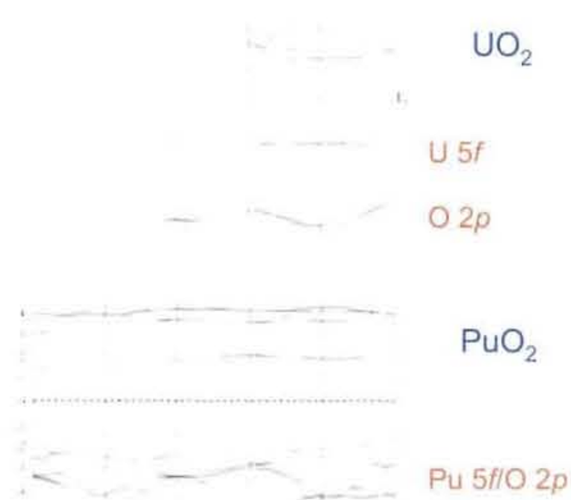
Goal 1: Test ionic vs. covalent behavior predicted in AnO_2





UO_2 looks like typical ionic solid; very little dispersion

$\Gamma \rightarrow X$; 190meV calculated; 130meV measured

PuO_2 shows much more hybridization; stronger band dispersion

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Goal 1: Epitaxial PuO_2 Films on YSZ

c-axis oriented - only 200 and 400 peaks

extremely high quality epitaxy - rocking curves 0.05°

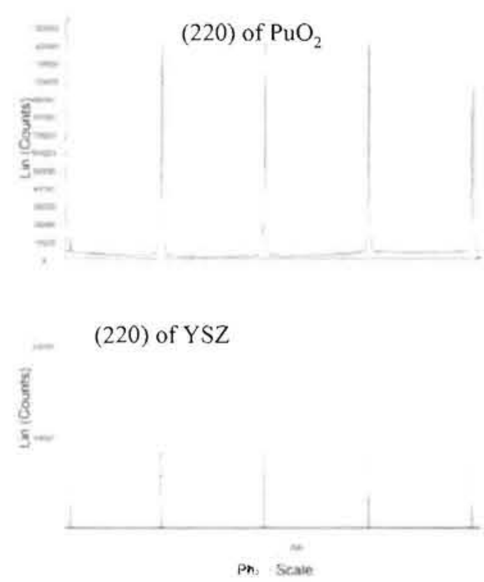
in plane orientation shown by Phi scan

(200) rocking curve 0.05°
shoulder – YSZ substrate

(400) rocking curve 0.05°
shoulder – $K\alpha_2$ line

(220) of PuO_2

(220) of YSZ



Phi Scan for in plane orientation

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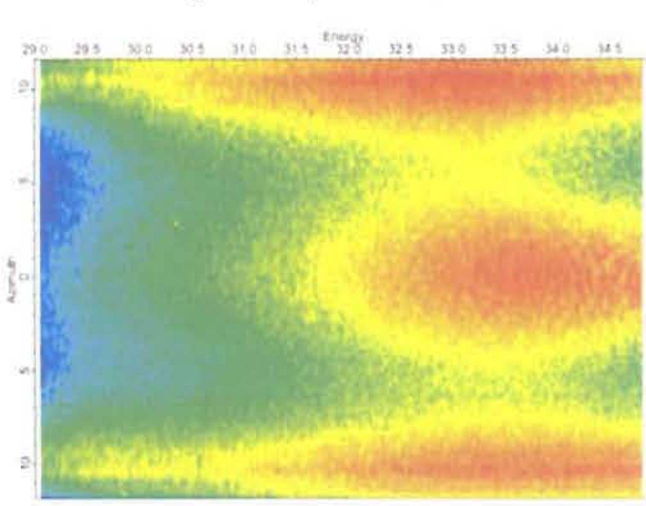
Goal 1: Photoelectron Spectroscopy for PuO_2

preliminary measurements



- Model predicts strong hybridization in Pu
  - merging of O 2p and Pu 5f
  - significant dispersion
- 1st ARPES shows **k**-dep. and hybridization

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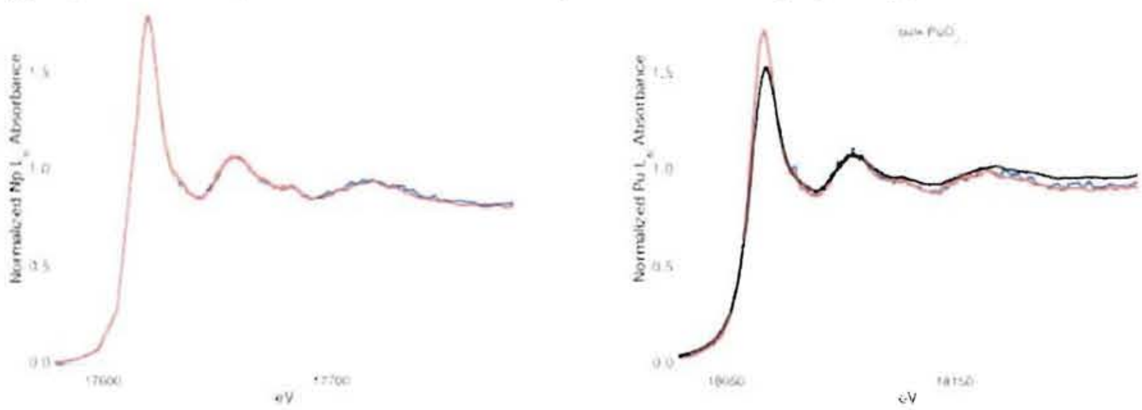
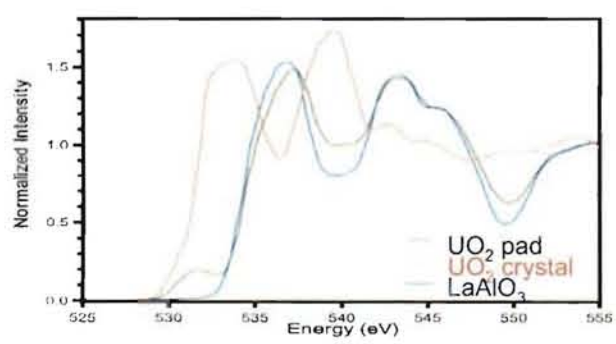
Goal 1: XAS for PuO_2

M $L_{2,3}$ edge: Good agreement between bulk sample and films for NpO_2, PuO_2 (YSZ)





O K-edge: UO_2 films (LAO):
substrate visible
(go to grazing incidence)
PuO_2 scheduled for June

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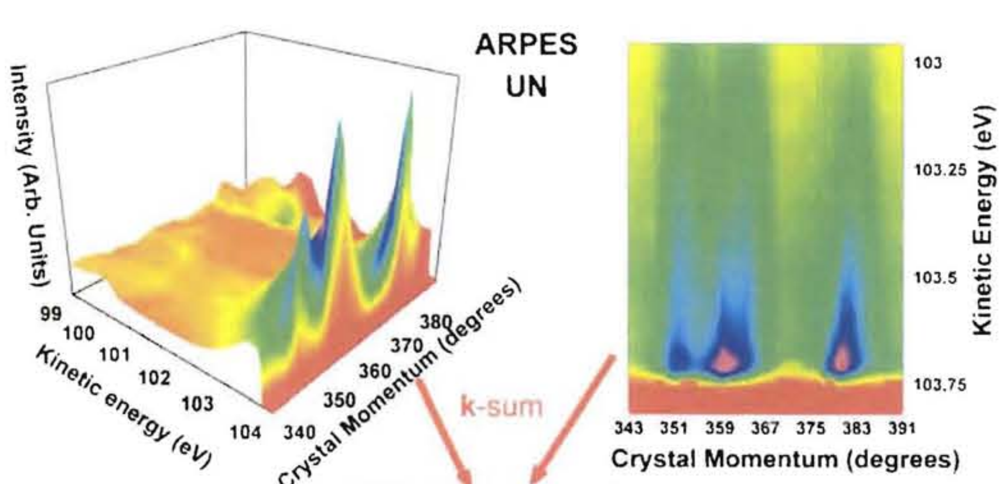
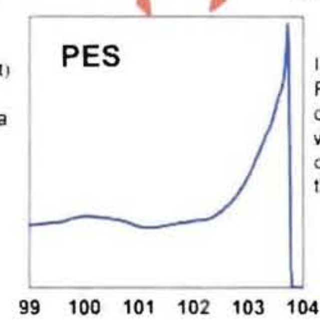
Goal 2: Correlated Metals



Basically, the PES spectrum (right) is the sum of the 25 independent E vs. **k** spectra in the ARPES data set (above)



In a one-electron picture, conventional PES relates the energy distribution curves to a density-of-states (DOS) while ARPES, which includes the crystal mometum (**k**) compares with the full band structure (E vs. **k**).

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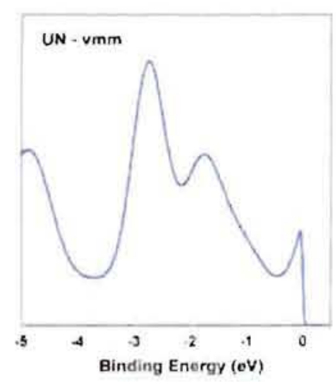
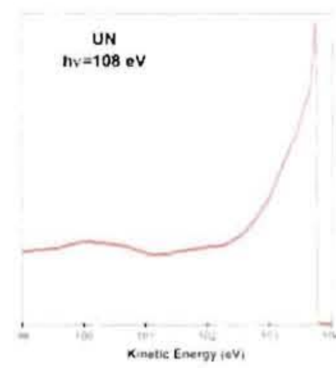
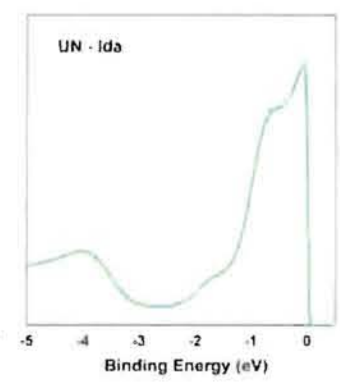
Goal 2: Correlated Metals



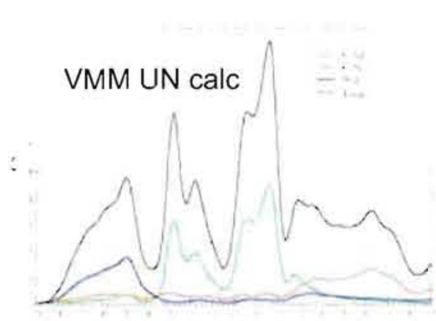
HSE (occupied DOS)



PES
U 5*f* component enhanced at 108eV



LDA(total DOS)



HSE (partial DOS)

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Theory efforts

Correlated metals

Functional development (Rice) DQMC extension (NCSU)

Applications (LANL)

Rice: investigating DFT/RPA in molecules; extending to solids
developing Hartree-Fock-Bogliubov / DFT method (**coupled pair mean field theory**)

NCSU: Diffusion Quantum Monte Carlo (DQMC): our gold standard;
extension to actinides completed;
in progress:
calculations on Cp_2AnL_2 (L=Cl, OH, NH_2, CH_3)
developing spin-orbit capability

LANL: accumulating experience with HSE for correlated metals:
in progress: AnN, AnN_2, An_2N_3; An = U, Np, Pu
HSE investigation of IM transition in VO_2
hybrid DFT calculations on Cp_2AnL_2 (L=Cl, OH, NH_2, CH_3)
developing pair/multiplet/DFT approaches

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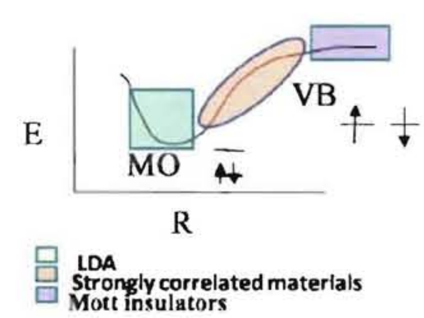
What is hybrid DFT missing?

DFT is a one-electron, **single determinant** approximation.
it cannot account for
proper magnetic correlations
Kondo singlets
multiplet states
Cooper pairs



Magnetic correlations:
$\Psi = \sigma^2 - \lambda\sigma^{*2}$
@ R_e $\lambda \sim 0$
@ large R $\lambda \sim 1$

Another problem DFT cannot do:
Van derWaals interaction:
He_2 at long distance;
arises from simultaneous dipole-dipole fluctuation
double excitations

$\Psi =$ $He_A(1s^2)$ x $He_B(1s^2)$ repulsive

$+ \alpha\, He_A(1s2p)$ x $He_B(1s2p)$ attractive

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How do we put these correlations in?

DFT/RPA (Rice)

Adiabatic connection fluctuation-dissipation theorem:
yields formally exact expression for E_c
depends on **frequency dependent density-density response $\chi_\lambda(\omega, x_1, x_2)$**
approximate χ in the RPA

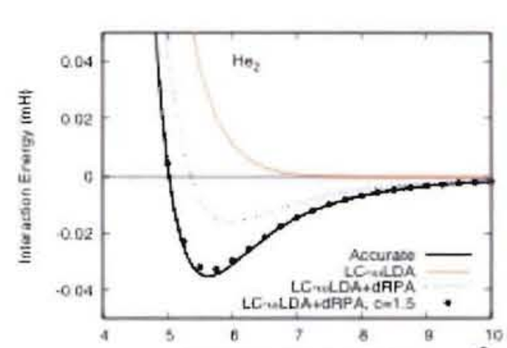
Langreth and Perdew, Solid State Comm. **17**, 1475 (1975) N
Furche, JCP **129**, 114105 (2008) N
Scuseria, et al, JCP **129**, 231101 (2008) N
equivalence of RPA with coupled cluster doubles (CCD) approach
continues theme of coupling DFT with wavefunction techniques

A path for hierarchical improvements to DFT now seems practical

THE JOURNAL OF CHEMICAL PHYSICS 130, 081105 2009
Long-range-corrected hybrids including random phase approximation correlation
Benjamin G. Janesko, Thomas M. Henderson, and Gustavo E. Scuseria

$$E_{xc} = E_{xc}^{\text{SR-LSDA}} + E_x^{\text{LR-HF}} + c_{\text{RPA}} E_c^{\text{LR-RPA}}. \quad (6)$$

Will screen HF exchange dynamically



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How do we put these correlations in?

GVB / DFT (CSU, LANL): preliminary

Generalized Valence Bond Theory:

include magnetic correlations through **multi-determinant reference state**

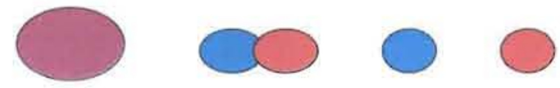
Ensemble DFT: Kait and Hoffmann, JCP **120**, 5005 (2004).

multi-determinantal reference allows us to treat multiplets

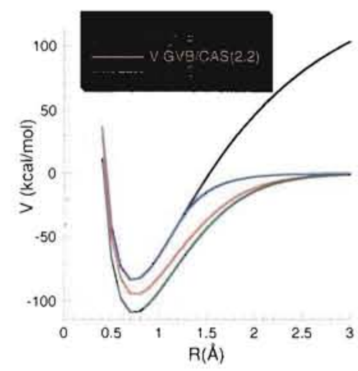
Magnetic correlations: $\Psi_{GVB} = (\phi_g\phi_g - \lambda\phi_u\phi_u) \quad (\alpha\beta-\beta\alpha)$

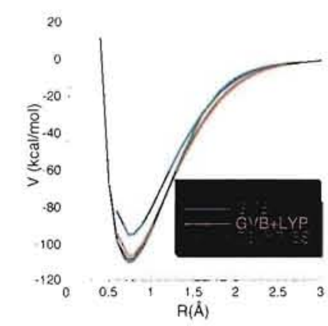
$= (\phi_g + \lambda_i^{1/2}\phi_u)(\phi_g - \lambda_i^{1/2}\phi_u)(\alpha\beta-\beta\alpha)$

$= \phi_1 \quad \phi_2 \quad (\alpha\beta-\beta\alpha)$



$\lambda=0$ $\lambda\sim 1/2$ $\lambda=1$





GVB:

$\Psi_{GVB} = A\,[\text{core}]\,\Pi_{i\,\varepsilon\,\text{active}}(\phi_i^2 - \lambda_i\phi_i^{*2})(\alpha\beta-\beta\alpha)$

antisymmetrized product of geminals

simple "one-electron" energy expression

GVB/DFT

add E_c and correct for overcounting

$$E = 2\sum_{i=1}^{nocc} f_i h_{ii} + \sum_{i,j=1}^{nocc}\left(a_{ij}J_{ij} + b_{ij}K_{ij}\right) + E_c(\rho) + \sum_{k=1}^{nactive} f_k\left[E_k^{self}(\rho_k) - E_k^{field}(\rho_k)\right]$$

$a_{ij},\ b_{ij} = f(\lambda)$

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How do we put these correlations in?

GVB / DFT : **preliminary**

Multiplets: Carbon atom (s^2p^2)

^3P: $\frac{1}{\sqrt{2}}(x\bar{y} + \bar{x}y)$, $\frac{1}{\sqrt{2}}(x\bar{z} + \bar{x}z)$, $\frac{1}{\sqrt{2}}(y\bar{z} + \bar{y}z)$

^1D: $\frac{1}{\sqrt{2}}(x\bar{y} - \bar{x}y)$, $\frac{1}{\sqrt{2}}(x\bar{z} - \bar{x}z)$, $\frac{1}{\sqrt{2}}(y\bar{z} - \bar{y}z)$, $\frac{1}{\sqrt{2}}(x\bar{x} - y\bar{y})$, $\frac{1}{\sqrt{6}}(x\bar{x} + y\bar{y} - 2z\bar{z})$

^1S: $\frac{1}{\sqrt{3}}(x^2 + y^2 + z^2)$

$$E = 2\sum_{i=1}^{nocc} f_i h_{ii} + \sum_{i,j=1}^{nocc}\left(a_{ij}J_{ij} + b_{ij}K_{ij}\right) + E_c(\rho) + \sum_{k=1}^{nactive} f_k\left[E_k^{self}(\rho_k) - E_k^{field}(\rho_k)\right]$$

Slater: tabulates atomic couplings: F^k, G^k
others easily derived

O: s^2p^4

Method	ΔE (ev) ^1D	ΔE (ev) ^1S	$\langle S^2 \rangle$ $M_s=1$	$\langle S^2 \rangle$ $M_s=0$
UHF	1.02		2.006	1.007
UBLYP	0.69		2.003	1.002
UB3LYP	0.73		2.002	1.002
ROHF	2.17	4.39	2.0	0.0
ROHF+LDA	1.84	3.34	2.0	0.0
ROHF+LYP	1.95	4.17	2.0	0.0
ROHF+TPSS	1.97	4.20	2.0	0.0
Exp. (J_{ave})	1.97	4.19	2.0	0.0

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Summary

Synthesis:
- PuO_2 synthesized; structure determined;
- U_3O_8 synthesized and gap measured; excellent agreement with theory

PES:
- UN ARPES completed;
- PuO_2 measurement in progress;

XAS:
- UO_2, NpO_2, PuO_2 (An $L_{2,3}$-edge) XAS in films compared to bulk (SSRL);
- UO_2 (O K-edge); will go to grazing incidence (June, LBNL)

Theory:
- AnN calculations progressing; GVB/DFT pair/multiplet approximations promising
- progress at Rice with DFT/RPA and Bogliubov/DFT pair approximations;
- DQMC for actinides in place; will begin with molecular bond energy benchmarks

Follow-ons:
- NNSA Pu Science Strategy (Dave Clark)
- BES (John Sarrao)
- Nuclear Energy programs (Sara Scott)

Los Alamos

Pentavalent Uranium: Capturing a Rare Oxidation State with Synthetic Chemistry

J. Kiplinger (MPA-CMMS)

For more than three decades, the actinide community as a whole considered pentavalent uranium compounds unstable towards redistribution to tetravalent U(IV) and hexavalent U(VI) species. The existence of pentavalent uranium has been debated; the few existing systems were discovered serendipitously and could not be reproduced. This left a noticeable gap in the uranium electronic continuum as these single-electron systems provide fertile ground for not only advancing theoretical capabilities, but also our fundamental understanding of actinide electronic structure, reactivity and bonding. However, a series of reports in 2007-2009 by our actinide chemistry team systematically overturned these long-held tenets by developing various routes—oxidation, salt metathesis, protonolysis or insertion—for synthesizing a suite of previously unknown U(V) complexes. These discoveries allowed us to collect a large amount of previously unavailable information on the chemistry and electronic structure of this rare oxidation state. The international impact of this work was substantiated by the explosion of activity in the field and large volume of follow-on papers on pentavalent uranium chemistry from other groups around the world. This work not only transformed pentavalent uranium chemistry, but also reinforced LANL's leadership role in actinide science.

Actinide Compounds with Soft Donor Ligands

A.J. Gaunt, S.D. Reilly, I. May, S. Kozimor (C-IIAC); E. Batista (T-1); M.P. Neu (ADCLES); B.L. Scott, J.M. Boncella (MPA-MC); A. Enriquez (PMT-10); G. Jarvinen (ADSMS); T. W.Hayton, D. Schnaars (UCSB); J.A. Ibers (Northwestern); K.I.M. Ingram, N. Kaltsoyannis (UCL)

Increasing our understanding of the structural preferences, reactivity, bonding and electronic preferences in actinide containing molecular compounds is of central importance to the design and implementation of advanced nuclear fuel cycle separation technologies and radioactive waste remediation strategies.

At LANL, we have a synthetic transuranic coordination chemistry capability dedicated to small-scale fundamental research and development activities, including a very rare example of a negative pressure inert atmosphere glovebox containing plutonium. We have focused upon studies of actinide metal complexation to soft donor atom ligands because extractant molecules containing N and S donor atoms have displayed a marked preference for actinide versus lanthanide selectivity with no proven explanation for this behavior. One of our primary aims is to elucidate bonding properties and differences in a systematic fashion across the 5f and 4f metals, and across a series of N, S, Se, and Te donor ligands. In addition, we are seeking to expand the available suite of non-aqueous transuranic precursors to facilitate more in-depth studies of soft donor bonding across the Np, Pu, Am actinide ions. We are moving towards adopting a multi-disciplinary approach (synthesis, structural analysis, spectroscopy, computational modeling) in an attempt to provide an unambiguous evaluation of the extent of covalency in the metal-ligand interactions and the relative participation of the 5f and 6d valence orbitals.

The ultimate goal is to be able to utilize the chemical bonding knowledge learned from our research to help guide ligand design for actinide selective chelators that will be suitable for novel separation processes in next generation fuel cycles.

Near-infrared Photoluminescence and Ligand K-edge X-ray Absorption Spectroscopies of $AnO_2Cl_4^{2-}$ (An: U, Np, Pu)

M.P. Wilkerson (C-NR); E.R. Batista, R.L. Martin (T-1); J.M. Berg (PMT-1); D.L. Clark (INST-OFF); S.D. Conradson (MST-8); S.A. Kozimor(C-IIAC); B.L. Scott (MPS-MC)

We have used photoluminescence and x-ray absorption spectroscopies to investigate electronic structures and metal-ligand bonding of a series of $AnO_2Cl_4^{2-}$ (An = U, Np, Pu) compounds. Recently, we reported the first observation and preliminary details of near-infrared photoluminescence from a plutonyl ion. Emission spectra measured between 6,000 and 10,000 cm^{-1} reveal more complicated spectra for $PuO_2Cl_4^{2-}$ than $NpO_2Cl_4^{2-}$ in terms of the number of transition peaks, which is consistent with the greater number of electronic states available to the plutonyl ion. Analyses of time-resolved photoluminescence decay waveforms measured from $PuO_2Cl_4^{2-}$ suggest complex decay kinetics. Ligand K-edge x-ray absorption spectroscopy (XAS) affords the opportunity to quantify the degree of covalency and assess the relative roles of 5f and 6d orbitals in actinide metal-ligand bonds. We will present XAS measurements and analyses of spectra collected from $UO_2Cl_4^{2-}$ and $PuO_2Cl_4^{2-}$ ions.

Alpha, Beta and Gamma Plutonium: Three Different Metals

Y. Suzuki, V.R. Fanelli, A. Migliori, J.B. Betts (MPA-CMMS); J. M. Mitchell, M.Ramos, F. Freibert (MST-16); C. H. Mielke (MPA-CMMS)

The elastic moduli of pure polycrystalline beta Pu were measured using resonant ultrasound spectroscopy between 415 K (above the transition from the alpha phase) and 491 K (below the transition to the gamma phase). Results will be compared with the elastic moduli of the alpha and gamma phases, measured on the same specimen, as well as the gallium-stabilized delta phase. The bulk modulus lies between those of the alpha and gamma phases as expected, but it has unusually small temperature dependence unlike that previously reported for the beta phase. The shear modulus is surprisingly nearly continuous between the beta and gamma phases. The Poisson's ratio shows typical metallic behavior. Overall, the elastic moduli we measured have higher values than any previous measurements, an indication of the higher quality of our sample.

New Actinide Intermetallics: Insight into the Role of f-electrons in Strongly Correlated Electron Materials

P.H. Tobash, E.D. Bauer, F. Ronning (MPA-CMMS); J.N. Mitchell (MST-16); J.A. Kennison (MPA-STC); B.L. Scott (MPA-MC); J.D. Thompson (MPA-CMMS)

The discovery of new strongly correlated electron materials is an essential piece of the materials strategy at LANL. Continuing the long-standing emphasis on discovering emergent phenomena and novel phases of matter through new materials, such as the discovery of heavy fermion superconductivity in UBe_{13}, UPt_3, and $PuCoGa_5$. We present the crystal structure and physical properties of three new actinide-containing intermetallic compounds, UIr_4Al_{15} and $Pu_2M_3Si_5$ (M = Co, Ni). The compounds have been synthesized from molten flux growth reactions and their crystal structures were established from single-crystal x-ray diffraction. UIr_4Al_{15} was found to be isostructural with the $NdRh_4Al_{15.4}$ structure type in the tetragonal space group $P4_2/nmc$ while $Pu_2M_3Si_5$ crystallized with the $U_2Co_3Si_5$-type in the orthorhombic space group Ibam. All three compounds exhibit heavy fermion behavior as suggested from the moderately enhanced Sommerfeld coefficient reaching approximately ~100 mJ/mol U(Pu)-K^2. Magnetic susceptibility studies reveal that UIr_4Al_{15} undergoes antiferromagnetic order at ~ 20K while the Pu-containing compounds show more complex magnetic ordering with successive antiferromagnetic and ferromagnetic transitions. Ultimately, these new compounds help us better understand the nature of the 5f electrons in strongly correlated electron materials.

Atomistic Modeling of the Corrosion of Actinides by Hydrogen

C.D. Taylor (MST-6); T. Lookman (T-1); R.S. Lillard (MST-6)

The introduction of hydrogen from the environment into metals can lead to performance reductions via surface pitting, spalling, embrittlement mechanisms, cracking and catalysis of void formation. The challenges associated with tracking hydrogen in a material are considerable, and are compounded when the focus is narrowed to the actinide materials. For these reasons atomistic modeling is a competitive tool for probing the mechanisms associated with hydrogen corrosion of actinides. By using density functional theory to evaluate hydrogen interactions with uranium and plutonium surfaces, intrinsic defects (vacancies, local strain) and chemical impurities, the energy barriers associated with the intermediate states associated with the hydriding reaction can be directly computed. Through the use of this technique we find that the trapping of hydrogen in defect states of uranium is critical for the nucleation of hydrides in the material, and that once this trapping state is formed, phase transformation is essentially a barrier-less process. Key defect states appear to be regions of local tensile strain (such as in the field of a dislocation, impurity states, or close to a grain boundary) as well as vacancies. The present modeling toolkit does not allow further selection between these sites, and new tools are presently being developed to allow extended molecular dynamics simulations of these defects in the larger materials context.

The Oxidation Characteristics of Plutonium in the Thin-Film Regime (< 0.05 m)

D.L. Pugmire, H.G. Garcia Flores, D.P. Moore, A.L. Broach (MST-16)

Historically, the oxidation/corrosion of plutonium has been studied by oxygen uptake inferred from mass gain measurements. Accuracy of these experimental setups likely limited measurements to oxide films thicker than ~ 0.05 to 0.1 m (50-100 nm). This is at the upper-limit of the thicknesses typically observed for oxide films on Pu metal substrates. The nature of these oxide films has historically been thought of as the growth of a dioxide (PuO_2) overlayer on the metal to a thickness at which the film begins to spallate (m's). It was later pointed out that thermodynamics argue for a thin layer of the sesquioxide (Pu_2O_3) at the dioxide/metal interface for thick oxide films. Several recent studies of the oxidation of plutonium with surface sensitive techniques under the controlled conditions of an ultra-high vacuum system concluded that the sesquioxide is present as a "transient" oxide layer during the initial stages of oxidation, or as a relatively thin layer at the oxide/metal interface. Significant questions remain as to whether these are realistic descriptions for the Pu-oxide, thin-film system.

X-ray photoelectron spectroscopy (XPS) is an ideal technique to study the surface of the Pu/oxygen system as the metal (0+), sesquioxide (3+), and dioxide (4+) species can be differentiated. In addition to information about the oxidation states of the plutonium species in the near surface region, XPS is also very useful for studying the relative atomic concentration of elements present at the sample surface. We are reporting our studies of the initial stages of plutonium oxidation with XPS. The results indicate that Pu_2O_3 can exist as a substoichiometric species on a metal substrate, and is probably best described as Pu_2O_{3-y}. It also appears that in this thin-film regime, PuO_2 exists as a relatively thin portion of the overall oxide-film thickness.

Resonant Ultrasound Spectroscopy Studies of Homogenization, Processing and Aging in Plutonium Alloys

T.A. Saleh, F.J Freibert, S. Richmond (MST-16); A. Migliori (MPA-CMMS)

Cast pucks of both alpha and delta plutonium were created as a part of R&D efforts at Los Alamos National Laboratory. The as-cast material was analyzed using a variety of characterization techniques, including resonant ultrasound spectroscopy (RUS), dilatometry and traditional microscopy. A brief overview of the experimental technique of RUS as it applies to plutonium will be presented. This poster will present the elastic moduli of alpha and delta phase plutonium alloys measured in as-cast and heat treated conditions. Furthermore, delta phase samples were loaded with hydrogen, and the impact on internal friction of inclusions and dissolved hydrogen on elastic properties will be presented. Sample quality, age, density and alloy content will be compared to the mechanical properties of plutonium alloys measured using this technique, focusing on changing properties as a function of homogenization and age.

New Synthetic Routes to Actinide Materials

M. McCleskey, A. Burrell (MPA-MC); Q. Jia (MPA-STC); R. Martin (T-1); J. Joyce (MPA-CMMS)

We have developed new routes for preparation of actinide materials. These materials are prepared in either bulk powders or ordered thin films. We use solution routes for the formation of order films of the actinide oxides and nitrides and unique fluoride based approaches for the formation of bulk nitride materials. These synthetic routes enable the formation of high purity materials with controlled composition by avoiding the use of carbothermic reactions conditions. The low temperature processing and high quality of the materials will enable accurate determination of many physical and electronic properties that are harder to obtain for materials prepared using other synthetic methods.

Irradiation Effects in a Multi-layer Dispersion Nuclear Fuel Surrogate

I.O. Usov, J.A. Valdez, J. Won, S. Valone, Y. Q. Wang, K.E. Sickafus (MST-8); R.M. Dickerson (MST-6); D.J. Devlin (MST-7); G.D. Jarvinen (ADSMS)

One of the promising directions in the development of new nuclear fuel forms is a transition from traditional single phase fuels such as UO_2 to fuel elements consisting of at least two phases: fissile and non-fissile phases. Dispersion of fissile components in a non-fissile matrix or alternatively, using non-fissile inclusions, may improve important properties of a nuclear fuel element, such as thermal conductivity, hardness and fracture toughness, diffusional release of fission gases, and corrosion resistance. Oxide ceramic materials are considered to be very attractive for use as non-fissile phases. Many radiation effects studies of ceramic oxides under conditions simulating nuclear reactor environments as well as in-pile irradiations have been reported. However, the majority of these studies were conducted on monolithic, single-phase materials.

The purpose of this study is to investigate ion irradiation effects in a dispersion nuclear fuel surrogate represented by MgO and HfO_2 thin film multi-layer structures. The HfO_2 is intended to simulate the fissile, UO_2 component of a dispersion fuel, while the MgO is intended to represent an inert matrix phase. To simulate radiation damage conditions in a nuclear fuel pellet, we irradiated our multi-layer structures with 10 MeV Au ions over a wide range of fluences and irradiation temperatures. In the bulk of the multi-layer structures (away from the interfaces between the layers), we observed radiation effects typical of the individual constituents, primarily, grain growth in the MgO, monoclinic-to-tetragonal phase transformation of the HfO_2, resistance to amorphization. On the other hand, structural changes such as formation of voids and amorphous regions were observed at the MgO/HfO_2 interfaces, even though MgO and HfO_2 individually do not show a tendency to void formation or amorphization upon irradiation.

Our conclusion is that irradiation effects in composites, consisting of dissimilar materials, are not always derived simply from their individual components. Therefore, irradiation effects in composites need to be investigated separately.

Microstructured Advanced Fuel Forms: Theory

X.-Y. Liu, S. Valone, C. Jiang, K. Sickafus (MST-8); C. Reichhardt (T-1); B. Uberuaga, I. Usov (MST-8)

By combining theory with experiment, we have achieved an improved understanding of the feasibility of the dispersion fuel concept, conceived for ease of waste separation and fuel reprocessing. A critical issue in the dispersion fuel concept is the tendency of fission products to reside in one phase or another of the composite. We use density functional theory (DFT) based first-principles modeling to understand the behavior of fission products in the fissile and inert phases, and the interface between them.

We find a matrix cation size effect—an inert phase with larger cation size can accommodate fission products (Xe, Sr, Cs) more easily than phases with smaller cation sizes. The Hubbard model based spin polarized DFT+U calculations are used to calculate the defects properties associated with fission products accommodation in stoichiometric, non-stoichiometry UO_2 oxide, and UO_2/inert phase interfaces.

During nuclear operation, cascade damage as secondary events from a fission track will occur throughout the material. Some of that damage will take place at the interface between the fissile and inert phases. To coordinate with the materials in the experiments, simulation cells are composed of surrogate HfO_2 in the fluorite structure and MgO in the rocksalt structure. Molecular dynamics simulations of cascade damage across interfaces of these materials shows Hf cations becoming kinetically trapped in the MgO phase. When the primary-knock-on atom energy is above a few hundred eV in the direction of the interface, the propensity for trapping is very high. Under these same conditions, an Mg cation will occasionally become trapped in the hafnia. Complementary electronic structure calculations indicate that Hf cations are thermodynamically unstable in MgO. These findings are consistent with our recent transmission electron microscopy where amorphitization at the MgO-HfO_2 interfaces was observed.

Immobilization of Fission Products in Complex Oxides: Example $(Ln)_2Tc_2O_7$ Pyrochlore to Immobilize Tc-99

M. Tang, M. Zhou (MST-8); T. Hartmann (University of Nevada, Las Vegas), G.D. Jarvinen (ADSMS), K.E. Sickafus (MST-8)

We have synthesized several pyrochlore-structured complex oxides, intended as host materials for the sequestration of the long-lived radiotoxic fission product, technetium (Tc) 99. Specifically, we synthesized $Ln_2Tc_2O_7$ compounds using five different lanthanides (Ln): Pr, Nd, Sm, Gd, and Lu. We performed x-ray diffraction and crystal structure Rietveld refinements, in order to quantify the cubic lattice parameter, a, for each compound, as well as the degree of cation order and the oxygen parameter, x. We also performed density functional theory calculations in which we determined theoretical values for a and x in fully-ordered $Ln_2Tc_2O_7$ compounds. In this presentation, we will compare and contrast the experimental and theoretical results described above. We will examine changes in ionic partial charge as the Ln species is varied in our $Ln_2Tc_2O_7$ pyrochlore compounds.

Tab 4

Materials Dynamics

A. Zurek (MST-8)

The materials strategy of Los Alamos National Laboratory maintains a balance of advancing the science in three theme areas: emergent phenomena, extreme environments and defects. The three theme areas interface with the Laboratory's three mission areas: nuclear deterrence, global thread reduction and energy security. We believe that our large scale science combined with small scale science, and associated experimental and theoretical capability, bridging wide ranges of temporal and spatial length-scales, from atomistic to nanoscale to microscale, and ultimately to continuum, places LANL as the leader in all three research areas.

The materials dynamics session of this review will illustrate ongoing activities that evaluate the dynamic material properties mainly relevant to the science campaigns, which provide direct impact on the weapons programs (the Lab's nuclear deterrent mission). The materials programs relevant to energy security were reviewed last year, and programs relevant to global thread reduction are reviewed this year in a separate session.

The first talk will focus on "small scale" science experiments on metals and high explosives. The second talk will illustrate our current mechanistic understanding of dynamic microstructural evolution and resultant damage processes. These insights are crucial in the development of predictive models that can accommodate large strain and high strain-rate processes. The third talk will illustrate the benefits of "large scale" science, by illustrating the insights provided by proton radiography at the Los Alamos Neutron Science Center (LANSCE) accelerator. The poster session will feature examples of the integration of mathematical descriptions with experimental validation of models over a wide range of lengths and time scales.

Materials Dynamics

Anna K. Zurek, Group Leader of MST-8

Materials Science and Technology Division

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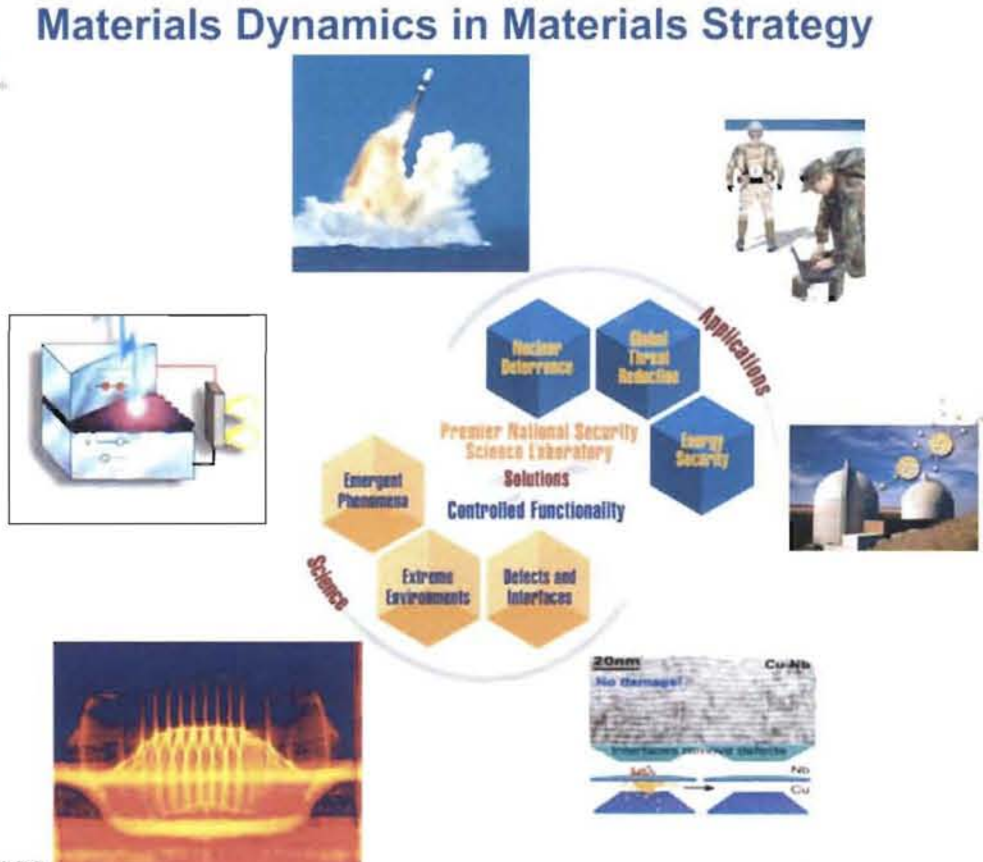
Materials Dynamics in Materials Strategy



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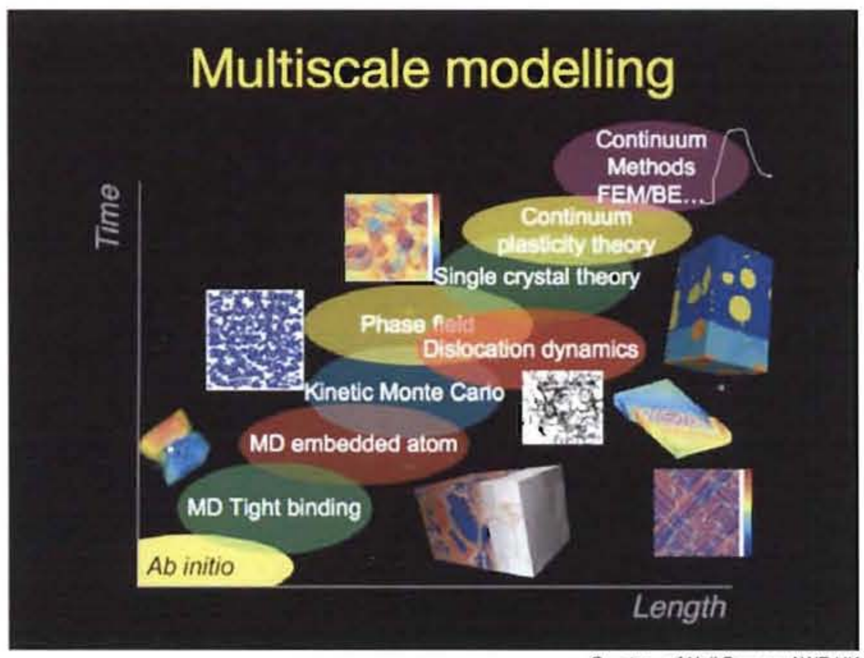
The response of materials at the continuum are linked to a behavior at the atomistic, nanoscale and microscale.



Courtesy of Neil Bourne, AWE UK

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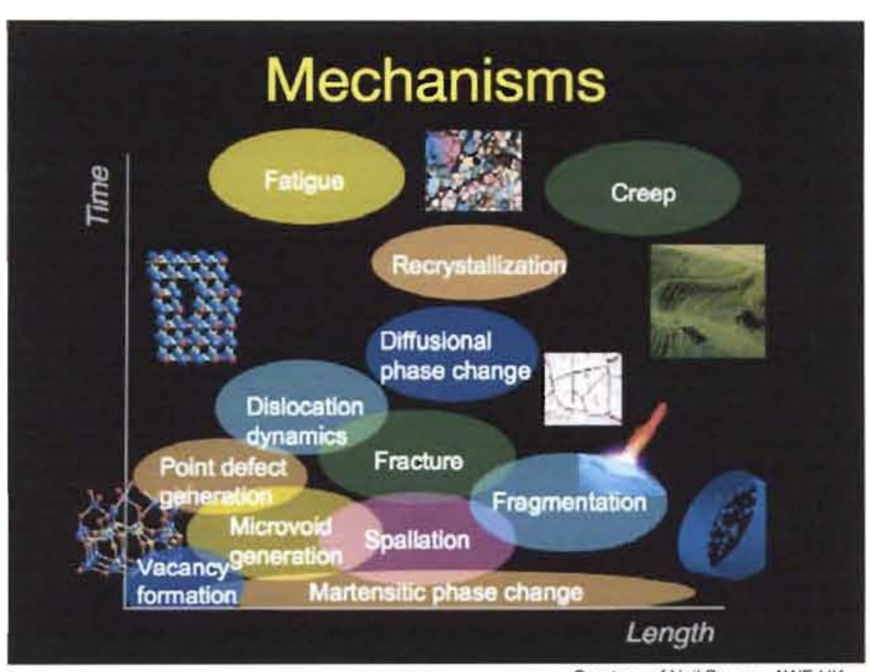
Verification of the multiscale modeling requires experiments ranging from small scale (gas guns) and integrated (p-Rad) tests.



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An Overview of Capabilities to Evaluate Dynamic Material Properties

R. Martineau (ADW)

The presentation will provide an overview of ongoing activities to evaluate the dynamic material properties of immediate interest to the science campaigns, which are provided directly to the weapons program. The overview will include the study of metals, high explosives, polymers and foams. The material presented is focused on obtaining the necessary thermodynamic data (equation of-state, phase diagram, etc.) and constitutive properties (spall, ejecta, yield strength, etc.) for materials and surrogates to the level of accuracy required to support the objectives of the stockpile program. The data are used to support our predictive capability framework and address uncertainties associated with stockpile certification.

An Overview of Capabilities to Evaluate Dynamic Material Properties (U)

Rick Martineau

Campaign 2 Program Manager

Materials Capability Review (U)

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Overview of LANL's Dynamic Materials Program (C2)

Objectives

- **Evaluate the dynamic material properties of**

plutonium, uranium, surrogates and other metal for strength, damage, failure, interfacial dynamics, EOS, phase transitions;

high explosives, foams and polymers for their influence of their dynamic properties on safety and performance of our weapon systems

Goals

LANL's dynamic materials program has both the breadth and depth to ensure the safety, security and reliability of the U.S. nuclear deterrent, reduce global threats, and solve other emerging national security challenges.

LANL's C2 Program funds over 50 groups in nearly 10 directorates

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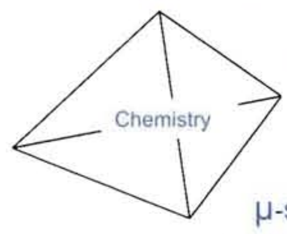
The stockpile materials are incredibly complex, each with a unique multiphase equation-of-state

1. Validation
2. Physics Insight
3. Fundamental data



Processing
- Wrought vs cast
- Heat treat

Properties
- mechanical properties
- damage evolution
- thermo-physical (EOS)
  - Mapping out the phase boundaries requires multiple capabilities
  - Complex loading allows one to sequentially probe multiple phases
  - A quantitative temperature diagnostic is key

μ-structure and loading
- microstructure and texture (grain size, phases)
- defects (twins, dislocations, voids, growth flaws)

MILESTONES

	FY11	FY12	FY13-15
EOS	• Obtain new data using the TA-55 gas gun	• Complete initial shock reshock experiments on cerium • Complete first set of high priority exp at Z • Provide baseline for EOS polymer data on existing and alternative materials	• Complete first experimental series using the large bore powder gun at U1a

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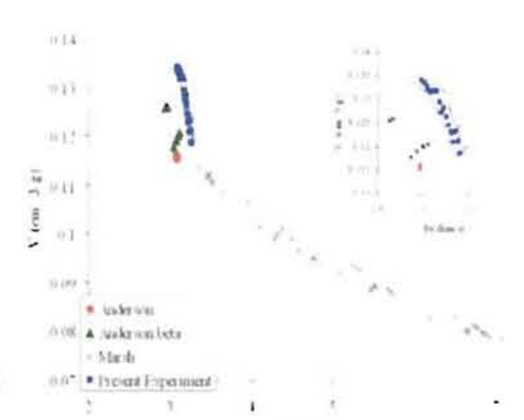
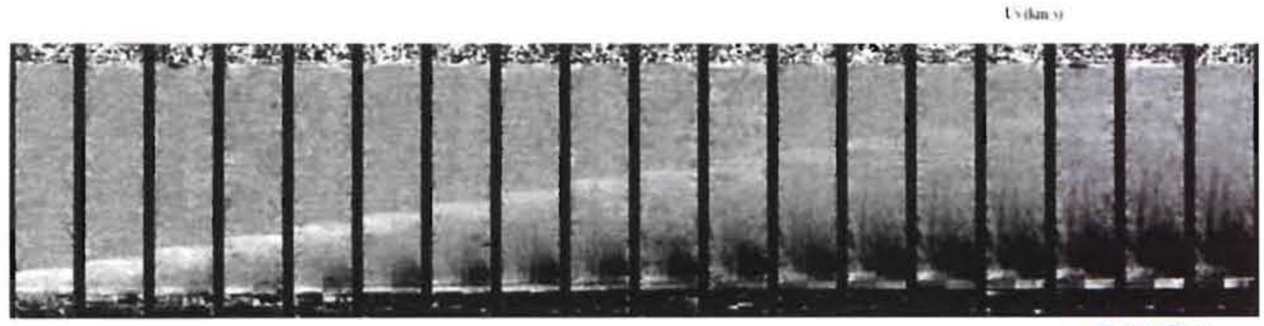
EOS

HE driven shock experiments with tin demonstrate a new technique to obtain EOS data at pRad (Schwartz)

- **Single experiment, provides multiple images to extract shock speed and density data, with 300 ns separation**
- **Technique will be useful for identifying phase transitions and may be applied to other materials of interest**
- **Imagine mapping out the entire hugoniot of material in one experiment**





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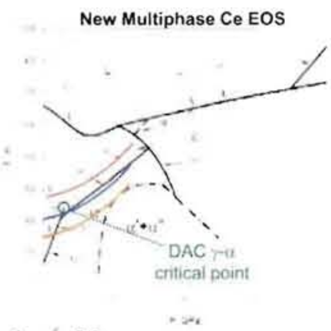
EOS

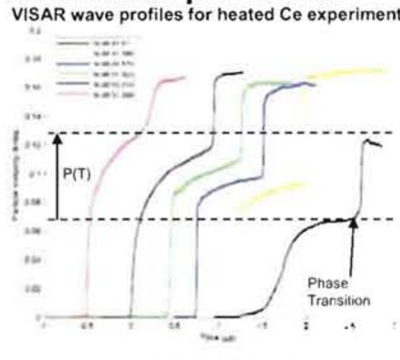
The gun impact experiments are used to locate phase boundaries off the principle Hugoniot for Cerium and other materials {Jensen}

- **Ce has a complicated phase diagram with multiple solid-solid boundaries.**
- **The low pressure γ-α boundary has been dynamically mapped using off-principle Hugoniot pre-heat experiments.**
  - Initial sample temperature ranged between 300K and 535K.
  - Phase transition stress increases with temperature.
- **The same low pressure γ-α boundary is also measured using shock-reshock experiments without pre-heat.**

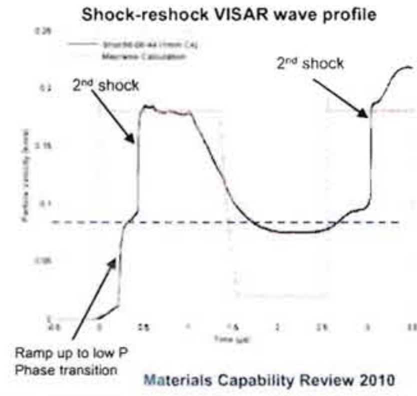
New Multiphase Ce EOS



VISAR wave profiles for heated Ce experiments



Shock-reshock VISAR wave profile



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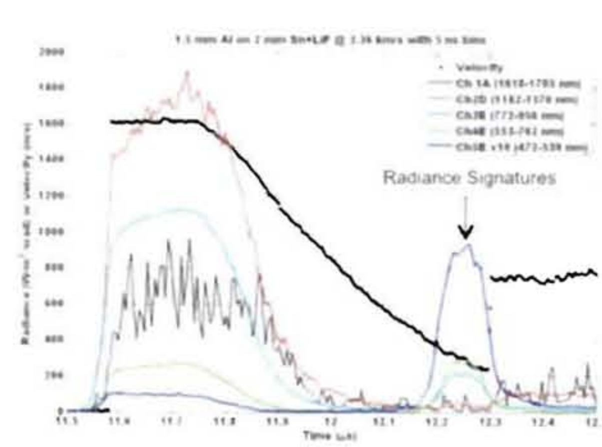
EOS

New diagnostics have obtained unique measurements of surface emissivity during a dynamic experiment {Holtkamp}

- **Experiments conducted using the 40 mm gun at Ancho Canyon**
- **Shock-release loading on tin**
- **Release off of the melt curve is readily apparent on multiple channels**
- **EOS calculations are consistent with measurements**
- **Calculated temperatures are within +/- 5% experimental uncertainty**
- **Broad application to dynamic events**



Resolving EOS uncertainties requires a quantitative assessment of temperature

Work conducted as part of an excellent collaboration between LANL, LLNL, and NSTec

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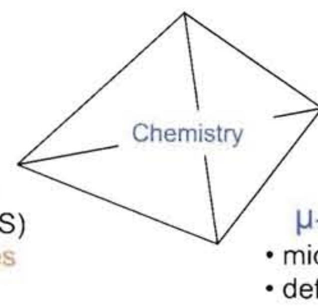
The dynamic behavior of a material obviously depends on constitutive properties, which in some cases are phase dependent

1. Validation
2. Physics Insight
3. Fundamental data



Processing
- Wrought vs cast
- Heat treat

Properties
- thermo-physical (EOS)
- mechanical properties
- damage evolution

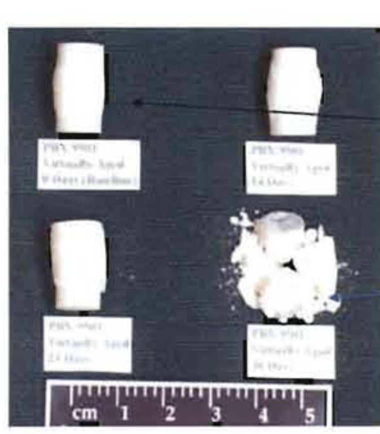
μ-structure and loading
- microstructure and texture (grain size, phases)
- defects (twins, dislocations, voids, growth flaws)

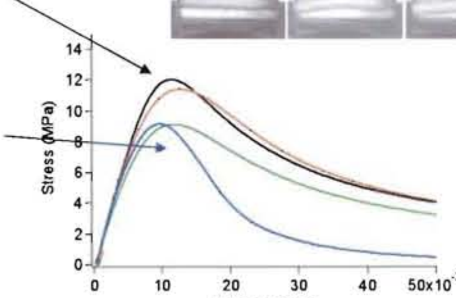
	FY11	FY12	FY13-15
Strength & Damage	• Initial assessment of extrusion using Ta and DU • Evaluate RT growth of Ta	• Complete initial strength and damage testing on Be • Complete report on Barolo Series	• Update phase specific strength using Kolsky and Quasi data • Assessment of phase specific spall using 40 mm • Deliver data on next generation HE thermal-mechanical and failure models

Prop & Damage

We are measuring the mechanical properties of artificially aged explosives {Idar}

- Compressive and tensile mechanical properties of plastic-bonded explosives (PBXs) and their constituents for physics based material model
- Taylor Anvil and SHPB testing of energetics, quasi-static testing of binders



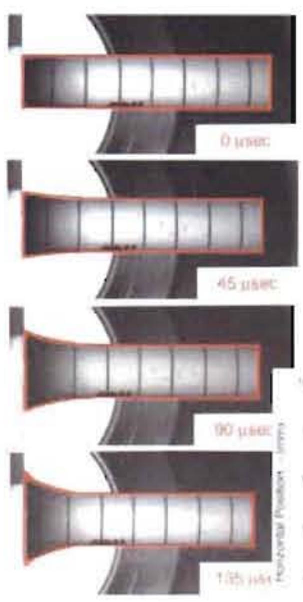


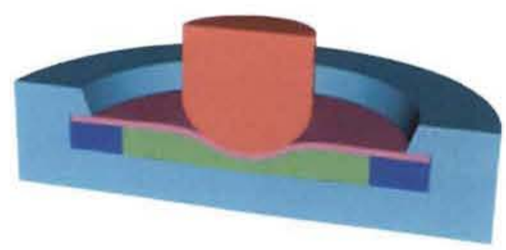
Used to baseline PBX continuum models for engineering assessments

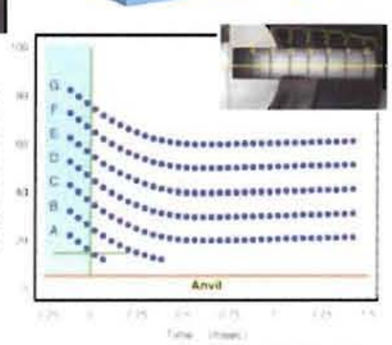
Prop & Damage

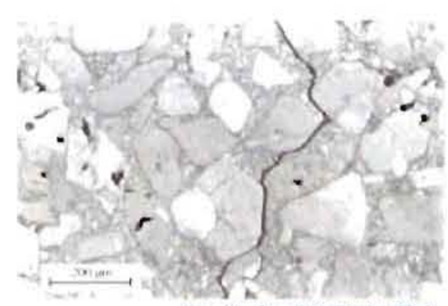
HE strength models are being developed to capture material response to load for dynamic response and initial conditions {Cheng-Lui}

ALE3D & Viscoscram simulations of experiments predict damage type, amount, location









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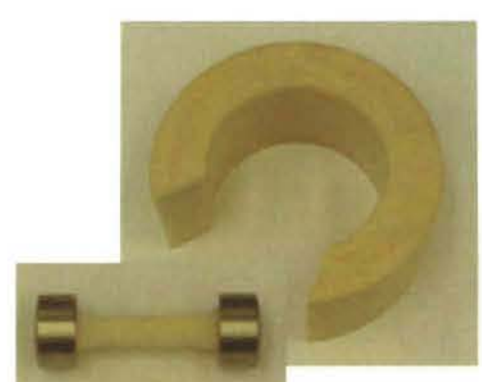
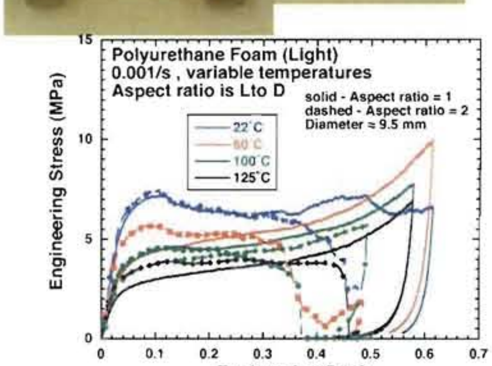
Prop & Damage

Compression and tension data of polyurethane foam informs constitutive models developed in stockpile systems {Dattelbaum/Cady}

- Polyurethane is a PMDI-based foam with initial density of 0.35 g/cm^3
- Compression tests performed at wide range of strain rates and temperatures
- Aspect ratio study in compression revealed different failure mechanisms
- Post-cure process resulted in apparent change in Tg
- There was no observable strain rate dependence in tension

Polyurethane foam mechanical properties are important for engineering assessments for existing and alternate material options and for material selection in future LEPs





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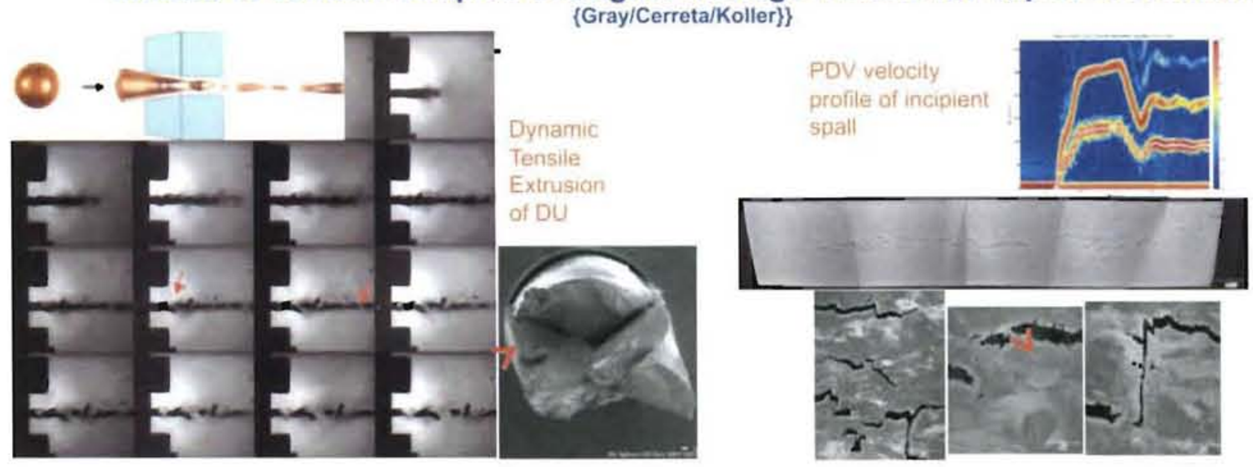
Prop & Damage

Dynamic tensile extrusion & incipient-spallation experiments are being utilized to validate coupled strength / damage models for depleted uranium

{Gray/Cerreta/Koller}}

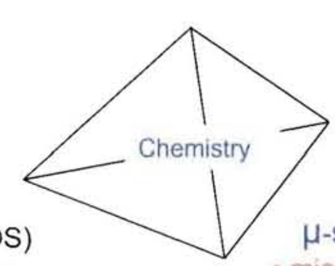


- Unlike Cu and Ta, DU appears to be shear dominated during dynamic extrusion
  - quasi-statically DU exhibits > 30% tensile strain to failure
- Incipiently spalled DU shows tensile cracking and severe plastic shearing often associated with inclusions
  - no evidence of microvoid formation and coalescence

Predictive modeling of dynamic damage evolution in DU requires complex shear processes to be described – these are currently not available in our models or codes

The dynamic behavior of a material obviously depends on chemistry, microstructure, physical properties and loading

1. Validation
2. Physics Insight
3. Fundamental data



Processing
- Wrought vs cast
- Heat treat

Properties
- thermo-physical (EOS)
- mechanical properties
- damage evolution

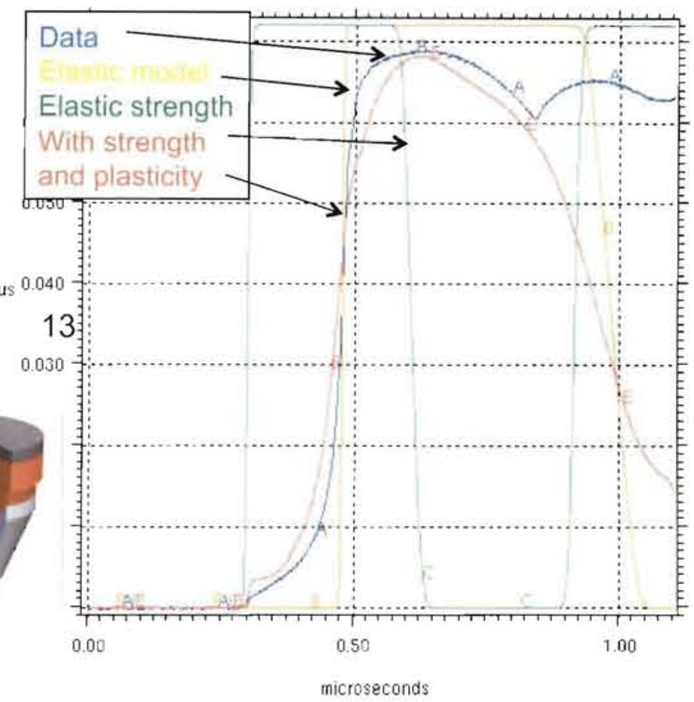
μ-structure and loading
- microstructure and texture (grain size, phases)
- defects (twins, dislocations, voids, growth flaws)

	FY11	FY12	FY13-15
μ-structure and loading	• Provide assessment of damage/drive relationship • Deliver high fi det and propagation data for confined geometries	• Complete second shock using Sn	• Provide damage data for Pu spall & inclusions

μ-structure

Beryllium under the relevant loading continues to challenge our understanding {Prime, Hull}

- **Our understanding of the EOS and yield strength for Be is relatively mature**
- **Damage under high pressure compressive loading remains a challenge**
  - Twinning, strongly rate dependent



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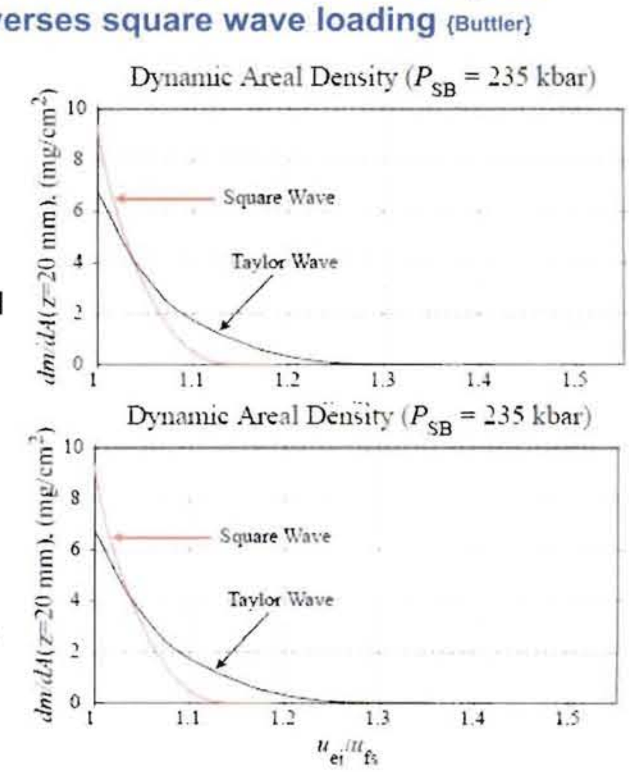
loading

Measured differences in mass and velocity distribution of ejecta production in Sn for Taylor verses square wave loading {Buttler}

- **Significant difference is observed in the mass distribution of ejecta for pressures greater than 21.5 GPa**
  - Similar mass distribution at low pressures
- **Comparisons of ejecta density indicates a different distribution based on the loading**
  - Difference is less obvious at lower pressures
- **Particle size distribution is likely to be dependent on the type of loading**
  - Would likely lead to different transport properties and breakup

Observations challenge our interpretation of the physics underlining ejecta production from gun experiments



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The dynamic behavior of a material obviously depends on chemistry, microstructure, physical properties and loading

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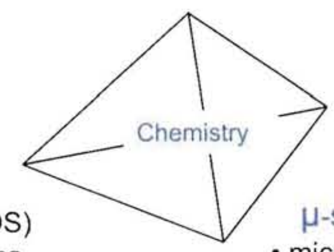

Processing
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Properties
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- damage evolution

μ-structure and loading
- microstructure and texture (grain size, phases)
- defects (twins, dislocations, voids, growth flaws)

	FY11	FY12	FY13-15
Processing	• Evaluate RT growth of TA	• Complete report on Barolo series • Deliver EC data for booster and main charge	• Provide damage data for Pu spall & inclusions

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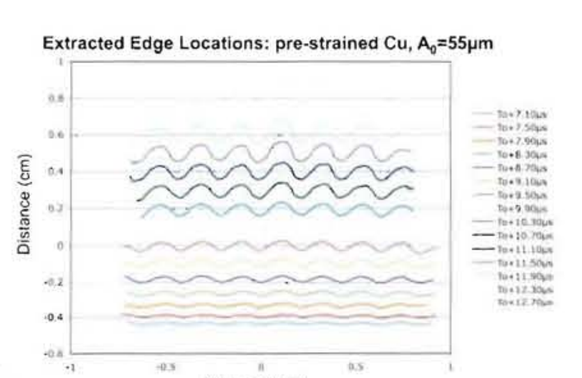
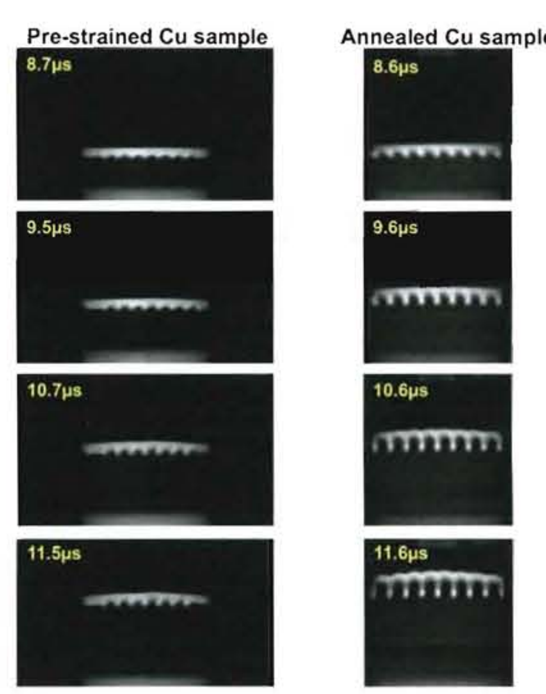
processing

pRad studies of perturbation growth rates as a function of time demonstrate a strong influence of materials processing (Olson)

- **Comparison between fully annealed and cold worked copper samples.**
  - 55μm sinusoidal initial perturbation imposed on each sample.
  - Identical sample acceleration.
- **Significant reduction in growth rate is observed for cold-worked Cu samples.**





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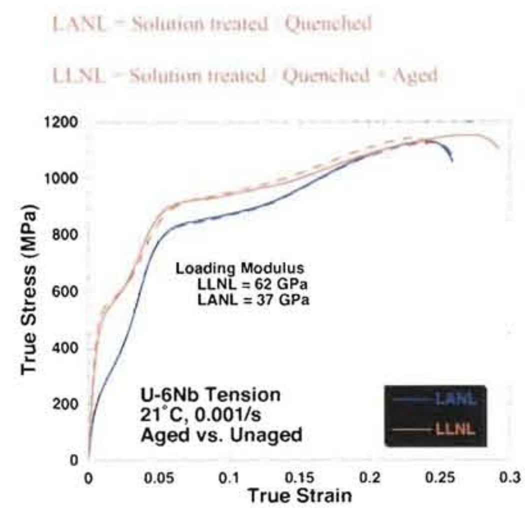
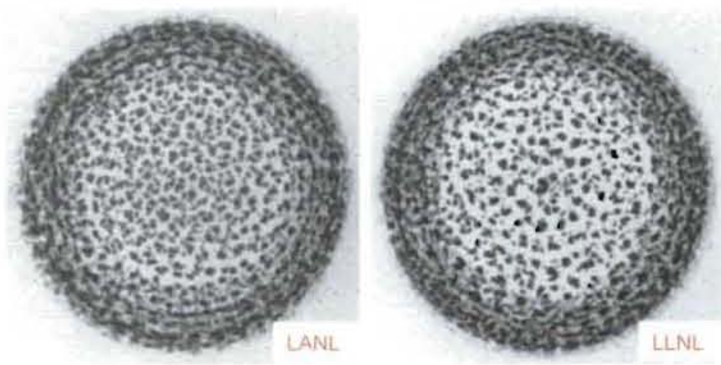
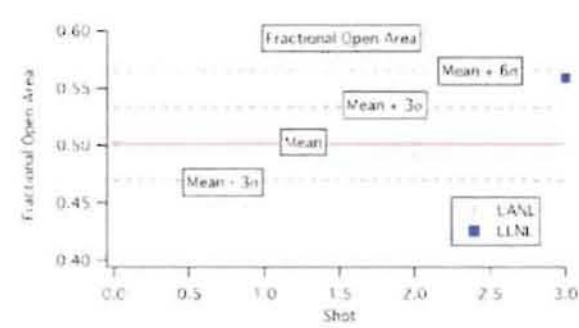
processing

Mechanical behavior fostered by processing and HE loading U-6Nb shows a strong influence of metallurgical state (Hull)



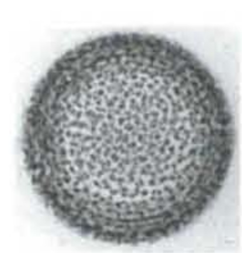




Understanding "process-aware" material response will enable design of materials for prescribed capabilities

LANL's dynamic materials program is well positioned to address near and long-term stockpile issues

- We have a healthy balance of fundamental, exploratory and validation experiments
- Our general approach is to probe materials of interest first through scaling and surrogates
- Our ASC codes are steadily becoming more capable with increased physics
- Out stockpile continues to age, which presents new challenges
- We must transform from process-based certification to product-based certification



Exciting opportunities exist for new and enhanced capabilities such as MaRIE

Damage Evolution under Dynamic Conditions—Experimentation and Modeling

J.F. Bingert (MST-8)

The response of materials under dynamic conditions may differ significantly from their equilibrium behavior. A mechanistic understanding of dynamic microstructural evolution and resultant damage processes is instrumental to the development of predictive materials models. These models, in turn, are critical enablers for meaningful predictive capabilities for large strain, high strain-rate processes. Within the Joint Munitions Program and Defense Programs Science campaigns, several investigations are underway focused on resolving some of the key features of damage initiation and growth processes. Highlights of these activities will be presented, including advanced in situ and post-mortem characterization of dynamically deformed and damaged material, along with the development of improved computational damage descriptions. Experimental examples will involve shear localization, incipient spall, and three-dimensional damage characterization. Examples of computational development will consist of strain localization, void growth, and shock damage modeling. Integration of experimentation, characterization, and model development and validation will be emphasized.

Damage Evolution under Dynamic Conditions – Experimentation and Modeling

J.F. Bingert, MST-8

Contributors:

MST-8: C. Cady, E. Cerreta, S.-R. Chen, R. Gray, R. Lebensohn, C. Liu, V. Livescu, M. Lopez, P. Rae, C. Tomé, C. Trujillo

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T-3: F. Addessio, C. Bronkhorst, H. Mourad

W-6: T. Mason DE-3: L. Hull XCP-5: D. Tonks ADW: E. Brown

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Outline

- **Motivation, Goals, and Relevance**
- **LANL's peers**
- **Examples of integrated experimental/modeling efforts**
  - I. Dynamic deformation – strain localization
    - Dynamic extrusion and modeling of strain localization
  - II. Microstructural effects on dynamic damage – anisotropy and voids
    - Experimental observations and dilatational plasticity modeling
  - III. Additional microstructural effects on damage – grains and twins
    - Shock damage in Cu & Ta and crystal plasticity damage modeling
  - IV. Dynamic response in polymers: example of phase transition
    - PTFE dynamic damage and modeling

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Motivation, Goals, and Relevance

- **Address Materials Strategy – Extreme thermomechanical environment theme.**
  - Move toward property-based requirements specification, in place of process-based qualification. ***From observation to control.***
  - Enable predictive capability for damage and failure processes during large-strain, high-rate processes.
- **Understand relationship between actual microstructures and damage evolution under dynamic loading.**
  - Incorporate fundamental knowledge into computational models that are capable of running in large-scale simulations.
- **Damage and failure behavior are critical determinants of material performance for National Security missions.**
  - Average material properties may be irrelevant in many scenarios.

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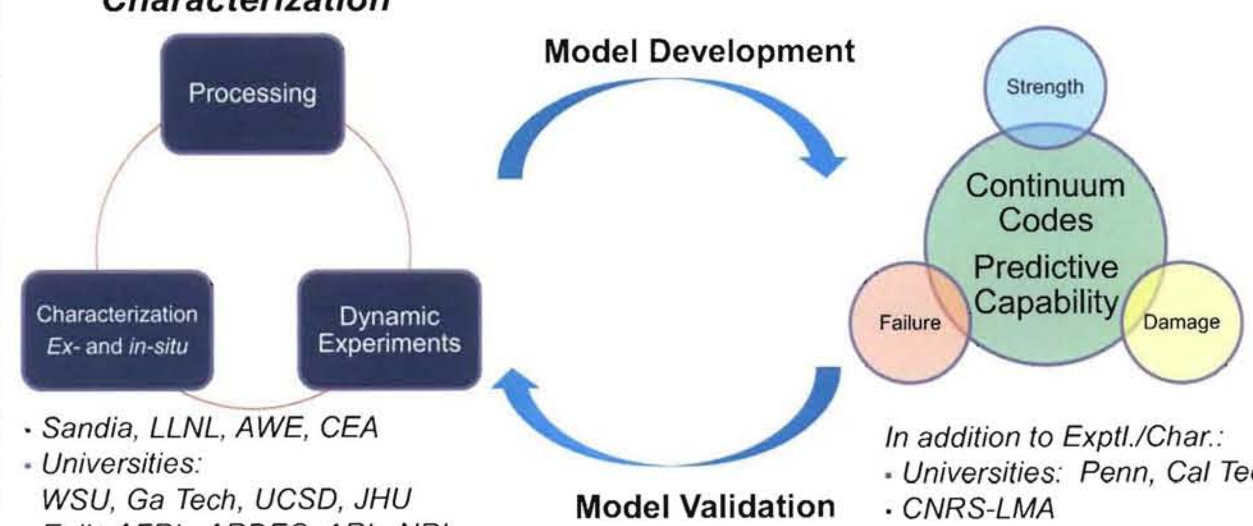
LANL's Peers: Many are also collaborators

Experimentation / Characterization ***Material Damage Modeling***



- *Sandia, LLNL, AWE, CEA*
- *Universities:*
  WSU, Ga Tech, UCSD, JHU
- *Eglin AFRL, ARDEC, ARL, NRL*

In addition to Exptl./Char.:
- *Universities: Penn, Cal Tech*
- *CNRS-LMA*

Our Strength: Tightly integrated experimental and theoretical project teams

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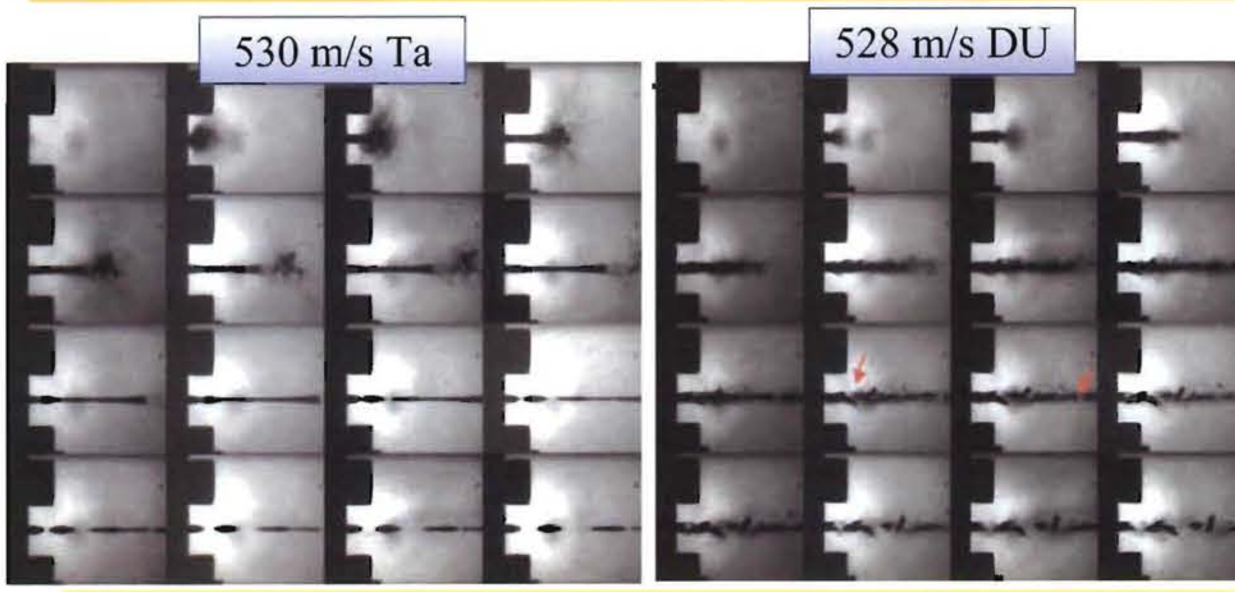
I. Dynamic Deformation – Observation of Localization



Failure/fragmentation mode is dictated by proclivity to strain localization. Can this behavior be predicted, and thus incorporated in design?

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I. Localization – Development of Predictive Capability

- **Localization phenomena involve a discontinuous strain field**
- **Conventional computational techniques**
  - Yield mesh-dependent results, unless mesh is sufficiently refined
  - Computation is prohibitively expensive, and requires *a priori* knowledge of the band location and orientation
- **Sub-grid computational technique**
  - Allows band orientation to be determined.
  - Allows smooth transition from uniform to localized deformation, and facilitates the use of different material models inside and outside the band
  - Part of the localization band is embedded inside an element, obviating the need for excessive mesh refinement
  - Localization band width is specified as a material parameter, not dictated by the mesh size

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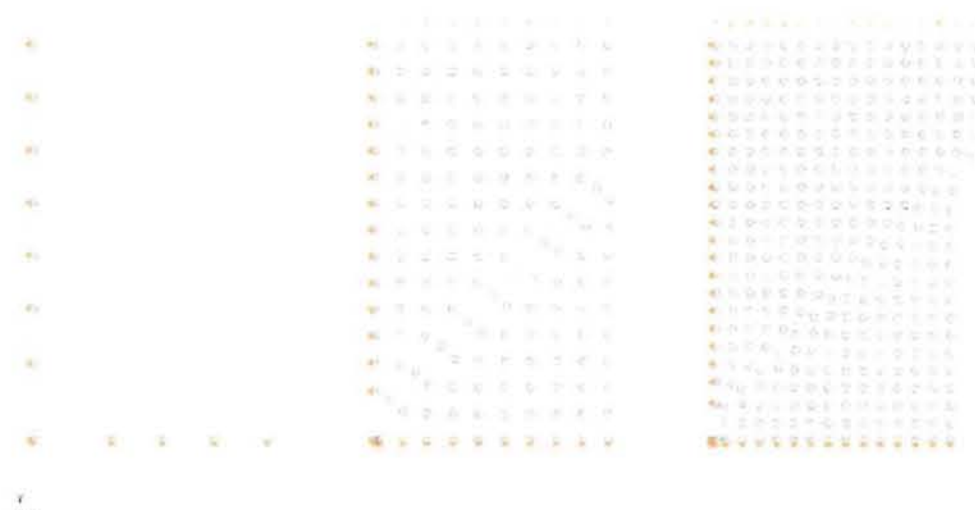
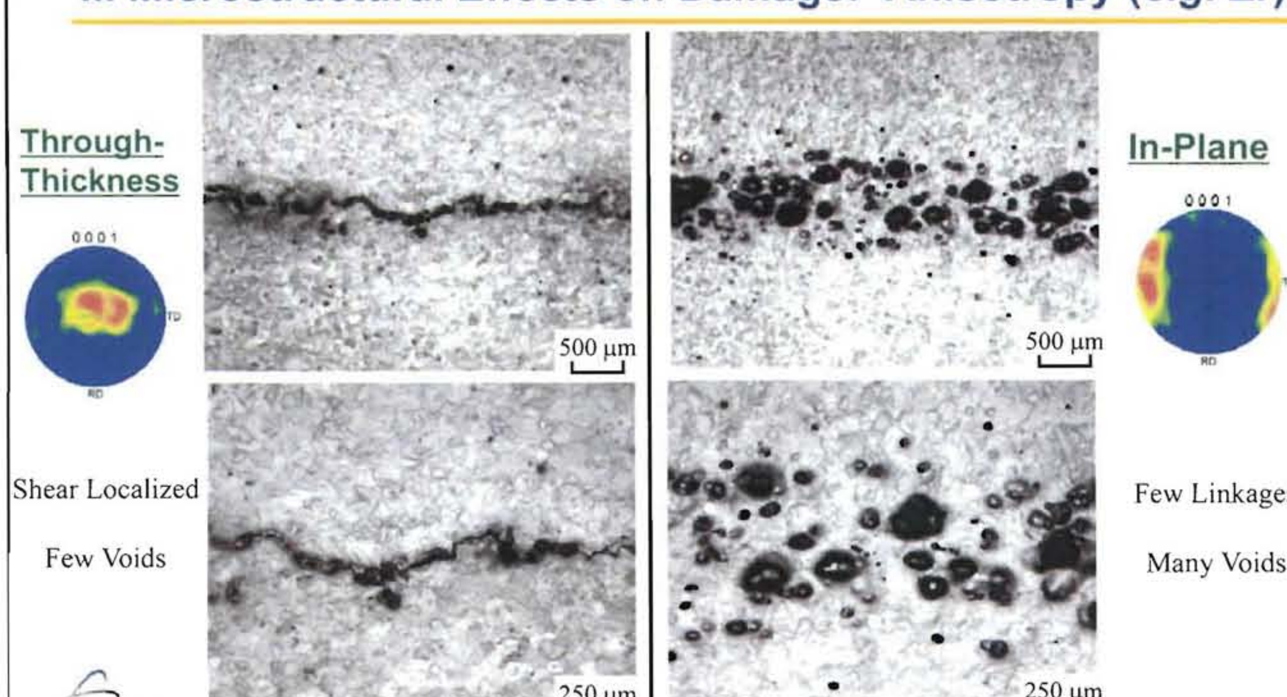
I. 2-Component (Sub-Grid) Localization Model



Location and orientation of band, and its effect on overall deformation, are captured reasonably well, even by coarsest mesh.

II. Microstructural Effects on Damage: Anisotropy (*e.g.* Zr)

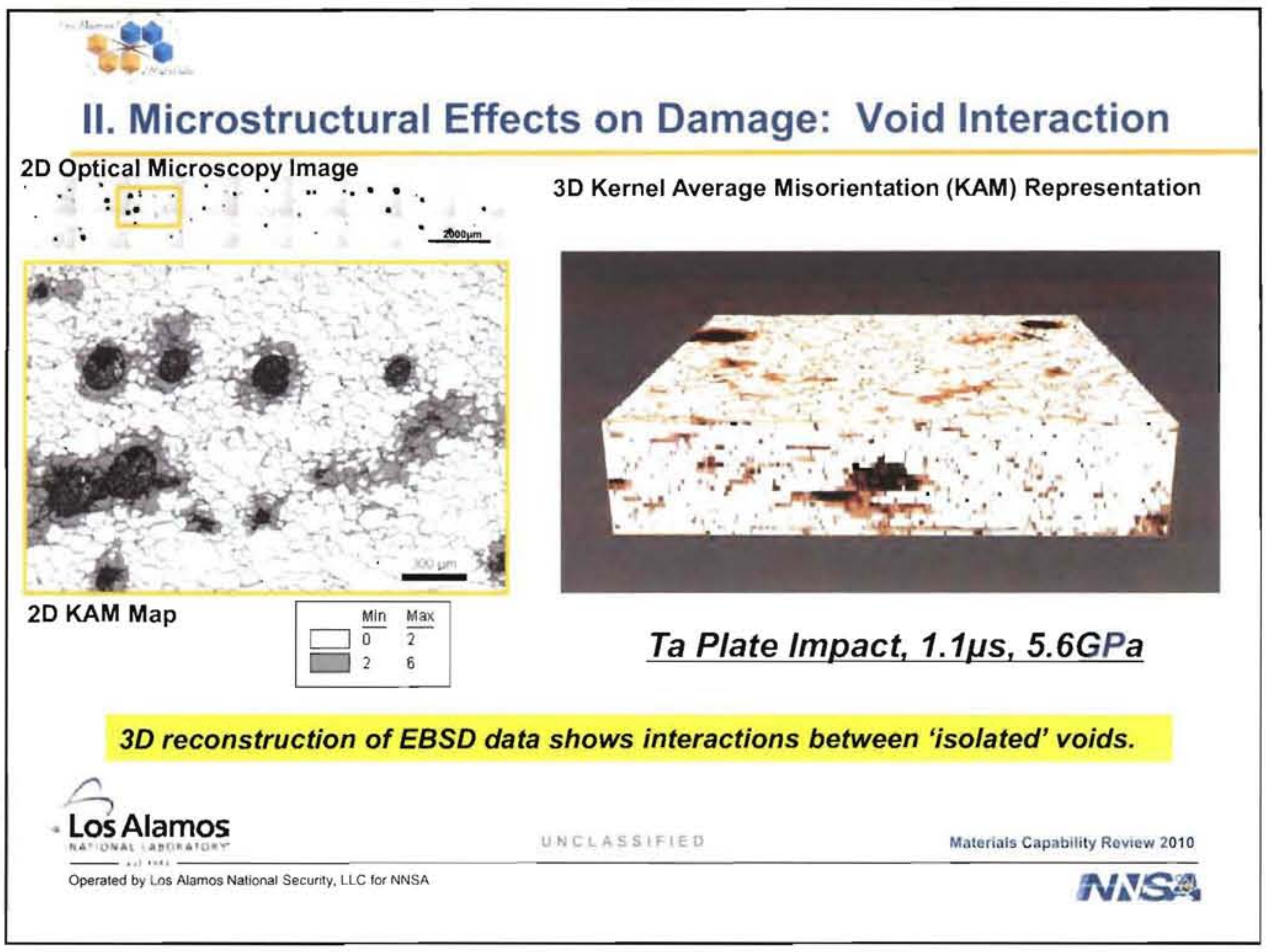


Shear Localized

Few Voids

Few Linkages

Many Voids


II. Microstructural Effects on Damage: Void Interaction
2D Optical Microscopy Image
2000μm
3D Kernel Average Misorientation (KAM) Representation
2D KAM Map
Min Max
0 2
2 6
Ta Plate Impact, 1.1μs, 5.6GPa
3D reconstruction of EBSD data shows interactions between 'isolated' voids.
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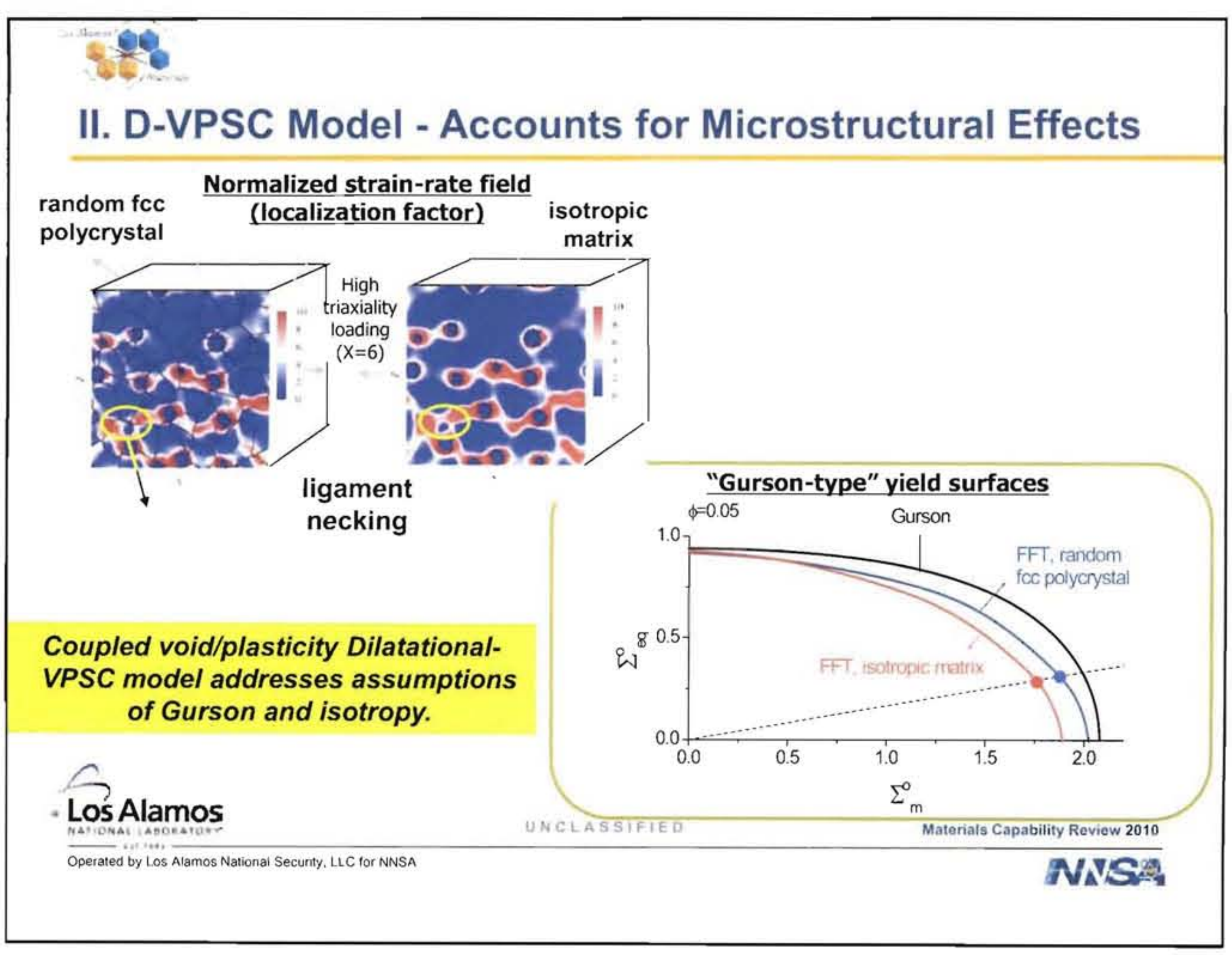
II. D-VPSC Model - Accounts for Microstructural Effects
random fcc polycrystal
Normalized strain-rate field (localization factor)
isotropic matrix
High triaxiality loading (X=6)
ligament necking
"Gurson-type" yield surfaces
ϕ=0.05
Gurson
FFT, random fcc polycrystal
FFT, isotropic matrix
1.0
0.5
0.0
1.5
2.0
Coupled void/plasticity Dilatational-VPSC model addresses assumptions of Gurson and isotropy.
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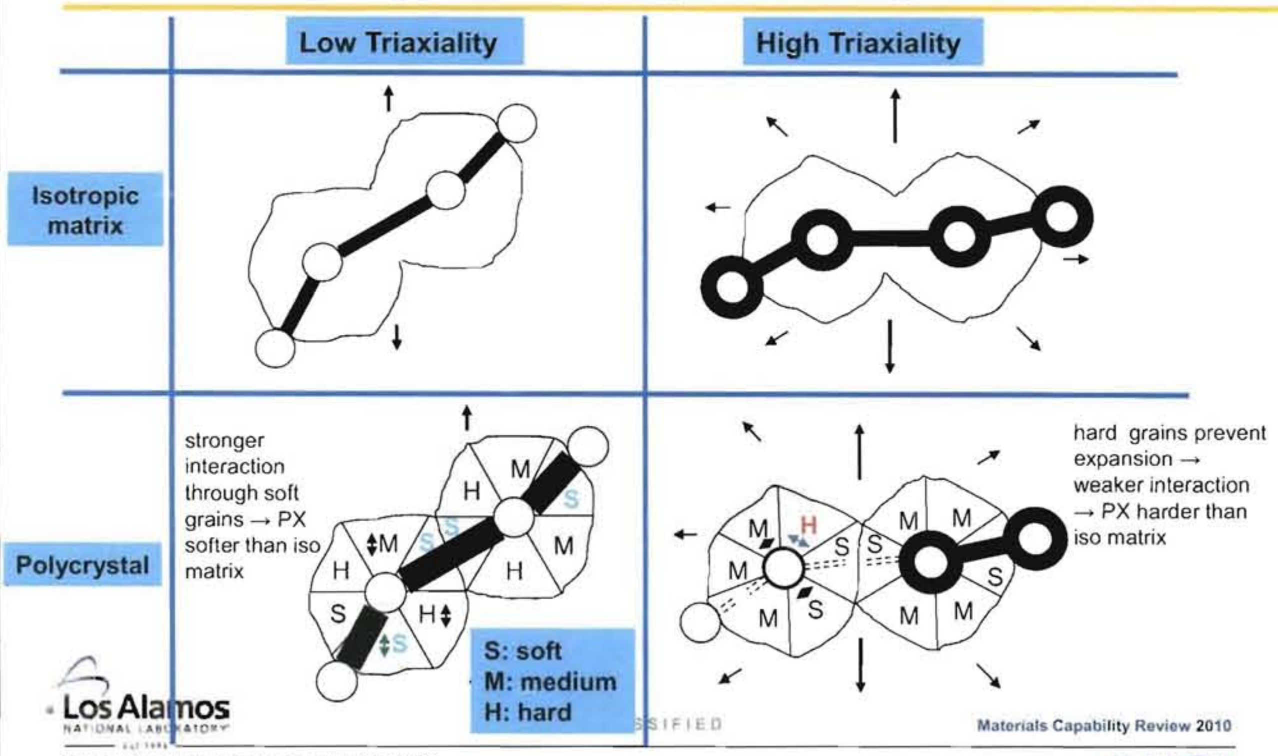
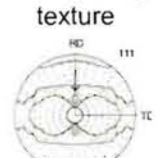
II. Anisotropy and Linkage in Damage Evolution

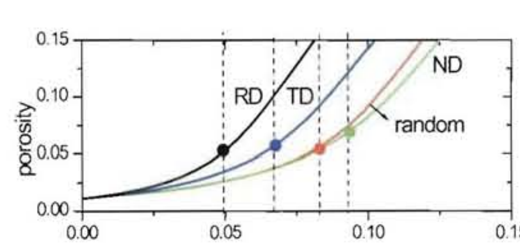


II. D-VPSC Results on Crystallographic Anisotropy

2) tension along harder direction → faster porosity evolution

X=2, n=10, sph voids, rolling texture

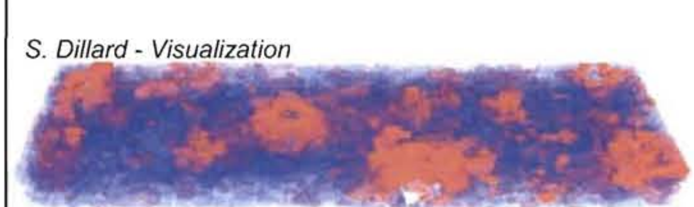




Mean field D-VPSC model accounts for damage evolution from void fields in anisotropic materials.

II. 3-D: D-VPSC Model and Experimental Results

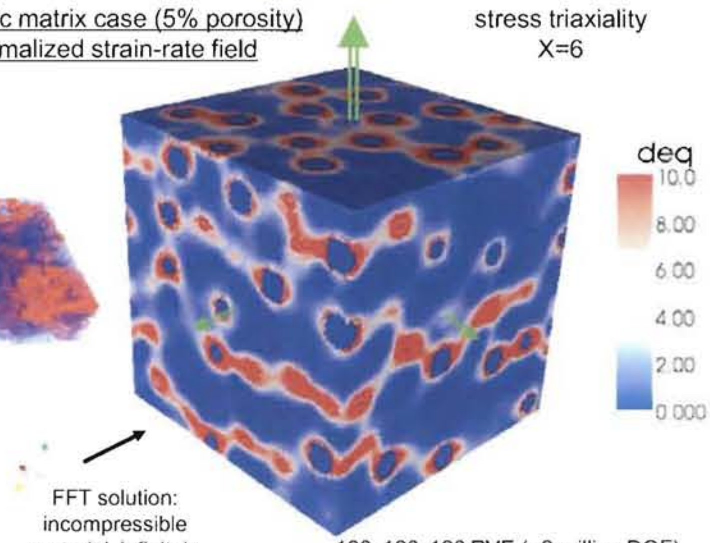
S. Dillard - Visualization



3D Reconstruction of misorientation field in shocked Tantalum

Isotropic matrix case (5% porosity) normalized strain-rate field

stress triaxiality X=6



FFT solution: incompressible material, infinitely compliant cavities

128x128x128 RVE (~2 million DOF), requires ~4 hours on a desktop

Future - Apply 3D characterization techniques to help validate 3D dilatational plasticity model.

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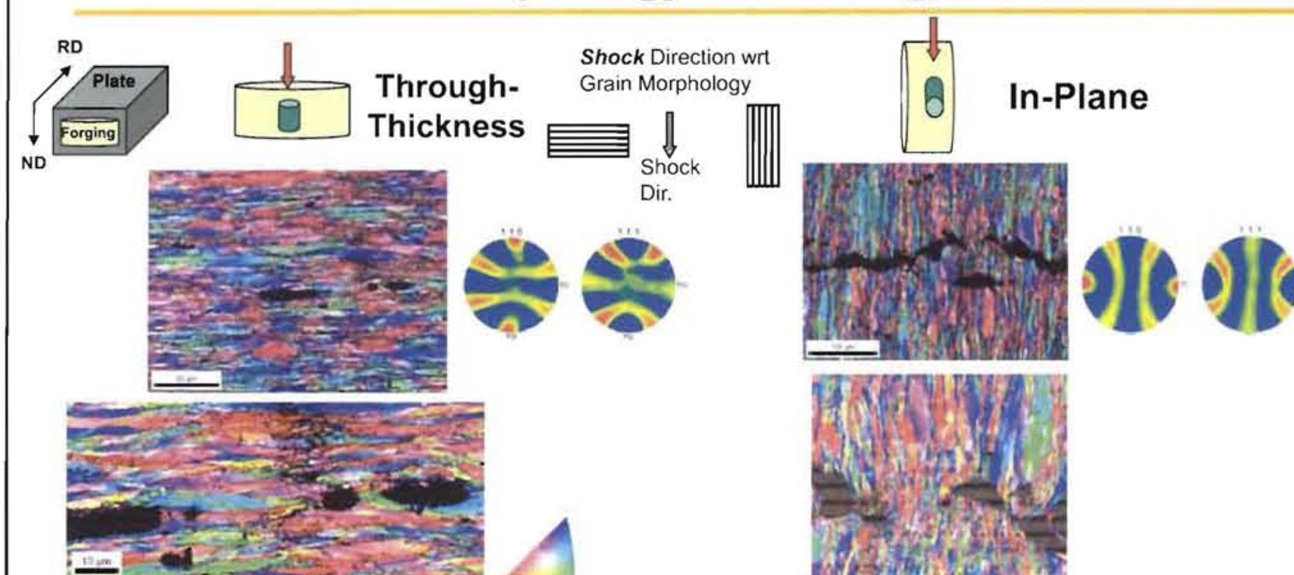
III. Grain Morphology and Damage in Cu



Complex interplay between anisotropic strength and morphology on damage evolution.

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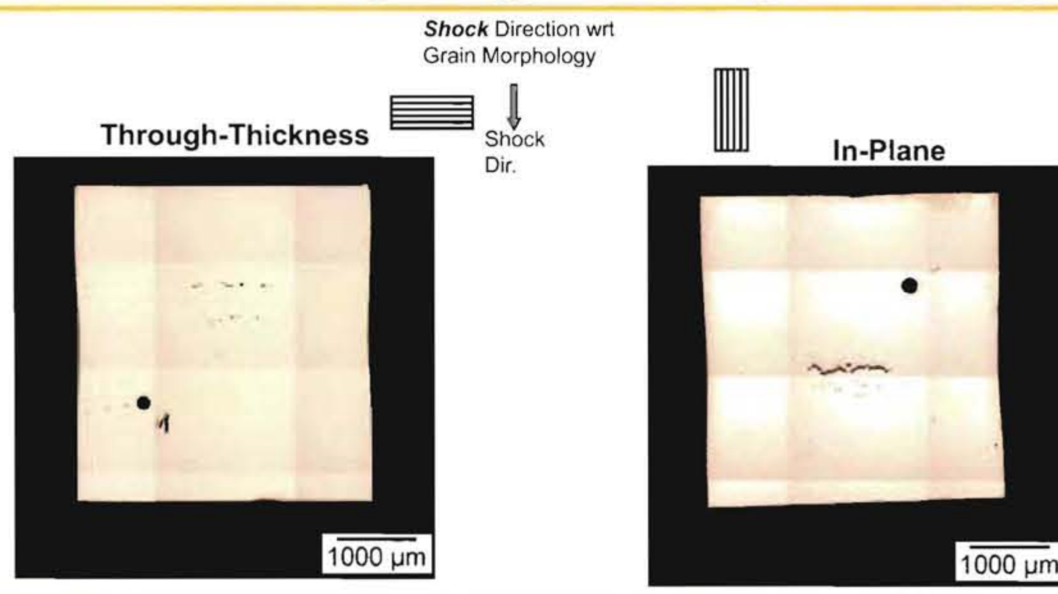
III. Interaction of Morphology and Strength on Damage



Significant effect of crystallographic and morphological anisotropy on damage evolution.

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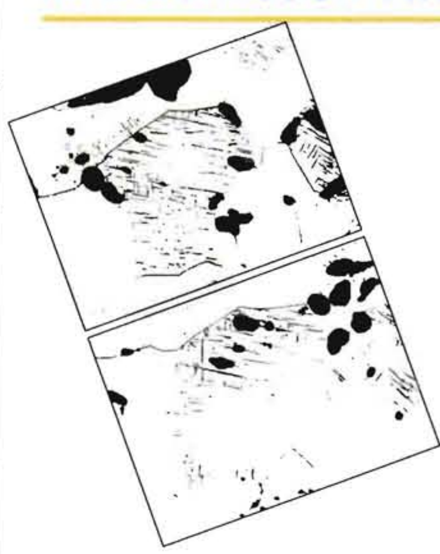
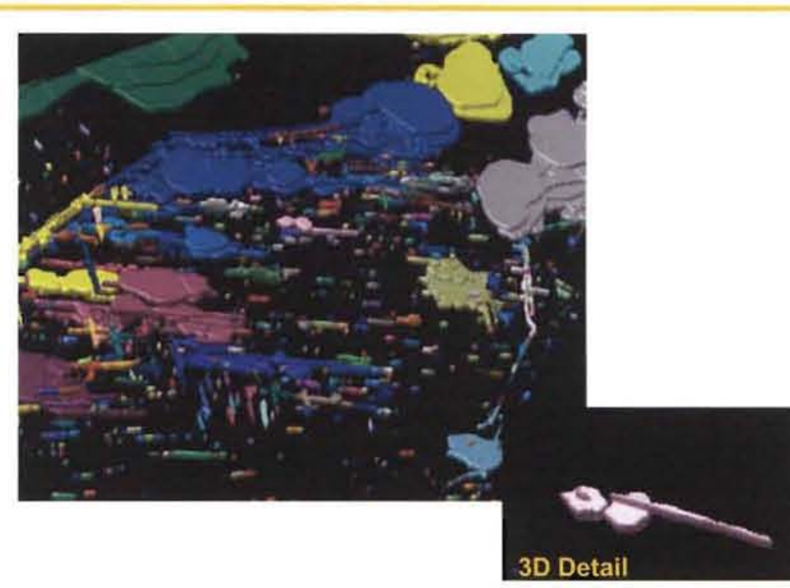
III. Deformation Twinning and Void Initiation in Tantalum





Volumetric reconstruction reveals role of twin intersections in void initiation.

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III. Incorporate Microstructural Details in Damage Model

Tonks Mesoscale Damage Model

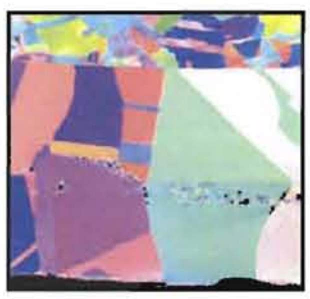
macroscopic shock damage model with crystal plasticity

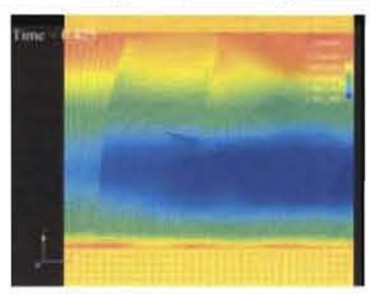
- **Large grained Cu, v = 225 m/s, P = 4.3 GPa.**
- **Single xtal plasticity model used in sample grains**
- **Each grain meshed individually**

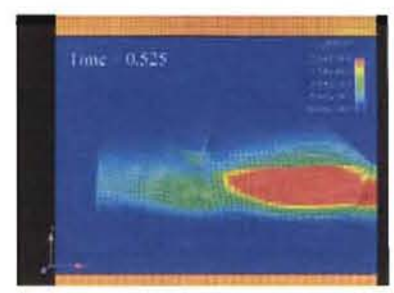
Koskelo LDRD team, Luo, Byler, Dickerson

Pressure (blue = negative)

Porosity







Indicates need for explicit treatment of GB for nucleation and fracture.

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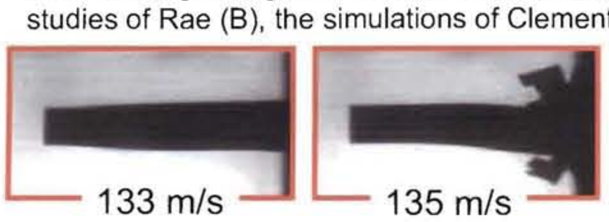
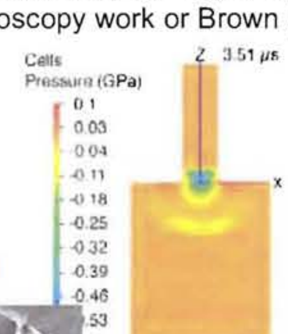
The ductile-brittle transformation observed in polytetrafluoroethylene (PTFE) in a Taylor impact experiment is correlated to crossing a solid-solid phase boundary.

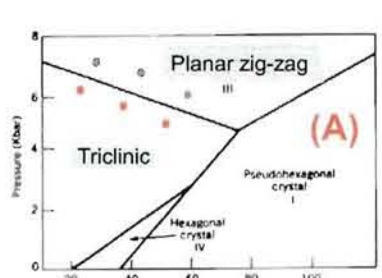
IV. Dynamic Response in Polymers: Phase Transition

Understanding the behavior of PTFE reactive materials requires understanding the detailed behavior originating from the solid-solid phase diagram (A) as illustrated by the Taylor impact studies of Rae (B), the simulations of Clements (C), and the microscopy work or Brown (D).



(B) Ductile to Brittle transition observed under Taylor impact loading





(D) Optical Studies: Brittle failure at 135 m/s

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Summary

- 2-Component model implementation will enhance our ability to predict material localization and failure at relevant time and length scales.
- D-VPSC development considers damage evolution in realistic material systems.
- Dynamic experimentation approaches integrated with model development; illuminate behavior that requires additional interrogation and understanding.
- Going forward, need improved nucleation models, continued extension to 3D models and data sets, and role of grain boundaries and local strain gradients.

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Proton Radiography: Studying Dynamic Properties of Shock-Loaded Materials and High Explosives

A. Saunders (P-23)

The Proton Radiography facility (pRad) at the Los Alamos Neutron Science Center (LANSCE) uses the unique properties of high-energy protons to generate multiple-frame radiographic movies of dynamic experiments, typically driven by high explosives or a powder gun. The high penetrating powers and low backgrounds associated with high-energy protons, as well as the capability of a linear accelerator such as LANSCE to continuously generate 50 ns proton pulses, make pRad a useful tool for studying several classes of experiments. Typical dynamic experiments include studies of high-explosive burn and detonation properties; nonlinear jet growth, including Richtmyer-Meshkov Instability growth; and material equation-of-state studies in shocked or other high-pressure situations. Recent development of static experiments has included the demonstration of pRad's ability to tomographically radiograph very high background static objects, such as spent nuclear fuel rods. The experimental techniques underlying pRad and results from recent examples of each of the above classes of experiments will be presented.

Proton Radiography: Studying Dynamic Properties of Shock-Loaded Materials and High Explosives

Alexander (Andy) Saunders

P-25

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Overview

- **How Proton Radiography works**
- **The key strengths of pRad**
- **And a few examples of recent work**
  - Fuel pin tomography (FFF)
  - Richtmyer-Meshkov Instability Growth (MPDH)
  - Tin Equation of State measurements (MPDH)

P-25: Eduardo Campos, Camilo Espinoza, Gary Hogan, Brian Hollander, Julian Lopez, Fesseha Mariam, Frank Merrill, Christopher Morris, Matthew Murray, Alexander Saunders, Cynthia Schwartz, T. Neil Thompson, Dale Tupa

DE-3: Joe Bainbridge, Robert Lopez, Mark Marr-Lyon, Paul Rightley

HX-4: Wendy McNeil

P-23: Gary Grim, Nicholas King, Kris Kwiatkowski, Paul Nedrow

LANSCE-NS: Leo Bitteker

NSTech: Douglas Lewis, Josh Tybo

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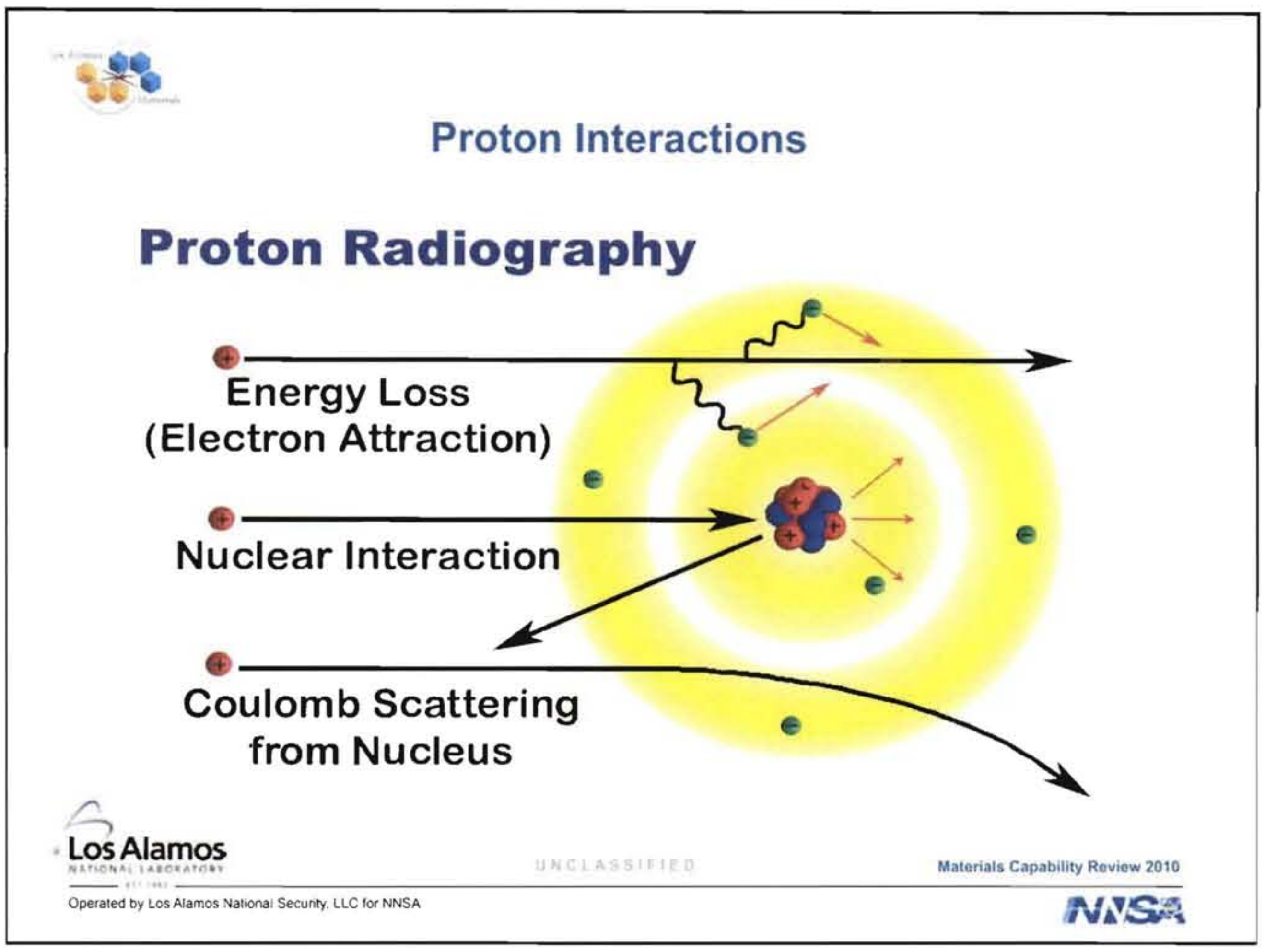
Proton Interactions
Proton Radiography
Energy Loss
(Electron Attraction)
Nuclear Interaction
Coulomb Scattering
from Nucleus
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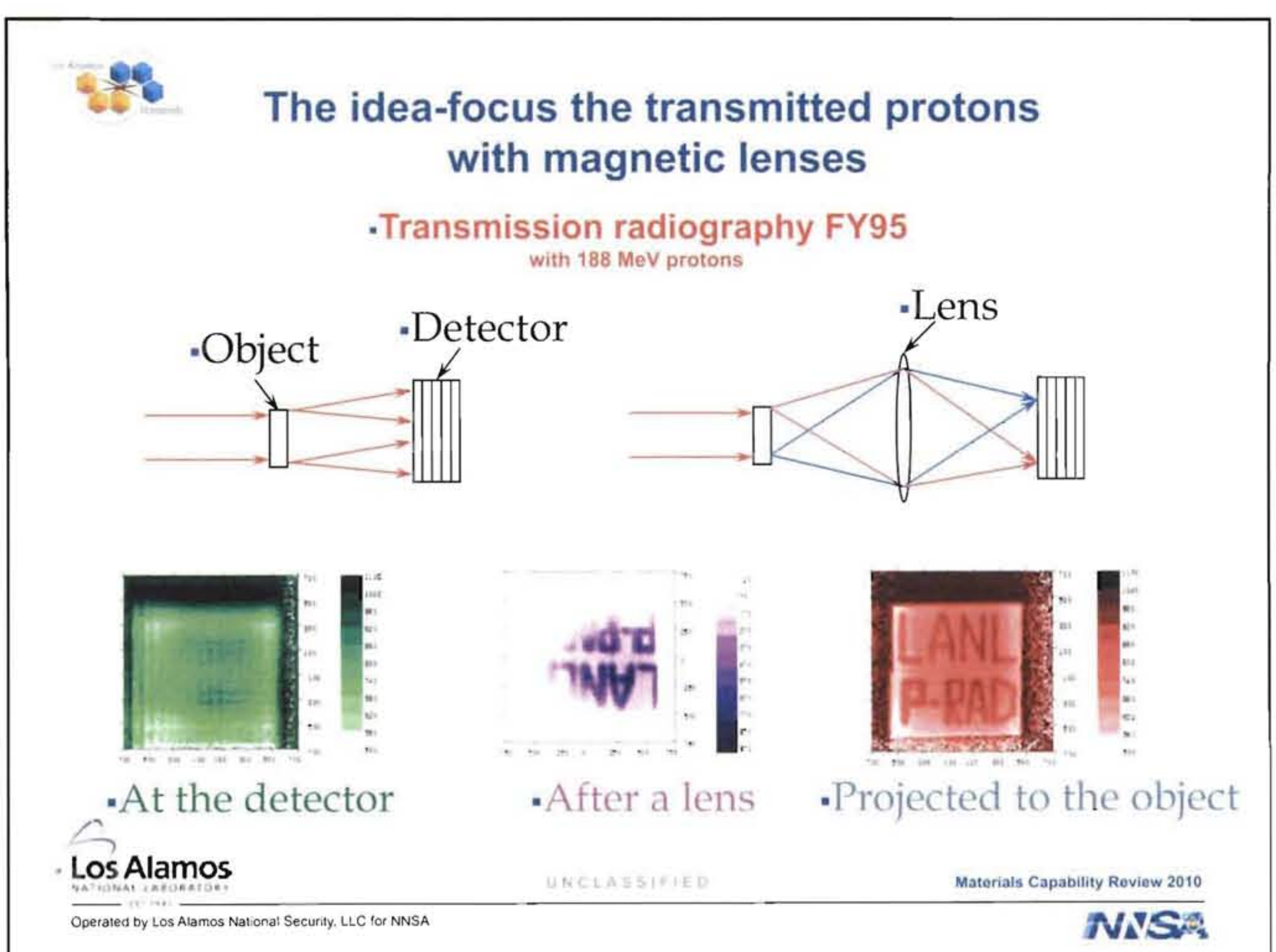
The idea-focus the transmitted protons
with magnetic lenses
▪Transmission radiography FY95
with 188 MeV protons
▪Object
▪Detector
▪Lens
LANL
P-RAD
▪At the detector
▪After a lens
▪Projected to the object
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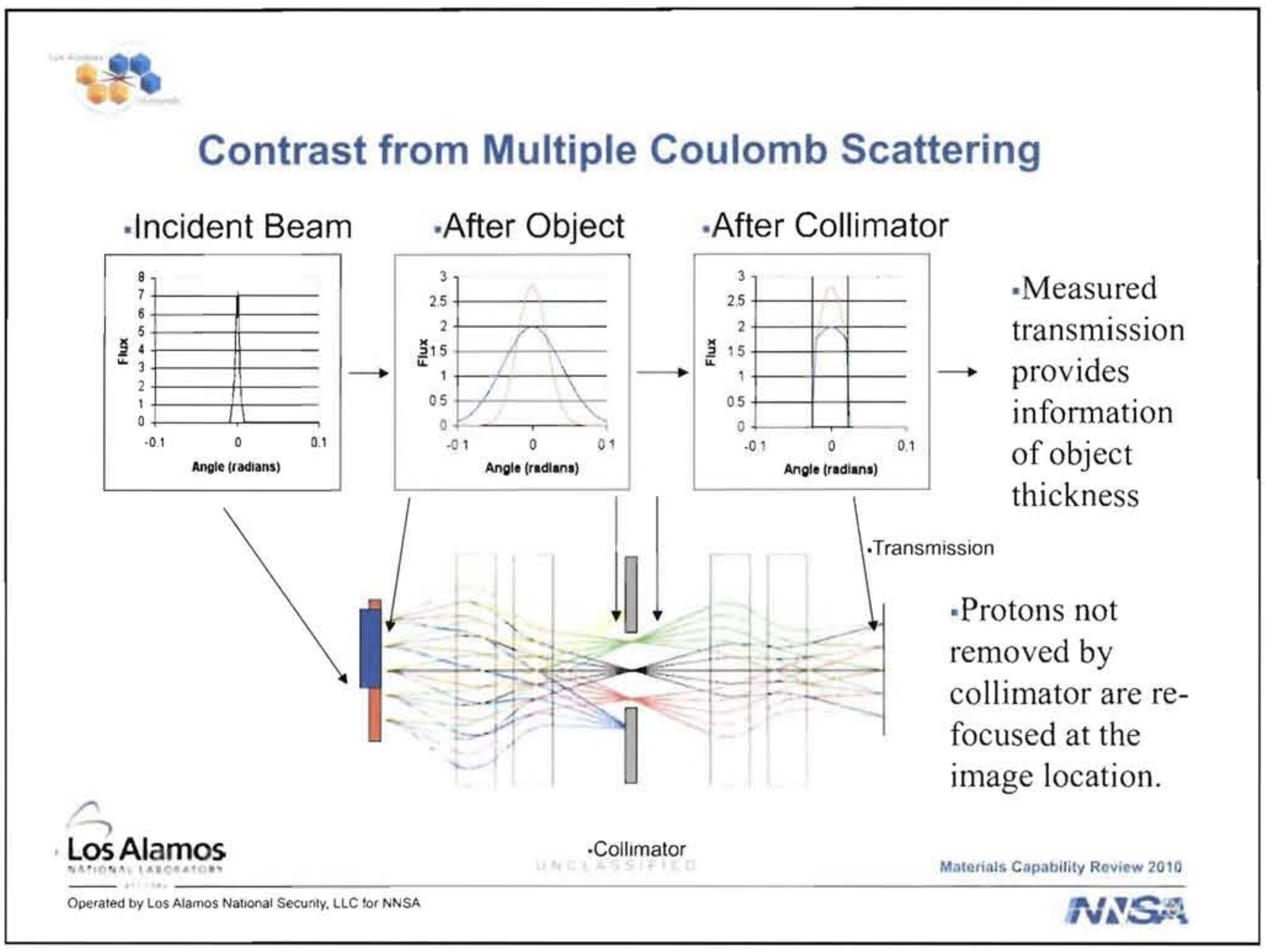
Contrast from Multiple Coulomb Scattering
•Incident Beam
•After Object
•After Collimator
Flux
Angle (radians)
•Measured transmission provides information of object thickness
•Transmission
•Protons not removed by collimator are re-focused at the image location.
•Collimator
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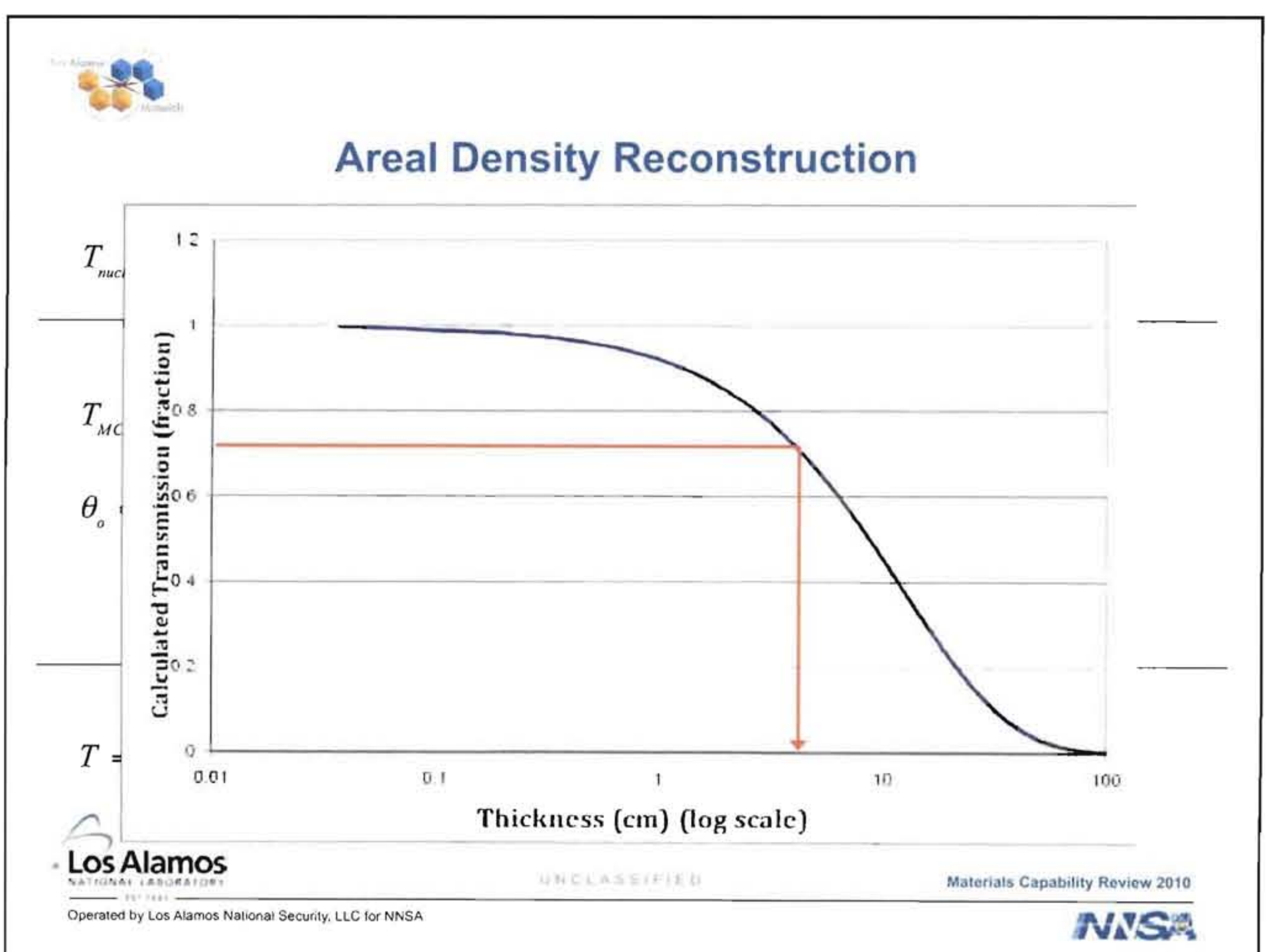
Areal Density Reconstruction
Calculated Transmission (fraction)
Thickness (cm) (log scale)
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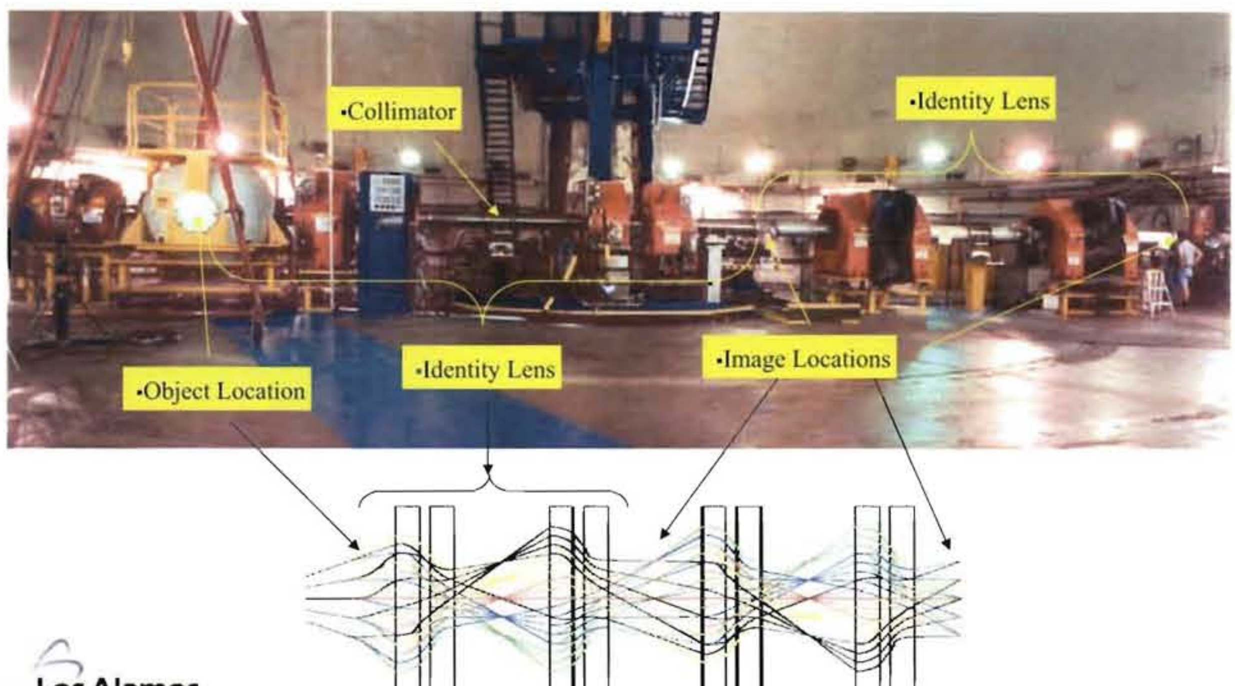
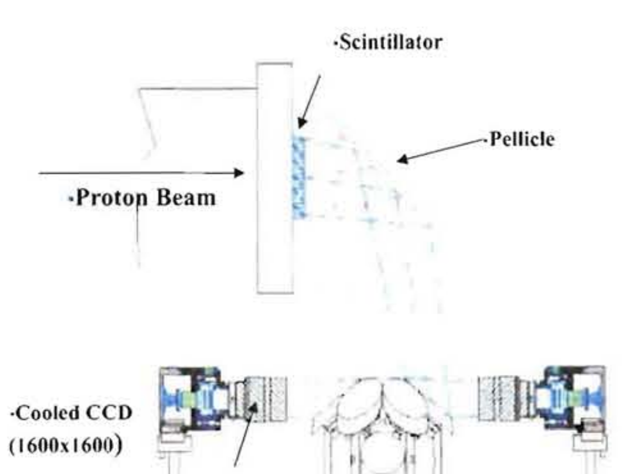
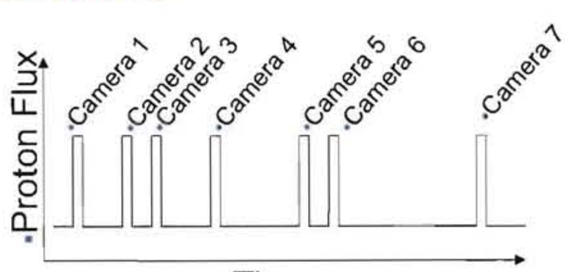
pRad Facility at LANSCE



Temporal Resolution

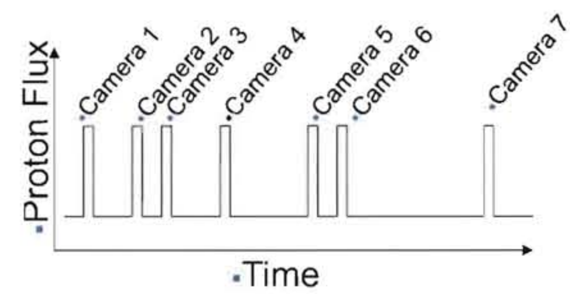




- **19** images at first station
- **22** images at second station
- Total **41** possible image times
- Typically **50 ns** exposure times
- Only limit is # of detectors

The Two Key Strengths of pRad

- Negligible backgrounds at detectors
- Many frames of flash quantitative radiographic data in a single shot
  - (and tunable interaction length, unlimited resolution improvement, etc. etc.)



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2009 pRad Experiments

- 38 Dynamic Experiments
- DE "Magic Cone" Detonator Tests (6)
- DE-9 HE Sandwich (2)
- Bacchus Prep Shots (3)
- Cookoffs (4)
- Equation of State, HE-driven (6)
- Hi-Fi Hockey Puck (6)
- High Strain Rate Instability (2)
- Equation of State, Powder Gun (3)
- RMI, HE-driven (4)
- RMI, Powder gun (2)

- Proton Interrogation of Cargo
- Muon Interrogation of Cargo
- Fuel Pin Tomography

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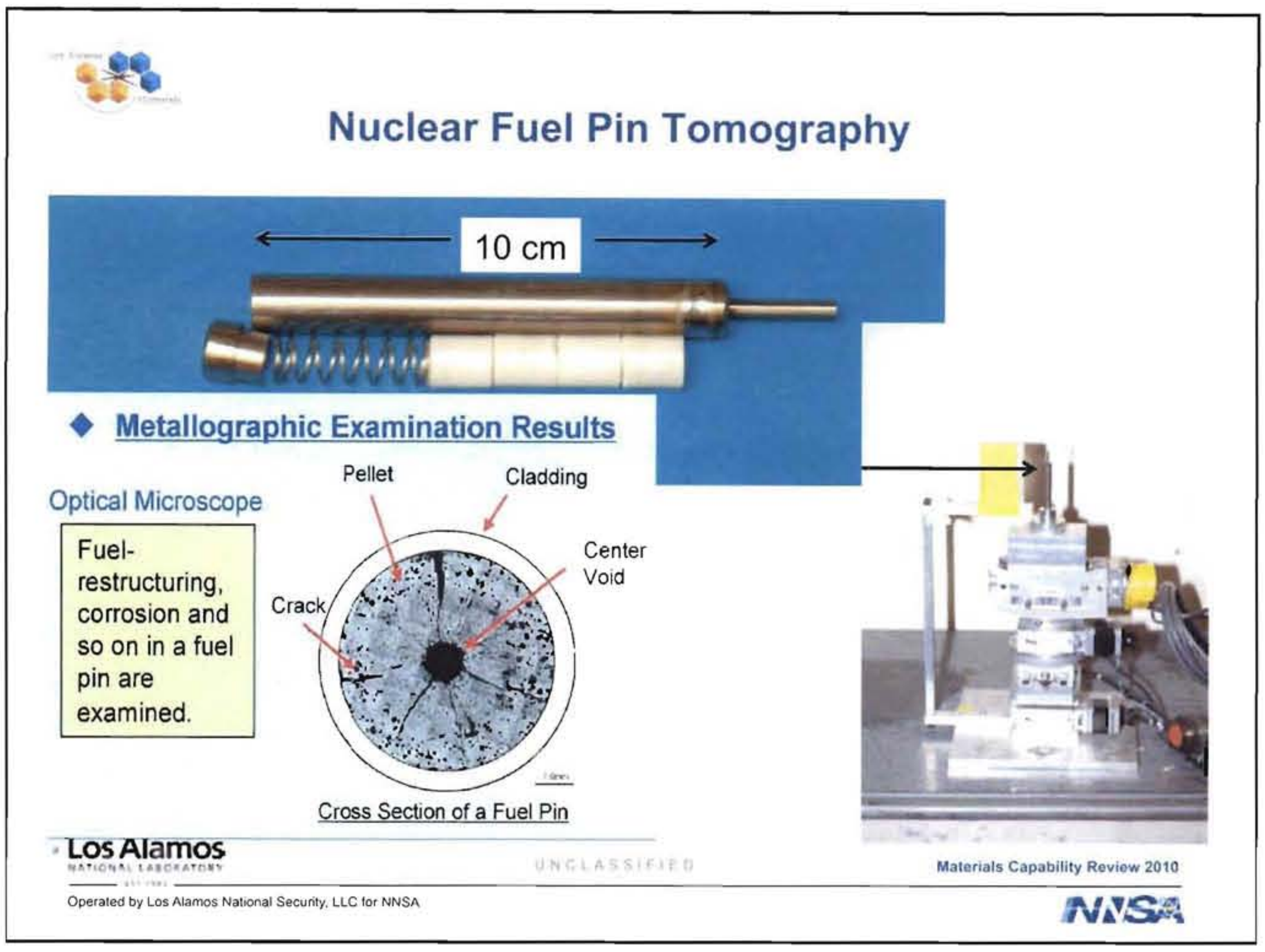
Nuclear Fuel Pin Tomography
10 cm
Metallographic Examination Results
Optical Microscope
Fuel-restructuring, corrosion and so on in a fuel pin are examined.
Pellet
Cladding
Center Void
Crack
Cross Section of a Fuel Pin
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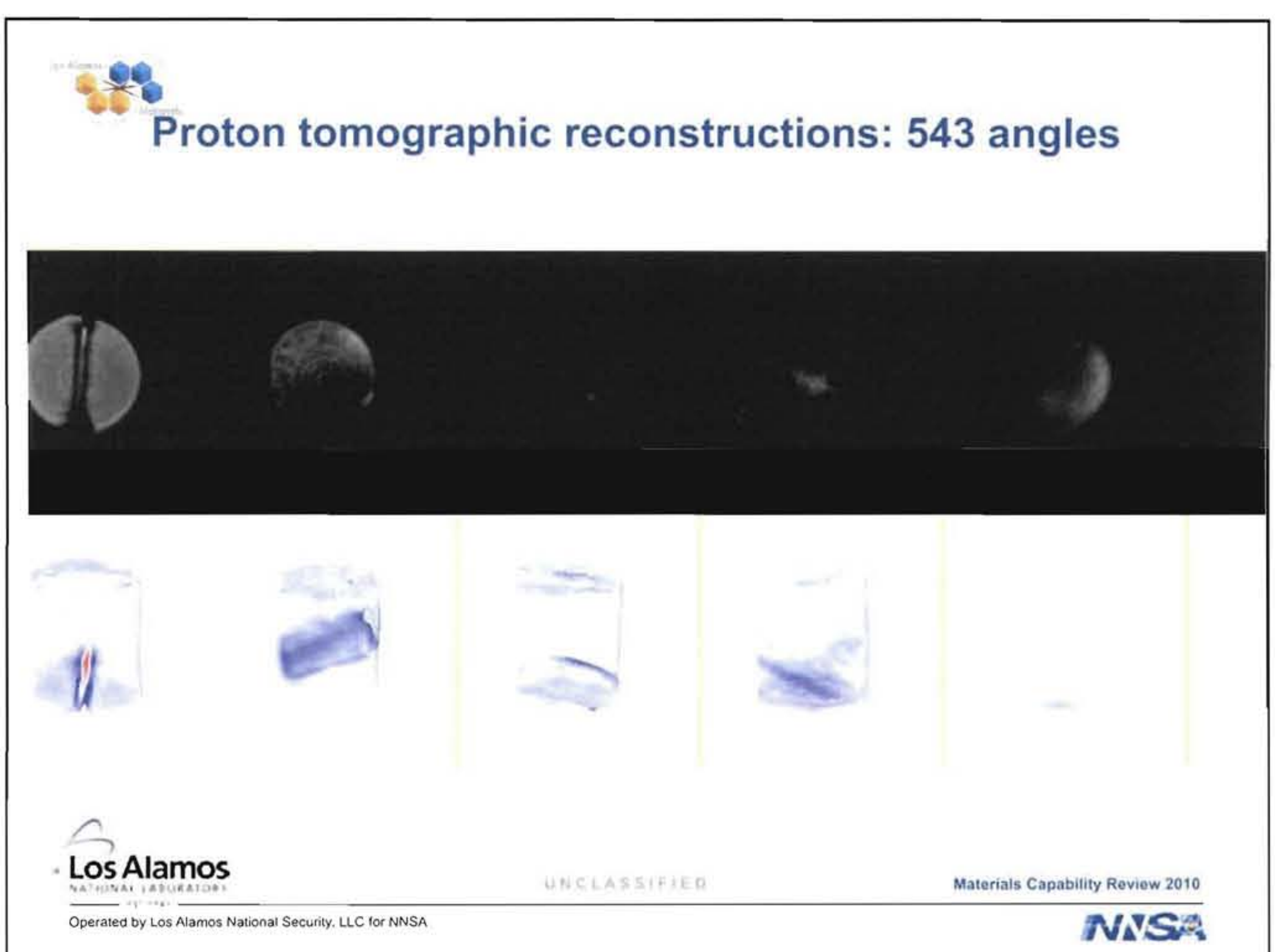
Proton tomographic reconstructions: 543 angles
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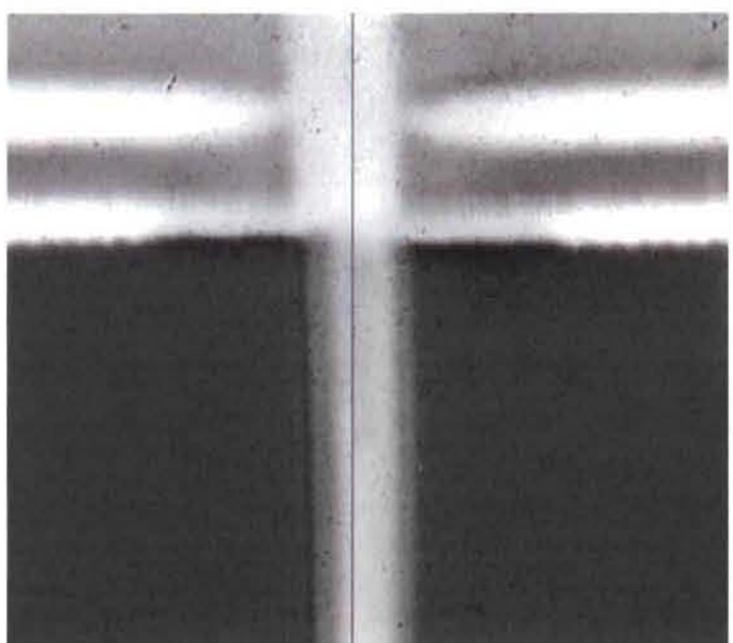
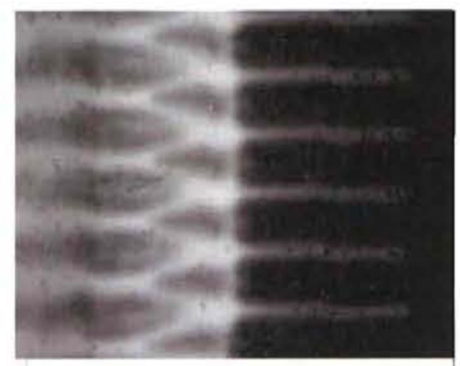
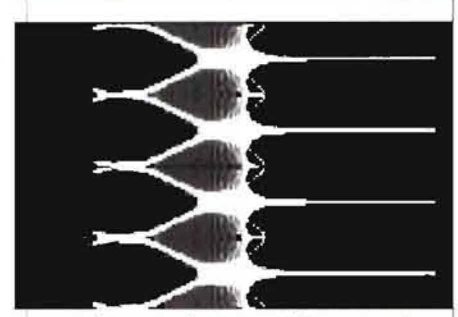
Richtmyer-Meshkov with uniform perturbation (RM) instability in molten tin (2004)





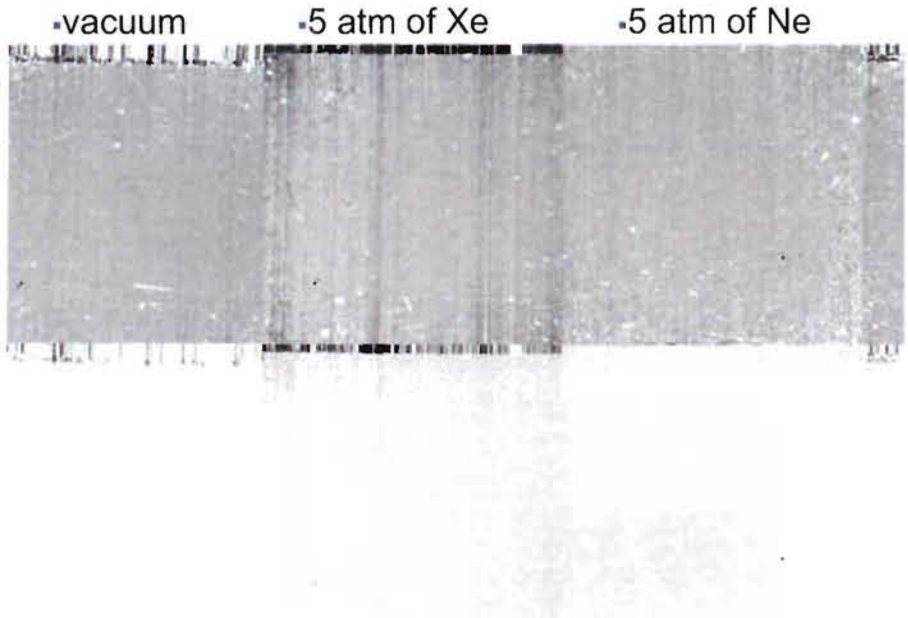


•Hydrodynamic Calculations

•(David Youngs et al.)

2009 RMI Results

•vacuum •5 atm of Xe •5 atm of Ne

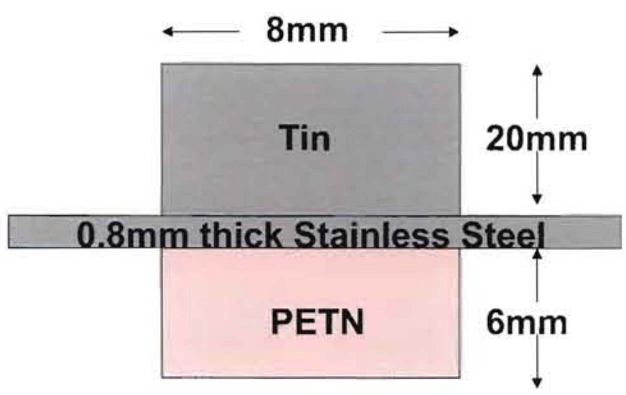


Enhanced Contrast

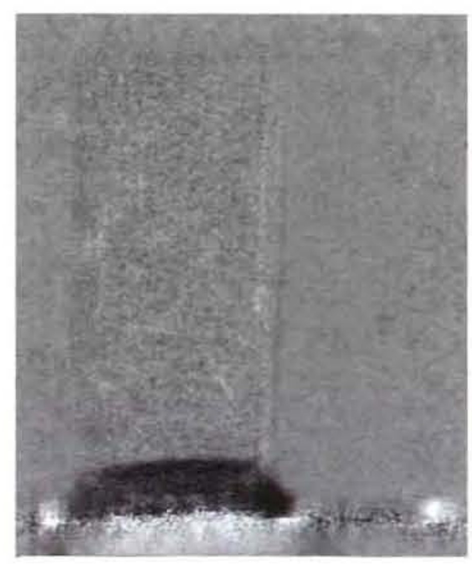
Regular Contrast

Taylor Wave-Driven Tin

- Explosive-driven "Taylor Wave" shock
- Multiple pressures, decaying over time
- Stainless steel membrane

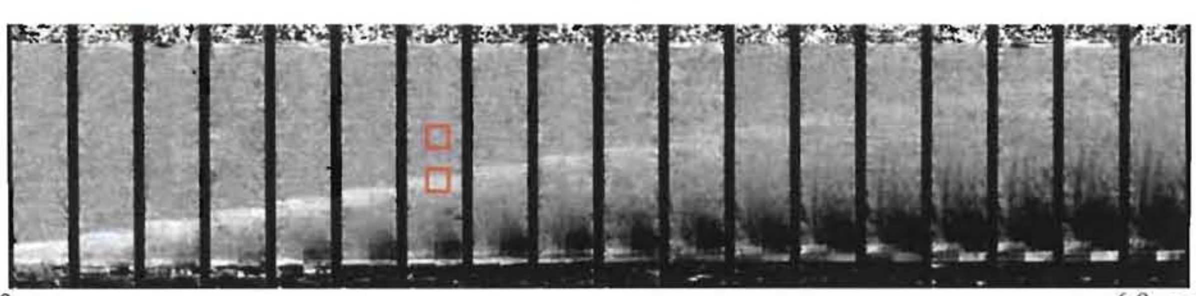


Rusty Gray provided "pristine" tin sample

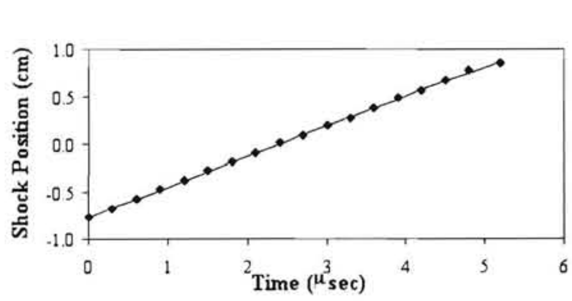


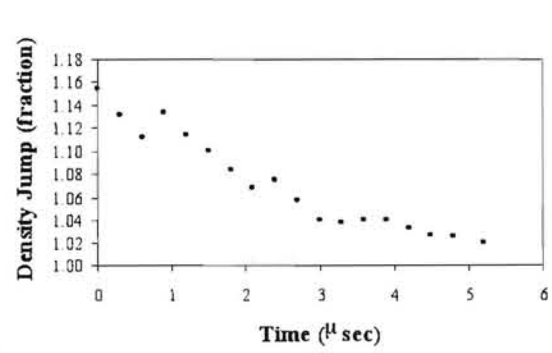
Dynamic / Static transmission radiographs

Position and Density Measurements



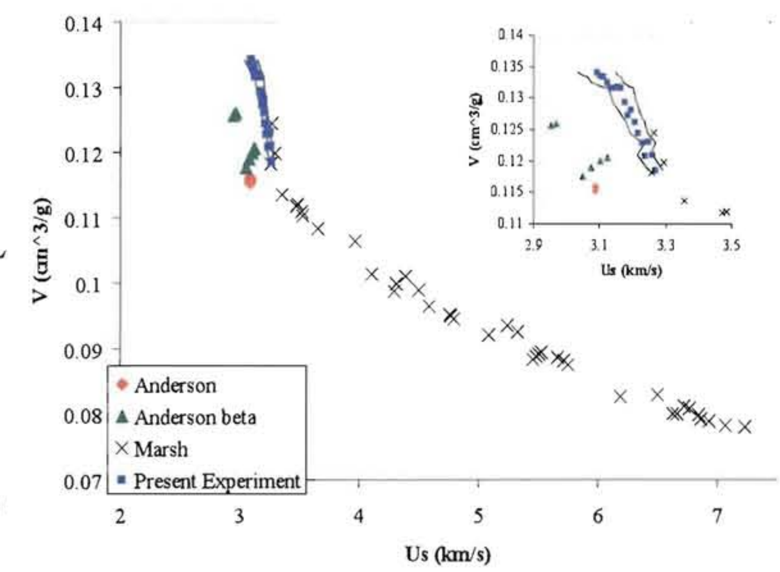
- 1.8μsec
- Time
- 6.9μsec





Single experiment, Multiple Measurements

- Single experiment measures many Hugoniot points
- Agreement with LASL Hugoniot data
- Hugoniot points measured from peak shock velocity down to nearly sound velocity



Next Cycle: measure release wave behind shock

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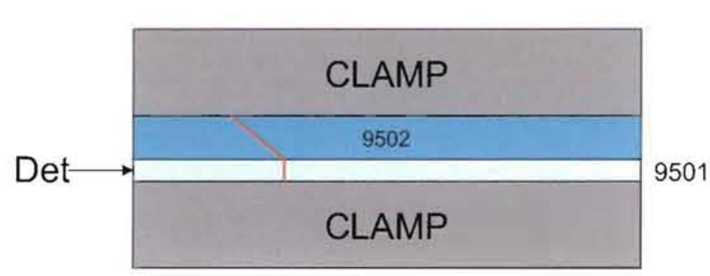
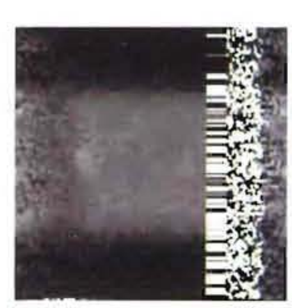
Conclusions

- **Proton Radiography has unique diagnostic capabilities**
- **~40 dynamic experiments in a typical year**
- **Material failure, Equation of State, HE burn**
- **And a growing static program for Threat Reduction and Nuclear Energy**





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Dynamical Simulations of Plutonium through an Atomistic Model

S.M. Valone (MST-8)

Dynamic responses of plutonium metal and alloys simulated with atomistic models are presented. A modified embedded atom method supplies the atomistic models for any combination of plutonium, gallium, and helium. Recent improvements to the model are described. The model describes some aging effects with helium.

Response of a $\Sigma 11$ Asymmetric Tilt Grain Boundary in Copper to an Applied Shear Stress at Finite Temperatures

S. Fensin (University of California, Davis); R. Hoagland, S. Valone (MST-8); M. Asta (University of California, Berkeley)

We present results of molecular dynamics simulations studying the temperature dependence of the structure and mechanical response to an applied shear stress for an asymmetric $\Sigma 11$-tilt grain boundary in copper. At higher temperatures a disordered liquid-like layer forms at the grain boundary and becomes wider in width as the melting temperature is approached from below. Upon application of shear stress the boundary undergoes incremental normal displacement, also known as coupled motion at low temperatures. This behavior is analyzed to determine the atomic mechanisms involved in the of the grain boundary. With increasing temperature, and associated disordering of the interface structure, the mechanical response switches to that of grain-boundary sliding at the highest temperatures, with more complex behavior being displayed at intermediate temperatures.

Dynamical Properties of Quasiparticles and Quasiparticle Aggregates in Hypervalent UO_2 and Other Complex Oxides

S.D. Conradson, A.D. Andersson, J.A. Bradley, J. Lezama-Pacheco (MST-8); K.S. Boland, S.A. Kozimor (C-IIAC); G. Rodriguez, D.A. Yarotski (MPA-CINT); S.A. Trugman (T-4); D.L. Clark (INST-OFF); L.L. Conradson (LANSCE-DO); A. Llobet, T.E. Proffen, F.R. Trouw (LANSCE-LC); F.J. Espinosa-Faller (Marista University, Merida, Mexico); and G. Seidler (University of Washington)

Uranium dioxide, known as urania, is used as fuel in nuclear reactors, and is also important as an environmental contaminant and as the form of uranium in the illegal trade in nuclear materials. It has the unusual chemical property that it can sustain a continuous U:O ratio from 1.5 to 3.0. Thus, instead the U ions all being identical can have different charges or oxidation states even within the same crystal. These differently charged U ions distort the geometry of their neighbor O ions, which are also disordered because the oxidation reactions cause extra O atoms to be incorporated into the material.

We have recently performed structural measurements that indirectly indicate that these polarons, as the combination of the differently charged U ion and its associated neighbor atoms that are displaced from their normal sites, are dynamical. Instead of being fixed in a single position in the crystal, the polaron easily moves or hops between different atoms in different locations. In this hypervalent urania, we know that the polaron is confined to a relatively small region because the material is not conductive, but it does shift rapidly within this volume. This is important because the dynamical structure includes chemical species with different reactivities and highly strained geometries that, despite their being transient on any given site, apparently are involved in the overall properties of the material. They may explain not only its oxidation and solubility, but also be critical in the fracture of fuel elements in nuclear reactors. We also have very recent evidence from ultrafast pump-probe optical reflectivity spectroscopy that the initial charge-separated excited state from above-the-gap excitation relaxes in around 400 psec to a long-lived 4 (μsec) state that is coupled to a U-O phonon.

Experimental and Theoretical Efforts to Examine the Multiphase Properties of Cerium

B.J. Jensen, F.J. Cherne (DE-9)

There is a scientific need to obtain new data to develop and validate new multi-phase equation-of-state (EOS) models for metals. Experiments are needed to locate phase boundaries, determine transition kinetic times, and to obtain EOS and Hugoniot data for relevant phases. The objective of the current work was to use complex loading and standard plate impact methods to access Hugoniot and off-Hugoniot states to probe different regions of the phase diagram for cerium. Cerium was chosen for this work because it exhibits a complex phase diagram at moderate pressure regimes readily accessible using standard shock wave methods. Data have been obtained to map the low-pressure solid-solid transition through the critical point, to determine melting transition for shock loading, and additional data to search for the higher pressure phases below melt. Details of the experimental methods and recent experimental results will be presented along with a discussion on how these results will inform a recently implemented multiphase EOS for cerium.

Phase Transformations During Shock Deformation of U-6wt.%Nb

R.D. Field (MST-6); E.K. Cerreta (MST-8); D. Dennis-Koller (DE-9); G.T. Gray, III, D. W. Brown (MST-8); H.M. Volz, A.M. Kelly, J.C. Lashley (MST-6); T.A. Mason (W-6); and D.J. Thoma (INST-OFF)

U-6wt%Nb is a shape-memory effect (SME) alloy that deforms by SME twinning mechanisms for the first ~7% of uniaxial deformation. Subsequent deformation is believed to occur via a mixture of slip and non-recoverable twinning. The processed alloy is inhomogeneous, with a compositional variation of approximately ± 1-2 wt.%. The transformation temperatures within this compositional range vary from approximately room temperature (RT) to a few hundred degrees Celsius, so that regions of the martensite microstructure (particularly high Nb regions) are on the cusp of stability with respect to the parent phase at RT. The parent to martensite transformation is accompanied by a small increase in volume. Thus, high rate/shock deformation that involves significant transients of hydrostatic compressive stress can result in reverse transformation to the parent phase as part of the plastic response of the material. The presentation will include a general discussion of SME and post-SME deformation along with experimental evidence of phase transformations during high rate/shock loading.

Understanding the Deformation Behavior of α-Uranium

R.J. McCabe (MST-6); C. Tomé (MST-8)

We are able to understand the deformation behavior of low-symmetry materials by combining advanced experimental characterization with state of the art polycrystal modeling. In this presentation, we detail the use of electron backscatter diffraction (EBSD) and the viscoplastic self-consistent (VPSC) model to understand the deformation behavior of α-uranium. Due to its low-symmetry, orthorhombic crystal structure, α-uranium exhibits complex deformation behavior including multiple slip and twinning modes, and its mechanical response is highly anisotropic and extremely challenging to interpret and predict. We use EBSD to analyze the primary deformation twinning modes and to monitor the texture evolution during deformation. The VPSC model is used to analyze the activities of all of the deformation modes while predicting the mechanical behavior and microstructural evolution. Model predictions of the deformation behavior and texture development are in reasonable agreement with the experimental measures.

Microstructure Based Heterogeneity Evolution Leading to Material Phase Transformation and Damage/Failure Events—A MaRIE First Experiment

C.A. Bronkhorst (T-3); J.L. Barber (T-1); I.J. Beyerlein (T-3); J. Boettger (XCP-5); G.T. Gray (MST-8); C.W. Greeff (T-1); E.M. Kober (LANL Institutes); P.A. Rigg (DE-9); A.B. Saxena (T-4); M.W. Schraad (T-3); B.L. Adams (Brigham Young University); N. Bourne (U.K. Atomic Weapons Establishment); S. Ghosh (Ohio State University); and G. Ravichandran (California Institute of Technology)

The large deformation, damage and failure process for many polycrystalline metallic materials is inherently ductile in nature. In general, this means that the material will choose four specific physics mechanisms for accommodation of imposed deformation field or resistance to loading–solid-solid phase transformation, large deformation plasticity, shear localization or adiabatic shear banding, and cavitation. At present, materials models to represent this damage process contain the elements of pore initiation or nucleation, pore growth, pore coalescence, and ultimate failure. The nucleation process is believed to depend heavily on microstructural-based heterogeneities and the spatial distribution of defects. These include grain boundaries, impurity inclusions, intersection of twin planes and dislocation sub-cells. The statistical spatial distribution of inherent (grain boundaries, inclusions, initial dislocations) or deformation induced heterogeneities (twinning, dislocation subcell) is believed to act in combination with the spatial and temporal intensity of loading to determine which of the weakest defect sites will initiate a pore. A nucleated field of pores will then grow in size until they become large enough such that the deformation field surrounding individual pores begins to overlap with neighboring pores–at which time the process of damage coalescence begins.

The coalescence phase is when the established pore field begins to join and when localization or adiabatic shear banding facilitates this process. Of course, ultimate failure will occur when the coalescence process brings about a percolated region of damage. For dynamic and shock loading conditions, these events occur within very small length and time spans so velocities and accelerations are very large. Therefore, in addition to spatial effects, local inertial effects must also be accounted for. This process is extremely complex, stochastic and inherently loading path/rate dependent and so we need new tools to be able to understand the three-dimensional link between the defect structure/ microstructure and detailed loading characteristics. This understanding will then be used to motivate new physically based models for micromechanical and continuum representation of these events. This understanding can also be used to design new materials and/or tailored processing of old materials for specific applications, which are based upon functional requirements and known physics. These are the motivations behind a MaRIE first experiment that will be discussed.

Microstructure in the Extreme Environment: Understanding and Predicting Dynamic Damage Processes

E.K. Cerreta (MST-8); D.D. Koller (DE-9); C.A. Bronkhorst, B.L. Hansen (T-3); R.A. Lebensohn (MST-8)

The Grand Challenge of Materials: Discovery Science to Strategic Application emphasizes the need to control material performance in extreme environments. This study examines the separate effects of kinetics (in the form of dynamic loading rate) from that of spatial effects (in the form of microstructural defect distributions). Recently, available mesoscale modeling techniques are being used to capture a physical link between kinetic and spatial influences on dynamic loading. This work contributes innovative new tools in the form of shock-wave shaping techniques for small-scale dynamic experimentation, three-dimensional materials characterization. The research lends insight into damage analysis at micron resolution as the Laboratory considers capabilities for MaRIE, and the capabilities for dynamic damage evolution based on the physics associated microstructure and strain rate effects. Such work positions the Laboratory to lead the way for the development of process-aware material performance and responds directly to two of the three scientific challenges of LANL's materials strategy: (1) defects and interfaces and (2) materials in extremes.

A fundamental understanding of length-scale and kinetic effects in the extreme environments of dynamic loading speaks directly to advancing understanding of emerging issues relevant to inclusion related failure in metals, grain size dependence on ejecta, and benefits of interfaces in mitigating defect development; issue central to C2, C4, and Office of Basic Energy Sciences (BES) Energy Frontier Research Center programs. Finally, the coupling of experimental techniques with theory and simulation is aimed at advancing damage modeling at LANL to position the Laboratory to the forefront of process-aware modeling as well as transitioning materials science from observation to property control.

Influence of Hot Spot Features on the Initiation Characteristics of Explosives

D.M. Dattelbaum, S.A. Sheffield, D.B. Stahl (DE-9); R. Menikoff (T-1); A.M. Dattelbaum (MPA-CINT); B. Patterson (MST-7)

The overwhelming consensus in the high explosive (HE) research community is that the generation of hot spots (highly localized regions of high temperature and pressure within which ignition occurs on a rapid time scale) is essential to the mechanism of initiation and detonation properties of most condensed phase high explosives. The potential origins of hot spots are numerous and include dynamic pore collapse, plastic shear band formation, friction from motion along closed cracks, or reflections from other in-situ interfaces. Despite many decades of research into the physics of high explosives, currently we only have a very basic understanding of the broad mechanisms underlying shock-induced hot-spot generation, hot-spot ignition, hot-spot interaction and reaction wave spread leading to HE initiation and detonation. Consequently, all current high explosive models treat hot-spot physics empirically. These models only work in limited regimes near calibration experiments; other applications require more substantial model recalibrations.

To gain insights into the role of hot spot features on initiation characteristics, well-defined micron-scale particles have been intentionally introduced into the homogeneous explosive nitromethane, providing a controlled model system for interrogating the influence of two types of hot spot origins, shock impedance mismatches and hollow microballoons, on initiation. In the presentation, we show the results of multiple series of gas gun-driven plate impact experiments on these mixtures. Detailed insights into the nature of the reactive flow have been obtained, and the data have been used to establish initiation mechanisms, and Pop-plots (run-distance-to-detonation versus shock input pressure) for the materials. Comparisons of sensitization effects and energy release characteristics relative to the initial shock front between the solid and hollow beads will be presented. These results are revealing new insights into how hot spots influence the reactive flow characteristics, initiation thresholds, and energy release in the chemical reaction zone behind the detonation front. In doing so, we are advancing our understanding of hot spots that may eventually lead to an ability to design explosives with tailored properties, as well as provide a credibly predictive capability for simulating explosives behavior. As such, the research supports LANL's missions in stockpile stewardship, threat reduction and homeland security, as well as DOE-DoD collaborative programs.

Recent Experimental and Modeling Observations of the Dynamic EOS, Yield, and Spall Strength Behavior of S-200F Beryllium

C. Adams, W. Anderson (DE-9); G. Gray, W. Blumenthal (MST-8); F. Freibert (MST-16); M. Prime (W-13); F. Addessio (T-3); L. Hull (DE-3)

In response to a renewed interest in the dynamic behavior of beryllium (Be), we have established a new capability for performing plate impact experiments on Be to study the dynamic equation-of-state (EOS), yield strength (Hugoniot Elastic Limit (HEL)), and spall strength of this material. We have conducted a series of symmetric and asymmetric plate impact experiments (peak stress between 2.1 and 19.0 GPa) and explosive (Taylor wave) loading experiments (peak stress of ~30 GPa) on vacuum hot-presssed (VHP) S-200F Be. Our EOS dataset obtained from the plate impact experiments for S-200F Be agrees well with that obtained decades earlier from experiments on S-200D and S-200E grades of Be. We see a significant influence of the Romanchenko correction on the magnitude of the spall strength (~0.81 - 0.90 GPa) for S-200F in the plate impact experiments and little dependence on strain rate amongst these experiments or when compared with spall strength data obtained from the experiments conducted with an explosive drive. Our dynamic yield strengths are significantly lower than observed in quasi-static experiments and we observe a progressive reduction in the HEL with increasing sample thickness. Reasonable agreement with modeling results is obtained depending on the particular EOS and strength, and/or, damage accumulation model employed in the simulations. We believe that twinning plays a significant role in the high strain rate deformation of VHP S-200F Be; a deformation mechanism not yet incorporated in the models.

The Study of High Speed Surface Dynamics using a Pulsed Proton Beam

W.T. Buttler (P-23)

A significant component of scientific research at LANL centers around the understanding of the failure modes of materials under extreme pressures. At these pressures of 10 GPa or more, materials can fracture and dislocate inhomogeneously, passing through multiple solid phases as the pressure wave releases to zero pressure into a solid or liquid phase. Often, the material surface is characterized by machining marks, or perturbatations that can cause the materials to eject metal fragments. In this case, there is an interest to understand how these ejected fragments, "ejecta," are formed and transported in gasses. To understand these failure modes, research often centers on theory and physics model development, combined with experiment, for incorporation of failure models into predictive hydrodynamic codes that model the behavior of materials at extreme pressures, which can exceed 100 GPa. Because surface failure modes that form ejecta are of interest, we have studied the failure phenomena in a variety of pressure loading extremes, which include shocking the materials in flyer plate experiments, referred to as supported or square wave loading experiments, and high explosive (HE) loading experiments, referred to as Taylor or triangular wave experiments.

The physics of pressure wave loading profiles attempts to link the shockwave profile to the underlying damage, where one case raises the material loading pressure to a sustained compression for some time, and the other is quickly raised to a high pressure that releases to lower pressures over longer time scales that cause tensile stresses on the materials near the surface. These different loading and release mechanisms cause the materials to fail in different manners, and understanding these different failure modes is of interest, but not necessarily required to develop relevant physics models. Considering the ejecta problem, the theory of the failure mode is thought to be linked to the formation of a special limiting extreme of a Richtmyer-Meshkov instability where the Atwood number is -1. In this model, as the shockwave releases from a few tens of GPa, if the material is a liquid on release, an instability will form that breaks up the material into small liquid droplets---ejecta. The ejecta will breakup further in the presence of a gas that is thought to be caused by drag forces, and in some cases Kelvin-Helmholtz (shear) instabilities. A predictive capability to model different materials that form ejecta is of interest. We study these phenomena with penetrating proton radiographs, and other mass measurement techniques. Other diagnostics include high-speed velocimetry to determine free-surface velocities, and the fastest ejecta velocities, and what is known as the bubble velocity as well.

I present a basic approach to experimental ejecta studies, and modeling approaches as well. The modeling approaches include simulations across multiple size scales. The experimental approaches that have led to the model development will be presented, and culminates in the presentation of dynamic proton radiographs of the instability formation and evolution in vacuum and two gasses. The movies are acquired over a time scale of about 10 microseconds, and the field of view is a cross sectional area of 40 millimeters by 40 mm. The instability velocities approach several km/s.

Copper Strength at High Strains and Strain-rates

R.T. Olson, D. L. Preston (P-23); A.M. Montoya, C. Morris (P-25); and A. Kaul (XCP-5)

Material strength models, such as Preston-Tonks-Wallace and Steinberg-Guinan, are constitutive models with parameters derived from data sets obtained primarily from quasi-static and Hopkinson-bar experiments. Consequently, the major predictive uncertainty of the models lies in the range of strain and strain-rate conditions where these experimental techniques are not well suited to yield data. These conditions, with strains up to several hundred percent at strain-rates between 10^5 and 10^8 s^{-1}, are precisely where explosive loading or high-velocity impact simulations utilize the models to predict the ensuing plastic deformation of metals.

A series of strength model validation experiments have been conducted that utilize flat copper samples with small perturbations of known wavelength and amplitude machined into one surface. A high-explosive plane-wave lens is used to generate shock-free, planar loading on the perturbed side of the plate and the amplitude of the Rayleigh-Taylor unstable perturbations are measured via a sequence of radiographs acquired as a function of time. The perturbation growth rate is inhibited by the dynamic strength of the metal and is compared directly to that predicted by various strength models via hydrodynamic simulations. Recently, acquired data shows the role material processing, and the resulting sample microstructure, has on bulk material strength under high strain and strain-rate deformation.

Pu Strength Experiments and Modeling

W.R. Blumenthal, S.R. Chen, (MST-8); T. Saleh, P. Contreras, (MST-16); M. Bange (WCM-DO)

The poster presents the integrated approach used for constitutive strength modeling of the various phases of plutonium. Both quasi-static and Kolsky bar uniaxial compression strength data are used in addition to other property measurements and validation tests (e.g. Taylor Anvil) to constrain constitutive strength models. This work is supported by Science Campaigns 1 and 2 and the materials capability programs.

Plutonium-Taylor Anvil Cold Test Facility

G.C. Kaschner, R.W. Ellis, T. Bell, M.L. Lovato, W.R. Blumenthal, (MST-8);
P.J. Contreras (MST-16); P. Than (University of California, Davis)

The Taylor cylinder-on-anvil impact test (also referred to as the Taylor Anvil) is a cost-effective, small-scale integrated compressive impact experiment used to validate constitutive strength and damage models for materials under high strain rate conditions and multi-axial stress conditions. During impact, a Taylor cylinder experiences large gradients of stress, strain, strain-rate, and temperature. Although the cylinder impact configuration is initially axi-symmetric, this test has been successfully used to account for the three-dimensional deformation behavior of anisotropic materials that are of interest to the nuclear weapons program.

This experimental technique is a critical link between small-scale fundamental plutonium experiments (such as the Kolsky bar, quasi-static compression, and the 40 millimeter launcher) and more costly large-scale integrated plutonium experiments that involve complex loading and require accurate material strength, damage, and equation-of-state models to simulate.

Taylor cylinders are typically 7-12 mm diameter by 25-40 mm long rods of the material of interest that are fired at moderate velocities (50 to 400 m/s) against a massive, rigid target (a very high hardness, polished steel anvil). The cylinder axial profile and impact footprint can be measured using in situ, high-speed photography and after impact using three-dimensional metrology. Additional post-test characterizations are used to understand the resulting deformation microstructures, how it evolved, and how it affects fundamental dynamic deformation behavior.

The gas gun and catch chamber for the Pu-Taylor anvil impact system have been assembled for cold test evaluation within the Materials Science Laboratory prior to installation at TA-55 and will be described.

The Multi-Probe Diagnostic Hall at MaRIE and the Science of Dynamic Extremes

C.W. Barnes (P-DO)

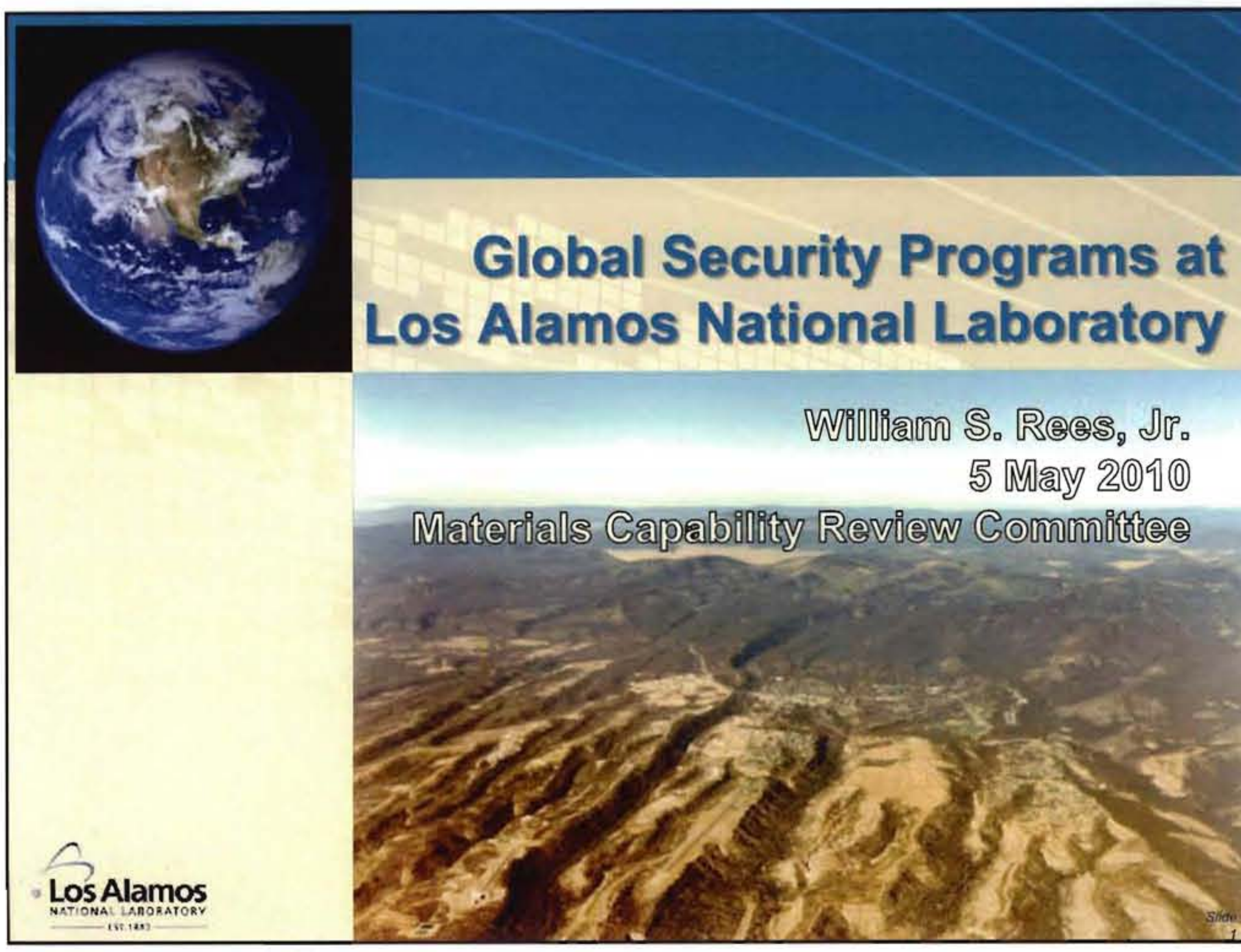
Defects and interfaces are the ultimate features that control materials performance, whether to limit or enhance it. The performance of materials in dynamics extremes, also known as compression science, is vital to a broad spectrum of engineering and defense applications related to LANL's national security science mission. To enable the transformation from the present era of observation to that of control of material's functionality and performance, new scientific tools are needed. The Matter-Radiation Interactions in Extremes (MaRIE) facility will provide dynamic observations of micro-structure that yield control of materials needed to reduce costs and increase confidence in the nuclear stockpile or advanced nuclear energy systems. There is a scientific need for *in-situ*, real-time, three-dimensional, experimental micro-structural quantification in extreme environments, allowing discovery of mechanisms and validation of simulations. A particular decadal challenge is transient and multiple measurements of the meso-scale at micron and nanosecond scales, what we call the micron frontier. The Multi-Probe Diagnostic Hall is being designed to address this and other compelling applications, such as multi-scale fluid dynamics or extreme electromagnetic field interactions with matter. The user-driven science case will be presented that define quantified scientific functional requirements. These requirements can then be met by functional facility requirements, and the current preferred alternative for the simultaneous and multiple x-ray, electron, proton, and neutron probes of matter will be described.

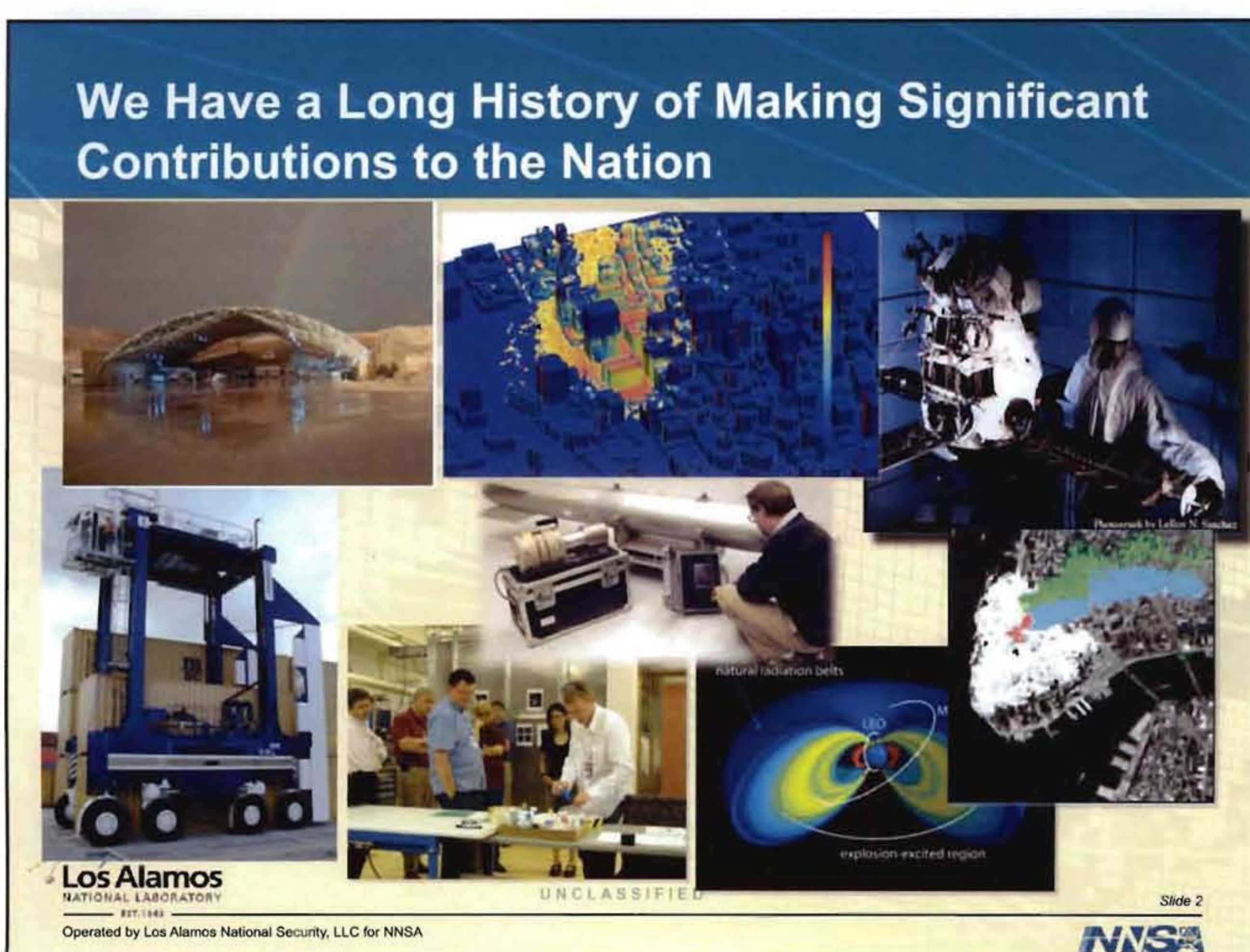
Tab 5

Global Security Programs at Los Alamos National Laboratory

W. Rees (PADGS)

Los Alamos National Laboratory has a long, and justifiably proud, history of science; not simply for the sake of itself, but devoted to the most pressing issues of national security. For the initial several decades of its existence, the mission was predominately dedicated to topics closely related to nuclear weapons. That component has remained the Laboratory's core mission, albeit consistently augmented by other tasks for the past 20 years. At the same time, the security challenges facing the nation have been trending annually upward at an increasing rate. In this environment, the Laboratory created the new position of Principal Associate Director for Global Security. The world in which we live is tumultuous and uncertain, with threats ranging from the inconvenient to the unthinkable. Security in such a world demands the fullest attention of the most talented citizens from all segments of society. LANL has a special technical leadership role to fulfill in this regard.


Global Security Programs at Los Alamos National Laboratory
William S. Rees, Jr.
5 May 2010
Materials Capability Review Committee
Los Alamos NATIONAL LABORATORY
Slide 1


We Have a Long History of Making Significant Contributions to the Nation
natural radiation belts
explosion excited region
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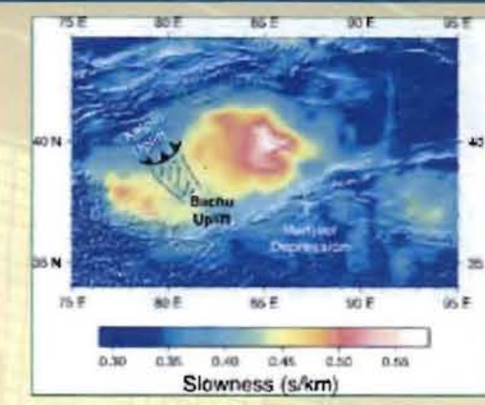
NNSA

Nuclear Nonproliferation

- LANL leads Fuel Fabrication Capability (FFC) portion of the NNSA Reactor Convert program.
- LANL/NNSA secures SNM at Mayak, world's largest nuclear storage facility
- LANL's Jim Doyle serves as key speaker in Carnegie Endowment verification conference
- HEU Blend Down Monitoring System upgraded, implemented at Russian sites, enables assurance of reactor fuel blend



Tarim Basin seismic event identification

HEU Blend Down Monitoring System

- New 3D method for CTBT seismic monitoring using joint inversion of surface wave velocity and gravity observations
- Coordinating with national (LEU-based) Mo-99 supply enterprise partners

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Slide 3

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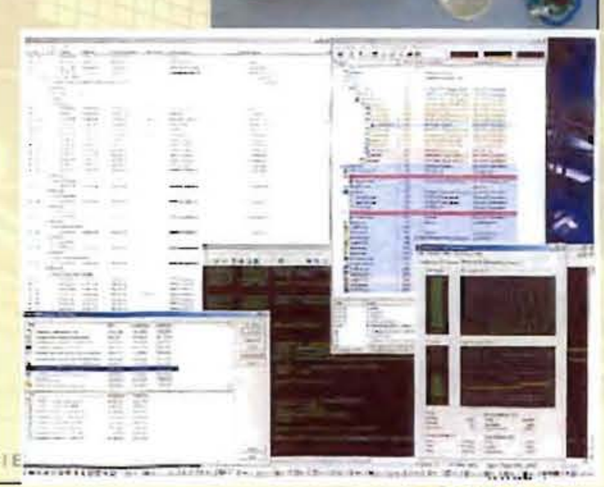
Cyber Systems

- Highly successful work with Intelligence Community partners
- Advancing the state of the art in areas of
  - Intrusion Detection
  - Reverse Engineering
  - Modeling and Simulation
  - Covert Communications
  - Knowledge Integration



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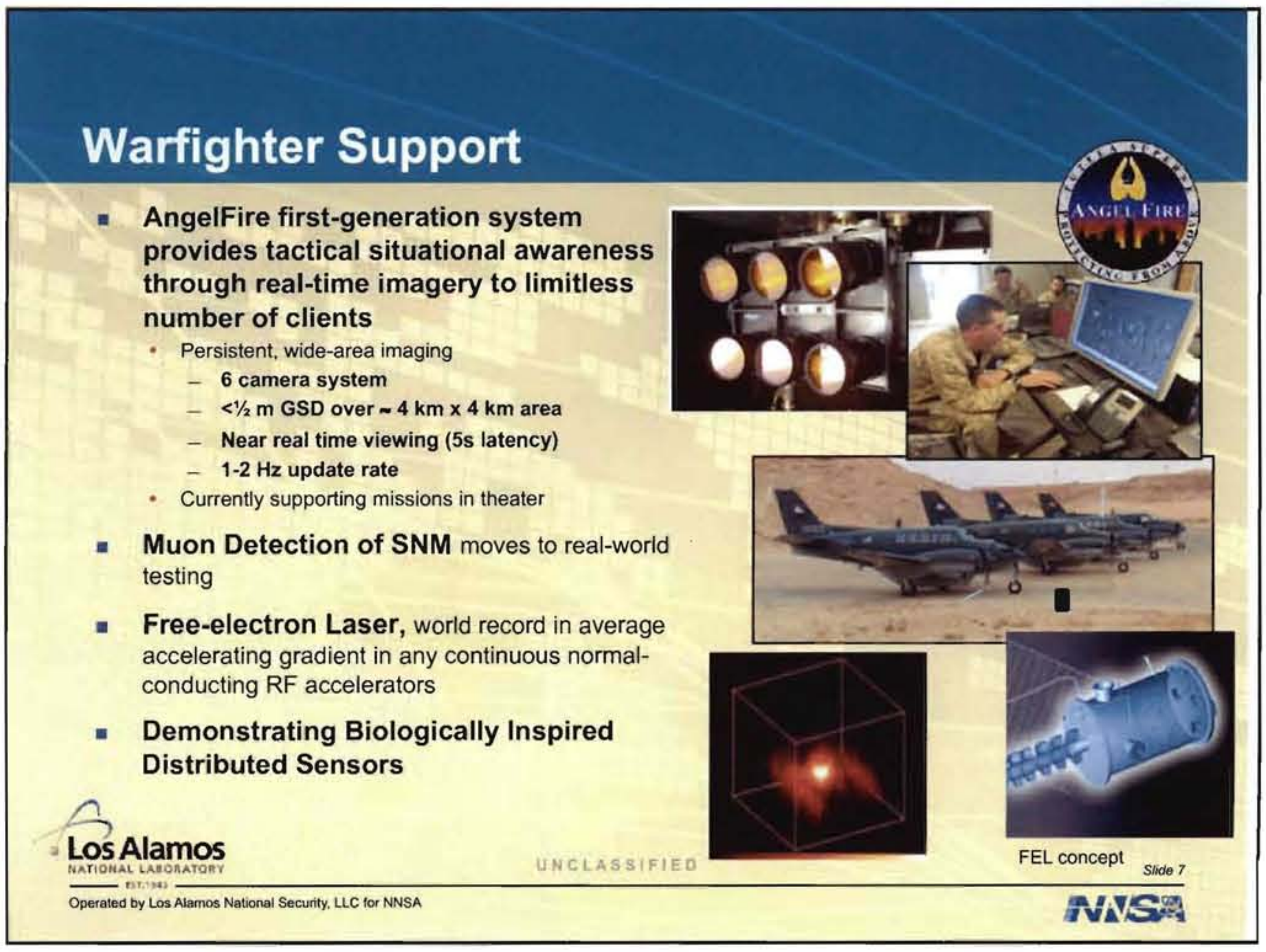
Warfighter Support
AngelFire first-generation system provides tactical situational awareness through real-time imagery to limitless number of clients
Persistent, wide-area imaging
6 camera system
<½ m GSD over ~ 4 km x 4 km area
Near real time viewing (5s latency)
1-2 Hz update rate
Currently supporting missions in theater
Muon Detection of SNM moves to real-world testing
Free-electron Laser, world record in average accelerating gradient in any continuous normal-conducting RF accelerators
Demonstrating Biologically Inspired Distributed Sensors
ANGEL FIRE
FEL concept
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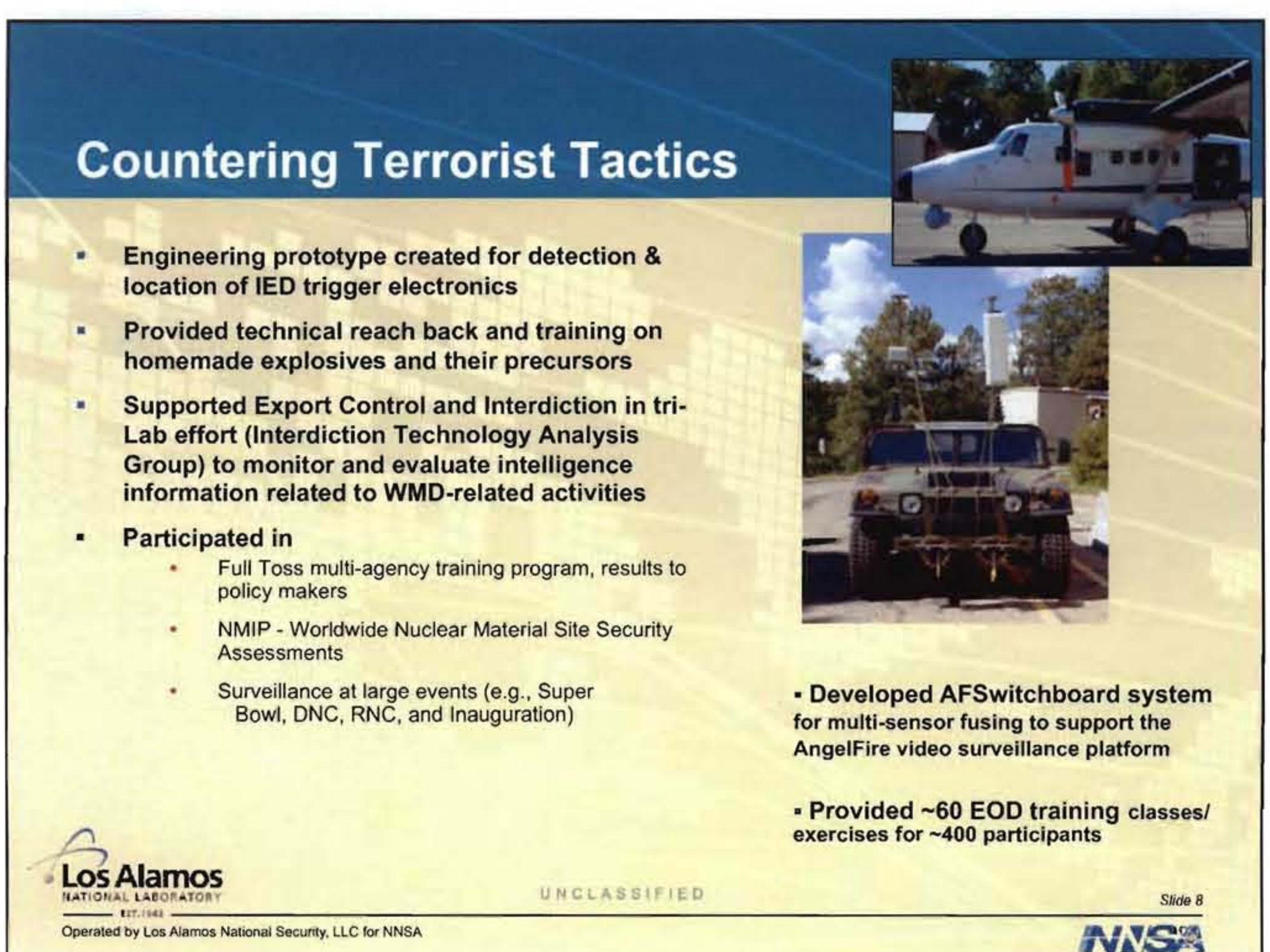
Countering Terrorist Tactics
Engineering prototype created for detection & location of IED trigger electronics
Provided technical reach back and training on homemade explosives and their precursors
Supported Export Control and Interdiction in tri-Lab effort (Interdiction Technology Analysis Group) to monitor and evaluate intelligence information related to WMD-related activities
Participated in
Full Toss multi-agency training program, results to policy makers
NMIP - Worldwide Nuclear Material Site Security Assessments
Surveillance at large events (e.g., Super Bowl, DNC, RNC, and Inauguration)
Developed AFSwitchboard system for multi-sensor fusing to support the AngelFire video surveillance platform
Provided ~60 EOD training classes/ exercises for ~400 participants
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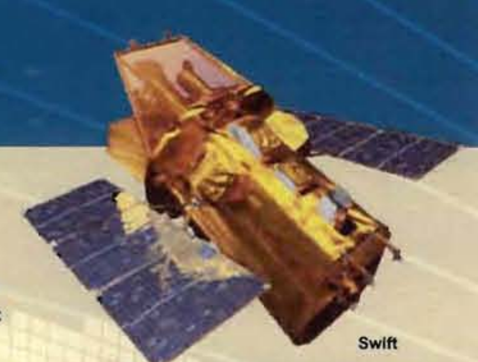
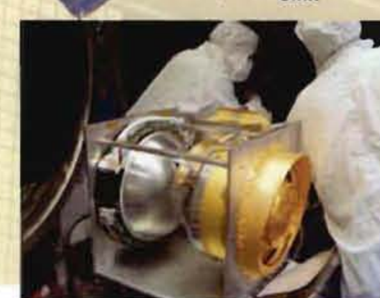
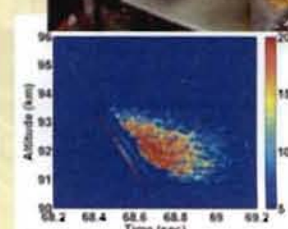
Space Systems

- Successful launch of IBEX, LANL instrument finds intriguing heliospheric results
- First unambiguous characterization of dust from the local interstellar medium using USAF Interferometric radar.
- NASA Swift Mission discovers most distant object in the universe.
- Patent application calculating the motion of radiation belt electrons ~ 1 million x faster.
- SABRS flight unit integrated, qualification unit delivered for testing,
- R&D 100 award for TeraOps Software Radio
- LANL instruments aboard final GPS Block IIR launch, and ground-based staff completes on-orbit assurance testing of six Block IIR EMP sensors


Swift


IBEX payload


Interstellar dust

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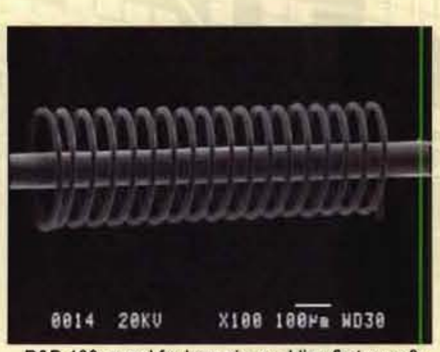
Intelligence Analysis, Integration and Exploitation

- $30M Funding for Tri-Lab Nuclear Intelligence Analysis and Capability Support
- 4 Nuclear weapons technology training classes for the intelligence community
- Completion of 5 Quick Response Capability (QRC) Deliveries


Cube-sat mini satellite



R&D 100 award for Lasonix, enabling first-ever 3-dimensional diodes, akin to the revolution of the first semiconductor devices in the late 1940s.

- Development started on two Cube-sat projects (inexpensive, rapid turn-around satellites) for tactical missions
- Nano and microengineered solutions team earned R&D 100 award for fabrication of 3-D electronics technology

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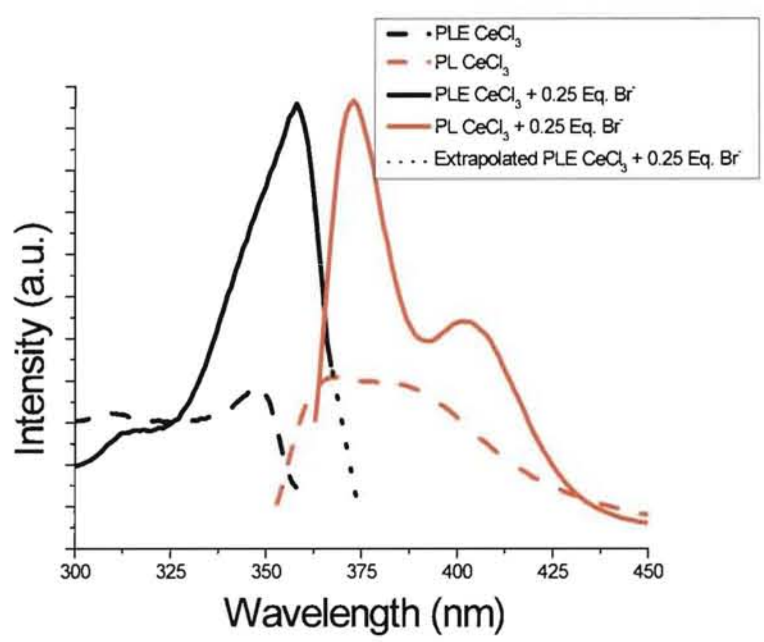

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Materials Capability Review 2010

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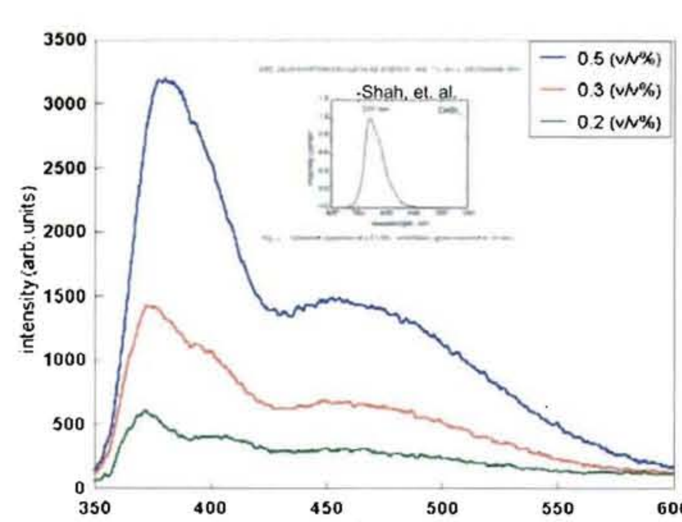
$CeBr_3$ Nanomaterial



- Optical Response to Ionizing Radiation is consistent with that for single crystal material

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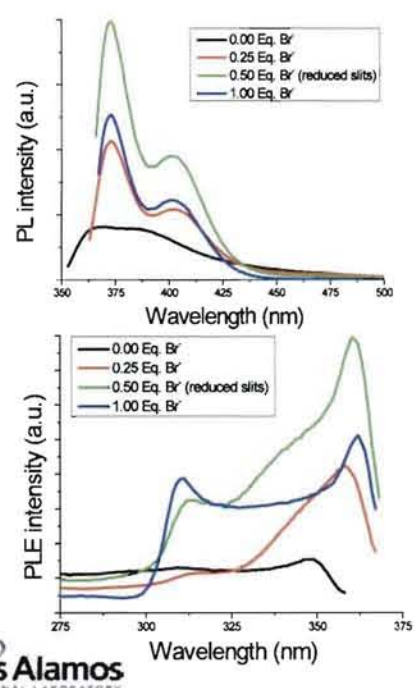
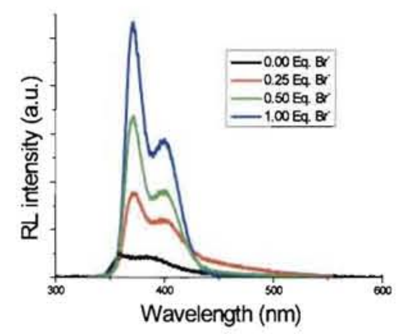
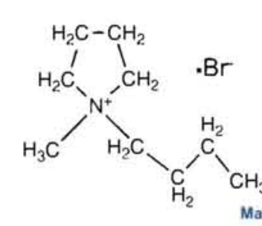




- Bromide salt addition to $CeCl_3$



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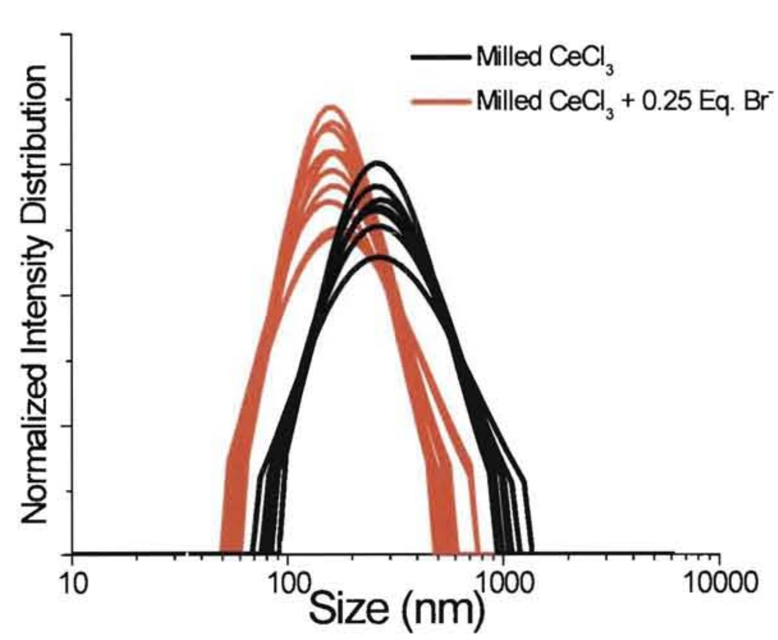

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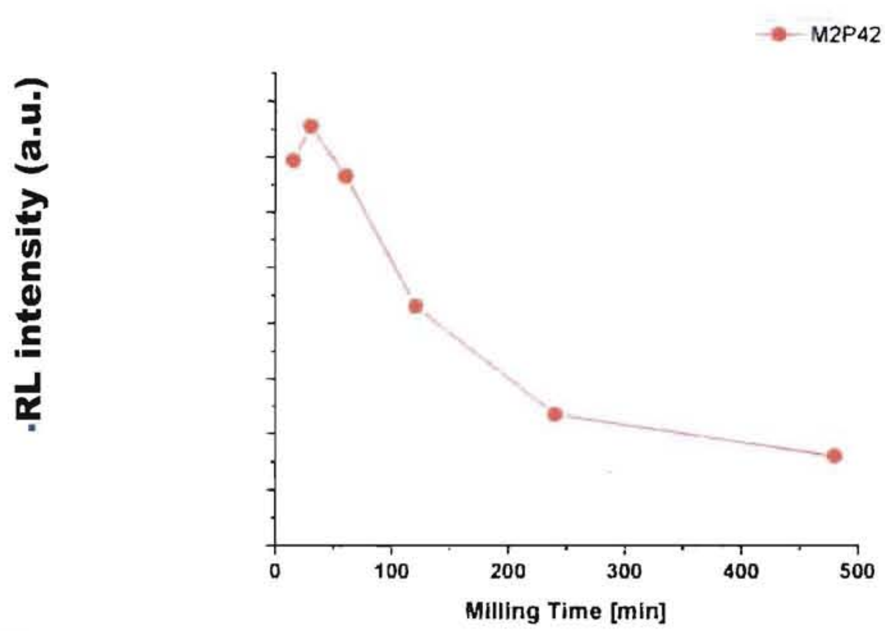

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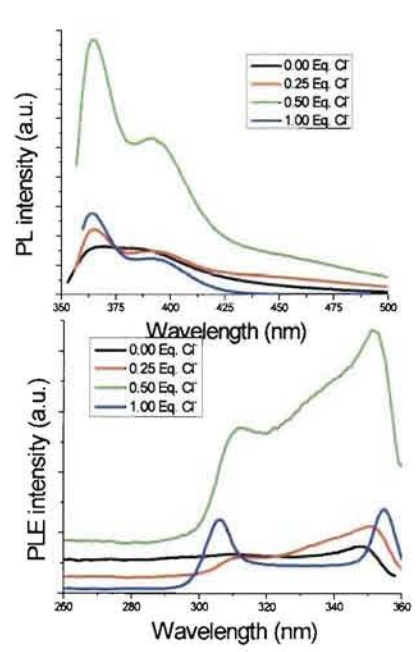
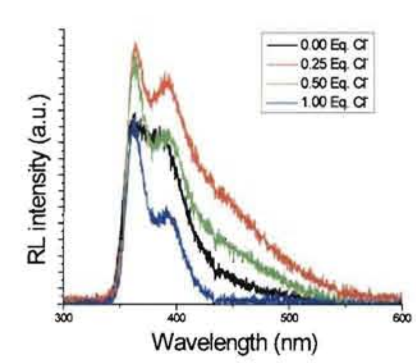
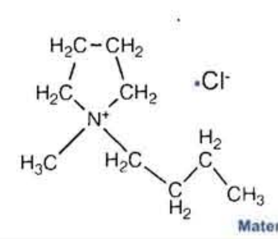




- Chloride salt addition to $CeCl_3$



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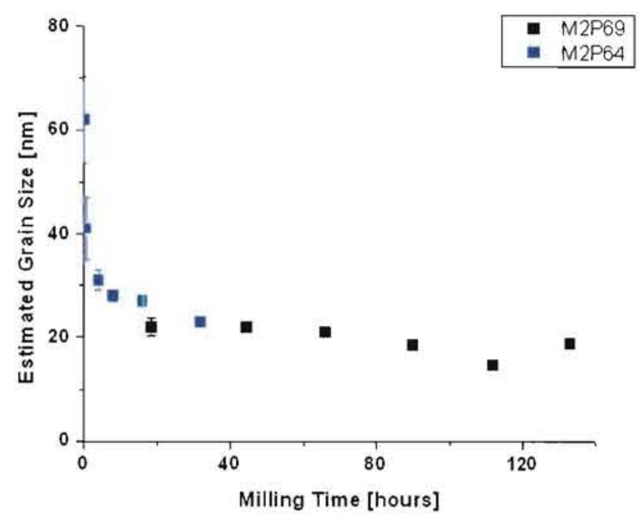

•Grain size as a function of milling time. Two independent milling runs

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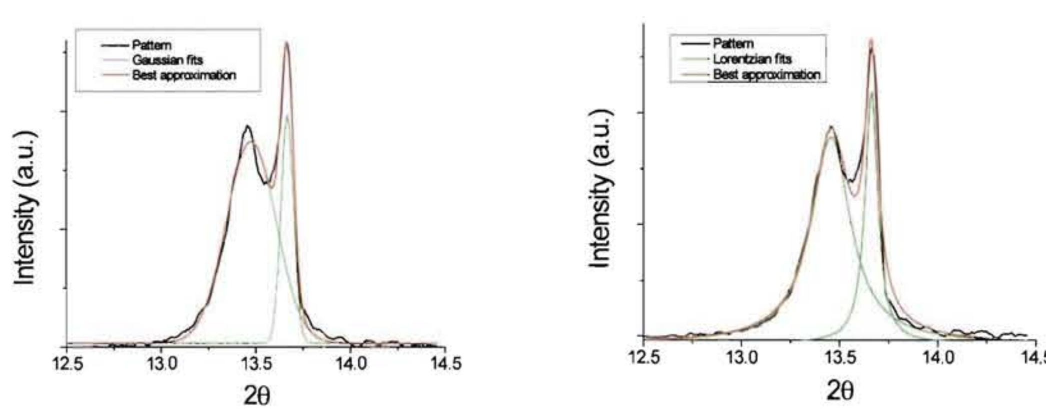

•Typically, XRD peaks are a mix of Gaussian and Lorentzian

	Peak A (Bulk)	Peak B (nano)
d-spacing:	0.6472 nm	0.6563 nm
Grain size:	> 100 nm	~30 nm

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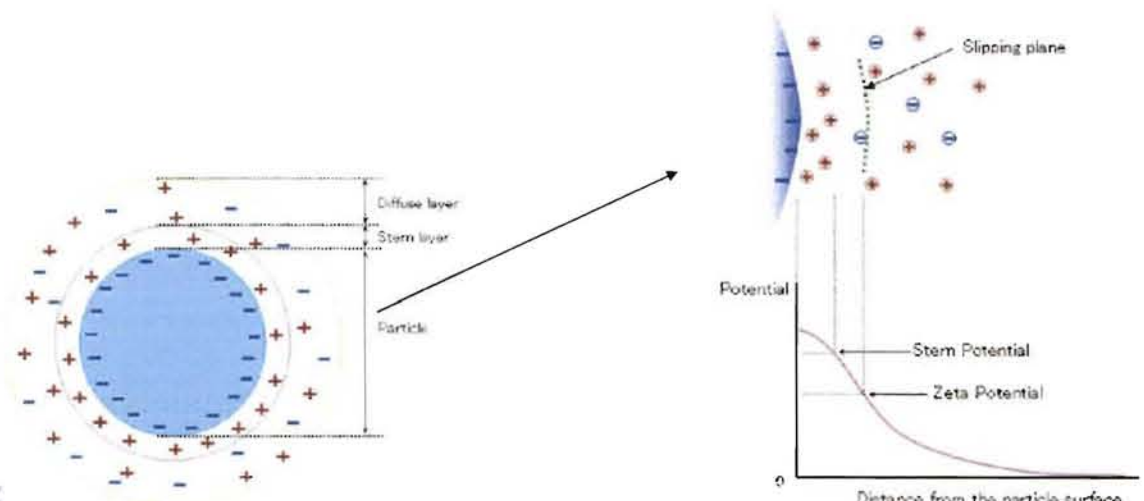
Zeta Potential

- **The zeta potential is the potential at the interface of charges that move with the particle and charges that do not**
  - This quantity is strongly correlated with the stability of dispersions



•Figures from Beckman Coulter Delsa Nano Manual

Industrial Scale Dispersion

•Mini-Cer

•150 ml grinding chamber

Mini-Cer is smallest practical bead mill, larger mills are also standard items

•Zeta RS

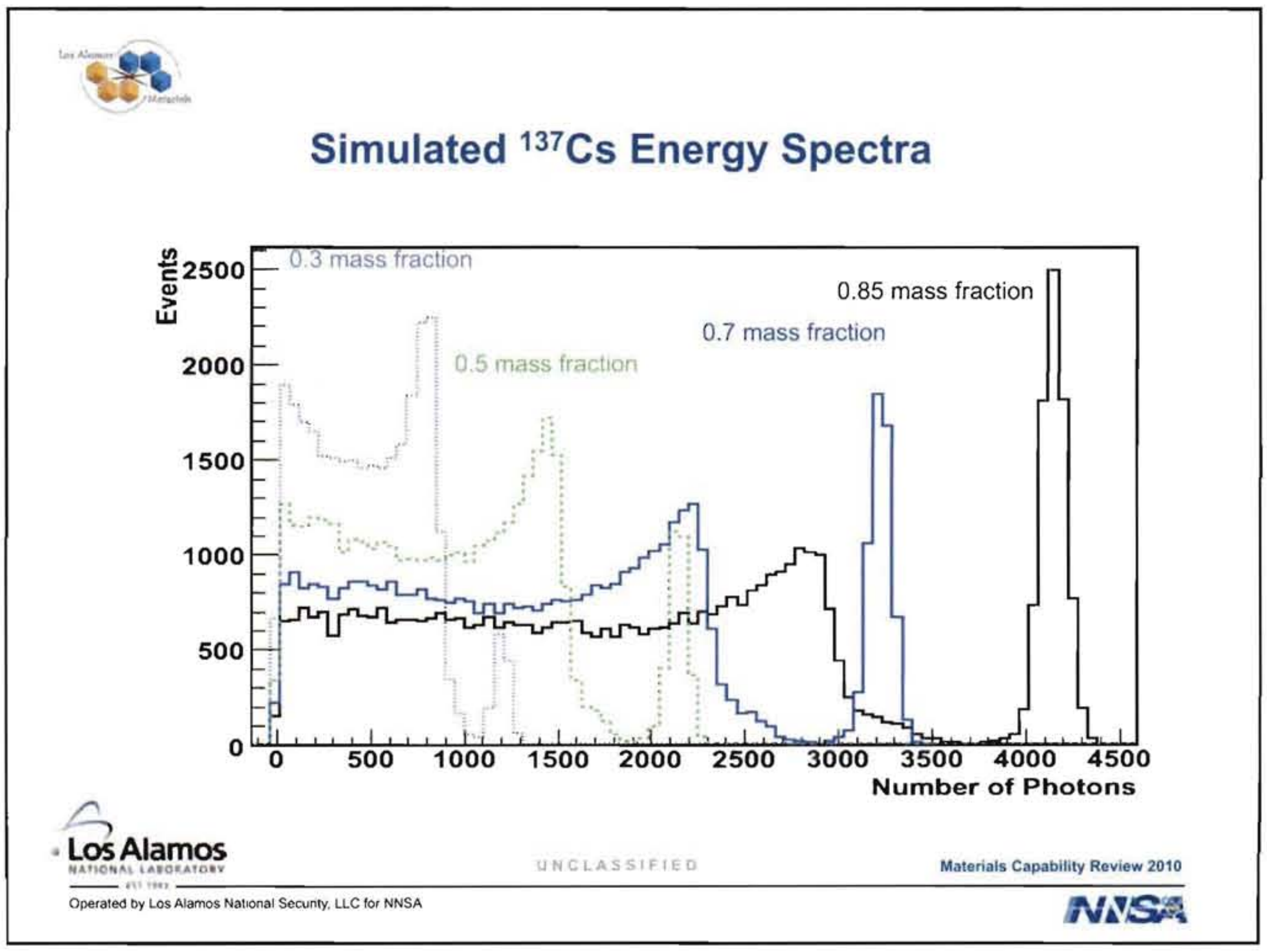
•4 liter grinding chamber
•Factor of 25 scale-up

•LMZ 25

•25 liter grinding chamber
•Factor of 165 scale-up

•LMZ 150

•150 liter grinding chamber
•Factor of 1000 scale-up


Simulated ^{137}Cs Energy Spectra
Events
2500
2000
1500
1000
500
0
0.3 mass fraction
0.85 mass fraction
0.7 mass fraction
0.5 mass fraction
0 500 1000 1500 2000 2500 3000 3500 4000 4500
Number of Photons
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Energy Deposition Model

- Uses NIST estar database for dE/dx and range tables
- Incorporates binomial statistics for particle sampling at each step
- Provides calculation of energy deposition in particles, ligand and matrix
- Assumes no interaction between constituents

$$E_p = \int_{range} f_v^p \frac{dE_p(E)}{dx} dx$$

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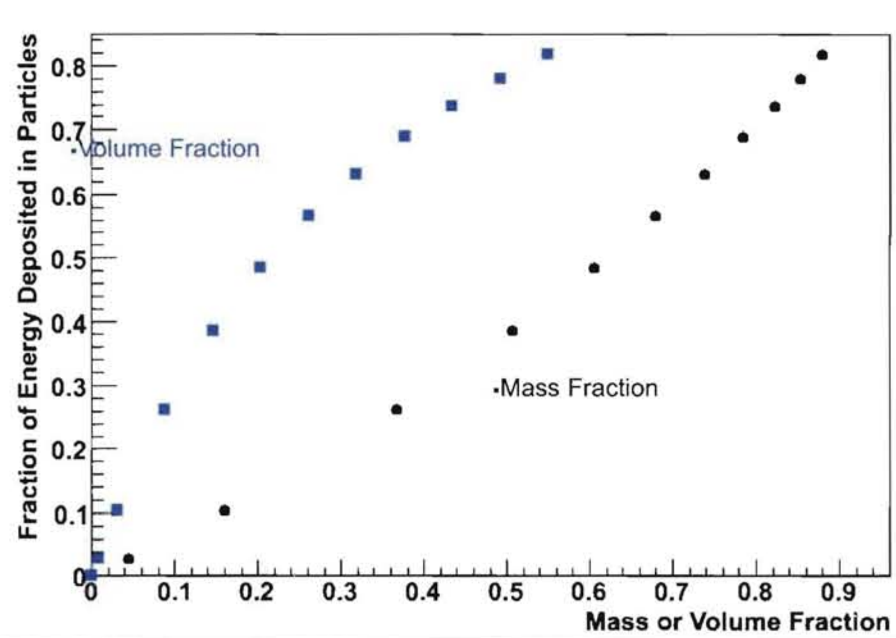
Calculated Energy Deposition



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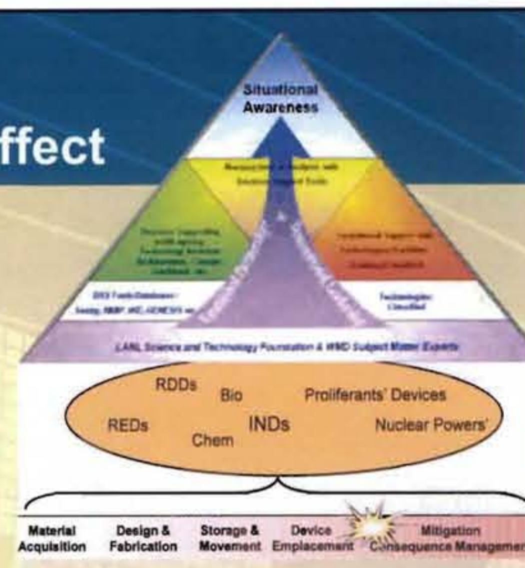
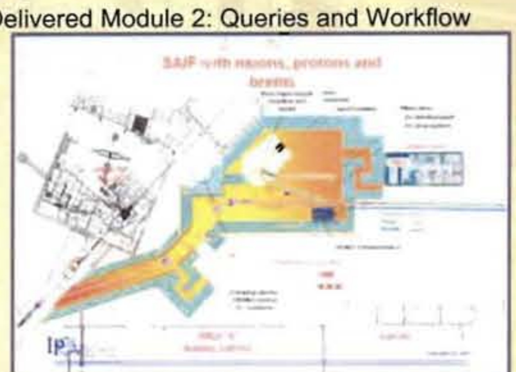
Counter Weapons of Mass Effect

- **Appointed as Lead Lab for CWAC/ DNDO**
  - A country-specific exercise (Joint DIA/DTRA/ DNDO)
  - Delivered suite of codes: signatures to probabilities
- **Appointed Lead Performer for NMIP Trinity**
  - Delivered Module 2: Queries and Workflow





- **Trained DoD** (4 Major Exercises)
- **Appointed DTRA/ONR Lead Lab** for Multi-Particle Stand-Off Detection
- **DHS Lead Center for** Gen-3 Bio Assay

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Slide 9

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Event Response

Preparing for ARG radiography

- **As of July 2009, LANL personnel had deployed for six real-world emergency-response events and 17 drills.**
  - **Supported presidential inauguration, conventions and other high-visibility events.**
- **Worked with NA-42 and the FBI supporting training, drills and hardware to establish the first Stabilization Operations capability for FBI Special Agent Bomb Techs in FY10.**
- **LANL personnel covered LLNL's JTOT Phase 2 obligations for most of FY09 until LLNL was able to demonstrate their ability to meet timelines.**
- **Participated in the "Fall Classic," at Nevada Test Site's Device Assembly Facility (DAF) involving measurements of high-fidelity Radiation Test Objects**
  - **Included measurements by JTOT and foreign entities (a first).**

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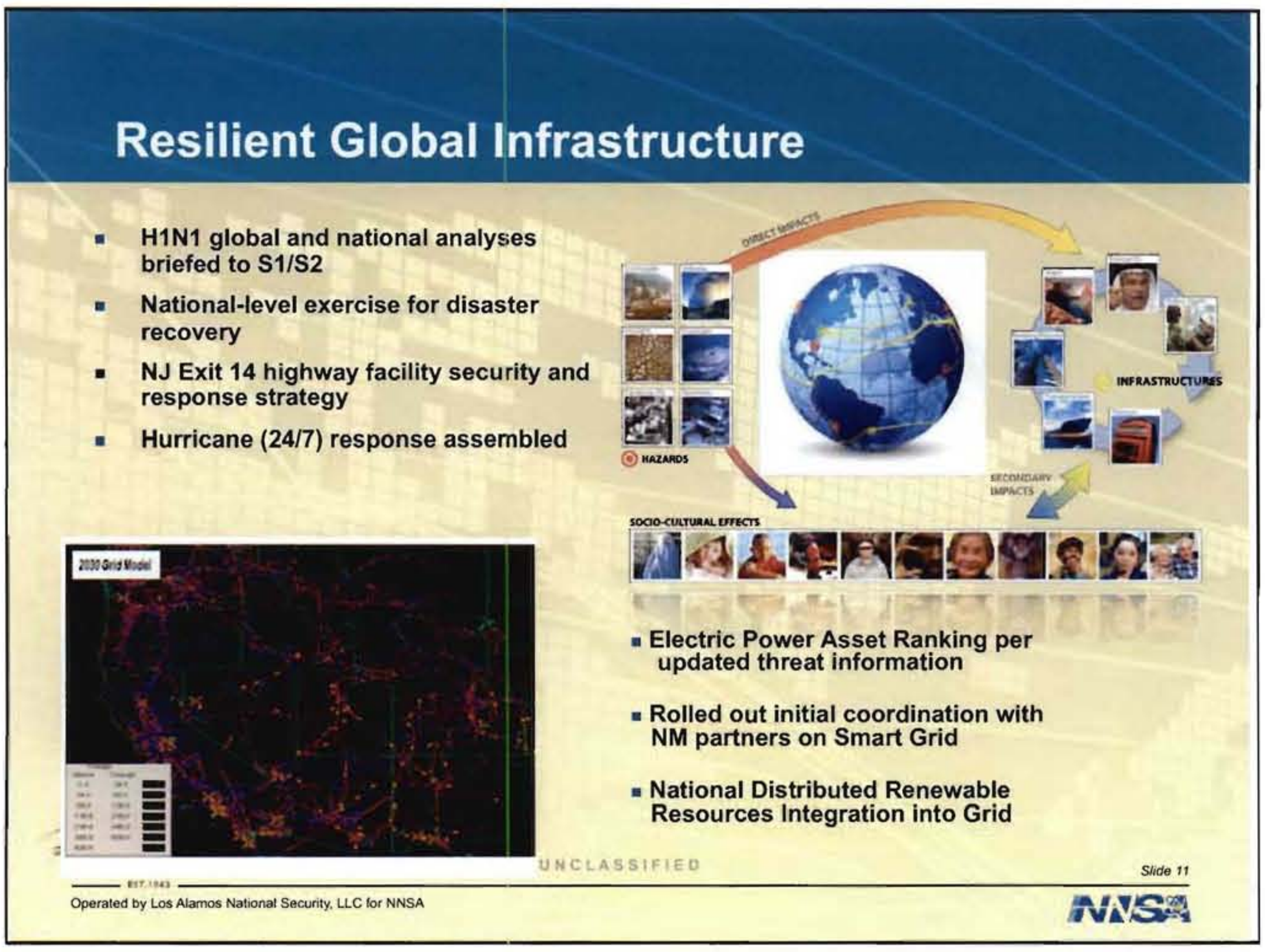
NNSA Slide 10


Resilient Global Infrastructure
H1N1 global and national analyses briefed to S1/S2
National-level exercise for disaster recovery
NJ Exit 14 highway facility security and response strategy
Hurricane (24/7) response assembled
DIRECT IMPACTS
INFRASTRUCTURES
HAZARDS
SECONDARY IMPACTS
SOCIO-CULTURAL EFFECTS
2030 Grid Model
Electric Power Asset Ranking per updated threat information
Rolled out initial coordination with NM partners on Smart Grid
National Distributed Renewable Resources Integration into Grid
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Introduction: Materials for Global Security

D.J. Thoma (INST-OFF, MDI)

National security is manifested in broad, programmatic efforts at Los Alamos National Laboratory. Starting in the last fiscal year, a new Principle Associate Directorate for Global Security has been formed, and the mission, structure, and thrust areas are evolving and maturing. Indeed, multi-disciplinary interactions are being defined and coordinated. Materials discovery and development play an important role to satisfy the programmatic requirements for national security missions. These areas include such topics as military applications, homeland security, and non-proliferation.

While the material requirements for global security are large and encompassing, this programmatic theme will focus upon topical areas of immediate programmatic opportunities. The topical focus will include nuclear detection and detection avoidance (camouflage). In nuclear detection, the theme will cover primary and secondary detection development, as well as merge into tertiary examinations such as nuclear forensics. Detection avoidance, although not necessarily in the nuclear regime, will focus on thrusts in metamaterials. The combined effort should provide a brief but cross-organizational view of programmatic efforts that rely on materials development to address national security demands.

Introduction: Materials for Global Security

Dan J. Thoma

Director-Materials Design Institute

Programmatic Element Theme Leader

Materials Capability Review May 5, 2010

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Materials for Global Security

- **Global Security is an evolving and maturing topic at LANL**
  - Dr. William Rees, Jr. presentation
  - Formation and organization of PADGS (over the past year)
- **Processes have begun to coordinate multi-disciplinary interactions and define key areas for LANL participation**
  - Workshops
  - Roadmaps
  - Team identification
  - Partnerships
- **Materials discovery and development play an important role to satisfy programmatic requirements for national security missions, for example**
  - Military applications
  - Homeland security
  - Non-proliferation, counter-proliferation
  - Treaty Verification

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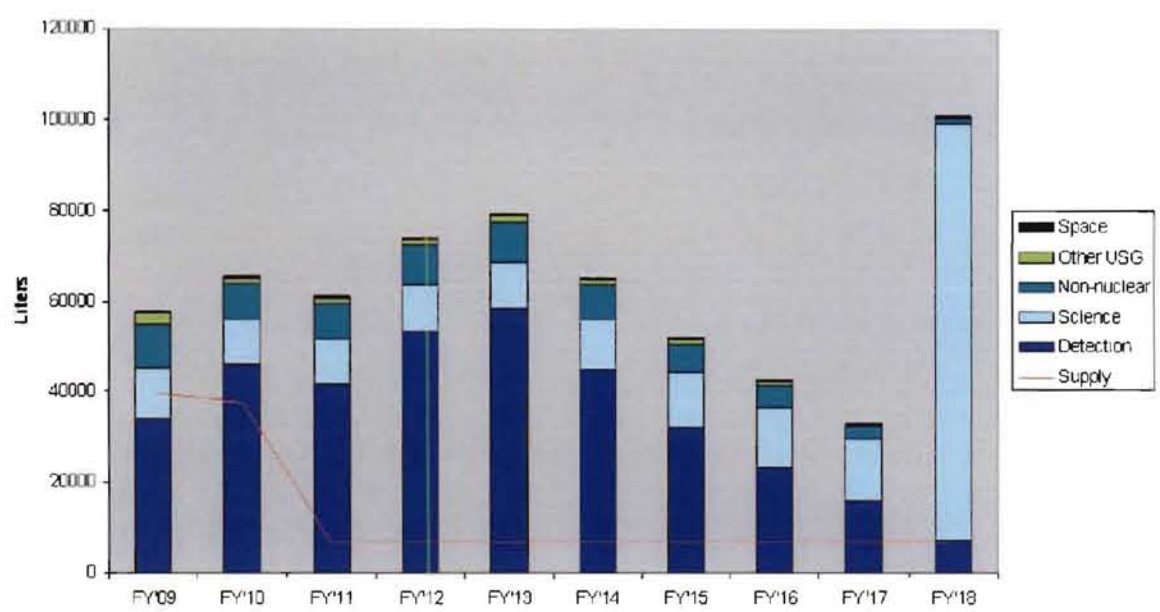
Example: He-3 Projected US Supply and Demand
(Without Action)



Materials for Global Security - Detection

While the materials development for Global Security is large and encompassing, the focus for the Review will be on recent thrust efforts and the potential for growth in these areas.

- **Detection/Surveillance/Treaty Verification**
  - Primary
    - Passive
    - Active
  - Secondary
  - Tertiary (Forensics)
- **Camouflage**
  - Metamaterials (applications only, link with emergent phenomena)

Nuclear Detection Materials

E. McKigney (N-1)

The current status of development of nanocomoposite scintillators at LANL will be outlined. The focus will be on the optical and radiation response properties of the nanomaterials, as well as an outline of the challenges associated with forming composites.

Nuclear Detection Materials

Bryan Bennett[1], Michael Blair[2], Leif Brown[3], Jon Cook[4], Rico Del Sesto[5], Rob Gilbertson[1], Andy Li*[4], Edward McKigney@[4], Ross Muenchausen[1], Nick Smith[1], Sy Stange*[4], Mark Wallace[6], Debra Wrobleski[1]

@ presenter *graduate student

[1] MST-7 [2] EES-14 [3] C-CDE [4] N-1 [5] MPA-MC [6] ISR-1

May 5, 2010

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Outline

- **Context – relevant mission needs and gap**
- **Approach – technical approach**
- **Results – highlight of one of the optical results**
- **Conclusions – current status and next challenges**

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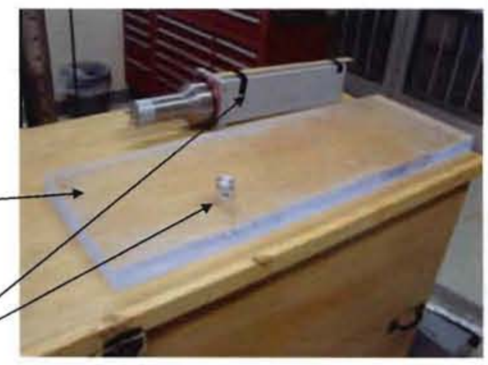
Conceptual Overview

•Nanocomposite scintillators will combine the performance of inorganic crystalline scintillators with the cost and processing of organic plastic scintillators.

•This will be accomplished by eliminating the need for crystal growth and synthesizing the materials using bulk chemical processing.



•Plastic Scintillator
•Low Cost
•Large Volume
•Poor Energy Resolution
•Poor Stopping Power

•Inorganic Crystalline
•Scintillator
•Medium-High Cost
•Small-Medium Volume
•Good Energy Resolution
•Good Stopping Power

•Straddle Carrier instrumented for scanning cargo containers

•Portal monitors for scanning vehicular or pedestrian traffic

•Hand-held radioisotope identifier for secondary inspection and search

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Optical Transparency

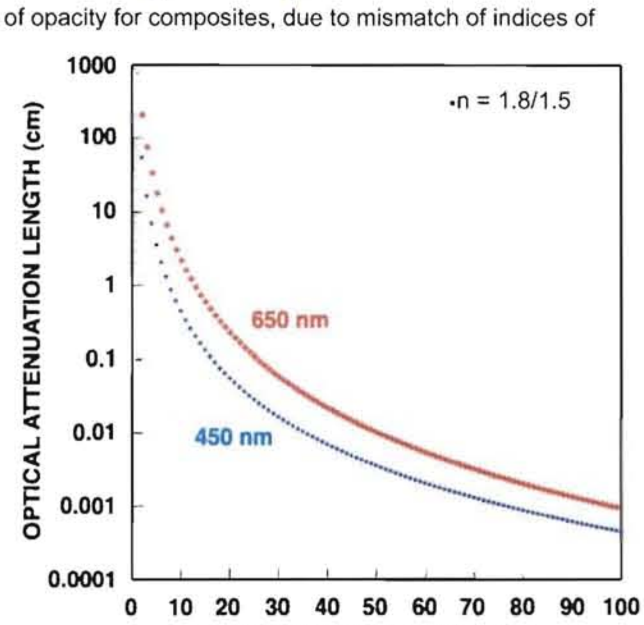
•Rayleigh scattering is an important source of opacity for composites, due to mismatch of indices of refraction between particle and matrix.

$$T = \frac{I}{I_0} = e^{-N\sigma x}$$

$$\sigma = \frac{2\pi^5}{3}\frac{d^6}{\lambda^4}\left(\frac{n^2-1}{n^2+2}\right)^2$$

$$N = \frac{v_{fraction}}{\frac{\pi}{6}d^3}$$

$$n = \frac{n_{particle}}{n_{matrix}}$$



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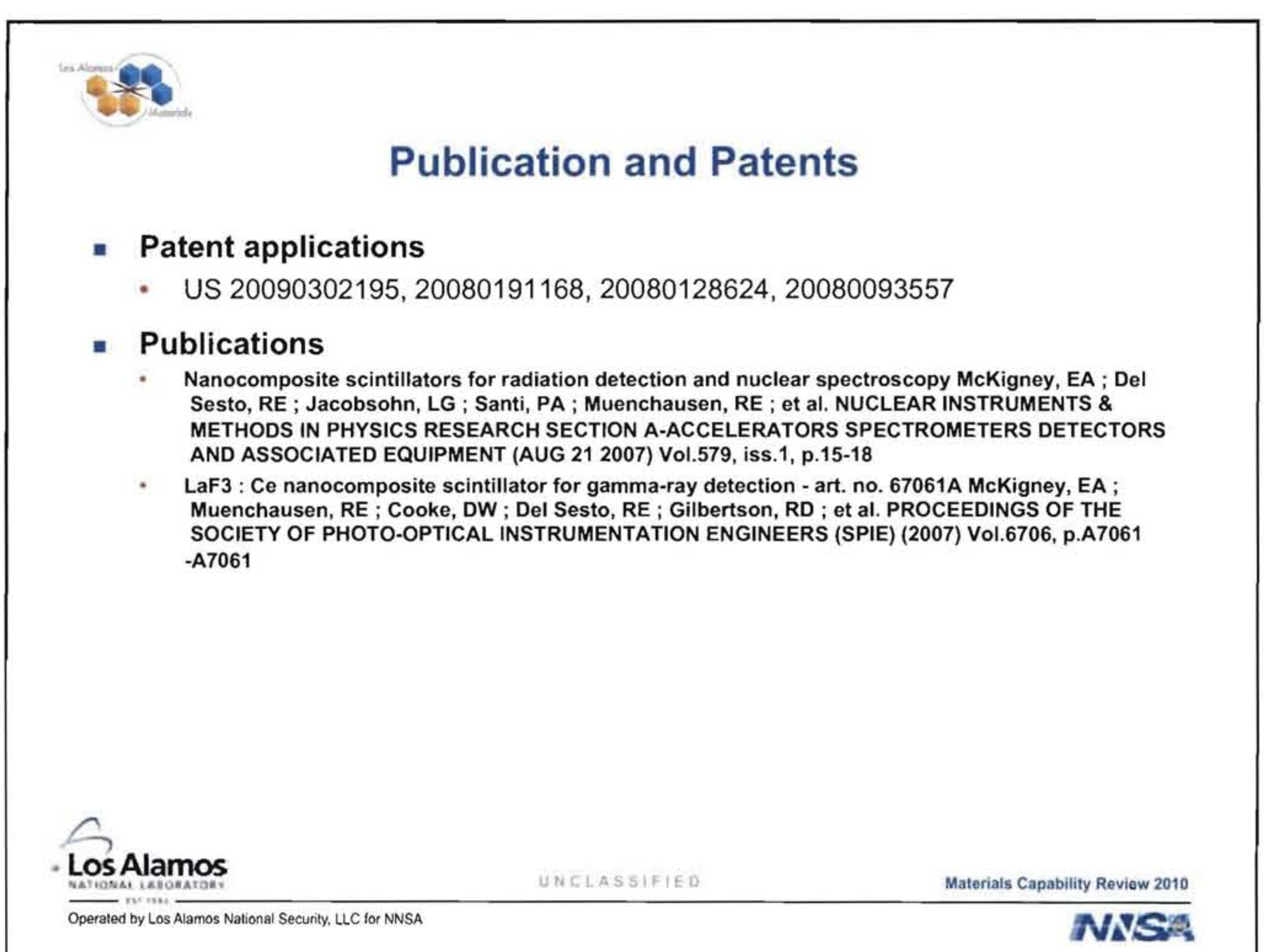
Publication and Patents
Patent applications
US 20090302195, 20080191168, 20080128624, 20080093557
Publications
Nanocomposite scintillators for radiation detection and nuclear spectroscopy McKigney, EA ; Del Sesto, RE ; Jacobsohn, LG ; Santi, PA ; Muenchausen, RE ; et al. NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT (AUG 21 2007) Vol.579, iss.1, p.15-18
LaF3 : Ce nanocomposite scintillator for gamma-ray detection - art. no. 67061A McKigney, EA ; Muenchausen, RE ; Cooke, DW ; Del Sesto, RE ; Gilbertson, RD ; et al. PROCEEDINGS OF THE SOCIETY OF PHOTO-OPTICAL INSTRUMENTATION ENGINEERS (SPIE) (2007) Vol.6706, p.A7061 -A7061
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Active Terahertz Metamaterials for Global Security

J. O'Hara, H.T. Chen, A. Azad, J. Zhou, K. Dani (MPA-CINT); E. Smirnova, D. Shchegolkov (ISR-6); A. Taylor (MPA-DO)

Nearly all global security priorities critically depend on electromagnetic technologies and, therefore, any major improvements in electromagnetic control can have a significant impact on LANL mission areas. Fairly recently, electromagnetic metamaterials have emerged as an approach to vastly improving control over electromagnetic waves, even enabling devices that would be impossible with natural materials. Metamaterials are artificial materials whose electromagnetic response is created by design, leading to controllable functionality well beyond what natural materials can offer. Numerous worldwide efforts have addressed metamaterials in the microwave and optical regimes with impressive results. One area of substantially less focus is the terahertz frequency regime, ironically an area of very poor technology development due to a lack of suitable natural materials for wave control. We present a brief overview of metamaterials and how they enable electromagnetic control. Then we show our work in developing active (or dynamic) terahertz active metamaterials. Our results prove that active terahertz metamaterials enable powerful methods to control electromagnetic waves in amplitude, phase, and polarization. In addition, this control is actively tunable, leading to new high-performance devices such as modulators and waveplates, which are described in detail. Finally, the impact of our work is discussed.

Active Terahertz Metamaterials for Global Security

J. O'Hara, H.-T. Chen, A. Azad,
J. Zhou, K. Dani, A. Taylor (MPA)

E. Smirnova, L. Earley, D. Shchegolkov (ISR)

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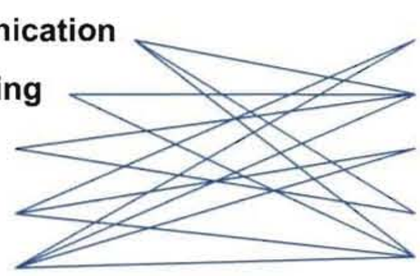
Electromagnetics in the LANL mission

Electromagnetic technologies

- Communication
- Computing
- Control
- Sensing
- Imaging



LANL missions

- Nonproliferation
- Space situational awareness
- Treaty monitoring
- Counterterrorism
- Intelligence support

Improved control over electromagnetic waves is foundational to LANL missions in Global Security.

Control through materials capability.

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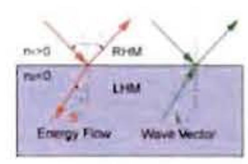
Electromagnetic metamaterials

Artificially constructed materials with properties derived from their sub-wavelength structures, not from the materials they are made of.

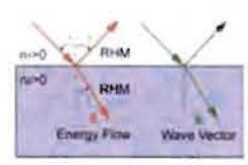
A material that exhibits an electromagnetic response not found in natural materials.

$$\mu < 0 \quad \varepsilon < 0 \qquad n < 0$$



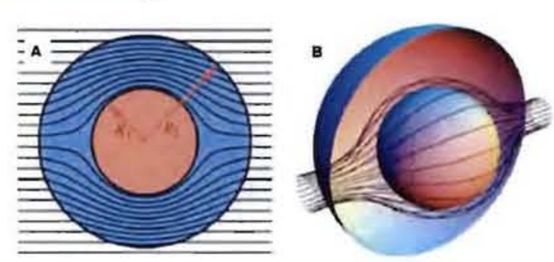
A material with a dynamically tunable electromagnetic response.

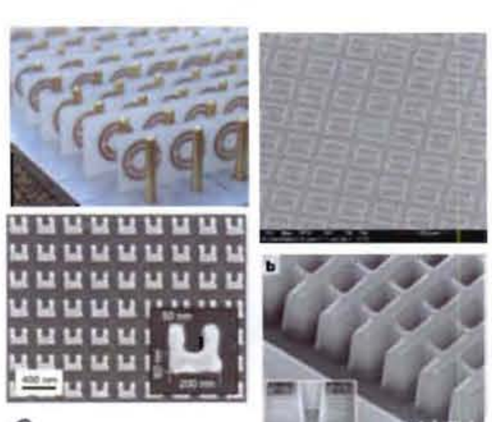
$$\varepsilon < 0 \longleftrightarrow \varepsilon > 0$$

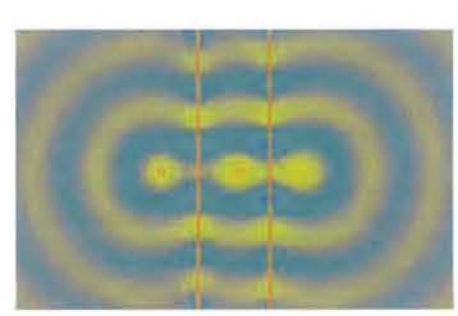


Designed functionality

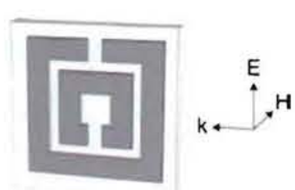
- **Response is scalable**
  - Radio waves to optical
- **Response is unique**
  - Perfect lens
  - Electromagnetic cloak

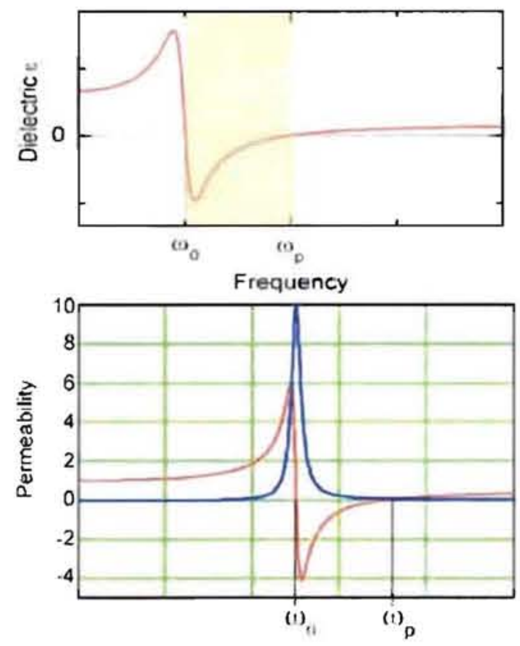




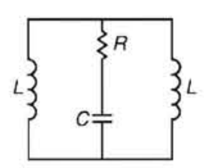


Controlling the effective electric and magnetic response





$$\varepsilon(\omega) = 1 - \frac{\omega_p^2 - \omega_0^2}{\omega^2 - \omega_0^2 + i\omega\Gamma}$$



$$\mu_{eff} = 1 - \frac{\frac{\pi r^2}{a^2}}{1 + \frac{2\sigma i}{\omega r \mu_0} - \frac{3}{\pi^2 \mu_0 \omega^2 C r^3}}$$

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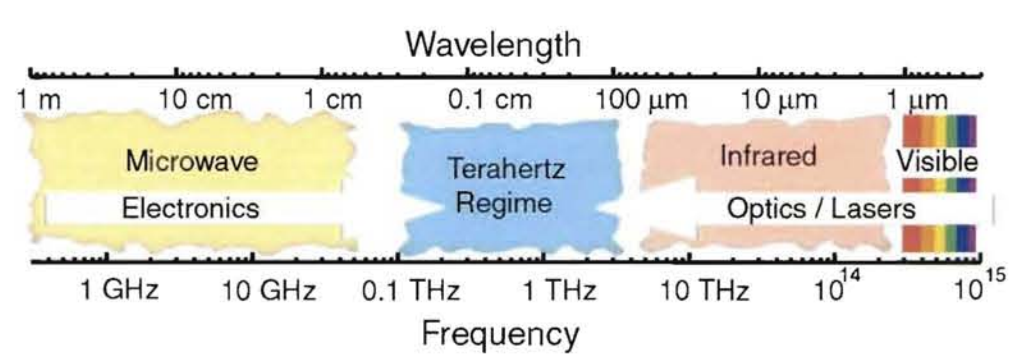
Our focus: terahertz



- **Electronic materials → semiconductors → radar, wireless comm**
- **THz materials → ??? → no practical devices**
- **Photonic materials → glasses, crystals → lasers, imaging arrays**

THz metamaterials = unique effort

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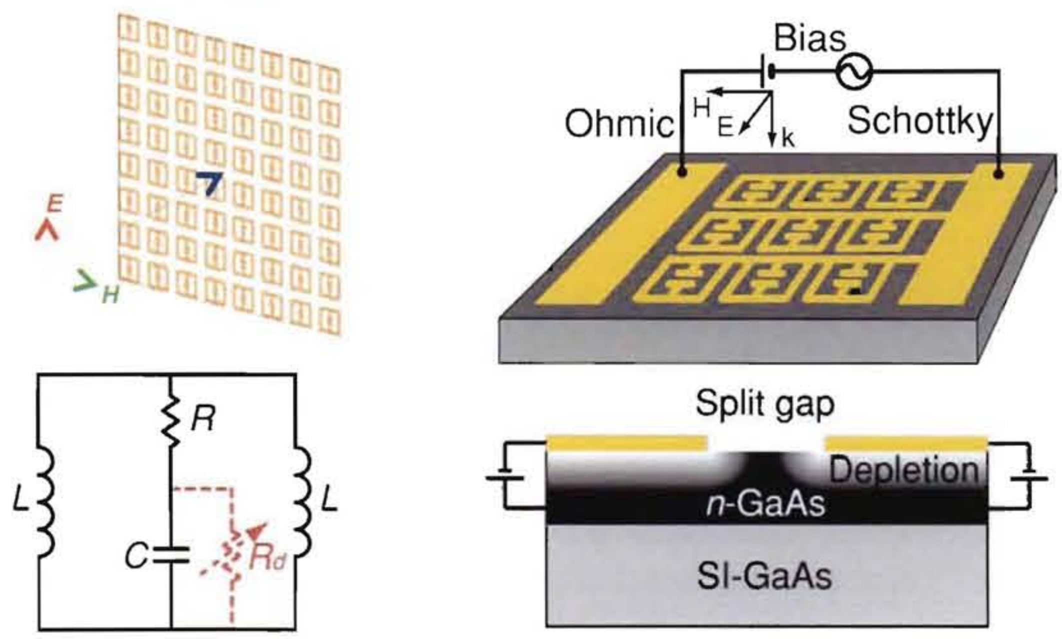
Electrical amplitude modulation of terahertz waves



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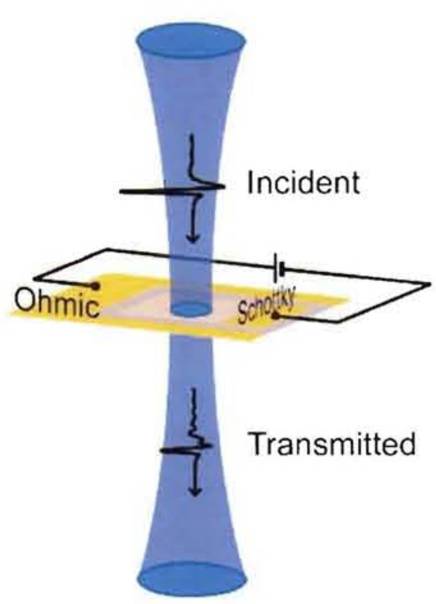
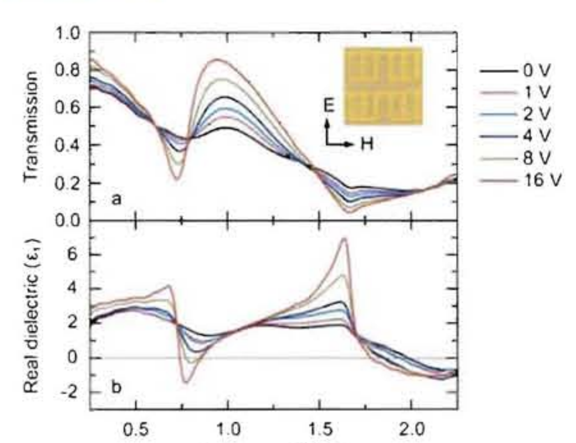
Performance





Results:
- THz switching efficiency: 70%, 2 MHz
- Switching ε between "+" and "-"
- Room temperature

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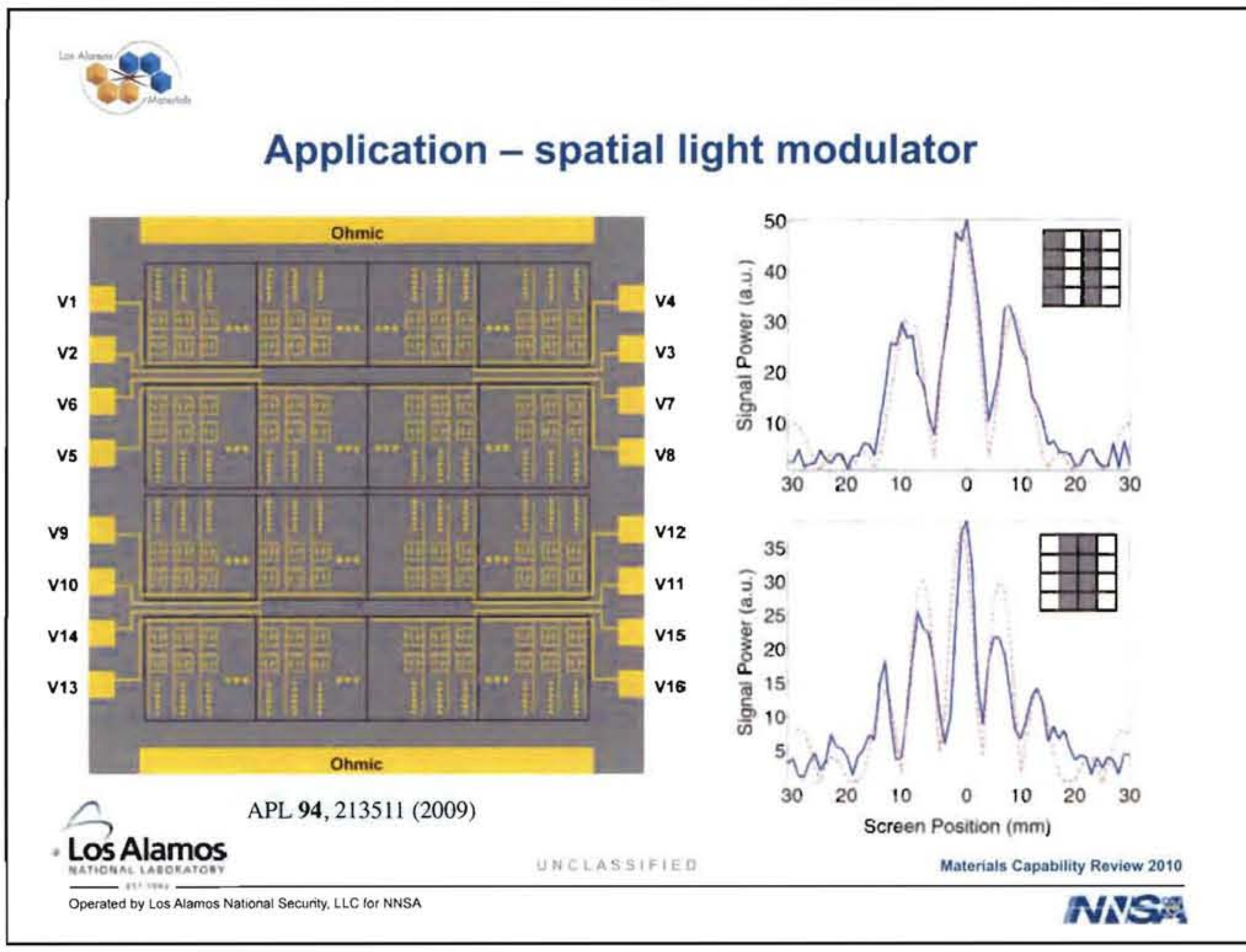
Application – spatial light modulator
Ohmic
V1
V2
V6
V5
V9
V10
V14
V13
V4
V3
V7
V8
V12
V11
V15
V16
Ohmic
Signal Power (a.u.)
Screen Position (mm)
APL 94, 213511 (2009)
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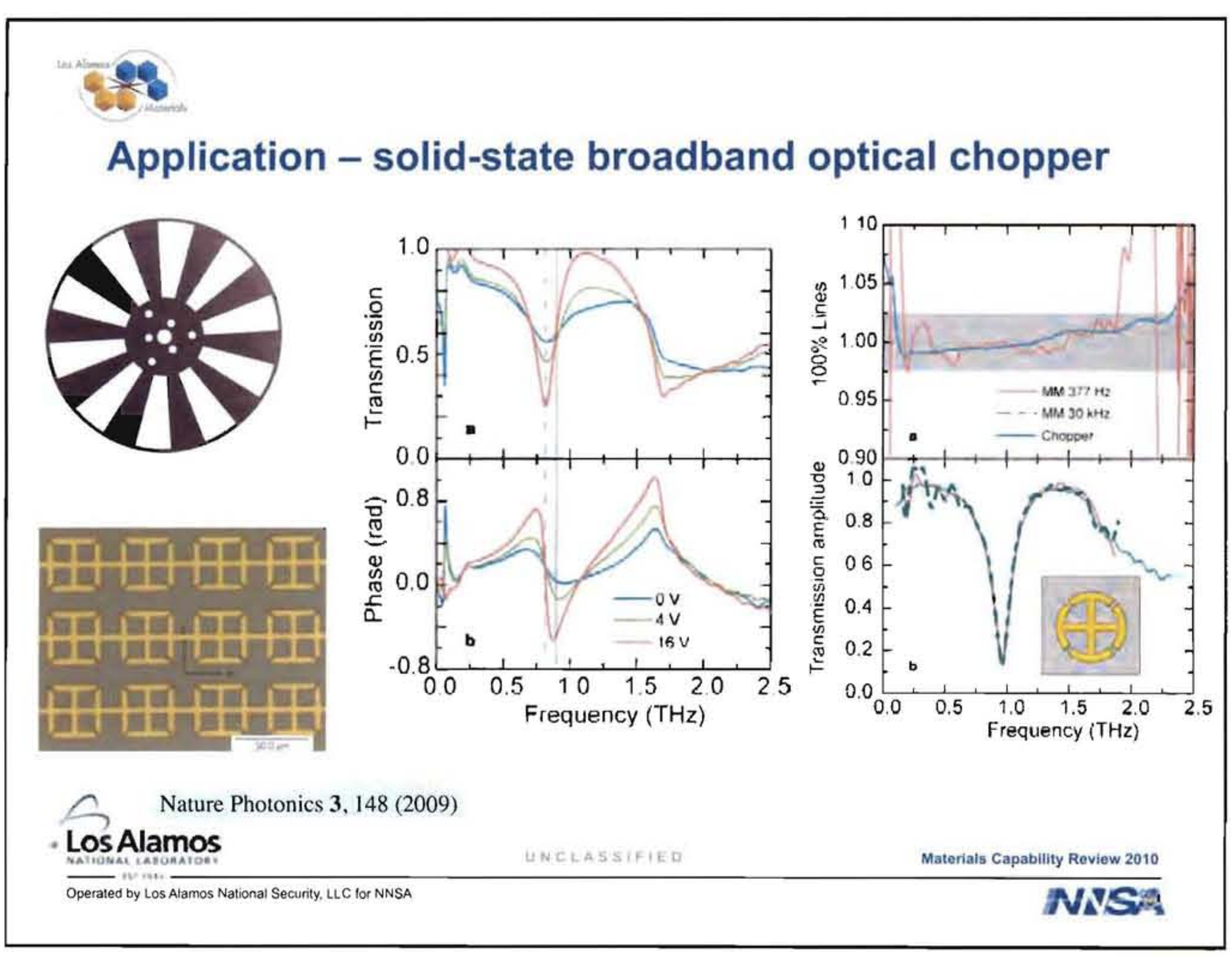
Application – solid-state broadband optical chopper
Transmission
Phase (rad)
Frequency (THz)
0 V
4 V
16 V
100% Lines
Transmission amplitude
MM 377 Hz
MM 30 kHz
Chopper
Frequency (THz)
Nature Photonics 3, 148 (2009)
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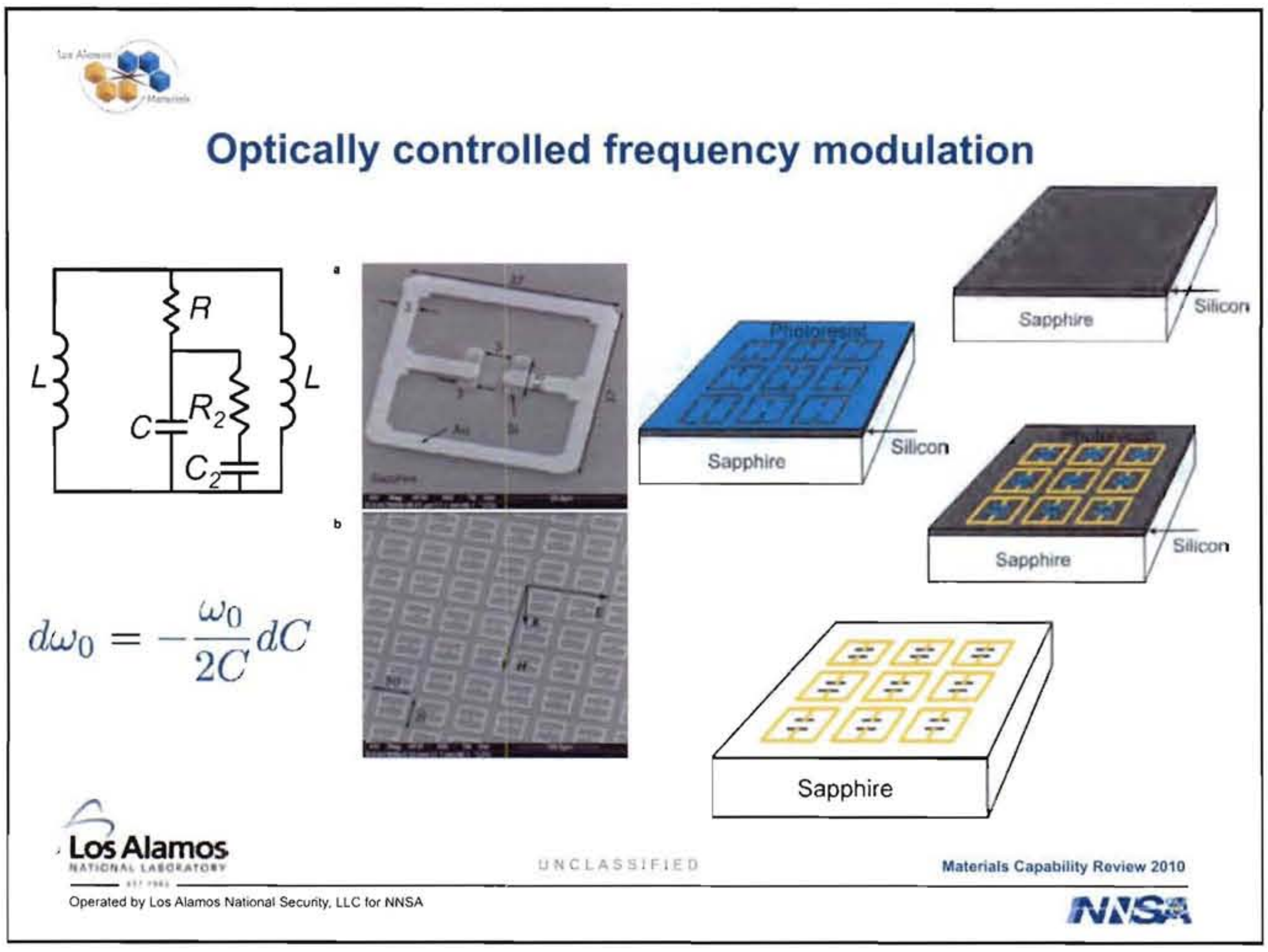
Optically controlled frequency modulation
R
L
L
C
R_2
C_2
$d\omega_0 = -\frac{\omega_0}{2C} dC$
a
b
Photoresist
Sapphire
Silicon
Sapphire
Silicon
Sapphire
Silicon
Sapphire
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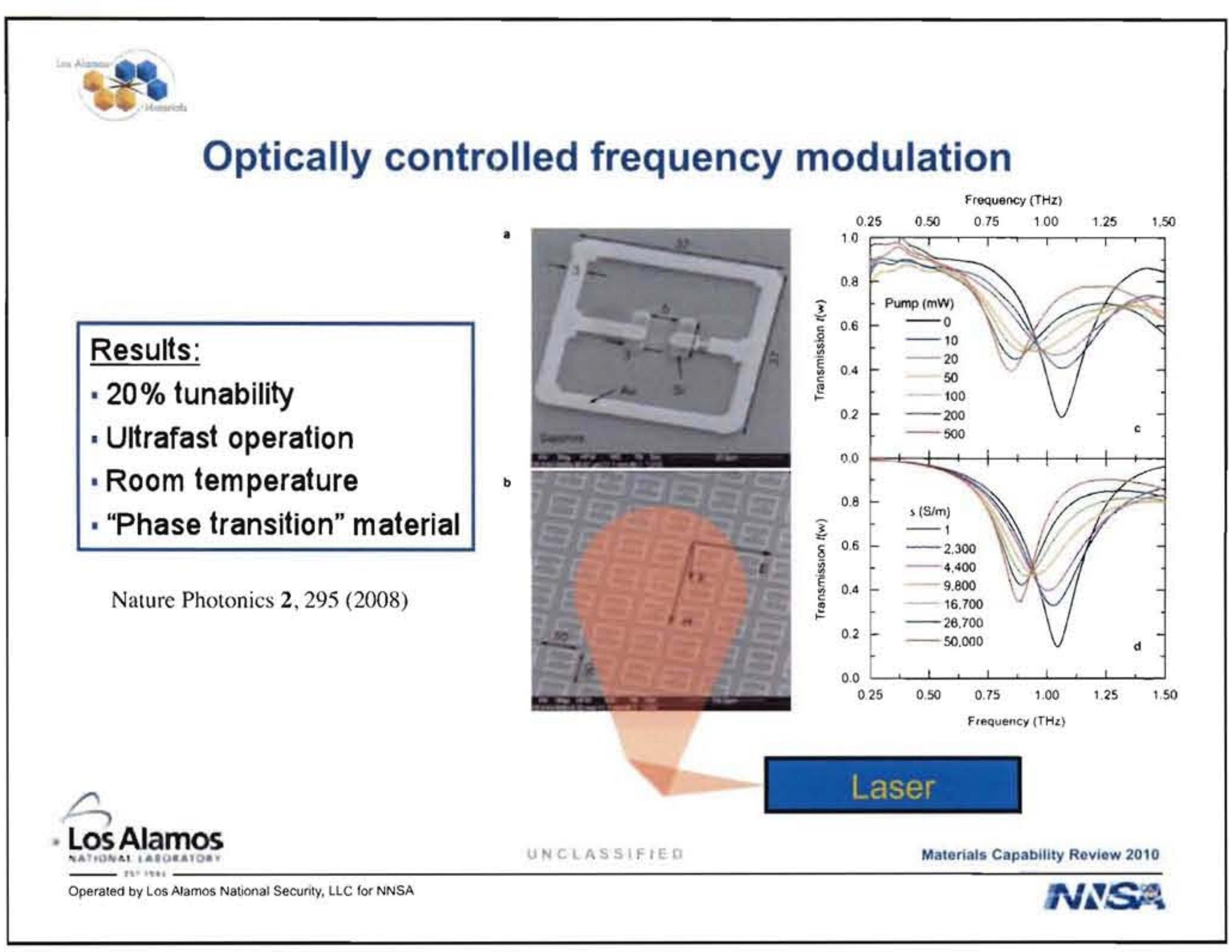
Optically controlled frequency modulation
Results:
▪ 20% tunability
▪ Ultrafast operation
▪ Room temperature
▪ "Phase transition" material
Nature Photonics 2, 295 (2008)
a
b
Frequency (THz)
Transmission
Pump (mW)
0
10
20
50
100
200
500
c
s (S/m)
1
2,300
4,400
9,800
16,700
28,700
50,000
d
Frequency (THz)
Laser
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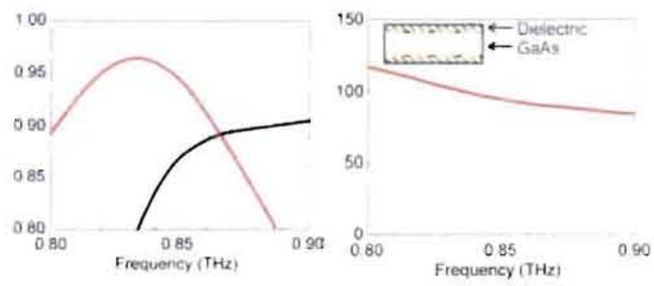
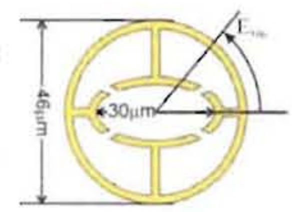
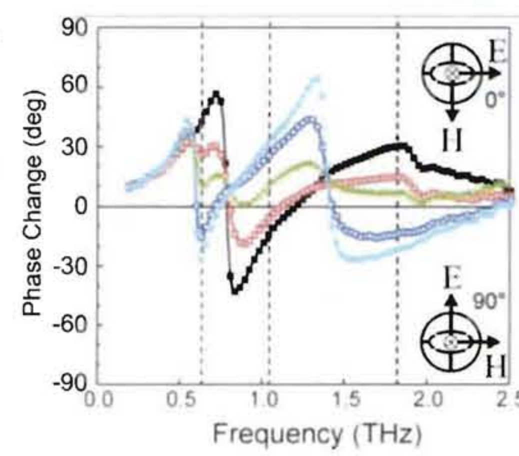
Polarization control



$\omega_H = (L_H C_H)^{-1/2}$

$\omega_V = (L_V C_V)^{-1/2}$



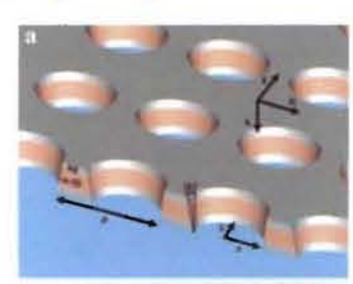


Results:
- Demonstrated polarization modulation
- Room temperature operation
- Only TWO metamaterial layers!

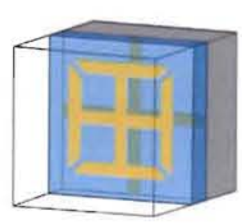
Optics Express **17**, 773 (2009)

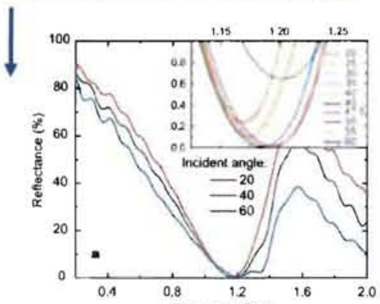
Other work completed and ongoing

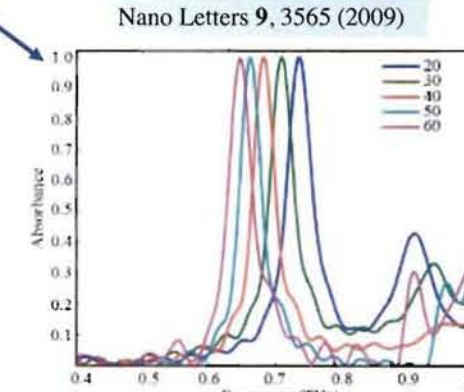
- Telecom ultrafast modulators
- Dynamic chiral terahertz metamaterials
- Ultra-thin perfect absorbers
- Compact terahertz sources
- Gradient index lenses
- Ultra-thin anti-reflection coatings



Nano Letters **9**, 3565 (2009)







Summary of efforts and relevance

- **Key points**
  - Leader in THz metamaterials
  - Leader in dynamic (active) metamaterials
  - Key roles in results of major players - LANL collaborators (BU, BC, OSU)

→ Google

- **Impact to LANL**
  - Basic materials capability → leveraged ultrafast materials leadership
  - Publications, presentations, media
    - >20 papers (incl. PRL, Nat. Photonics)
    - >15 invited talks, > 30 media reports
    - International Workshop for Electromagnetic Metamaterials (IWEM)
  - A successful example of LDRD:
    - WFO - $513k, IC Postdoctoral Fellow - $240k, DARPA - $1.8M
  - Applications to Global Security
    - Interest of external GS customers
    - Emergent phenomena leading to real-world devices

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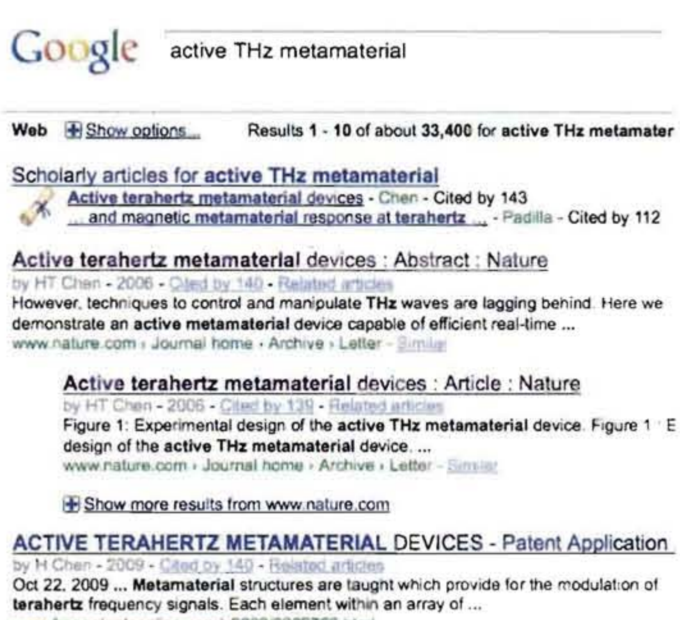
Dominant coverage over first several pages...



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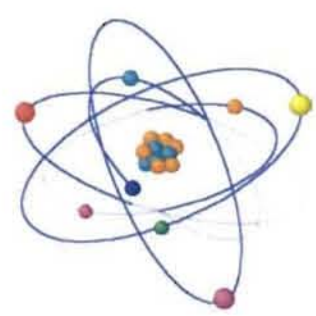
A new regime of control

Natural materials

- $a \ll \lambda$
- N > 10^9 atoms/λ^3
- $d\varphi \ll \pi/100$ rad/atomic layer
- loss = very low / atom



Metamaterials

- $a \lesssim \lambda$
- N ~ 10^3 'atoms'/λ^3
- $d\varphi > \pi/2$ rad/meta-layer
- loss = high / 'atom'

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Possible Experiments on Verification of Cherenkov Radiation in Metamaterials

E.I. Simakov, D. Yu. Shchegolkov (ISR-6); A. Azad, J.F. O'Hara (MPA-CINT)

The field of left-handed materials has blossomed recently with many new theoretically predicted electromagnetic phenomena being experimentally verified. Those include the most basic properties, such as the negative index of refraction and negative phase velocity, and more advanced experiments, demonstrating sub-wavelength "perfect lens" imaging. However, the gap in knowledge exists in the field of interaction between the charged particle beams and electromagnetic waves in left-handed materials. In particular, the effect of the Reverse Cherenkov Radiation (RCR), which was predicted back in 1968, has never been experimentally demonstrated. Meanwhile, apart from the obvious fundamental importance, applications of the RCR effect may range from novel higher-order-mode suppressors in microwave and millimeter-wave sources to improved particle detectors for satellite non-proliferation missions. We propose to conduct the first RCR experiment at our mm-wave laboratory at LANL. The experimental configuration represents a circular waveguide filled with a metamaterial with simultaneously negative permittivity and permeability, in which the electromagnetic wave with a frequency of 95 GHz will interact with an electron beam. We have demonstrated that for certain values of effective permittivity and permeability, only the backward-propagating mode can be excited by the electron beam. We also consider other possible experiments with potential threat reduction applications. In particular, the inherently secure encryption of an electromagnetic signal appears to be possible via chaos masking of an electron beam inside of a metamaterial waveguide.

Composites for Radiation Detection

T.M. McCleskey (MPA-MC)

The search for new robust phosphors is an ongoing endeavor as phosphors play key roles in materials from light-emitting diodes (LEDs) to radiation detection. We have discovered a new class of inorganic phosphors with high quantum yields and short lifetimes based on modified photonic crystals (PCs). Using a new process developed at LANL called polymer assisted deposition (PAD), which allows us to coat inverse opal PCs without blocking the pores we applied coatings of Zr and Hf within the pores of PCs. The result is a new class of highly emissive phosphors stable to water and temperatures up to 500 °C. This emission was completely unexpected from Hf and Zr as their d^0 configuration and the large bandgaps associate with ZrO_2 and HfO_2 preclude emission from the zirconium or hafnium layer directly. In fact, there are no other literature reports of emission in the visible from HfO_2 or ZrO_2 to our knowledge. The use of PCs offers a dramatic change from traditional solid particle phosphors in that the refractive index and optical properties of the phosphor can be manipulated by changing the PC base material and the architecture respectively. The linked cavities of inverse opal PCs can be filled with high index materials to from transparent composites. We are currently exploring the potential of such composites for radiation detection.

Development of Molecular Scintillator Materials

R. Del Sesto, D. Ortiz-Acosta, R. Feller, M. McCleskey, A. Burrell, K. Ott (MPA-MC); R. Gilbertson (MST-7); R. Muenchausen, S. Tornga, B. Bennett (MST-8); E. McKigney, E. Esch, M. Bacrania (N-1); M. Blair (EES-14); L. Brown (C-CDE); R. Martin, L. Roy (T-12); D. Smith, M. Graf (T-11)

The development of phosphor materials for applications such as lighting, imaging, and detection has become an important area of materials research in the 21st century. Phosphor materials have a particular motivation in the area of new radiation detection technology. The improvement of existing phosphors, as well as the development of new phosphor based materials, to improve both efficiency and light yield has provided sophisticated materials that can be used to detect the illicit movement of radioactive materials. Through a combined approach of materials synthesis and theoretical modeling we can design new, more efficient optical materials and model their luminescent behavior to understand the processes involved in scintillation and energy conversion. The synthesis of new, modular, molecular and supramolecular materials containing phosphors allows us to control the size and dimensionality of such materials and provides us with new insights into the scintillation process. The understanding of how molecular phosphor materials work through synthesis, characterization, and theoretical modeling provides a platform for the design of more efficient detector materials.

Functionalized Metal Nanofoams for Radiation Detection

A. Mueller (C-CDE); B. Tappan (DE-6); J. Veauthier (C-IIAC)

Recent investigations into the use of functionalized metal nanofoams as photoactive electrochemical electrodes for fuel production has yielded promising results. Redox reactions driven by the absorption of optical photons give rise to easily measured electrical currents. Functionalization of these foams by coating with semiconductor films or alloying of the foams with other metals using polymer assisted deposition (PAD) has allowed for the exploration of more complex materials systems for the purpose of photo-electrochemical (PEC) hydrogen production.

The versatility of the foam synthesis allows for the preparation of a wide variety of elemental and binary compound foams. Recently, cerium nitride foams were produced, creating a radioluminescent material. The combination of PAD and the metal nanofoam synthesis will allow for the production of more scintillating foams for γ-ray or neutron detection, depending upon the material system employed. The advantage of the geometry provided by the nanofoams is that the e-h pairs generated by absorption within the bulk of the foam are always near the surface, ready to interact with the detecting medium. As such, the foam may be made thick, providing a significant path-length of interaction for the radiation without leading to self-absorption of the generated signal. This allows for the preparation of the foams from high-Z elements (such as the CeN foam) resulting in an increased stopping power and higher loading than doped glasses or plastics.

A New Spinel: Ce Scintillator for Gamma Ray Detection

C.F. Chen, H.M. Volz (MST-6); F.P. Doty, R.J.T. Houk, P. Yang (Sandia National Laboratories)

We are reporting on a new polycrystalline ceramic scintillator for possible use in gamma ray detection and medical imaging applications. The goal was to develop a cerium doped spinel ($MgAl_2O_4$:Ce), which can be processed utilizing ceramic forming techniques. High purity $MgAl_2O_4$ powders were used as the starting materials. Lithium fluoride (LiF) was used as a sintering aid and CeO_2 powder was used as the dopant. The mixed and dried powders were hot pressed in a vacuum environment to achieve a high density $MgAl_2O_4$:Ce.

The hot pressed sample shows a transparent polycrystalline appearance. The x-ray diffraction (XRD) shows a single phase without any secondary phase. The microstructure shows a highly dense structure with a small amount of residual pores within the microstructure. The grain size has a wide range of sizes ranging from 3 to 50 microns with an average grain size of about 20 microns. The polished sample has a high IR transmission at roughly 86 percent. The in-line transmission within the visible range is about 50 percent and about 40 percent at the excitation peak of 410 nm. The excitation and emission were centered at about 300 and 401 nm, respectively, which matches well with the in line transmission results. The $MgAl_2O_4:Ce_{0.005}$ has a very short decay time at about 4.55 ns, which is much faster than either $LaBr_3:Ce^{3+}$ and $LaCl_3:Ce^{3+}$.

Theory and Modeling of Scintillator Materials

M. Graf, D. Smith (T-4); R. Martin, E. Batista (T-1)

We are developing a theory to understand the mechanisms of radiation absorption, charge transfer, non-radiative processes and scintillation in existing and new materials. Understanding the processes from bulk down to molecular scales will allow the design of next generation materials for radiation detection. Through a combined theoretical and materials synthesis approach, we propose to develop novel composite materials through a bottom-up approach to synthesis and modeling of scintillation behavior when exposed to ionizing radiation. The models range from the atomic to macroscopic scales and can reveal specific processes that enhance or degrade scintillation efficiency, allowing us to tune modifications to optimize light output and resolution.

Remote Detection of the Uranium and Plutonium Content of a Nuclear Reactor

A.C. Hayes (T-2); J. Hu (N-4); W.B. Wilson (EES-12)

We have developed concepts for monitoring the fissioning uranium and plutonium content of a nuclear reactor from outside the reactor during operation using the emission of noble gases and antineutrinos. The growth rate of 239Pu is, to first order, proportional to the magnitude of the thermal peak of the neutron flux and inversely proportional to the 235U enrichment of the fuel. The production of 136Xe is determined by two components, one directly as a fission product, and one by capture of thermal neutrons on

135Xe. This second contribution scales with the magnitude of the thermal neutron peak, and thus, the production of 136Xe scales inversely with the growth rate of 239Pu. Our second monitoring scheme relies on the fact that plutonium emits about 50 percent fewer detectable anti-neutrinos per fission than does uranium. Thus, as the plutonium growth rate increases, the anti-neutrino rate decreases. With knowledge of the thermal power of the reactor, the anti-neutrino emission rate can be used to determine the plutonium content of the reactor fuel. The emission of 136Xe and anti-neutrinos provide powerful tools for monitoring the plutonium and uranium content of a reactor, and when taken together, become very difficult to spoof.

Molecular Forensic Science of Nuclear Materials

M.P. Wilkerson, C.J. Burns, W.S. Kinman, D. Podlesak, L.R. Riciputi, H.D. Selby (C-NR); A.D. Andersson, S.D. Conradson (MST-8); J.M. Berg (PMT-1); K.S. Boland, A.L. Costello, S.A. Kozimor (C-IIAC); D.L. Clark (INST-OFF); D.E. Hobart, P.T. Martinez, L. Tandon (C-AAC); S.A. Kinkead (DE-3); J. Mitchell (MST-16); C. Mora (EES-14), M.T. Paffett (MST-6); K.D. Rector, G.L. Wagner (C-PCS)

We are applying our understanding of actinide chemical structure and bonding to broaden the suite of analytical tools available for nuclear forensic analyses. Uranium- and plutonium-oxide systems form under a variety of conditions, and these chemical species exhibit some of the most intriguing behavior of metal oxide systems known. Environmental studies have shown the value of utilizing the chemical signatures of actinide oxide materials to understand transport following release into the environment. Chemical speciation of actinide oxide samples may also provide clues as to the age, source, process history, or transport of the material. The scientific challenge is to identify, measure and understand those aspects of actinide speciation that carry information about material origin and history most relevant to forensics.

We describe our efforts in material synthesis and analytical methods development to characterize actinide oxide molecular structures for forensics science. Initial results to measure structural variability of uranium oxide samples using synchrotron-based x-ray absorption fine structure and other techniques will be presented.

Microcalorimetry

M. Rabin (ISR-2)

Detect, locate, identify, characterize, and respond—these few words describe the essential challenges for countering nuclear proliferation and the threat of weapons of mass destruction. Science and engineering research has transformative potential for the technical aspects of each of these challenges, relying on advances in materials science, detector innovation, advanced algorithms, and information technology. Simulation plays a key role in assessing the validity of new ideas in this field. In this presentation, I will briefly describe some of the relevant advanced materials, intriguing unconventional detectors, and algorithms for extracting and quantifying nuclear signatures. New scintillators will improve detection and discrimination of nuclear material; instruments based on coded apertures and Compton imagers are emerging to provide directionality and enhance the ability to locate radioactive sources; and rapid spectral analysis tools are evolving to identify them. Advanced materials include insulators (perhaps based on nanophosphors or scintillators discovered through combinatorial chemistry) semiconductors (low-inclusion CdZnTe), and superconductors.

Our work has focused on the application of superconducting device technology to problems in international nuclear safeguards and nuclear forensics. Cryogenic microcalorimeter detectors provide unprecedented energy resolution for the measurement of x-rays, gamma-rays, and alpha particles, directly improving the precision and accuracy of nuclear materials characterization. Energy resolution in the 100 keV region of the x- and gamma-ray spectrum can be as much as an order of magnitude better than planar high-purity germanium detectors (best conventional technology). The high-energy resolution is derived from operation at temperatures below 100 mK, a temperature range now accessible with commercial technology without liquid cryogens. The detector technology is well suited to analyze materials with complex spectra presenting closely spaced spectral peaks. To increase detection efficiency we are pursuing the fabrication of large arrays of sensors. Beginning with a single pixel prototype device in 2005, we have rapidly advanced to the present operation of a 256-pixel array. This is the largest array of this type ever produced, and presents challenges in fabrication, operation, and calibration. I will discuss the operation and performance of the 256-pixel array, and present results of a recently conducted head-to-head comparison of isotopic determination measurements with high-purity germanium. The ultra-high resolution obtained from microcalorimeter detectors benefits a number of charged-particle detection applications related to nuclear forensics, nuclear safeguards, environmental monitoring of actinides, and nuclear data measurements. Detailed isotopic analysis of complex alpha spectra from mixed-actinide sources and preliminary results on electron spectrometry for beta-decay and conversion-electron measurements will be presented.

Nonproliferation of Uranium Metal

R. E. Hackenberg (MST-6)

This research examined the feasibility of exploiting trace elemental impurities and controlled microalloy additions to metallic uranium for the potential end uses of forensics, safeguards, and counterproliferation. A significant microalloy and processing experimental matrix was done. The flow of elemental impurities into and out of metallic uranium as well as associated microstructural signatures—their rise, persistence, and annihilation—through various melting, casting, and thermo-mechanical processing routes pathways was characterized using bulk chemical analysis and various microscopy methods. This exploited the hitherto untapped information contained in the uranium metal's internal microstructure, particularly how certain elements are inhomogeneously distributed and sequestered as second-phase inclusions. This project is funded by the weaponization portfolio of NA-22, the DOE Office of Nonproliferation R&D.

Proliferation-resistant Monolithic LEU Fuel Fabrication Development

A.J. Clarke, R.D. Field, (MST-6); D.R. Korzekwa (MST-16); D.L. Hammon, D.J. Alexander, K.D. Clarke, R.J. McCabe, C.T. Necker, P.A. Papin, A.M. Kelly, R.T. Forsyth, J.C. Foley, R.M. Aiken, P. Burgardt, A.N. Duffield, B. Aikin, V.D. Vargas, D.A. Korzekwa, R.R.Trujillo, J.A. Balog, T.V. Beard, I.P. Cordova, H. Swenson, K.C. Rau, R.L. Edwards, J.D. Katz, D.E. Dombrowski, D.F.Teter, P.S. Dunn (MST-6)

This presentation summarizes recent modeling, experimental, and fabrication results for monolithic, low enriched uranium (LEU)-10wt.%Mo fuel fabrication. This work supports the Global Threat Reduction Initiative to reduce the worldwide usage and availability of highly enriched uranium. LANL and MST-6 are collaborating with Idaho National Laboratory and Y-12 National Security Complex in process development for research reactor replacement fuel elements. These fuel elements will be fabricated in the Sigma Complex at LANL. In addition to the necessary fabrication facilities, LANL expertise in advanced characterization and modeling are supporting process development efforts.

Nonlinear Perovskites for High Power Microwave Generation and other Applications

D. Reagor (MPA-STC); C. Chen (MST-6); S. Russell (ISR-6)

Electromagnetic transmission lines loaded with nonlinear dielectrics are known to be high power and weight efficient up-converters of slower electromagnetic pulses into high power microwave (HPM) pulses. These nonlinear transmission line sources of HPM promise to be an order of magnitude smaller in terms of size and weight than conventional vacuum sources. The best nonlinear dielectrics known are Perovskites with ferroelectric transitions near the operating temperature. The Perovskite structure has non-optimum bond lengths, and at some sites of high symmetry, the atoms are not ideally bonded. This leads to a structural instability where the atoms can displace, and via interactions, produce a collective displacement, or ferroelectric state. The collective displacement is often described as an optically active phonon mode softening to zero frequency at the ferroelectric transition. At temperatures near the ferroelectric transition of a pure sample the dielectric constant is often greater than 10,000 at small fields, decreases 50% with electric fields less than 1 kV/mm, and sharply peaked in temperature. Capacitor manufacturers introduce disorder to disrupt the formation of the collective polarization. This reduces the nonlinearity and produces a broader peak in the temperature dependence of the dielectric constant. In this proposed project, our primary goal is the opposite: to maintain the nonlinearity while broadening the temperature dependence of the response. We will be developing processes using graded compositions than do not nanostructurally phase separate or otherwise disrupt the collective behavior, but instead manipulate the collective polarization in a controlled manner.

Utilizing Laser CVD to Incorporate Carbon Nanotubes in Composite Materials

J. Maxwell, S. Sisntay (IAT-2)

Laser-assisted chemical vapor deposition (LCVD) is a technique that uses heat intensity created by a laser beam to induce solid-state deposition of materials. The unique

mechanical and electrical properties of carbon nanotubes (CNTs) make them attractive components of any composite material. Using LCVD, metastable materials, such as diamond-like carbon, and functionally graded materials can be grown. Additionally, growth of normally—immiscible materials, such as tungsten mercury alloys, are also possible. CNTs can also be grown using LCVD and this presents an opportunity to leverage their unique properties in the design of nanoscale composite materials.
We have demonstrated growth of CNTS on many types of materials including W and Hf wires, Si substrates, and Al_2O_3 bundles of fibers. LCVD is an attractive processing technique because it is able to produce aligned CNTs that can be co-deposited within a surrounding matrix material. For example, aligned CNTs could be co-deposited with Au, Ag, or Cu, such that the composite has enhanced properties over and beyond the matrix. Through co-deposition, we anticipate potential materials such as Cu with enhanced conductivity, brittle materials such as ceramic or glass microwires with improved toughness. Co-deposition also presents new opportunities to explore the performance of novel micro-composites such as CNTs embedded in a radiological matrix. Presented here are results showing growth and co-deposition of CNTs with various matrix materials, and on various substates using LCVD.

Tab 6

Overview: Electronic and Photonic Materials Research at LANL

D. Smith (T-4)

This talk will present a brief overview of electronic and photonic materials research at LANL and will introduce the talks and posters that will be presented on this topic later during the review. Some general characteristics of electronic and photonic materials research at LANL will first be described. The connection of this research with LANL's missions will be discussed. Specific technical accomplishments in four selected research areas will be highlighted: spin physics, composite nanomaterials, complex oxides, and organic semiconductors. The following talks and posters will expand upon our work in these four research areas.

Overview: Electronic and Photonic Materials Research at LANL

Darryl Smith
T-4: Physics of Condensed Matter and Complex Systems
Theoretical Division

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Application Inspired Materials Research

Design, synthesize/grow, and measure new electronic/photonic materials with novel properties that can be utilized in electronic/photonic devices

Understand the physical process that occur in the materials so that materials and devices can be effectively designed and controlled

Design, fabricate and test devices that take advantage of novel material properties

Various applications require different material properties and device geometries, but there is synergy in the basic physical processes that must be understood and controlled

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Research in Several Divisions and Centers

Synthesis, fabrication, measurement and theory approach

- Materials Physics and Applications (MPA)
- Materials Science and Technology (MST)
- Los Alamos Neutron Scattering Center (LANSCE)
- Chemistry (C)
- Theoretical (T)
- International Space and Response (ISR)
- Nuclear Nonproliferation (N)

Strong overlap with review categories

- Global Security
- Emergent Phenomena

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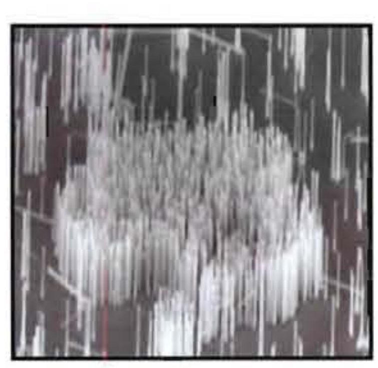
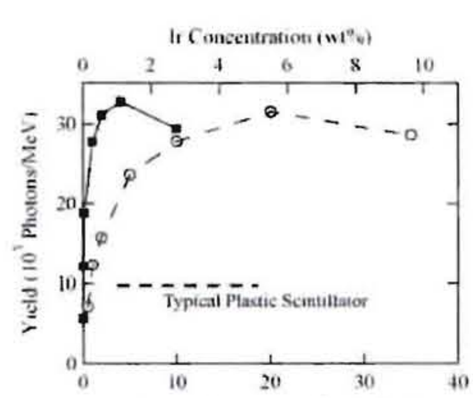
Connection to Laboratory Missions

- Energy Security
  - Solar cells
  - Thermoelectrics
  - Superconductivity
  - Energy efficiency
- Global Security
  - Radiation detectors
  - Optical detectors
  - Quantum technology
  - Information technology
  - Sensing technologies



Ge nanowire array

Nanostructured materials for solar cell/thermoelectric applications



Triplet harvesting for γ detection scintillators

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Role of Defects and Interfaces

Spin Physics

Spin injection/detection at Fe/GaAs Interfaces

- Physical structure
- Electronic structure
- Magnetic structure
- Interface doping profiles

Artificially Structured Materials

- Interface trap states
- Charge and energy interface transport
- Interface scattering
- Interface energy levels
- Surface contact potentials

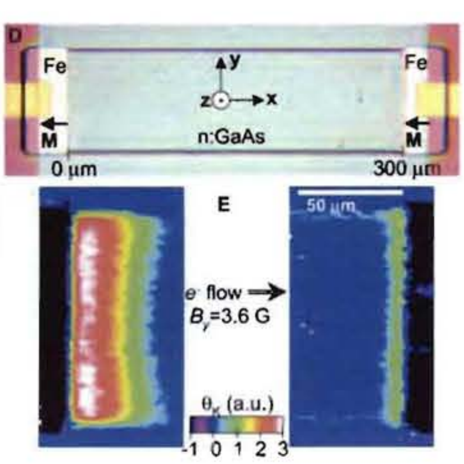
Complex Oxides

- Phase segregation
- Interface strain
- Strains and ferroelasticity
- Vortex pinning

Organic Semiconductors

- Inorganic/organic interfaces
- Organic/organic interfaces
- Manipulating interface energy levels
- Electrical transport/trapping
- Disordered composites

Spin Physics



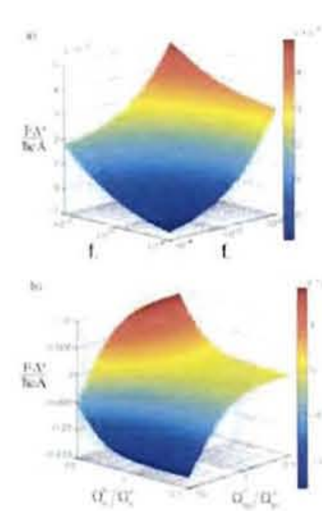
From: "Imaging spin transport in lateral ferromagnet/semiconductor structures", S. A. Crooker, et al., Science **309**, 2191 (2005); Cited: 115

Global Security
- Quantum technology
- Information Technology

Some Significant Publications

- "Electrical spin injection into semiconductors", D. L. Smith and R. N. Silver, Phys. Rev. B **64**, 045323 (2001); Cited: 127
- "Imaging spin flows in semiconductors subject to electric, magnetic, and strain fields", S. A. Crooker, et al., Phys. Rev. Lett. **94**, 236601 (2005); Cited: 75
- "Electrical detection of spin transport in lateral ferromagnet-semiconductor devices", X. H. Lou, et al., Nature Phys. 3, 197 (2007); Cited: 127
- "Bias-controlled sensitivity of ferromagnet/semiconductor electrical spin detectors", S. A. Crooker, et al., Phys. Rev. B **80**, 041305 (2009)
- "Spin noise of conduction electrons in n-type bulk GaAs", S. A. Crooker, et al., Phys. Rev. B **79**, 035208 (2009)
- "Spin Noise of Electrons and Holes in Self-Assembled Quantum Dots", S. A. Crooker, et al., Phys. Rev. Lett. **104**, 036601 (2010)

Artificially Structured Materials



From: "Casimir-Lifshitz theory and metamaterials", F. S. S. Rosa, D. A. R. Dalvit, P. W. Milonni, Phys. Rev. Lett. **100**, 183602 (2008); Cited: 20

- Energy Security
  - Solar cells
  - Thermoelectrics
  - Energy efficiency
- Global Security
  - Radiation detectors
  - Quantum technology
  - Sensing technologies

Some Significant Publications

- "Energy-transfer pumping of semiconductor nanocrystals using an epitaxial quantum well", M. Achermann, et al., Nature **429**, 6992 (2004); Cited: 189
- "Photoinduced charge transfer between CdSe nanocrystal quantum dots and Ru-polypyridine complexes", M. Sykora, et al., JACS **128**, 9984 (2006); Cited; 46
- "Spectrally resolved dynamics of energy transfer in quantum-dot assemblies: Towards engineered energy flows in artificial materials", S. A. Crooker, et al., Phys. Rev. Lett. **89**,186802 (2002); Cited: 187

- "Hybrid Photovoltaics Based on Semiconductor Nanocrystals and Amorphous Silicon", B. Sun, et al., Nano Lett. **9**, 1235 (2009).
- "Ultrafast electron and hole dynamics in germanium nanowires", R. P. Prasankumar, et al., Nano Lett. **8**, 1619 (2008).
- "Surface contact potential patches and Casimir force measurements", W. J. Kim, et al., Phys. Rev. A **81**, 022505 (2010)

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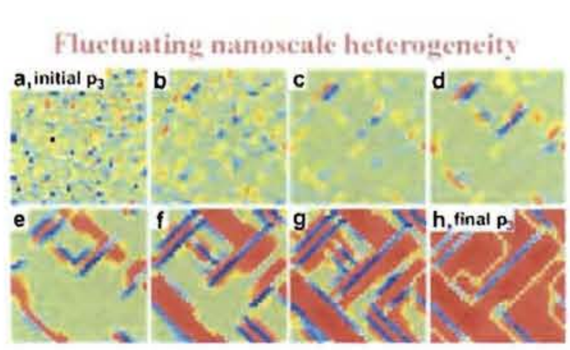
Complex Oxides



From: "Strain-induced metal-insulator phase coexistence in perovskite manganites", K. H. Ahn, T. Lookman and A. R. Bishop, Nature **428**, 401 (2004); Cited: 209

- Energy Security
  - Superconductivity
- Global Security
  - Sensing technologies

Some Significant Publications

- "Strongly enhanced current densities in superconducting coated conductors of $YBa_2Cu_3O_{7-x}$+$BaZrO_3$", J. L. Macmanus-Driscoll, et al., Nature Materials **3**, 439 (2004); Cited: 325
- "Angular-dependent vortex pinning mechanisms in $YBa_2Cu_3O_7$ coated conductors and thin films", L. Civale, et al., Appl. Phys. Lett. **84**, 2121 (2004); Cited: 107
- "Ferroelastic dynamics and strain compatibility", T. Lookman , et al., Phys. Rev. B **67**, 024114 (2003); Cited: 65

- "Interfaces in ferroelastics: Fringing fields, microstructure, and size and shape effects", M. Porta, et al., Phys. Rev. B **79**, 214117 (2009).
- "Defect-induced incompatibility of elastic strains: Dislocations within the Landau theory of martensitic phase transformations", R. Groger, et al. Phys. Rev. B **78**, 184101 (2008).
- "Synergetic combination of different types of defect to optimize pinning landscape using $BaZrO_3$-doped $YBa_2Cu_3O_7$", B. Maiorov , et al., Nature Materials **8**, 398 (2009).

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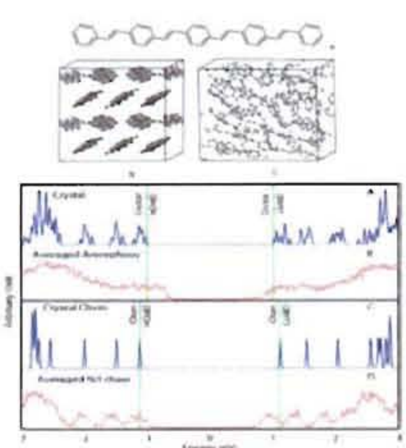
Organic Semiconductors



From: "Effect of Intra-molecular Disorder and Inter-molecular Electronic Interactions on the Electronic Structure of PPV", P. Yang et al., Phys. Rev. B 76, 241201R (2007)

- Energy Security
  - Solar cells
  - Energy efficiency
- Global Security
  - Radiation detectors
  - Optical detectors
  - Sensing technologies

Some Significant Publications

- "Direct measurement of conjugated polymer electronic excitation energies using metal/polymer/metal structures", I. H. Campbell, et al., Phys. Rev. Lett. **76,** 1900 (1996); Cited: 277
- "Physics of organic electronic devices", I. H. Campbell, et al., Solid State Physics **55**, 1 (2001); Cited 73
- "Molecular and solid-state properties of tris-(8-hydroxyquinolate)-aluminum", R. L. Martin, Phys. Phys. B **61**, 15804 (2000); Cited 93
- "Quantum efficiency of ambipolar light-emitting polymer field-effect transistors", J. Zaumseil, et al., J. Appl. Phys. **103**, 064517 (2008).
- "Energy level alignments and photocurrents in crystalline Si/organic semiconductor heterojunction diodes", I. H. Campbell and B. K. Crone, J. Appl. Phys. **108**, 113704 (2009).
- "A near infrared organic photodiode with gain at low bias voltage", I. H. Campbell and B. K. Crone, Appl. Phys. Lett. **95**, 263302 (2009).

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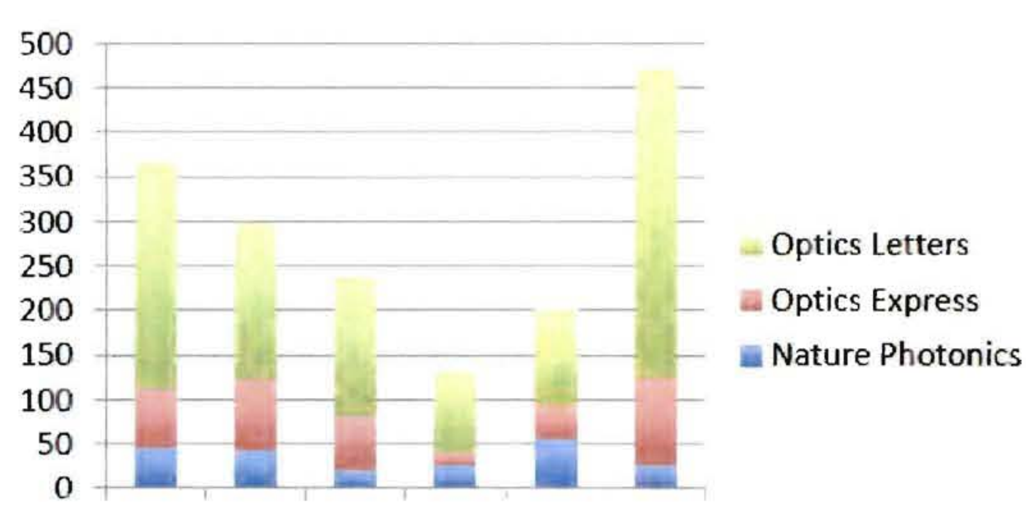
Publications in Photonic Journals 2004-2009



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Presentations and Posters

Presentations

Scott Crooker MPA-CMMS "Imaging Electron Spin Transport in Semiconductor Spintronic Devices"

Diego Dalvit T-4 "Casimir Interactions"

Posters

Spin Physics
- Mike Fitzsimmons
- Athanasios Chantis

Artificially Structured Materials
- Shadi Dayeh
- Milan Sykora

Complex Oxides
- Turab Lookman
- Quanxi Jia
- Rohit Prasankumar
- Leonardo Civale

Organic Semiconductors
- Ian Campbell
- Sergei Tretiak

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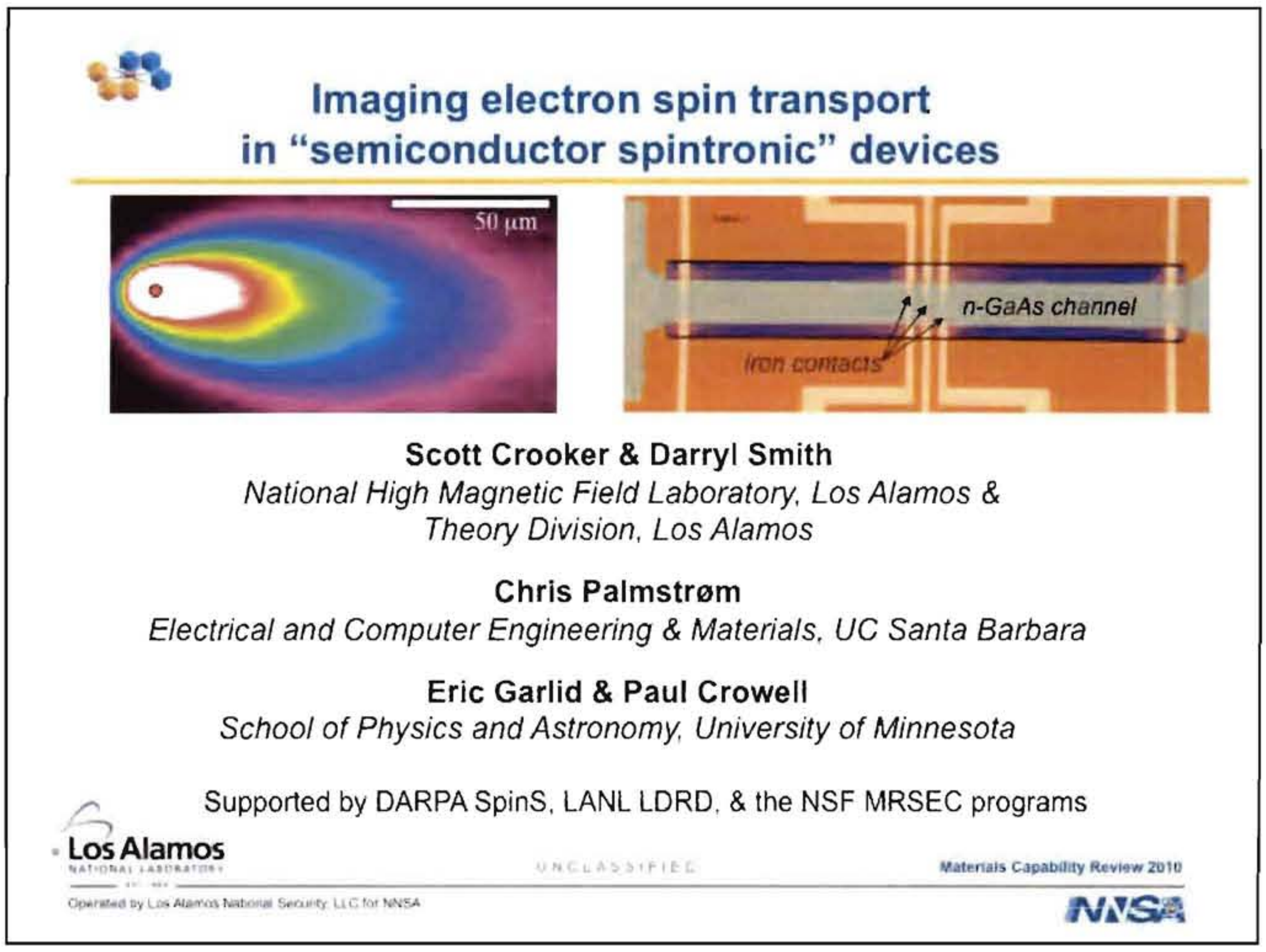
Imaging Electron Spin Transport in Semiconductor Spintronic Devices

S.A. Crooker (MPA-CMMS); D.L. Smith (T-4)

The field of semiconductor spintronics is focused on exploiting an electron's spin degrees of freedom in order to achieve additional functionality in future electronic devices. Three essential elements of a semiconductor spin transport device are: an efficient mechanism for electrically injecting spin-polarized electrons into a semiconductor; a practical means for spin manipulation and transport; and a simple electronic scheme for detecting the resulting spin polarization. This talk will address each of these three elements using data from low-temperature, magneto-optical scanning Kerr microscopy studies. In these experiments, we directly image the drift, diffusion, and precession of spin-polarized electrons flowing laterally in hybrid GaAs devices having iron (Fe) electrical contacts that form a special Schottky tunnel-barrier at the ferromagnet-semiconductor interface. The two dimensional images reveal efficient electrical spin injection extending out to 120 microns in the n:GaAs channel, and an accumulation of spins within a spin diffusion length of a drain contact. All these experiments are conducted in a geometry that is sensitive only to electron spin precession, allowing for detailed theoretical modeling of spin transport in the channel based on spin drift-diffusion equations. Moreover, optical and all-electrical studies show that these Fe/GaAs interface contacts can also be used as tunable electrical spin detectors in addition to their role as spin injectors.


Imaging electron spin transport
in "semiconductor spintronic" devices
50 μm
n-GaAs channel
iron contacts
Scott Crooker & Darryl Smith
National High Magnetic Field Laboratory, Los Alamos &
Theory Division, Los Alamos
Chris Palmstrøm
Electrical and Computer Engineering & Materials, UC Santa Barbara
Eric Garlid & Paul Crowell
School of Physics and Astronomy, University of Minnesota
Supported by DARPA SpinS, LANL LDRD, & the NSF MRSEC programs
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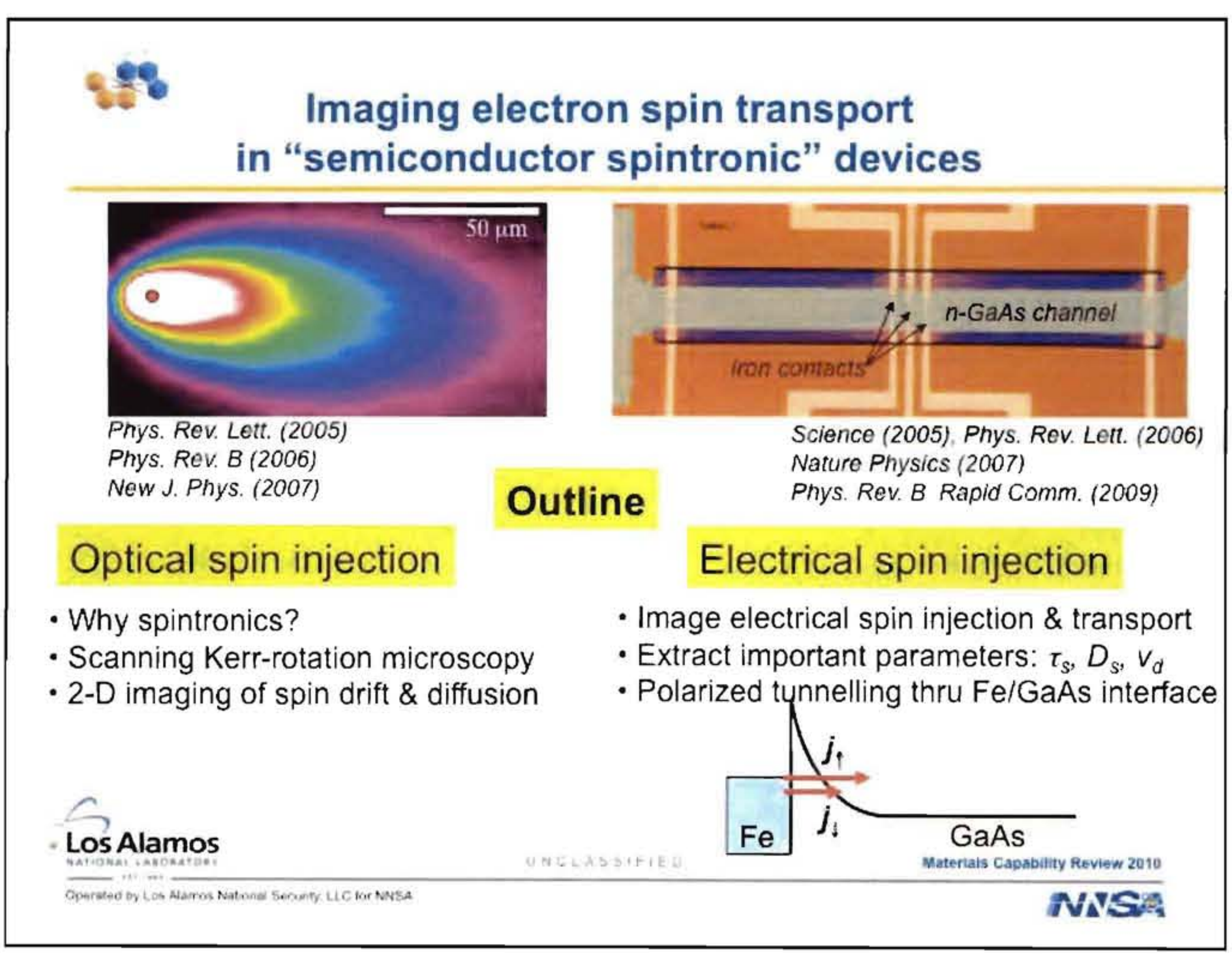
Imaging electron spin transport
in "semiconductor spintronic" devices
50 μm
n-GaAs channel
iron contacts
Phys. Rev. Lett. (2005)
Phys. Rev. B (2006)
New J. Phys. (2007)
Outline
Science (2005), Phys. Rev. Lett. (2006)
Nature Physics (2007)
Phys. Rev. B Rapid Comm. (2009)
Optical spin injection
• Why spintronics?
• Scanning Kerr-rotation microscopy
• 2-D imaging of spin drift & diffusion
Electrical spin injection
• Image electrical spin injection & transport
• Extract important parameters: τ_s, D_s, v_d
• Polarized tunnelling thru Fe/GaAs interface
$j_\uparrow$
$j_\downarrow$
Fe
GaAs
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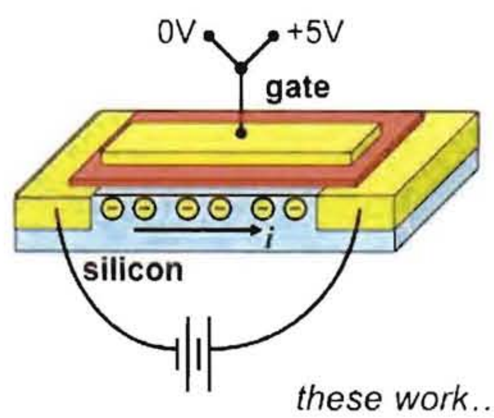
"Semiconductor spintronics"

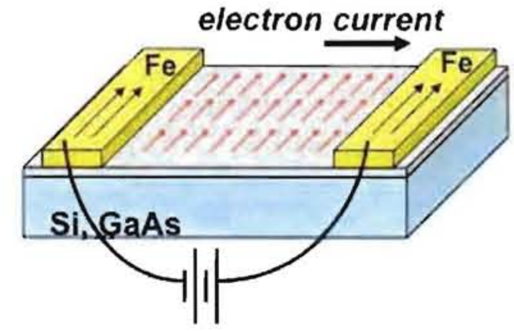
- A (proposed) new generation of "spintronic" devices that derive functionality from electron *spin* degrees of freedom (not charge).

Conventional field-effect transistor (FET)



these work...

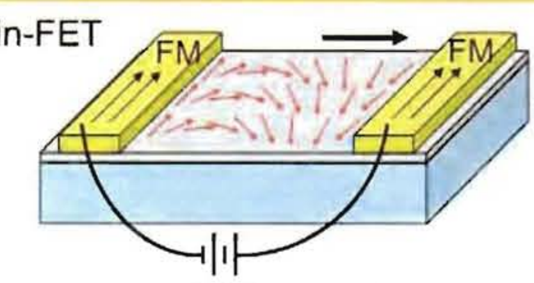
"spin-FET"



these don't... (yet?)...

Prototype lateral spin transport devices

spin-FET

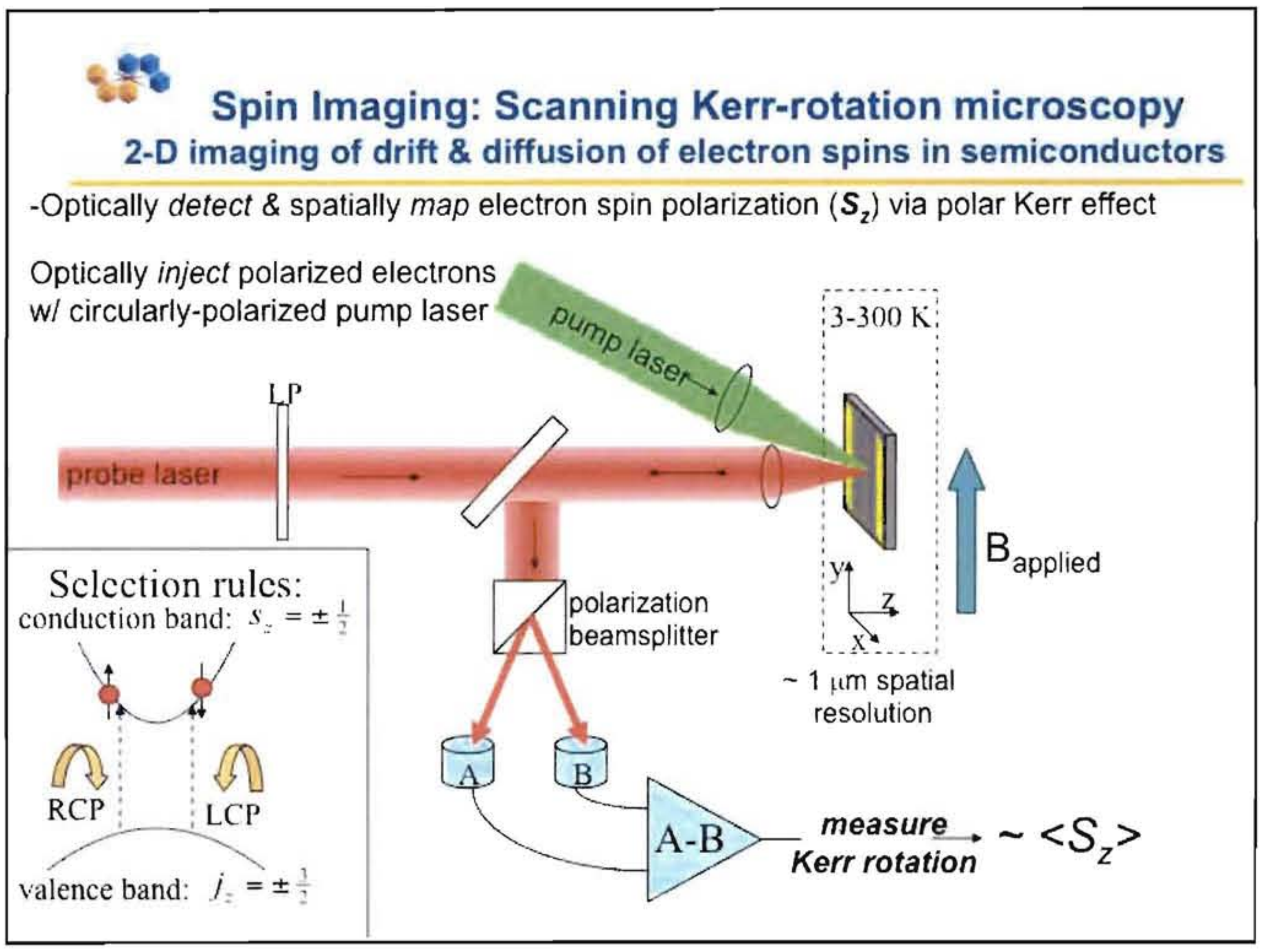


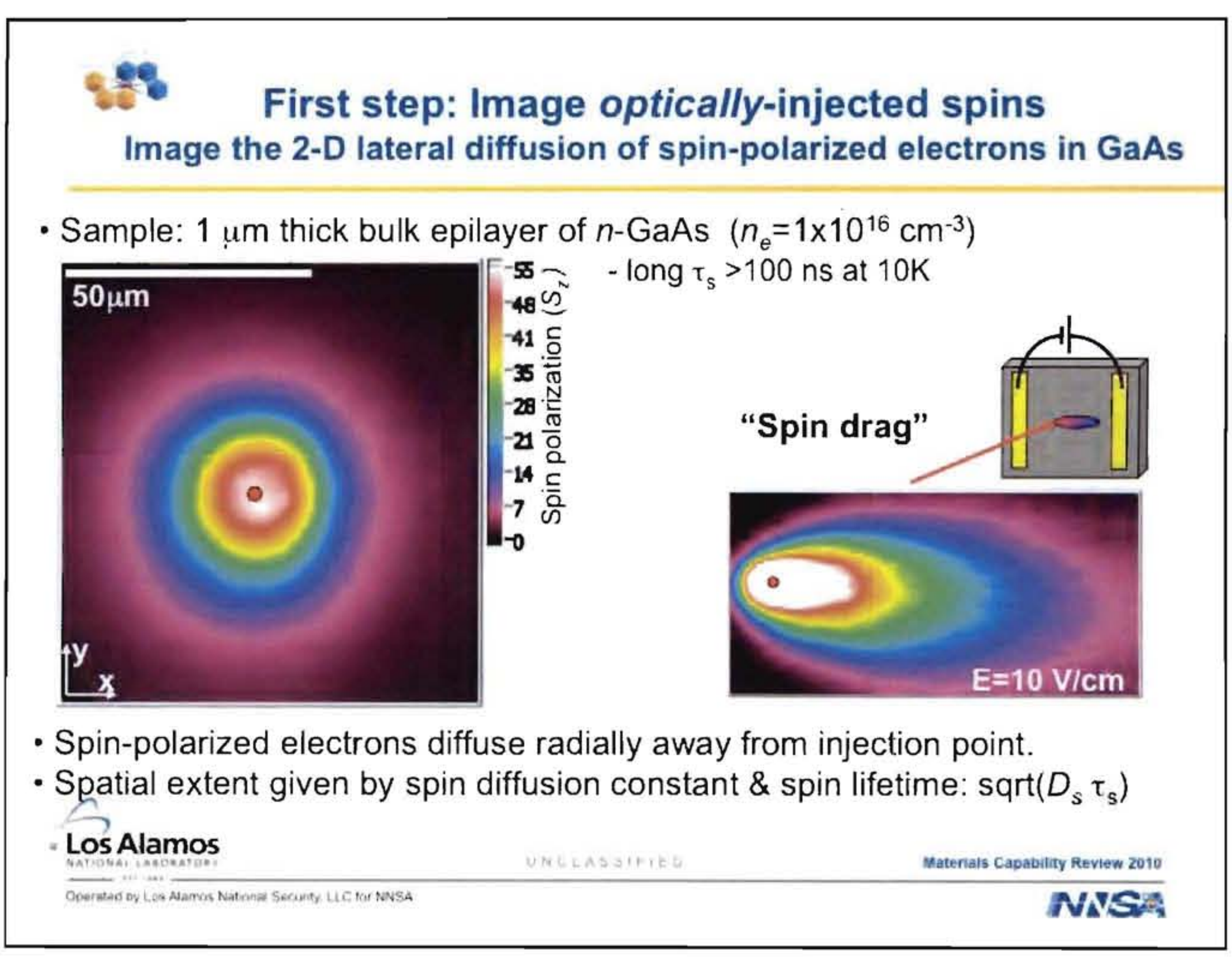
GaAs (this work, Regensburg)
Silicon (NRL, U. Maryland)
Graphene (Netherlands)
Organics (Japan)

Many proposals! All generally require four things:

- Electrical ***injection*** of spin-polarized electrons into semiconductors
- ***Transport*** of spins from one point in device to another
- Means to ***manipulate*** spins w/ external fields (***B***, ***E***, strain, ??)
- ***Electrical detection*** of spin-polarized currents

Physics goal: Image these processes via optical techniques & understand spin tunnelling across Fe/GaAs interface


Spin Imaging: Scanning Kerr-rotation microscopy
2-D imaging of drift & diffusion of electron spins in semiconductors
-Optically detect & spatially map electron spin polarization (S_z) via polar Kerr effect
Optically inject polarized electrons w/ circularly-polarized pump laser
pump laser
3-300 K
LP
probe laser
Selection rules:
conduction band: $s_z = \pm\frac{1}{2}$
RCP
LCP
valence band: $j_z = \pm\frac{3}{2}$
polarization beamsplitter
y
z
x
~ 1 μm spatial resolution
$B_{applied}$
A
B
A-B
measure Kerr rotation ~ $<S_z>$


First step: Image optically-injected spins
Image the 2-D lateral diffusion of spin-polarized electrons in GaAs
• Sample: 1 μm thick bulk epilayer of n-GaAs (n_e=1x10^{16} cm^{-3})
- long τ_s >100 ns at 10K
50μm
55
48
41
35
28
21
14
7
0
Spin polarization (S_z)
"Spin drag"
E=10 V/cm
y
x
• Spin-polarized electrons diffuse radially away from injection point.
• Spatial extent given by spin diffusion constant & spin lifetime: sqrt(D_s τ_s)
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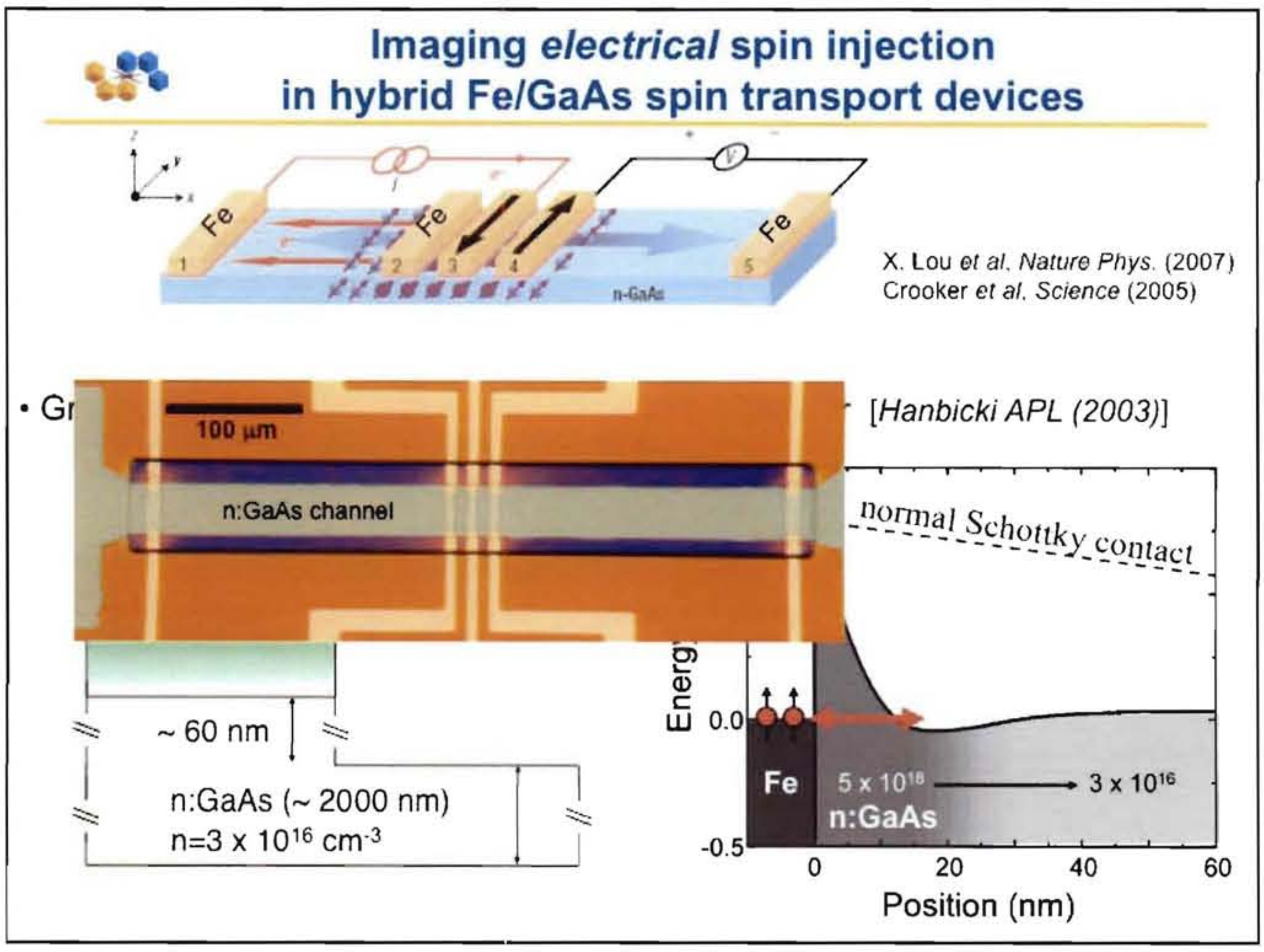
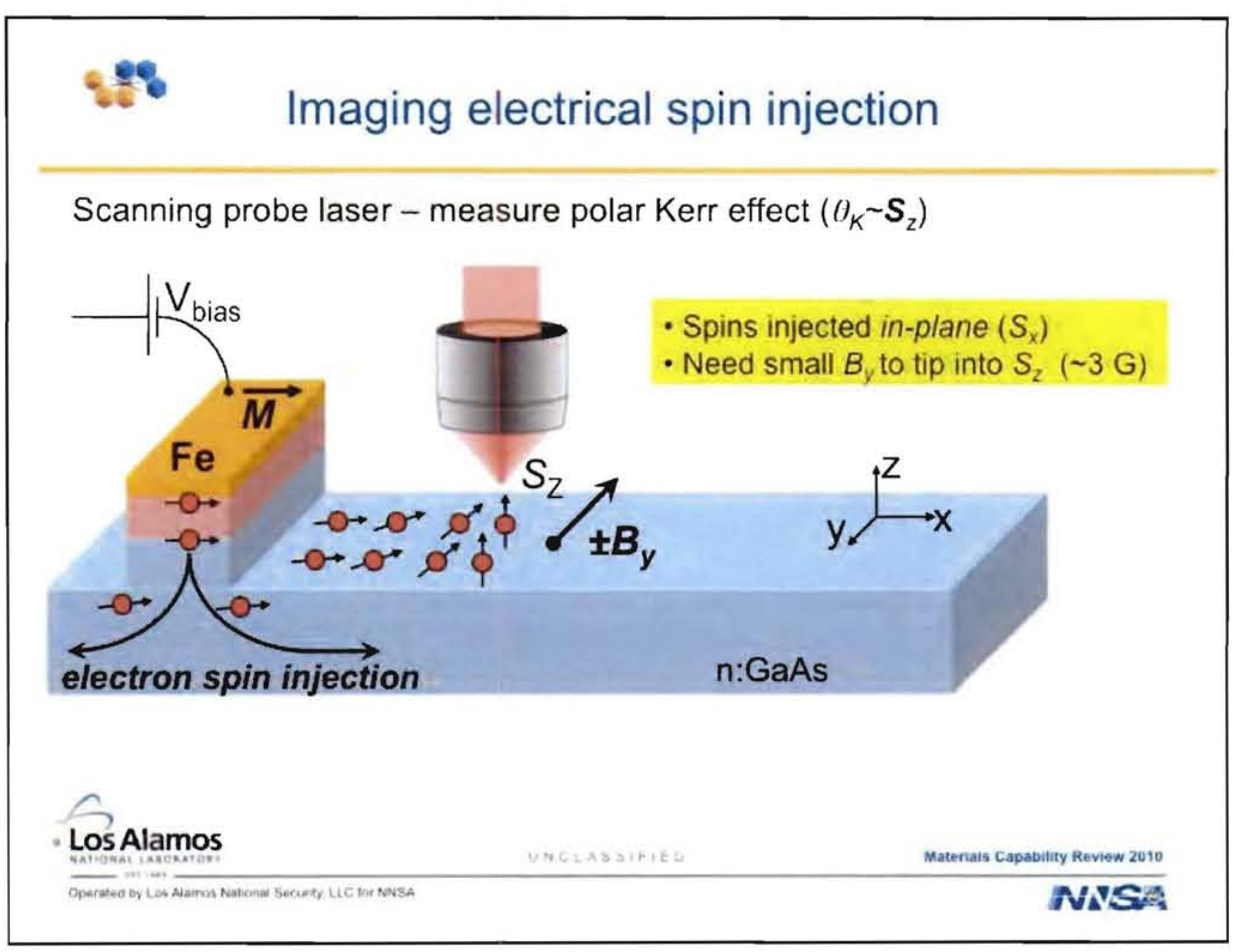

Imaging *electrical* spin injection
in hybrid Fe/GaAs spin transport devices
Fe
Fe
Fe
n-GaAs
X. Lou *et al. Nature Phys.* (2007)
Crooker *et al. Science* (2005)
• Gr
100 μm
n:GaAs channel
[Hanbicki APL (2003)]
normal Schottky contact
~ 60 nm
n:GaAs (~ 2000 nm)
n=3 x 10^16 cm^-3
Energ
0.0
-0.5
Fe
5 x 10^18
3 x 10^16
n:GaAs
0
20
40
60
Position (nm)


Imaging electrical spin injection
Scanning probe laser – measure polar Kerr effect (θ_K~S_z)
V bias
• Spins injected *in-plane* (S_x)
• Need small B_y to tip into S_z (~3 G)
M
Fe
S_Z
±B_y
z
y
x
electron spin injection
n:GaAs
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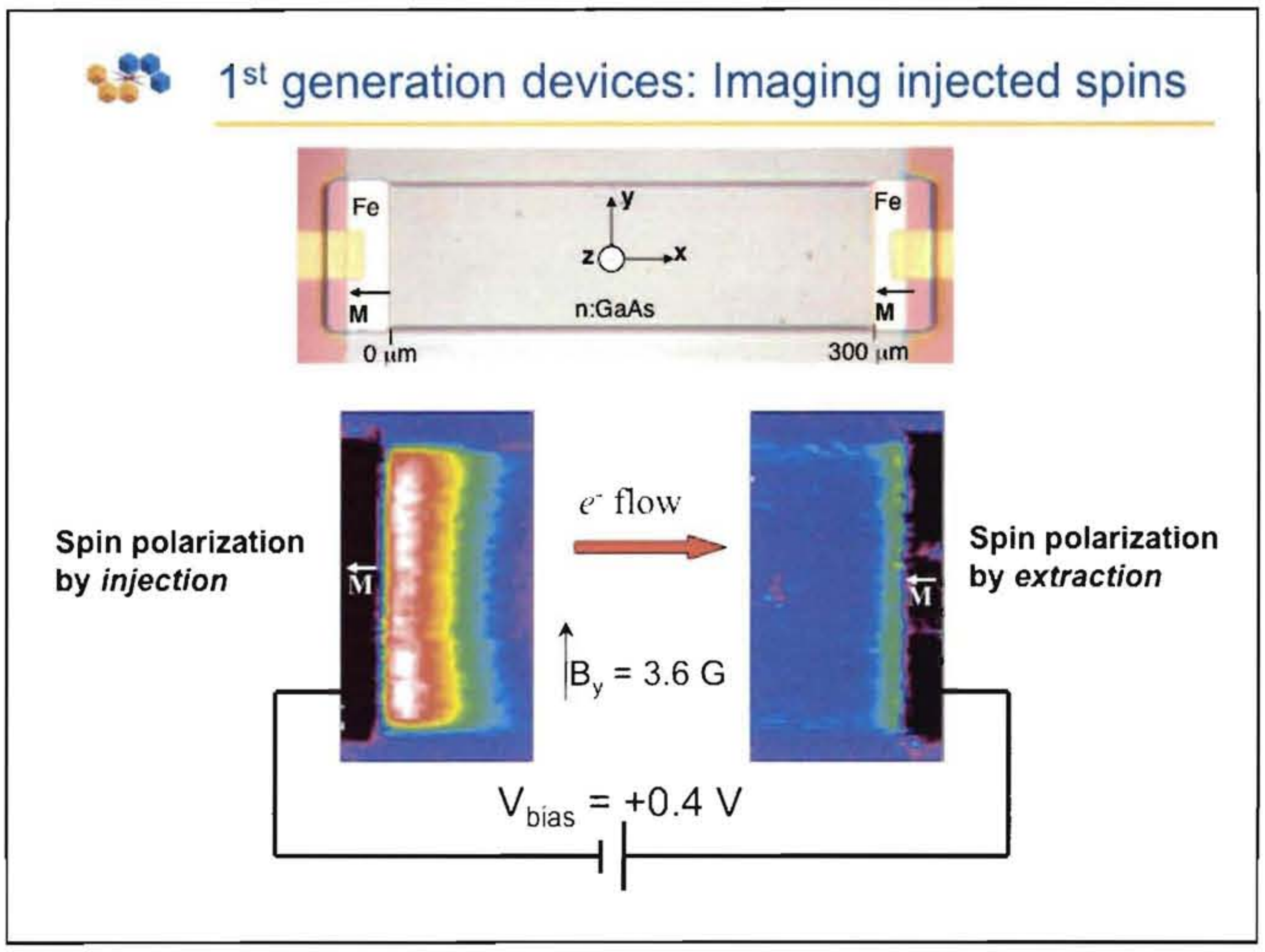
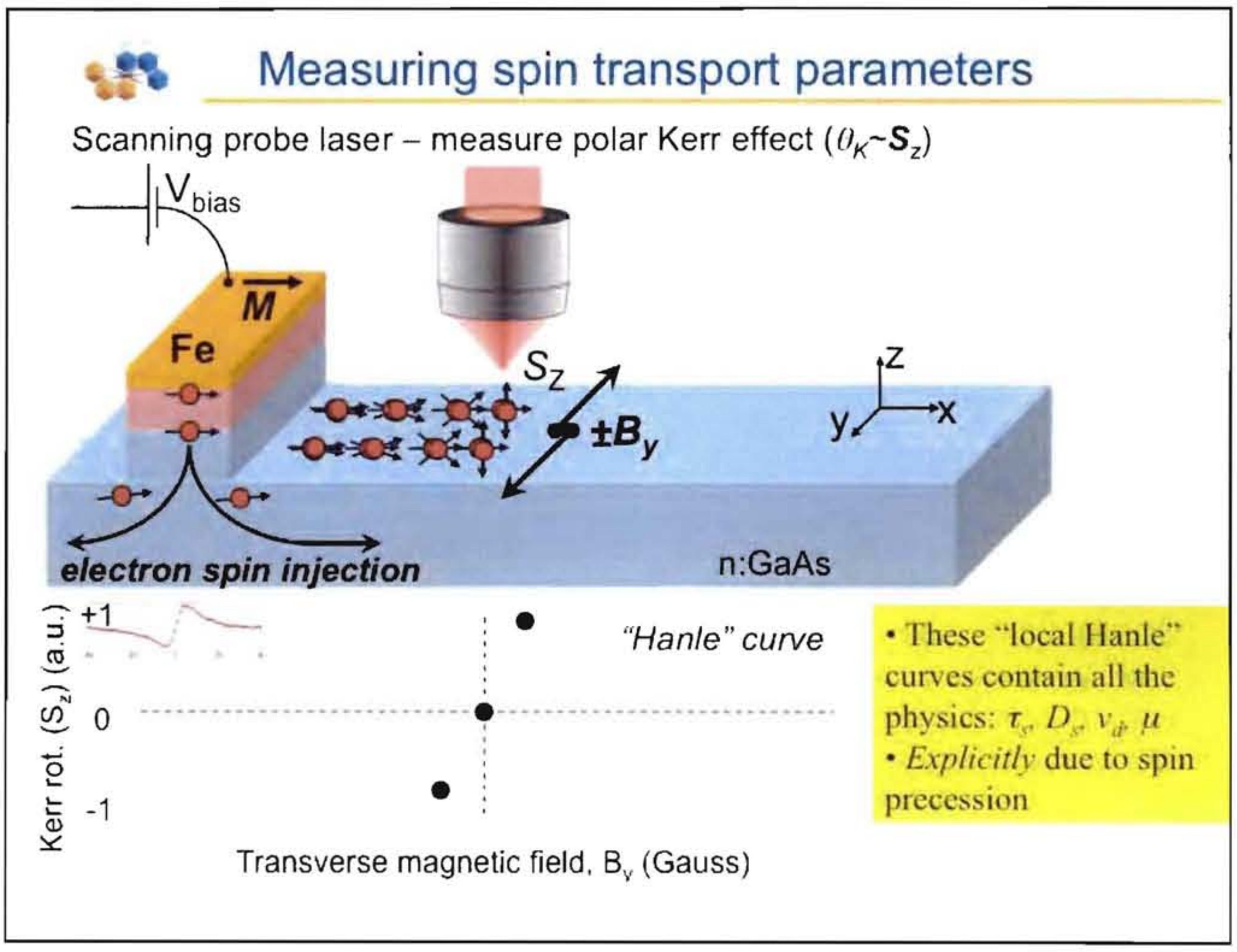
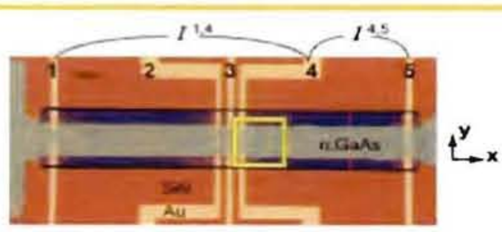
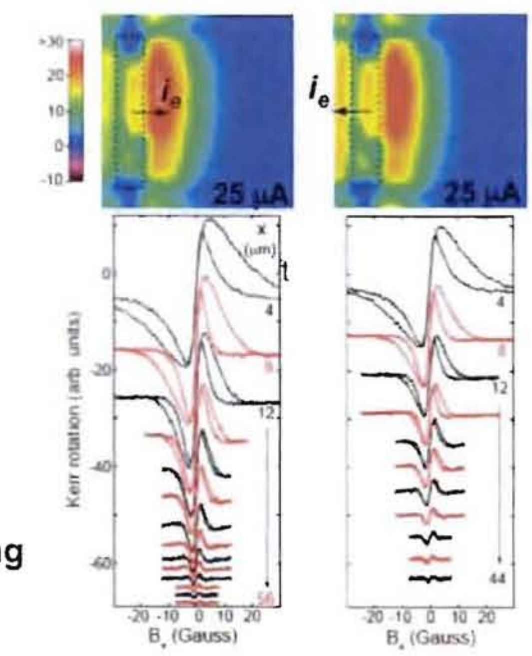

1st generation devices: Imaging injected spins
Fe
Fe
y
z
x
M
n:GaAs
M
0 μm
300 μm
Spin polarization by injection
M
e- flow
M
Spin polarization by extraction
By = 3.6 G
Vbias = +0.4 V


Measuring spin transport parameters
Scanning probe laser – measure polar Kerr effect (θK~Sz)
Vbias
M
Fe
Sz
±By
z
y
x
electron spin injection
n:GaAs
Kerr rot. (Sz) (a.u.)
+1
0
-1
"Hanle" curve
Transverse magnetic field, By (Gauss)
• These "local Hanle" curves contain all the physics: τs, Ds, vd, μ
• Explicitly due to spin precession

Measuring spin transport parameters



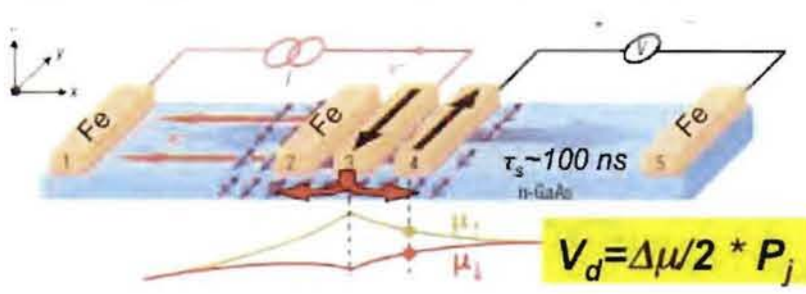


Fit Hanle data to obtain spin transport parameters:

$D = 10\ cm^2/s$
$v_d = 7000\ cm/s$
$\tau_s = 90\ ns$

Extremely useful for interpreting all-electrical spin-valve data!!

Fe/GaAs lateral spin injection, transport, & detection devices

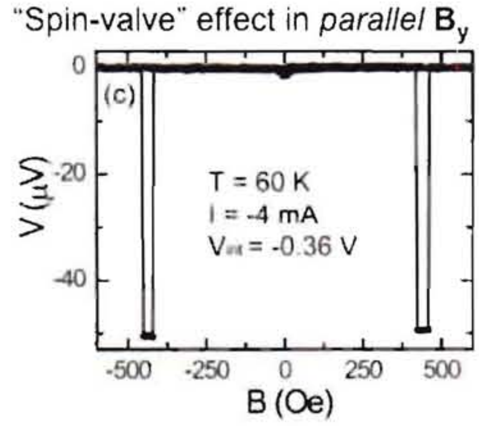


they work!
(detector at zero bias)

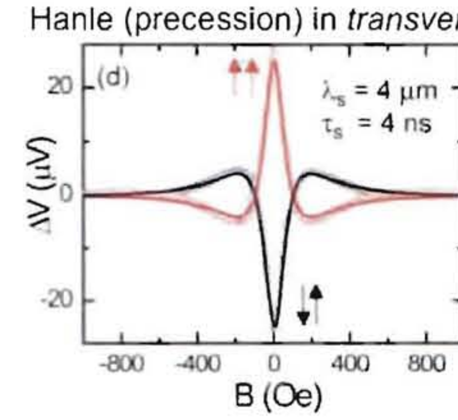
X. Lou *et al. Nature Phys.* (2007)

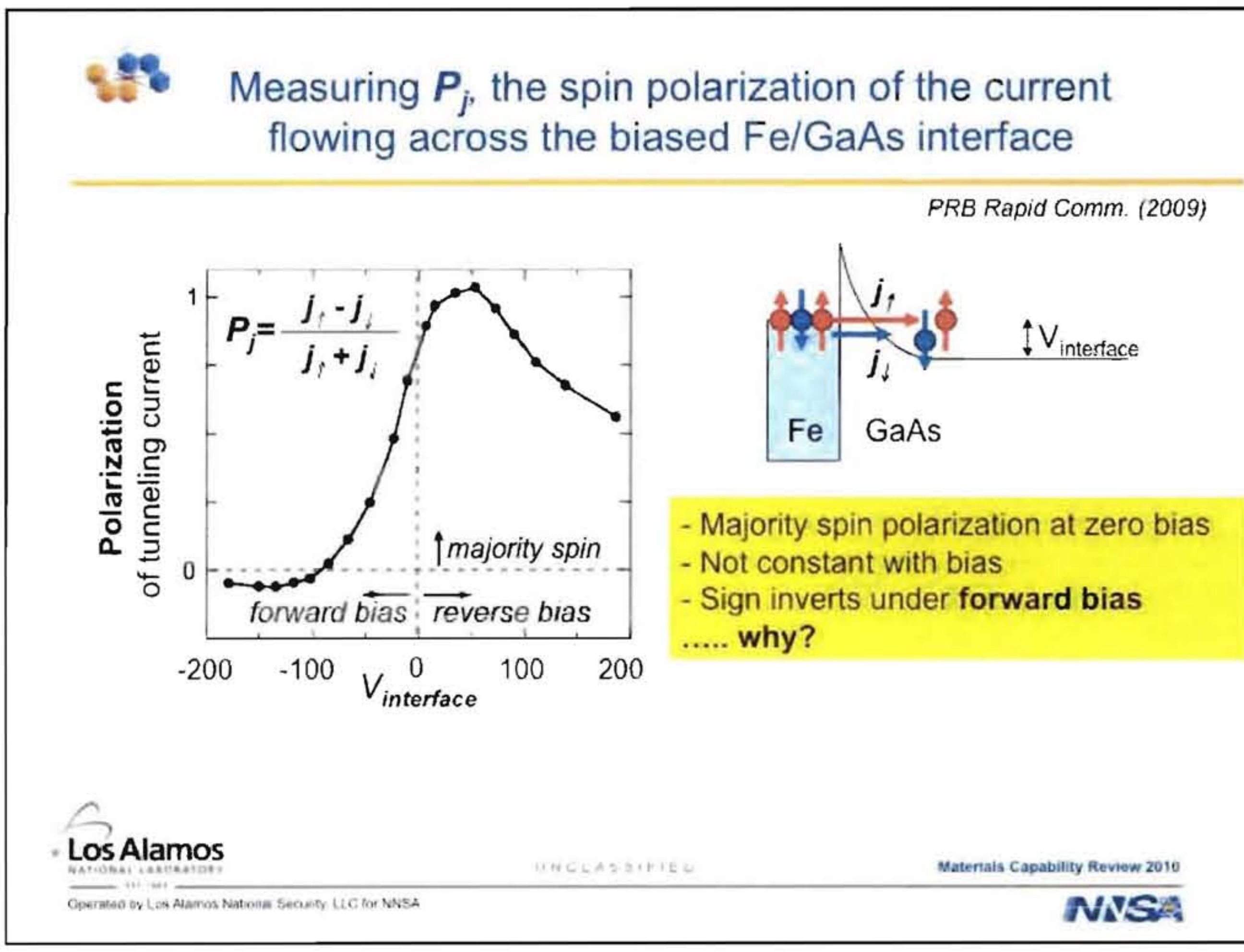
- Devices use a third 'non-local' *detection* electrode through which *no* current flows *[Johnson & Silsbee (1985); Jedema (2002); Valenzuela (2004)]*
- Transport studies show:

"Spin-valve" effect in *parallel* B_y



Hanle (precession) in *transverse* B_z




Measuring P_j, the spin polarization of the current flowing across the biased Fe/GaAs interface
PRB Rapid Comm. (2009)
$P_j = \frac{j_\uparrow - j_\downarrow}{j_\uparrow + j_\downarrow}$
Polarization of tunneling current
majority spin
forward bias
reverse bias
-200
-100
0
100
200
$V_{interface}$
$j_\uparrow$
$j_\downarrow$
$V_{interface}$
Fe
GaAs
- Majority spin polarization at zero bias
- Not constant with bias
- Sign inverts under forward bias
..... why?
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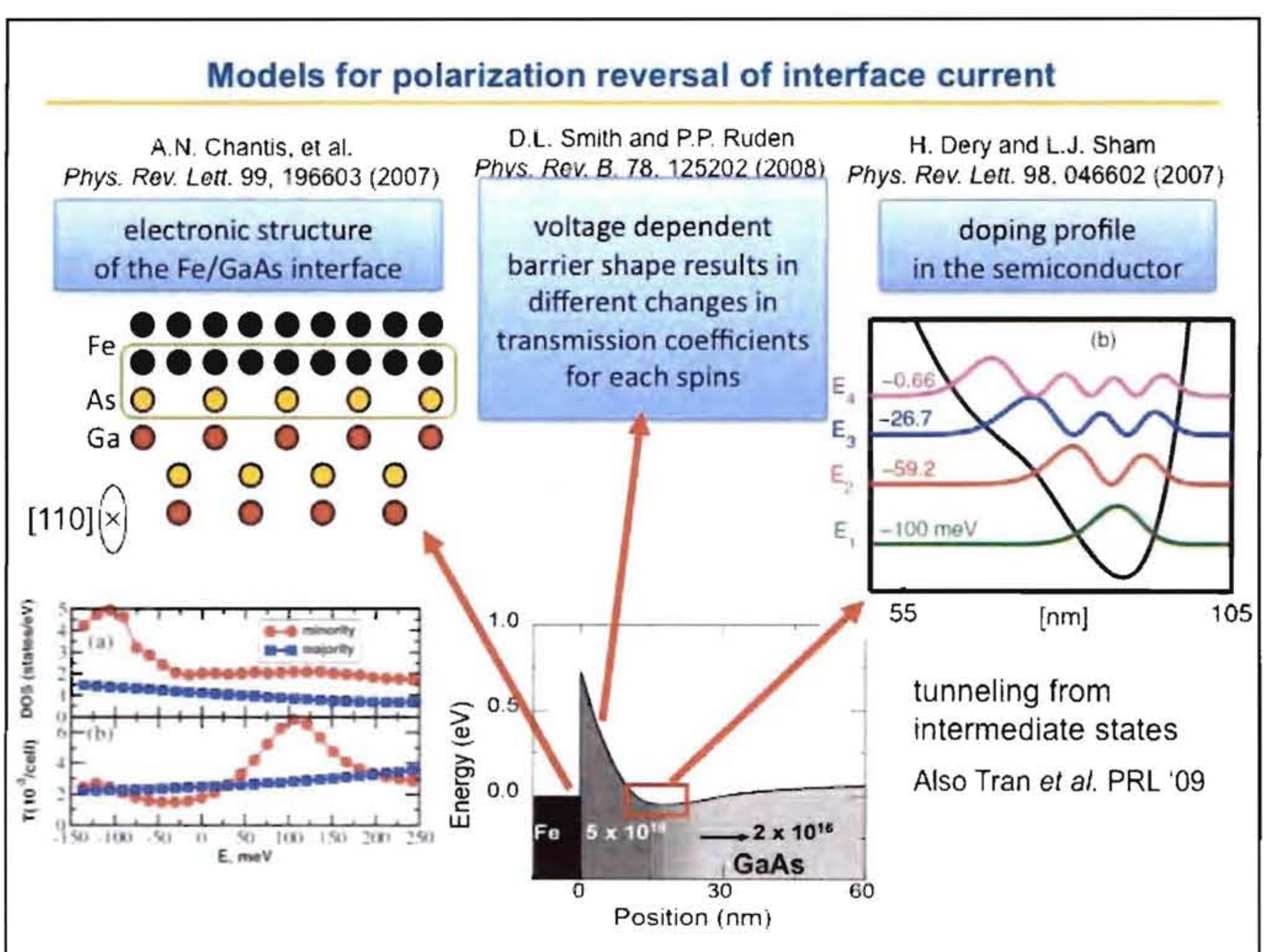
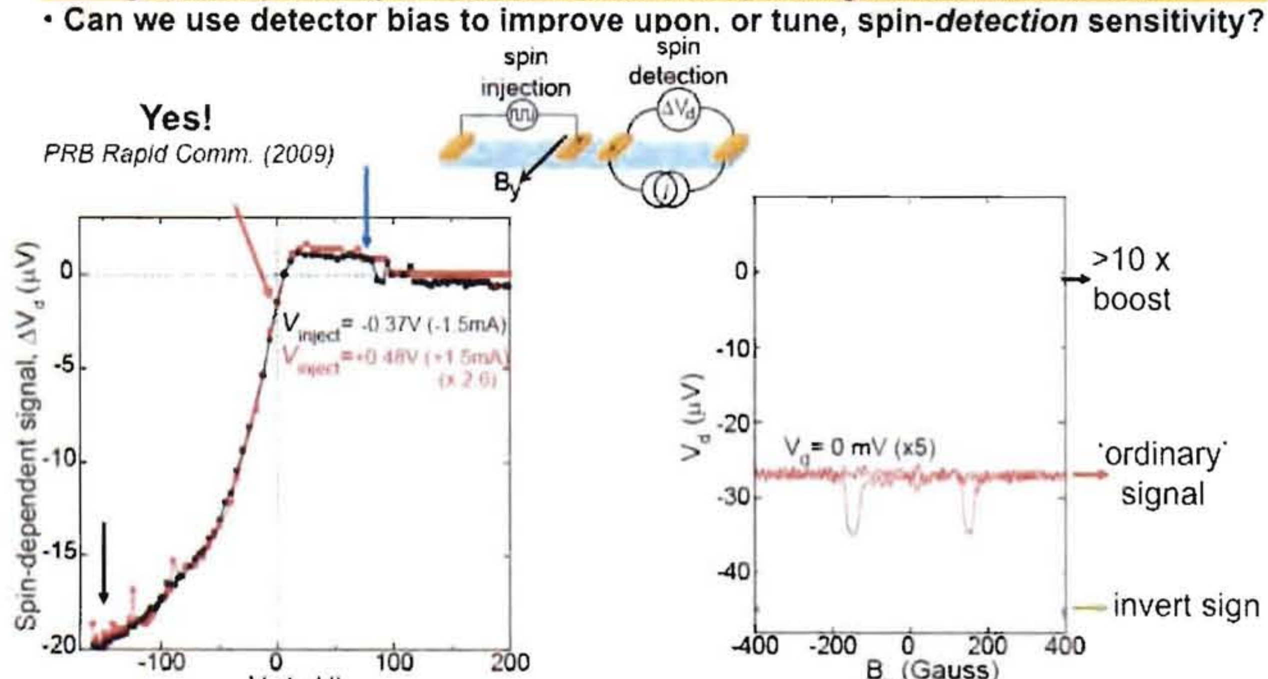

Models for polarization reversal of interface current
A.N. Chantis, et al.
Phys. Rev. Lett. 99, 196603 (2007)
electronic structure of the Fe/GaAs interface
D.L. Smith and P.P. Ruden
Phys. Rev. B 78, 125202 (2008)
voltage dependent barrier shape results in different changes in transmission coefficients for each spins
H. Dery and L.J. Sham
Phys. Rev. Lett. 98, 046602 (2007)
doping profile in the semiconductor
Fe
As
Ga
[110]
minority
majority
E, meV
(b)
-0.66
-26.7
-59.2
-100 meV
55
[nm]
105
1.0
0.5
0.0
Energy (eV)
Fe
5 x 10¹⁸
2 x 10¹⁶
GaAs
0
30
60
Position (nm)
tunneling from intermediate states
Also Tran et al. PRL '09

Implications for spin *detection?*

- All "non-local" studies of electrical spin detection in lateral devices (in GaAs, Si, graphene) used spin detection electrodes operating at *zero* interface bias.
- **Can we use detector bias to improve upon, or tune, spin-*detection* sensitivity?**

Yes!
PRB Rapid Comm. (2009)



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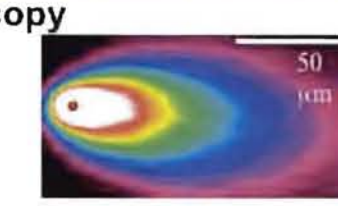
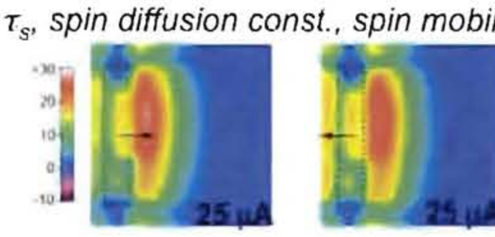
Summary

- **Image spin drift & diffusion w/ scanning Kerr microscopy**
  - *Both optically- and electrically-injected electron spins*
  - *Spin transport in E, B, and* **k***-dependent spin-orbit fields*



- **Fe/GaAs lateral spin transport devices**
  - *Image spin drift & diffusion, both 'downstream' and 'upstream' of the current path*
  - *Independent measure of τ_s, spin diffusion const., spin mobility, drift velocity*



- **Inversion of spin injection at finite bias across Fe/GaAs barrier**
  - *Spin-polarized tunneling across Fe/GaAs interface varies w/ bias*
  - *Consequence: tune sign and magnitude of spin-detection sensitivity*

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Casimir Interactions

D.A.R. Dalvit (T-4)

Casimir interactions are a macroscopic manifestation of the quantum vacuum. They arise from topological constrains of quantum vacuum electromagnetic fluctuations. Casimir forces represent a challenge for nanotechnology, as they are both responsible for stiction in micro- and nano-electromechanical machines, and also an opportunity, as they provide the possibility of non-contact force transmission via the quantum vacuum.

The sign and magnitude of the Casimir force depends on the geometry and material composition of the structures involved. The goal of our research program is to engineer Casimir forces with metamaterials, with three specific metrics: measurement, neutralization, and dynamic control. Metamaterials are artificially structured materials with designer electromagnetic properties, and offer several knobs to control the electromagnetic response of a material structure.

This project is a LANL/Sandia Laboratories partnership through the Center for Integrated Nanotechnologies (CINT), and is funded by the Defense Advanced Research Projects Agency (DARPA) under its Casimir Effect Enhancement program. It is a cross-disciplinary project leveraging materials/quantum, and involves theory, fabrication, and characterization. Our work impacts LANL's mission on basic science and technology, and contributes to LANL material strategy on emergent phenomena at interfaces.

Casimir Interactions

Diego Dalvit, Peter Milonni, Felipe da Rosa (T)

John O'Hara, Toni Taylor, Jianfeng Zhou (MPA)

in collaboration with I. Brener, P. Davids, M. de Boer, and S. Howell (Sandia)

discover LDRD

DARPA

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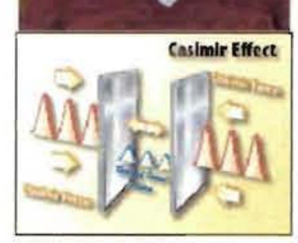
The Casimir force

- **Macroscopic manifestation of the quantum vacuum**
  - Originates from changes in quantum vacuum fluctuations imposed by material boundaries.
  - Predicted by the Dutch physicist Hendrik Casimir in 1948.
  - Typically an attractive force.
  - Related to van der Waals force.

$$E = \frac{1}{2}\sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \Rightarrow \boxed{\frac{F}{A} = \frac{\pi^2}{240}\frac{\hbar c}{d^4}}$$

$(130\mathrm{nN/cm}^2 \ @\ d = 1\mu\mathrm{m})$

  - Not small, nN is a large force on the microscale $\approx 10^{13} F_{\mathrm{grav}}$



- **Magnitude and sign depend on geometry and composition of materials**

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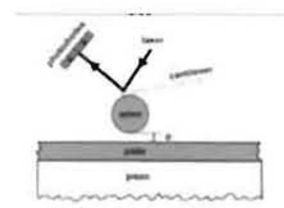
Modern Casimir force experiments

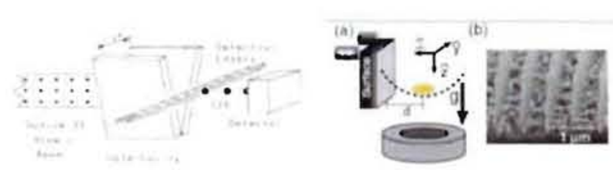
- **Torsion pendulum**

- **AFM**



- **MEMS and NEMS**

- **Atom deflection/reflection**



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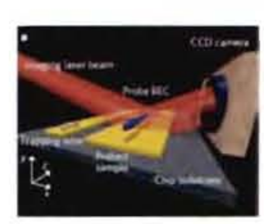
Examples of relevant applications

- **Nanotechnology**
  - MEMS and NEMS
    - Casimir force limiting factor to stiction in nanomachines
    - Quantum levitation via repulsive Casimir
  - Casimir actuation
    - Contactless force transmission via lateral Casimir
    - Quantum friction between materials in relative motion

- **Quantum science and technology**
  - Casimir atom-surface interactions
    - Precision measurements with ions, neutral atoms
    - Quantum technologies: e.g. atom chips



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Materials aspects of Casimir force

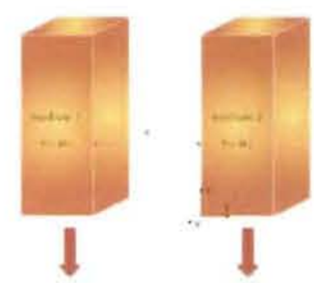
- **Casimir force manipulation requires the ability to tailor the electric and magnetic properties of a material over the electromagnetic spectrum**
  - Material properties included via reflection matrices in Lifshitz formula

$$\frac{F}{A} = 2\hbar \, \mathrm{Im} \int_0^\infty \frac{d\omega}{2\pi} \int \frac{d^2\mathbf{k}_\parallel}{(2\pi)^2} K_3 \mathrm{Tr} \frac{\mathbf{R}_1 \cdot \mathbf{R}_2 e^{2iK_3 d}}{1 - \mathbf{R}_1 \cdot \mathbf{R}_2 e^{2iK_3 d}}$$

$$\mathbf{R}_i[\epsilon(\omega), \mu(\omega), \ldots] \qquad K_3 = \sqrt{\omega^2/c^2 - k_\parallel^2}$$

  - Sum over all possible quantum fluctuations: broad-band, all angles of incidence, all polarizations.

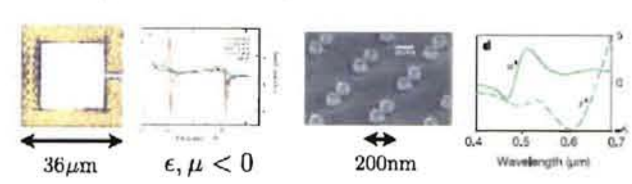
- **Goal of this project: Casimir force engineering with metamaterials**
  - Measurement
  - Neutralization
  - Dynamical control



$\epsilon_1 \gg \mu_1$ $\mu_2 \gg \epsilon_2$

Why metamaterials?

- **Artificial structured composites with designer EM response**
- **Novel material properties:**
  - Independent tuning of $\epsilon(\omega)$ and $\mu(\omega)$
  - High frequency magnetism
  - Chirality
- **Largely unexplored design space**
- **Dynamic (electronic/photonic) control of material response**



THz MM: SRR Optical MM: nanopilars

- **Requirements for MM approach for Casimir force control are challenging:**
  - High $\mu(\omega)$, low $\epsilon(\omega)$ (for neutralization/repulsion)
  - Isotropy: scalar $\epsilon(\omega)$, $\mu(\omega)$
  - Role of E-B coupling (chiral MMs)
  - Homogeneity (eff. medium)
  - Broadband

$$\begin{bmatrix} \mathbf{D} \\ \mathbf{B} \end{bmatrix} = \begin{bmatrix} \varepsilon & \xi \\ \zeta & \mu \end{bmatrix} \begin{bmatrix} \mathbf{E} \\ \mathbf{H} \end{bmatrix}$$

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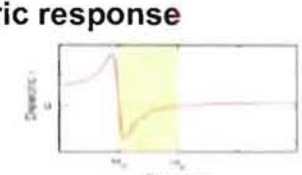
Effective EM response of MMs

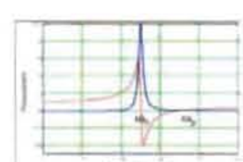
- **Effective medium approximation**
  - MM is probed with EM wavelengths much larger than unit cell
  - MM describable by effective homogeneous optical parameters

- **Effective electric response**

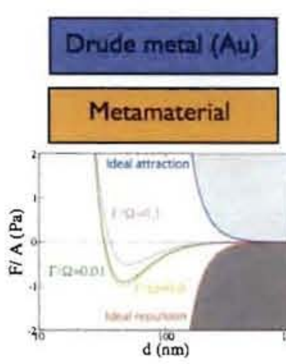


$$\varepsilon(\omega) = 1 - \frac{\omega_p^2 - \omega_0^2}{\omega^2 - \omega_0^2 + i\omega\Gamma}$$

- **Effective magnetic response**



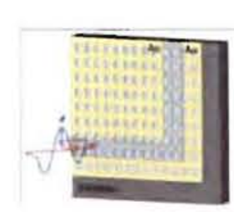
$$\mu_{eff} = 1 - \frac{\pi r^2 / a^2}{1 + \frac{2\sigma i}{\omega r \mu_0} - \frac{3}{\pi^2 \mu_0 \omega^2 C r^3}}$$

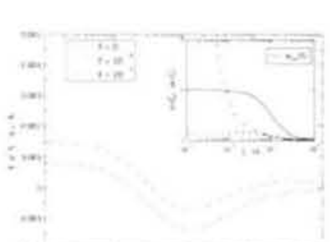


Repulsion-attraction

Casimir force with metallic-based MMs

- **Fishnet designs**
  - Demonstrated magnetic response at optical frequencies
  - Continuous Drude metal good for dynamic switching
  - Deleterious for Casimir neutralization/repulsion





$$\epsilon(\omega) = 1 - f\frac{\Omega_D^2}{\omega^2 - i\omega\gamma_D} - (1-f)\frac{\Omega_e^2}{\omega^2 - \omega_e^2 + i\gamma_e\omega}$$

f : filling factor

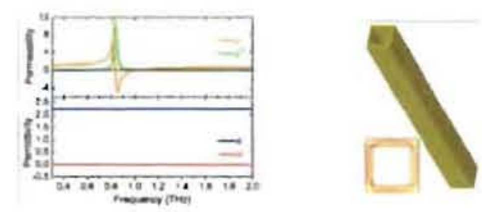
$$\mu(\omega) = 1 - \frac{\Omega_m^2}{\omega^2 - \omega_m^2 + i\gamma_m\omega}$$

Phys. Rev. Lett. **100**, 183602 (2008); Phys. Rev. A **78**, 032117 (2008)

- **MMs with diminished permittivity**

Other MM possibilities for Casimir control

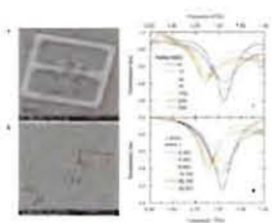
- **All-dielectric metamaterials**
  - Path to magnetism without metals
  - No Drude background, low permittivity
  - Requires high index contrast



- **Chiral metamaterials**
  - Mixing of E-H fields

$$\mathbf{D}(\mathbf{r},\omega) = \epsilon(\omega)\mathbf{E}(\mathbf{r},\omega) - i\kappa(\omega)\mathbf{H}(\mathbf{r},\omega)$$
$$\mathbf{B}(\mathbf{r},\omega) = i\kappa(\omega)\mathbf{E}(\mathbf{r},\omega) + \mu(\omega)\mathbf{H}(\mathbf{r},\omega)$$

  - Path to neutralization w/ strong chirality
  - Anisotropy: generalization of Lifshitz
- **Active control**
  - Dynamics MMs made of metals and semiconductors
  - Photonic or electronic dynamic control of EM response: frequency, amplitude, phase



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EMA approach to Casimir enhancement using MM

- **Calculation of force-displacement curves**
  - Inclusion of real optical data

$$\varepsilon(i\xi) = 1 + \frac{2}{\pi}\int_0^{\infty}\frac{\omega\varepsilon''(\omega)d\omega}{\omega^2+\xi^2}, \quad \mu(i\xi) = 1 + \frac{2}{\pi}\int_0^{\infty}\frac{\omega\mu''(\omega)d\omega}{\omega^2+\xi^2}$$

  - Casimir-Lifshitz force between two slabs

$$F(a) = -\frac{1}{\pi A}\sum_{p=te}^{tm}\sum_{n=0}^{\infty}{}' \int_0^{\infty} dk\, k\,(k^2+\xi_n^2/c^2)^{1/2} \times \frac{r_p^{(1)}(\xi_n,\mathbf{k})r_p^{(2)}(\xi_n,\mathbf{k})e^{-2a(k^2+\xi_n^2/c^2)^{1/2}}}{1-r_p^{(1)}(\xi_n,\mathbf{k})r_p^{(2)}(\xi_n,\mathbf{k})e^{-2a(k^2+\xi_n^2/c^2)^{1/2}}}$$

  - Reflection coefficients

$$r_{tm}^{(i)} = \frac{\epsilon_i\sqrt{k^2+\frac{\xi_n^2}{c^2}} - \sqrt{k^2+\epsilon_i\mu_i\frac{\xi_n^2}{c^2}}}{\epsilon_i\sqrt{k^2+\frac{\xi_n^2}{c^2}} + \sqrt{k^2+\epsilon_i\mu_i\frac{\xi_n^2}{c^2}}} \qquad r_{te}^{(i)} = r_{tm}^{(i)}, \quad \epsilon \leftrightarrow \mu$$

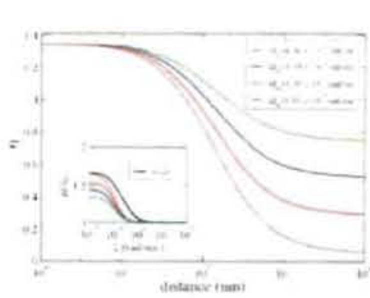

Fig. III.7: Normalized Casimir force between a Au plate and a Au-based non-connected MM for different magnetic resonance frequencies.

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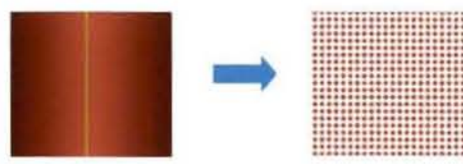
Beyond effective medium approximation

- **For Casimir EMA not enough: feature sizes comparable to wavelengths**

Homogeneous medium $\epsilon_{\text{eff}}(\omega)$ $\mu_{\text{eff}}(\omega)$



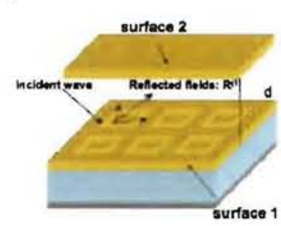
Non homogeneous medium $\epsilon(\mathbf{r},\omega)$ $\mu(\mathbf{r},\omega)$

- **Exact numerical methods for Casimir force in complex material structures**
  - Green function approach: computation of Casimir stress tensor (FDTD)
  - Scattering approach: computation of Casimir energy (RWCA)

$$\frac{E(d)}{A} = \hbar \int_0^\infty \frac{d\xi}{2\pi} \log\det\left[1 - \mathcal{R}_1 e^{-\mathcal{K}d} \mathcal{R}_2 e^{-\mathcal{K}d}\right]$$

$$-ik\frac{\partial \mathbf{E}_t}{\partial z} = \nabla_t[\chi \hat{e}_3 \cdot \nabla \times \mathbf{H}_t] - k^2 \mu \hat{e}_3 \times \mathbf{H}_t$$
$$-ik\frac{\partial \mathbf{H}_t}{\partial z} = -\nabla_t[\zeta \hat{e}_3 \cdot \nabla \times \mathbf{E}_t] + k^2 \epsilon \hat{e}_3 \times \mathbf{E}_t$$

$$-ik\frac{\partial \Psi_{m'n'}}{\partial z} = \sum_{mn} H_{m'n',mn} \Psi_{mn}$$



Fabrication, characterization, and measurement

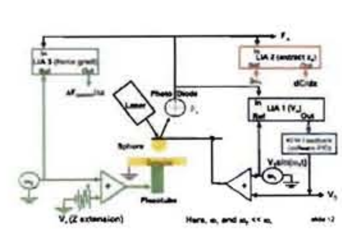
- **Nanofabrication at CINT-LANL with state-of-the-art electron-beam writer**

SRR: Au on InSb (3-12 um)

Fishnets: Al on BaF2 (7-12 um)

- **Complex T&R (angle resolved) and n&k (ellipsometry)**

- **Casimir force measurement with AFM**



Calibration via Coulomb forces
Measurement of contact potentials
Measurement of Casimir force

Relevance to LANL & materials strategy – Key points

- **Impact to LANL missions on basic science and technology**
  - Applications to nanotechnology and quantum: stiction, actuation, atom chips
- **Contribution to LANL materials strategy**
  - Emergent phenomena at interfaces : materials controlled functionality for Casimir force manipulation.
- **Key points of our project**
  - Casimir force engineering with metamaterials.
  - High profile publications (PRL, Nature) and media coverage (New Scientist, IEEE).
  - Partnership between LANL and Sandia: leverages CINT, cross-disciplinary.
  - Initial work funded by LDRD-ER. Transitioned to external DARPA funding. A program development success.
  - >20 white papers, only 5 funded proposals nationwide.
  - Organized international conference on Casimir force control.
  - Book on Casimir physics, to be published by Springer.

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The Influence of Growth Temperature and Annealing on the Magnetization of a Ferromagnetic/Semiconductor Interface

M.R. Fitzsimmons (LANSCE-LC); S. Park (Pusan National University); C.F. Majkrzak (National Institute of Standards and Technology); B.D. Schultz (International Technology Center); C.J. Palmstrom (University of California, Santa Barbara)

The magnetization depth profiles of three FeCo/GaAs samples grown at different temperatures and measured before and after annealing were obtained using polarized neutron reflectometry. Prior to annealing, the sample grown at 95 °C had the thickest magnetically degraded interfacial region between the FeCo film and the GaAs substrate. For the sample grown at -15 °C, the magnetic interface was sharp. For all samples, annealing promoted thicker interfacial regions with suppressed magnetization and distinct boundaries with the adjoining (FeCo or GaAs) material. Thus, the magnetic structure of the FeCo/GaAs interface was very sensitive to the conditions of growth and annealing.

Bias Dependence of Spin Transport at Ferromagnet/Semiconductor Tunnel Junctions

A.N. Chantis, D.L. Smith (T-4)

Recent experiments have established that electrical spin injection and detection using ferromagnet/semiconductor Schottky tunnel barriers exhibit strong bias dependence. In this poster, we present theoretical studies that explain these experimental observations. Using a combination of first-principles electronic structure methods and theoretical modeling we have shown that the observed bias-dependence originates from two distinct physical mechanisms: the bias dependence of electron spin-dependent tunneling, which is of microscopic origin and depends on the specific electronic properties of the interface; and the macroscopic electron-spin transport properties in the semiconductor. We have demonstrated that the second mechanism allows one to tune the spin-detection sensitivity in ferromagnet/semiconductor tunnel contacts over a wide range. These theoretical results are in good agreement with the recent experimental observations.

Heterostructured Si/Ge Nanowires for High Performance Electronics

S.A. Dayeh, S.T. Picraux (MPA-CINT)

Heterostructured nanowires composed of Si and Ge in axial and core-shell configurations with electrical doping and composition control are enabling new approaches to nanoscale devices. We have developed an in-situ growth procedure for implementing 100% doping and composition modulation of Ge/Si heterostructure nanowires in three dimensions with unprecedented control over their structure, morphology, and properties. In this vapor-liquid-solid growth approach a low temperature "gold-blocking" layer that changes the interfacial energy between the gold growth seed and the nanowire is deposited, thereby preventing gold diffusion on its sidewalls and enabling the complete *in situ* growth of such heterostructures.

Composition modulation along the axial direction, which is typically the charge transport direction, has resulted in the highest performance asymmetric tunnel transistors ever achieved, with 10^5-10^7 I_{on}/I_{off} ratios and high current drives. This performance is enabled by these unique asymmetric devices made possible by semiconductor nanowire heterostructures that allow a Ge source for efficient tunneling of charge carriers into the channel with high current drives and a Si drain for low reverse tunneling into the channel and therefore low off currents. Radial heterostructured core-shell nanowires have shown significantly increased field-effect mobility values and current drives (both up to two times) over those transistors made with nanowires that have Au diffusion on their sidewalls. These high performance devices promise high-speed electronics, high linearity amplifiers, low power operation, and low standby power dissipation, potentially suitable for radar and satellite communications and high performance and durable portable electronics. These studies are currently being extended to core-shell photovoltaic nanowire arrays and spin injection and transport devices.

Interfacial Energy and Charge Transfer in Assemblies Consisting of CdSe Nanocrystals and Ru-polypyridine Complexes

M. Sykora, A.Y. Koposov (C-PCS); T. Cardolaccia, T.J. Meyer (University of North Carolina); V.I. Klimov (C-PCS)

Understanding of energy and charge transfer processes at the semiconductor/liquid junction interfaces is important for design of new type of electronic and solar energy conversion devices. Quantum confined semiconductor nanocrystals (NCs) represent an important group of materials with the potential to significantly enhance performance of related applications. To develop a better understanding of energy and charge transfer processes involving semiconductor NCs we have studied interactions between CdSe NCs and series of Ru-polypyridine complexes. Using ATR-FTIR spectroscopy, we show that complexes functionalized with carboxylic acid functionality chemically bind to the surface of NCs, whereby the carboxylic acid is deprotonated in the process. The analysis of the concentration dependence of photoluminescence (PL) quenching using Langmuir model reveals that surface coverage of the NCs with the complexes can be effectively controlled by variation of the complex/NC ratio in solution. We show that in the NQD/Ru-complex assemblies the NC PL is quenched with efficiencies up to 100%. The mechanism of quenching is either ET or CT, depending on the NC size. In the case of small NCs, the dominant interaction mechanism is dipole-dipole type ET enabled by large overlap of the NC PL and the absorption spectrum of the complex. For large NCs, the overlap of the NC PL and the absorption spectrum of the complex is small and the dominant interaction mechanism is rapid CT. Demonstrated sensitization of complexes with NQDs opens interesting opportunities for designing new types of photocatalytic materials for solar energy conversion applications.

Intrinsic Inhomogeneity in Functional Materials

T. Lookman (T-4); K.H. Ahn; A.R. Bishop; M. Porta (T-4); A. Saxena (T-4); S.R. Shenoy

The presentation will discuss the interplay of spin-charge and lattice results in intrinsic inhomogeneity, which leads to functionality in a wide class of materials with complex unit cells, including multiferroics, manganites, relaxor ferroelectrics and high Tc superconductors. The role of strain as an elastic template, leading to long-range anisotropic interactions, is fundamental to understanding the emergence of multiple competing states and sensitivity to perturbation (e.g. doping, external fields) in these materials. Local anisotropic constraints that can result in frustration can also manifest such global consequences. I will review a number of examples from our work on multiferroic and perovskite materials that illustrate this emerging theme.

Tailoring the Morphology of Carbon Nanotube Arrays: From Spinnable Forests to Undulating Foams for Stretchable Conductors

Y.Y. Zhang, G.F. Zou, S.K. Doorn, J. Y. Zhai (MPA-CINT); H. Htoon (C-PCS); L. Stan (MPA-STC); M.E. Hawley (MST-8); J. Xiong (MPA-CINT); C.J. Sheehan (MPA-STC); and Q.X. Jia (MPA-CINT)

Directly spinning carbon nanotube (CNT) fibers from vertically aligned CNT arrays is a promising way for the application of CNTs in the field of high-performance materials. However, most of the reported CNT arrays are not spinnable. We have systematically studied the correlation between the catalyst pretreatment, the CNT morphology, and the CNT spinnability. By controlling catalyst pretreatment conditions, we have demonstrated that the degree of spinnability of CNTs is closely related to the morphology of CNT arrays. Shortest catalyst pretreatment time led to CNT arrays with the best spinnability, while prolonged pretreatment resulted in coarsening of catalyst particles and nonspinnable CNTs. By controlling the coalescence of catalyst particles, we have demonstrated the growth of undulating CNT arrays with uniform and tunable waviness. The CNT arrays can be tuned from well-aligned, spinnable forests to uniformly wavy, foam-like films.

By embedding continuous CNT ribbons in poly(dimethylsiloxane) (PDMS), we have successfully fabricated transparent stretchable conductors that can maintain stable conductivity under repetitive stretching. The CNT/PDMS film fabricated by this approach shows good transparency, excellent flexibility, and stable resistance with application of strains up to 100%. Furthermore, the resistance and the transparency of this material can be controlled by varying the quality of CNT forests (e.g. height, single-wall or multi-walled), the layers of CNT ribbons (more layers, more conductive, but less transparent), and the matrix polymers.

Ultrafast Phenomena in Complex Oxides

R.P. Prasankumar (MPA-CINT)

Complex oxides, such as high-T_c superconductors (HTSC), multiferroics, and colossal magnetoresistance manganites, display a variety of unique phenomena throughout their phase diagrams. However, despite the substantial attention given to these systems over the past 25 years, many important questions remain unresolved, motivating the application of novel techniques to these fascinating materials. The technique of ultrafast optical spectroscopy (UOS) in particular is capable of temporally resolving quasiparticle dynamics in these systems on a femtosecond time scale, which has shed much light on their fundamental properties.

In this work, we have utilized UOS to temporally resolve carrier dynamics in a variety of complex oxides, ranging from multiferroic materials to oxide superlattices. For example, optical pump, mid-infrared (IR) probe measurements on the charge-and-orbital ordered manganite $Nd_{0.5}Sr_{0.5}MnO_3$ revealed the presence of intrinsic phase inhomogeneities throughout the measured temperature range through polaron dynamics. We have also used UOS to study polaron dynamics in multiferroic $LuFe_2O_4$, a material that has generated much recent interest due to its strong magnetoelectric coupling. Here, temperature-dependent experiments revealed the influence of charge and spin ordering on polaron dynamics as well as the coupling between polaronic and on-site excitations. In addition, we have recently performed UOS studies of HTSC/manganite superlattices, novel oxide heterostructures that offer a high degree of control over material properties. These measurements revealed the dominant influence of the HTSC layers at early timescales, which was supplanted by the manganite layers at longer times.

Finally, we have recently demonstrated a novel ultrafast optical system that is capable of directly pumping low energy excitations in complex oxides and probing the photoinduced changes in their properties with terahertz pulses. This system has been benchmarked through mid-IR-pump, THz-probe measurements on InSb and will be used in the near future to unravel the coupling between different degrees of freedom (e.g., electrons and phonons) in complex oxides.

Vortex Physics in Oxide and Pnictide High Temperature Superconductors

L. Civale, B. Maiorov, S.A. Baily, H. Zhou, T.G. Holesinger, N. Haberkorn, M. Miura (MPA-STC); M. Jaime. F. Balakirev (MPA-CMMS)

Vortex physics has been a topic of continuous interest since the discovery of the oxide high temperature superconductors (HTS). The fascinating vortex phenomenology in the oxide HTS, such as their complex phase diagram and their rich non-equilibrium dynamics, arises from the strong influence of thermal fluctuations, which in turn is a consequence of the small superconducting coherence length (x) and the large crystalline anisotropy (g). Although this behavior strongly contrasts with the much simpler vortex phenomenology in conventional low temperature superconductors (LTS), there is no sharp boundary between vortex physics in LTS and HTS. The discovery of the FeAs-based superconductors provided a perfect opportunity to "bridge the gap" by investigating vortex matter in a whole new family of materials spanning broad ranges of T_c and g. While the high T_c and consequent small x in some of them result in large fluctuation effects similar to those found in the oxides, such as the appearance of vortex liquid phases and fast dynamics, the multi-band superconductivity in the FeAs compounds introduces a new level of complexity, requiring a re-evaluation of the concept of anisotropy in the vortex behavior.

We will present comparative studies of vortex matter in oxide- and FeAs-based superconductors. From angular dependent resistivity studies at high fields (both pulsed and DC) we extract information about the upper critical field (H_{c2}) and the presence of vortex solid-liquid phase transitions in single- and multi-band anisotropic superconductors. Using angular dependent nonlinear transport we determine critical currents and investigate vortex pinning mechanisms, and using time relaxation (flux creep) studies we explore the vortex dynamics and the characteristics of the depinning excitations.

Near Infrared Organic Photodiodes with Gain at Low Bias Voltage and High Visible Transparency

I.H. Campbell (MPA-11)

Organic photodiodes are of interest for many applications due to their simple, low temperature processing, high quantum efficiency, compatibility with large area, flexible and curved substrates, and low cost. To date, organic photodiode research is focused on solar energy applications. Despite this, most organic photodiodes and solar cells are sensitive only in the visible spectrum. For solar energy, communication, and imaging applications, it is desirable to extend organic photodiode sensitivity into the near infrared (NIR).

The research demonstrates two types of near infrared organic photodiodes: One is diodes with photoresponse out to ~1100 nm and with a gain of ~10 at 1000 nm under 5V reverse bias. The second is diodes with a transparency of ~80% throughout the visible spectrum with ~100% external quantum efficiency in the NIR. The diodes employ soluble naphthalocyanines (Nc) with peak absorption coefficients of $\sim 10^5$ cm^{-1} in the NIR. In contrast to most organic photodiodes, no exciton dissociating material is used in diode 1. At zero bias, these diodes are inefficient with an external quantum efficiency of ~1%. In reverse bias, large gain occurs that is consistent with a photoconductive gain mechanism. The transparent photodiodes are heterojunctions of Nc/C_{60}. At zero bias, these diodes have ~100% internal quantum efficiency that increases in reverse bias due to photoconductive gain. The potential of these materials and devices for solar cells is discussed.

Modeling of Electronic Structure, Photoinduced Dynamics and Energy Transfer in Conjugated Molecules

S. Tretiak (T-1/CINT)

Prediction and understanding of photoinduced processes in molecular- and nano-materials is fundamental to a myriad of technological applications, ranging from sensing, imaging, solar energy harvesting, to future optoelectronic devices. This poster overviews several applications of quantum-chemical approaches aimed to model photoinduced dynamics of excitons and charges in a number of molecular materials over multiple length and time scales. In the amorphous clusters of conjugated polymers, we analyze the nature of electron and hole traps induced by conformational disorder and inter-molecular electronic interactions, which will affect carrier mobilities in the polymeric materials. To explore ultrafast dynamics and exciton transport in several conjugated molecular systems, our calculations use the CEO semiempirical package combined with the Tully's fewest switches algorithm for surface hopping probing non-adiabatic processes. Our analysis shows intricate details of photoinduced vibronic relaxation and identifies the conformational degrees of freedom leading to ultrafast dynamics and energy transfer. This theoretical modeling allows us to understand and to potentially manipulate energy transfer pathways in molecular materials suitable for solar energy conversion.

Tab 7

Emergent Phenomena–CINT Overview

D.E. Morris (MPA-CINT)

The Center for Integrated Nanotechnologies (CINT) is one of five U.S. DOE Nanoscale Science Research Centers (NSRC). As CINT is a national user facility, it is jointly operated by Los Alamos National Laboratory and Sandia National Laboratories. Among its many distinguishing characteristics is its affiliation with the host National Nuclear Security Administration (NNSA) labs and its focus on integration nanoscience. A brief overview of the structure and characteristics of CINT will be provided along with some performance statistics in relation to the other NSRCs. The science focus of CINT will be described with emphasis on ongoing work pertinent to the emergent phenomena theme and. more broadly, to the strong overlap between CINT science and the materials strategy at LANL. The relationship between CINT and the host labs is a key metric for our success, and the strong synergy that exists will be described in terms of mutual benefits and direct links to NNSA mission science.

Emergent Phenomena – CINT Overview

David E. Morris

Co-Director and Center Leader

Center for Integrated Nanotechnologies

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Overview

- **Introduction to the Center for Integrated Nanotechnologies**
  - Distinguishing Characteristics
  - Some Performance Statistics and Comparisons
- **Scientific Structure and Focus of CINT**
  - The CINT Thrusts
  - Mapping to the Materials Strategy
  - Examples of Emergent Phenomena from the Thrusts
  - CINT Signature Initiatives
- **The Role of CINT in the NNSA Mission**
  - CINT / LANL Relationship
  - Mission-specific Research
- **Summary of the Emergent Phenomena Session**

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CINT: Distinctive Among the Five DOE Nanoscale Science Research Centers

- **A joint venture between Los Alamos National Laboratory and Sandia National Laboratories**
  - Two Laboratory – Single Center Model
- **Only NSRC associated with NNSA – all others at Office of Science labs**

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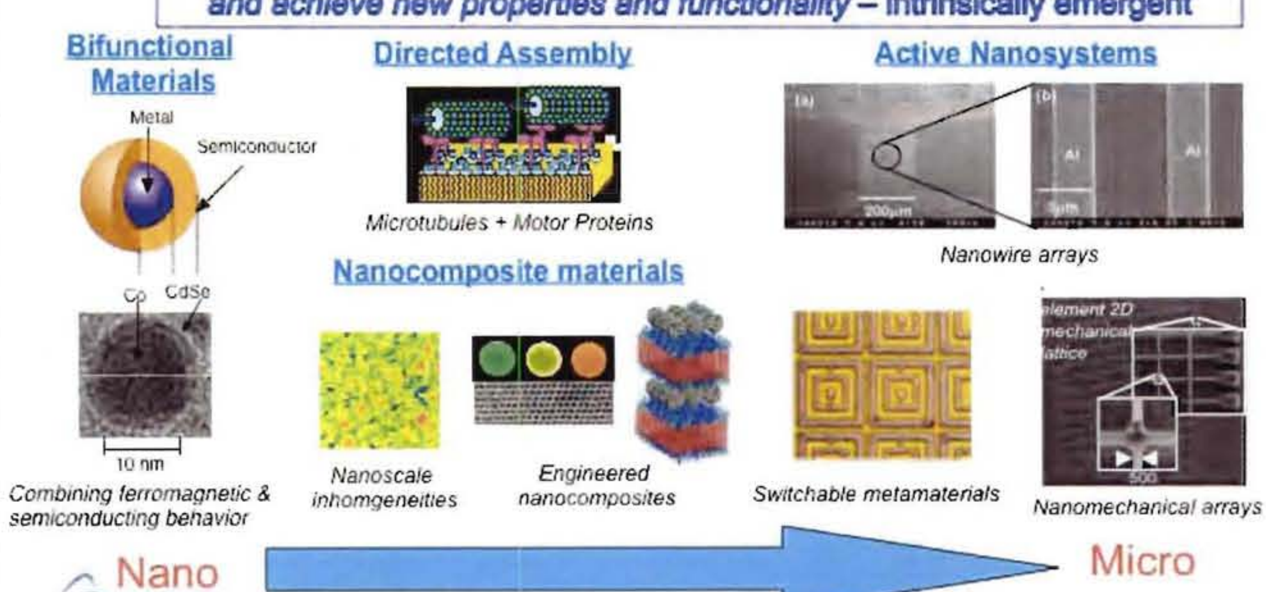
CINT Signature: Focus on Nanoscience Integration

Assembling diverse nanoscale materials across length scales to design and achieve new properties and functionality – intrinsically emergent



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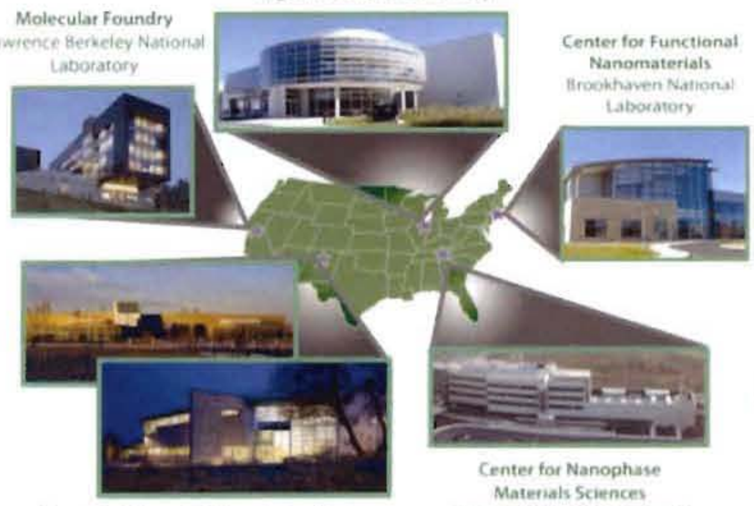
The Five DOE NSRCs and Co-located DOE User Facilities

Advanced Photon Source
Center for Nanoscale Materials
Argonne National Laboratory

Advanced Light Source
Molecular Foundry
Lawrence Berkeley National Laboratory

National Synchrotron Light Source
Center for Functional Nanomaterials
Brookhaven National Laboratory



LANSCE Lujan Center + NHMFL and MESA
Center for Integrated Nanotechnologies
Los Alamos National Laboratory & Sandia National Laboratory

Spallation Neutron Source
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

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CINT Technical Staffing (LANL & SNL)

- Scientists – 36 (all 0.5 FTE or higher *)
- Postdoctoral Researchers – 66 total
  - CINT supported – 17
  - Distinguished Fellowship – 12
  - Lab leveraged & CINT mentored – 37
- Graduate Students – 7
- Technologists – 14

Recent CINT Scientist Hires:
Quanxi Jia, Stephen Doorn, Nathan Mara

* *Other support from BES Core, LDRD, programmatic, etc*

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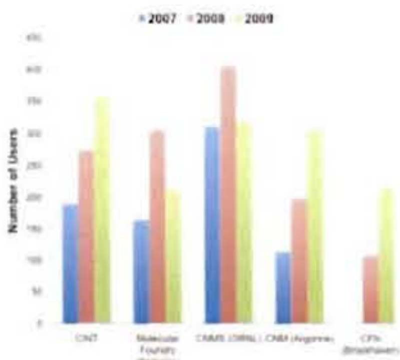
NSRC Comparison: Key Statistical Areas

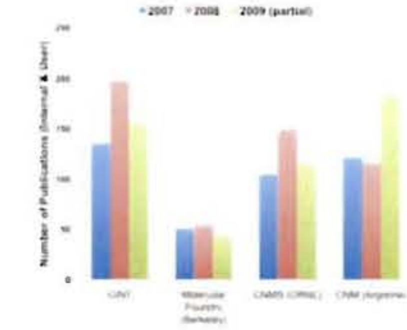
(individual NSRC web sites)

Users

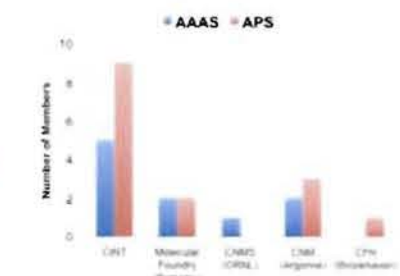


(http://www.sc.doe.gov/bes/users.htm)

Publications



Society Recognition



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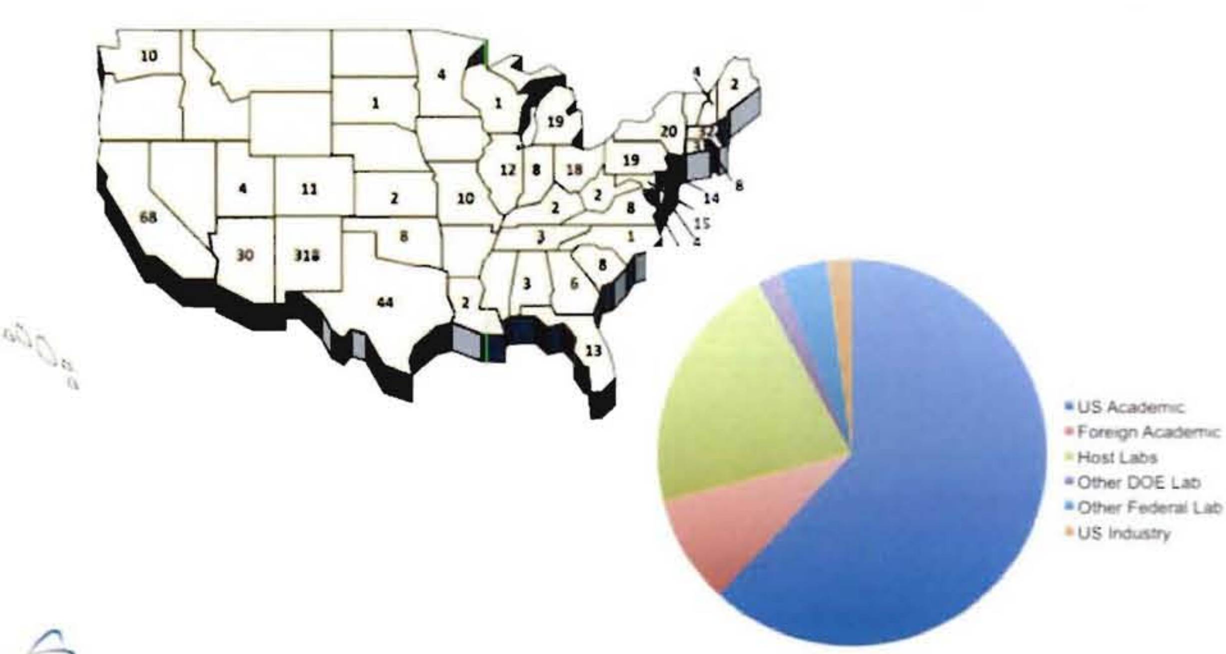
CINT: User Facility Demographics



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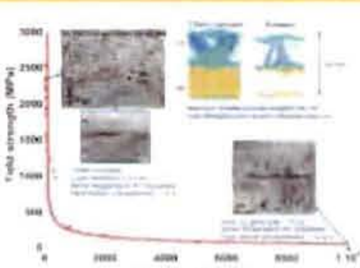
CINT: International Gateway to Nanoscience

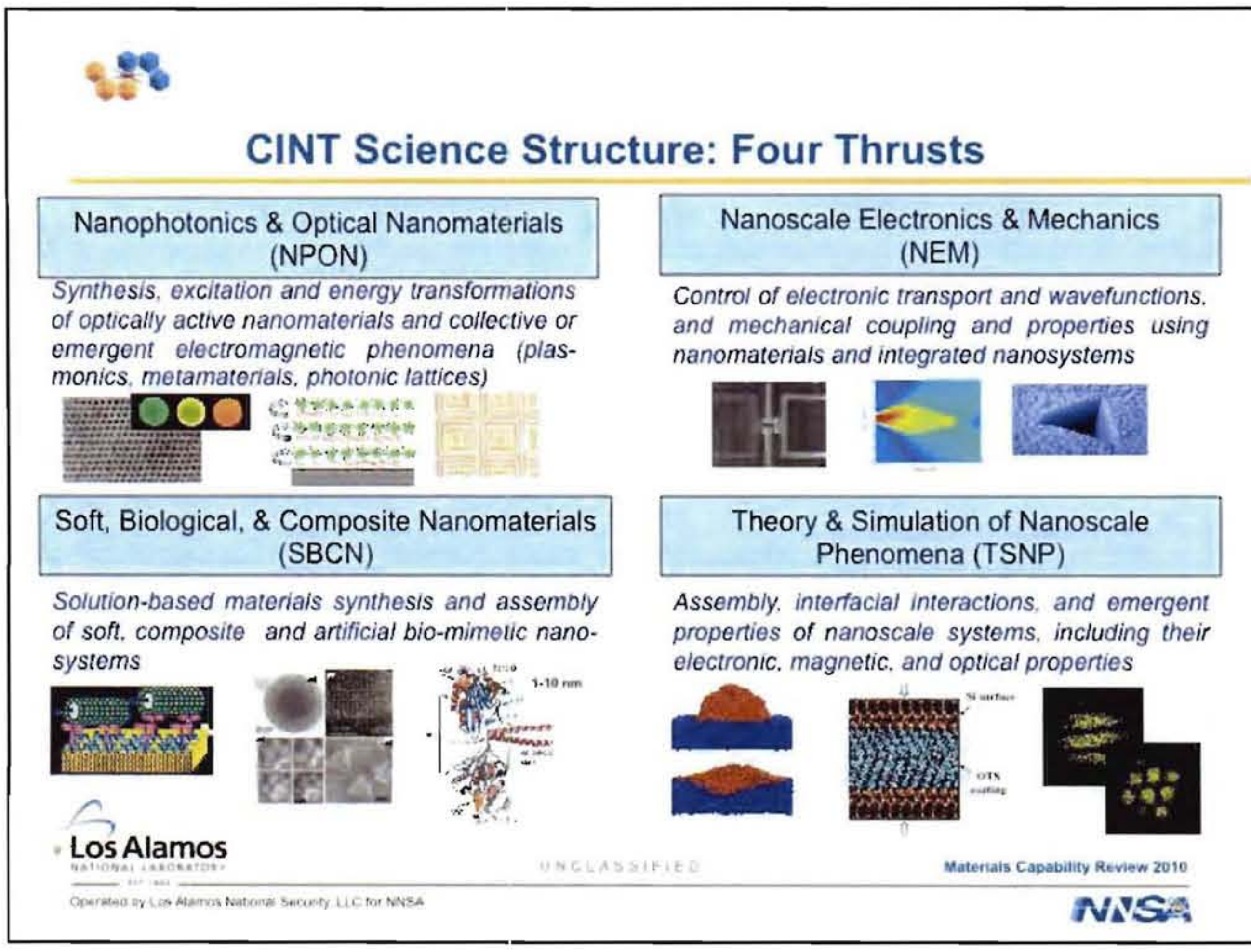
- *User Program and Postdoctoral / Student Staffing give CINT a true international flavor*
- *NNSA foreign national requirements are not a limiting factor*

CINT: A Key Role in the EFRC Initiative

- **CINT-led EFRCs**
  - Center for Materials at Irradiation and Mechanical Extremes (MIME)
    - PI: Mike Nastasi (w/ LLNL, UIUC, MIT)
  - Center for Advanced Solar Photophysics
    - PI: Victor Klimov (w/ NREL, Rice, UC...)



- **CINT Partnering Roles**
  - Science of Precision Multifunctional Nanostructures for Electrical Energy Storage
    - PI: Rubloff, U. Maryland (Hwang, Picraux)
  - EFRC for Solid State Lighting Science
    - PI: Simmons, Sandia (Prasankumar)
  - Photosynthetic Antenna Research Center
    - PI: Blankenship, Wash. Univ. (Montano)


CINT Science Structure: Four Thrusts
Nanophotonics & Optical Nanomaterials (NPON)
Synthesis, excitation and energy transformations of optically active nanomaterials and collective or emergent electromagnetic phenomena (plasmonics, metamaterials, photonic lattices)
Nanoscale Electronics & Mechanics (NEM)
Control of electronic transport and wavefunctions, and mechanical coupling and properties using nanomaterials and integrated nanosystems
Soft, Biological, & Composite Nanomaterials (SBCN)
Solution-based materials synthesis and assembly of soft, composite and artificial bio-mimetic nanosystems
Theory & Simulation of Nanoscale Phenomena (TSNP)
Assembly, interfacial interactions, and emergent properties of nanoscale systems, including their electronic, magnetic, and optical properties
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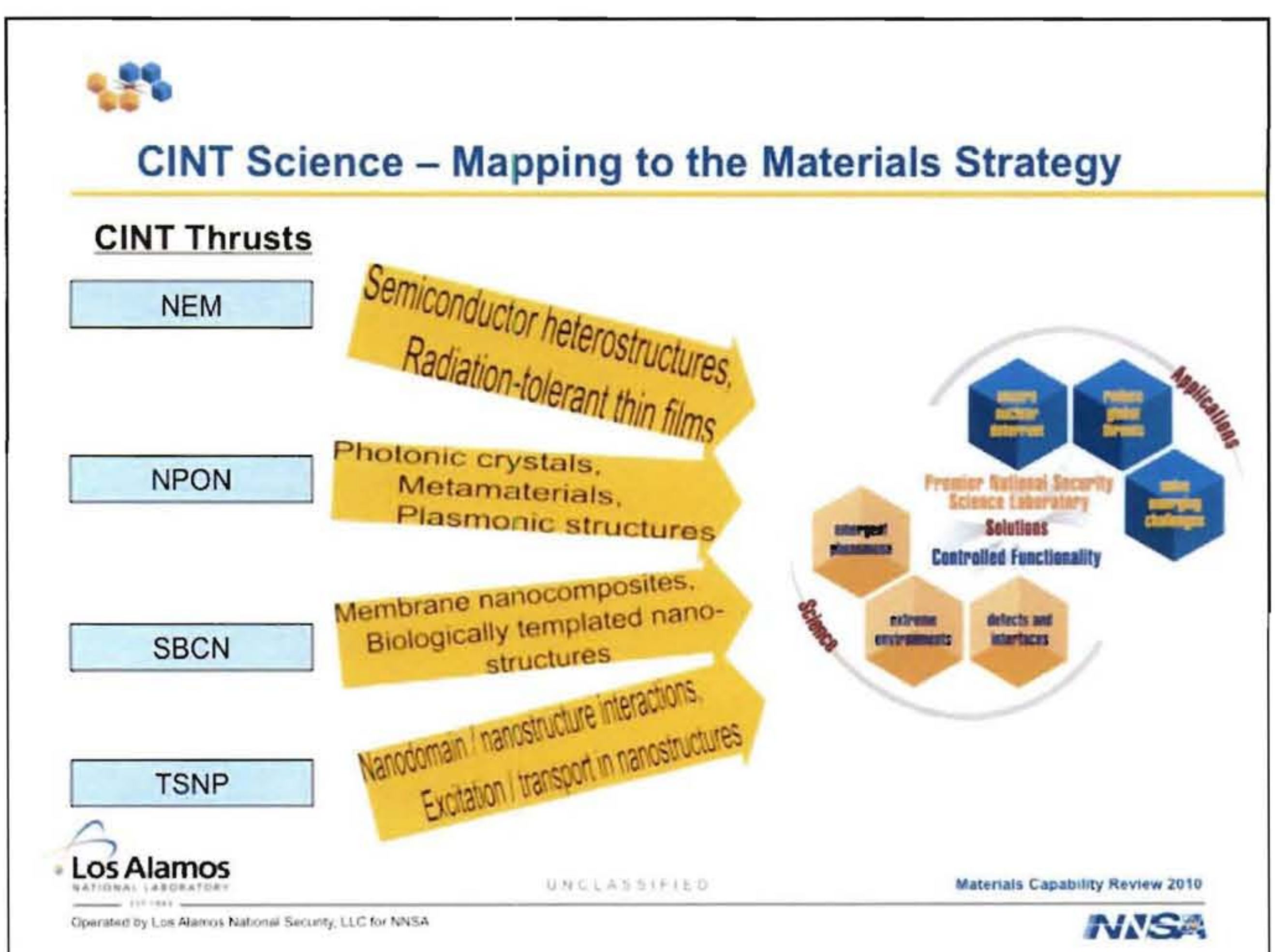
CINT Science – Mapping to the Materials Strategy
CINT Thrusts
NEM
Semiconductor heterostructures, Radiation-tolerant thin films
NPON
Photonic crystals, Metamaterials, Plasmonic structures
SBCN
Membrane nanocomposites, Biologically templated nanostructures
TSNP
Nanodomain / nanostructure interactions, Excitation / transport in nanostructures
Applications
Solutions
Controlled Functionality
Science
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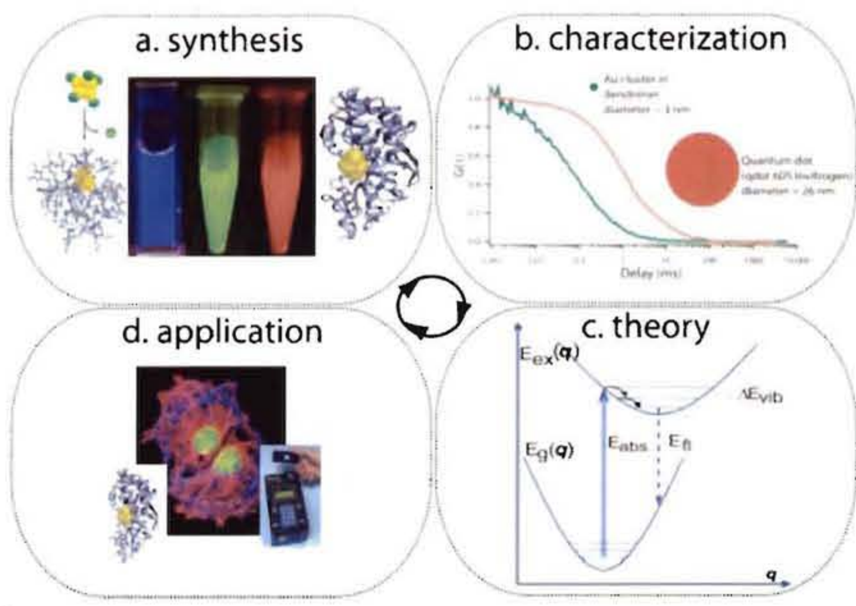
Emergent Phenomena – SBCN Thrust Example

Predictive Design of Noble Metal Nanoclusters – Jen Martinez, PI



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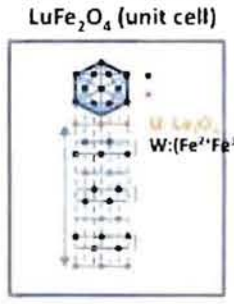
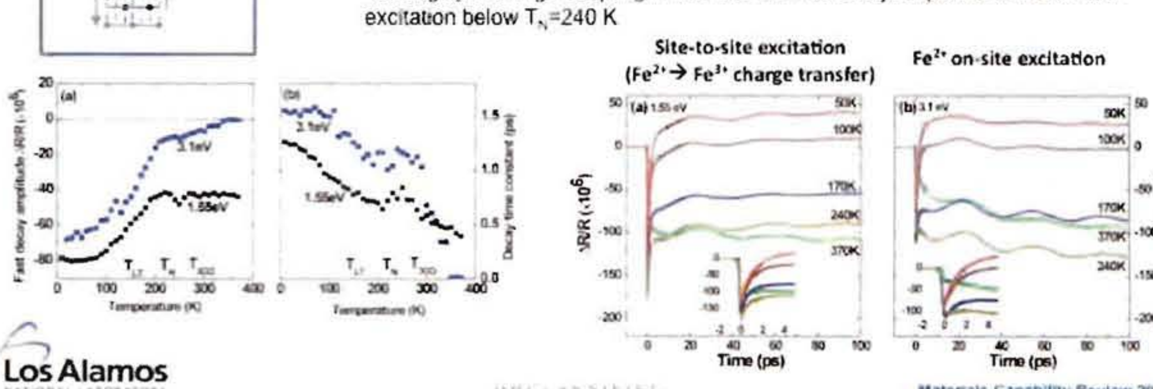
Emergent Phenomena – NPON Thrust Example

Ultrafast Polaron Dynamics in Multiferroic $LuFe_2O_4$ – R. Prasankumar, PI

Crystal structure of $LuFe_2O_4$ (unit cell)



- First ultrafast optical experiments on this intensely studied multiferroic system reveal influence of charge and spin order on polaron dynamics
- $LuFe_2O_4$ is a frustrated multiferroic material with strong magnetoelectric coupling, even at room temperature
- ~100 fs difference in the initial decrease in ΔR/R between site-to-site and on-site excitation
- Frustrated triangular lattice leads to longer polaron redressing time (~1 ps compared to 500 fs in cubic systems)
- Strong spin-charge coupling influences the fast decay amplitude of the on-site excitation below T_N=240 K



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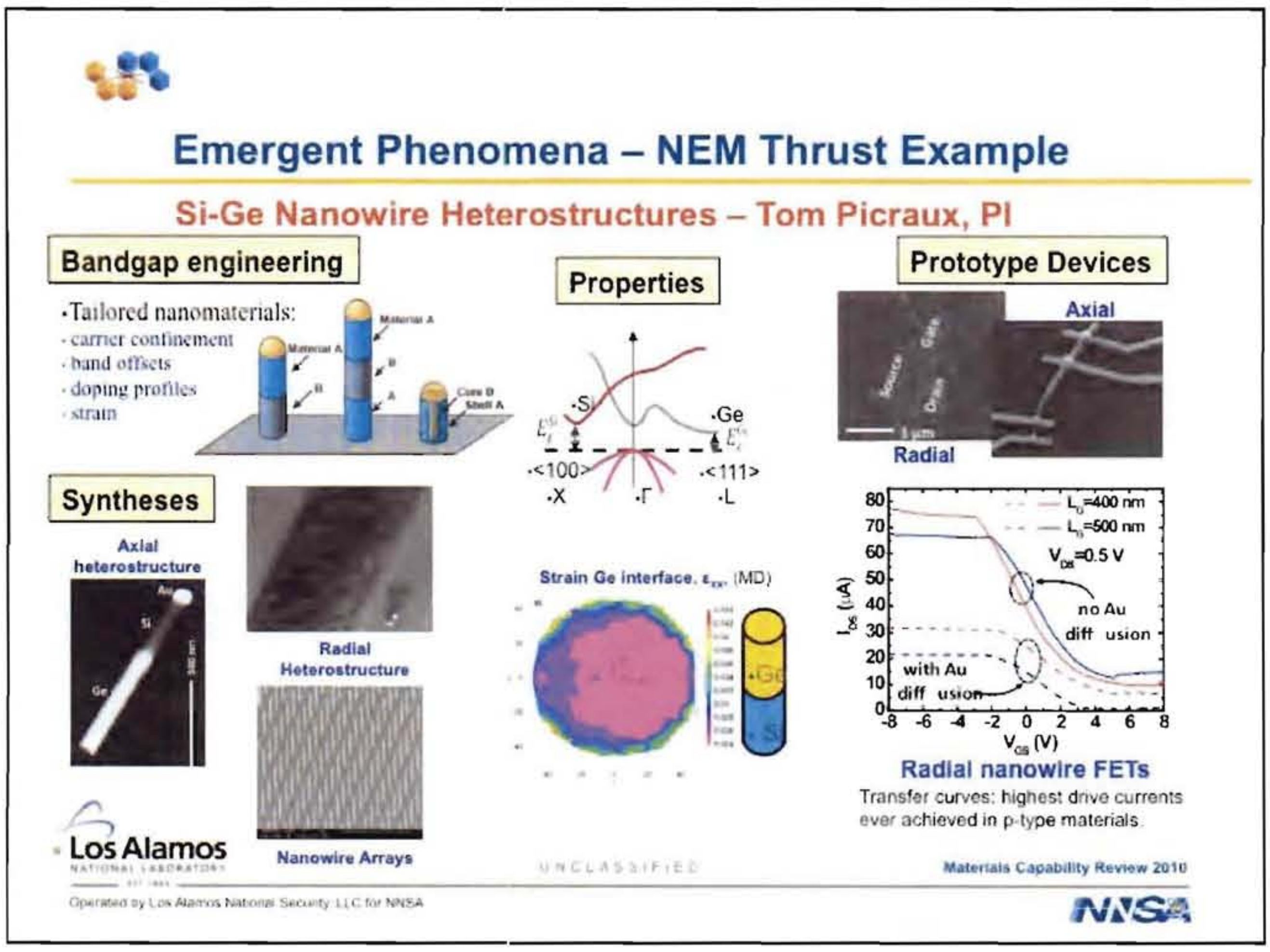
Emergent Phenomena – NEM Thrust Example
Si-Ge Nanowire Heterostructures – Tom Picraux, PI
Bandgap engineering
•Tailored nanomaterials:
· carrier confinement
· band offsets
· doping profiles
· strain
Properties
•Si
•Ge
•<100>
•<111>
•X
•Γ
•L
Prototype Devices
Axial
Radial
Syntheses
Axial heterostructure
Radial Heterostructure
Nanowire Arrays
Strain Ge interface
L=400 nm
L=500 nm
no Au diff usion
with Au diff usion
Radial nanowire FETs
Transfer curves: highest drive currents ever achieved in p-type materials.
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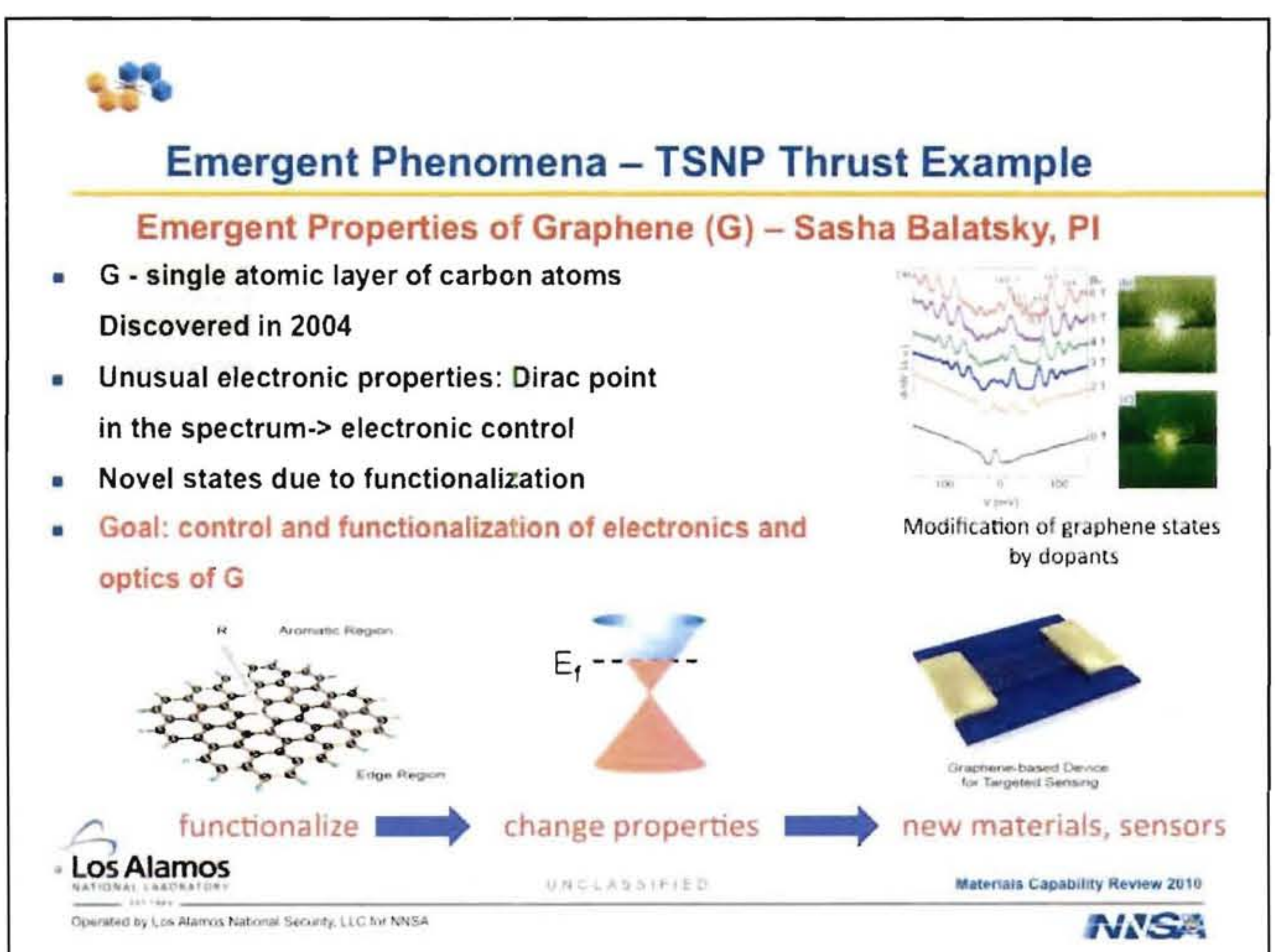
Emergent Phenomena – TSNP Thrust Example
Emergent Properties of Graphene (G) – Sasha Balatsky, PI
G - single atomic layer of carbon atoms
Discovered in 2004
Unusual electronic properties: Dirac point
in the spectrum-> electronic control
Novel states due to functionalization
Goal: control and functionalization of electronics and
optics of G
Modification of graphene states
by dopants
Aromatic Region
Edge Region
E_f
Graphene-based Device for Targeted Sensing
functionalize
change properties
new materials, sensors
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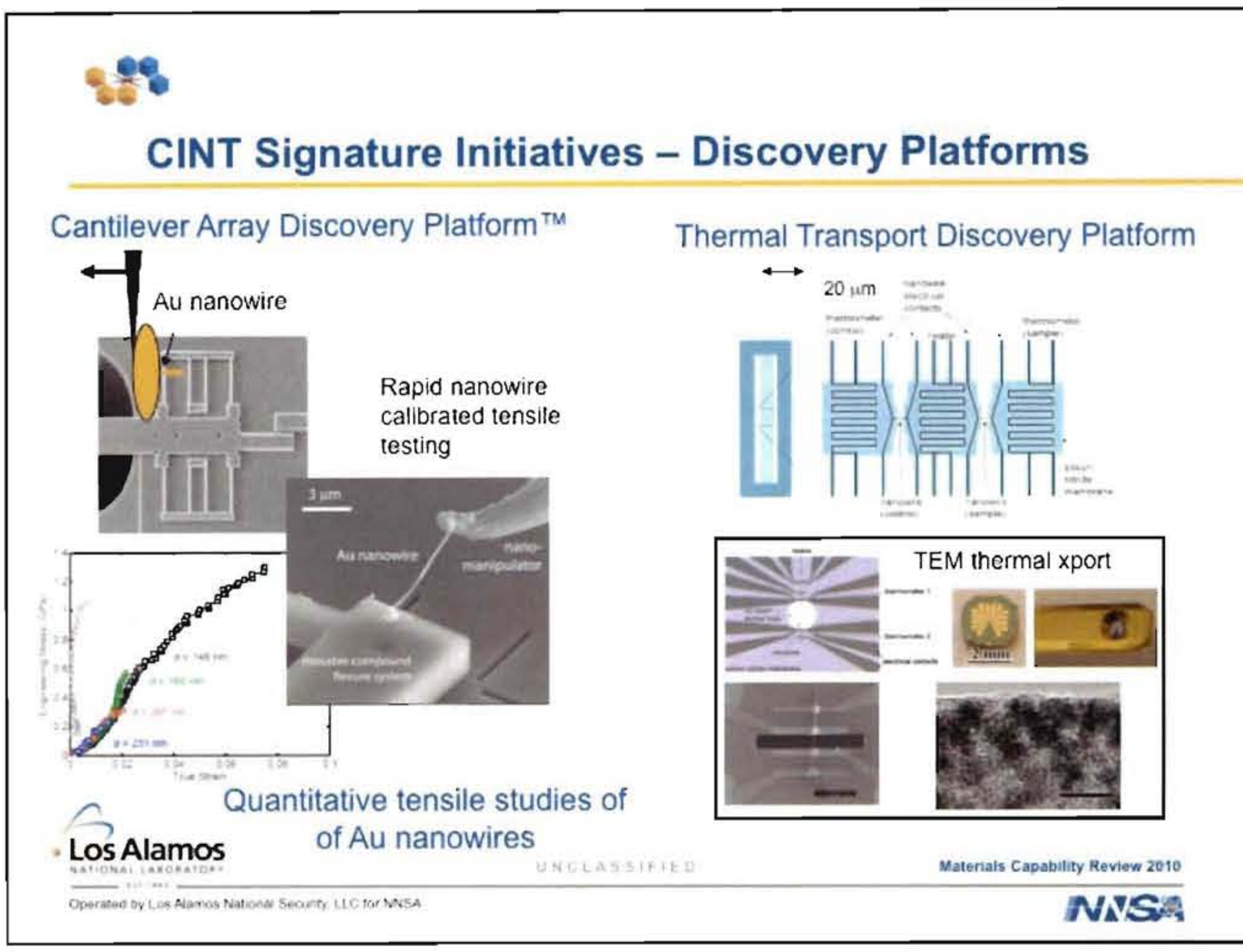
CINT Signature Initiatives – Discovery Platforms
Cantilever Array Discovery Platform™
Au nanowire
Rapid nanowire calibrated tensile testing
3 µm
Au nanowire
nano-manipulator
Quantitative tensile studies of of Au nanowires
Thermal Transport Discovery Platform
20 µm
TEM thermal xport
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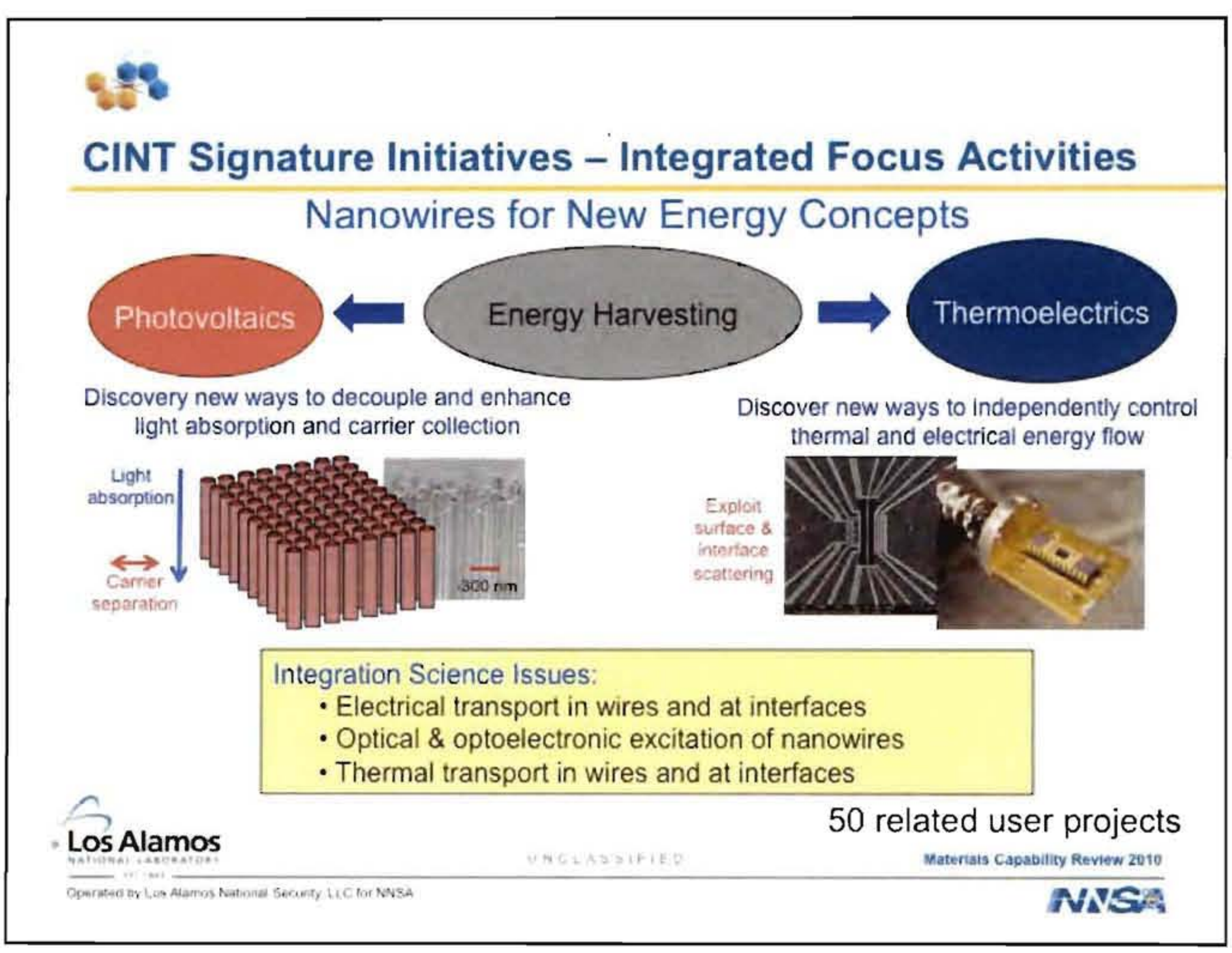
CINT Signature Initiatives – Integrated Focus Activities
Nanowires for New Energy Concepts
Photovoltaics
Energy Harvesting
Thermoelectrics
Discovery new ways to decouple and enhance light absorption and carrier collection
Discover new ways to independently control thermal and electrical energy flow
Light absorption
Carrier separation
300 nm
Exploit surface & interface scattering
Integration Science Issues:
• Electrical transport in wires and at interfaces
• Optical & optoelectronic excitation of nanowires
• Thermal transport in wires and at interfaces
50 related user projects
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The Symbiotic CINT / LANL Relationship

- Value of CINT to LANL
  - Outstanding people, expertise, capabilities
  - LANL access to CINT facilities and expertise
  - Enabling new programs (BES, Energy, TR)
  - Partnership with Sandia
  - Strong connections to LANL Materials Strategy and MaRIE
- Value of LANL to CINT
  - Access to LANL capabilities and facilities including Lujan and NHMFL
  - Connections to LANL Institutes and Centers for outreach and science enhancement
  - Competitive engagement in LDRD process
  - Programmatic opportunities to extend CINT science

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CINT: A Valued Enabler of Mission Relevant Research

Examples of Recent CINT User Projects led by LANL PIs

- **Nuclear Deterrence**
  - Quantum control of initiation in nanoenergetics [Dave Moore DE-9]
  - Nanoscale plasticity within energetic single crystals [Kyle Ramos, DE-9]
  - Physical and optical characterization of thin-films for laser-driven shock compression experiments [Dan Eakins, DE-9]
  - Mechanical properties of nanocrystalline substructures in regions of shear localization [Ellen Cerreta, MST-8]
  - Nanomechanics of irradiated materials [Peter Hosemann, MST-8]
- **Global Threat Reduction**
  - A versatile protein-based nanobio sensor [Dung Vu, C-PCS]
  - Agile plasmon filters [Amy Ross, MST-16]
  - Visualization applied to molecular scintillator design [Rich Martin, T-1]
  - Morphology and composition of gamma-ray glass scintillators [Markus Hehlen, C-CDE]

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Emergent Phenomena

- **Oral Presentations**
  - Novel Functional Semiconductor Nanocrystal Quantum Dots and Nanowires for Applications Involving Energy Conversion – Jennifer Hollingsworth, C-PCS
  - Nanoscale Features in Graphene – Sasha Balatsky, T-4
- **Poster Presentations**
  - Supported Lipid Membranes on Nanoporous Metals – Andrew Dattelbaum, MPA-CINT
  - Gold and Silver Nanoclusters for Detection of Biological Materials -- Tim Yeh, MPA-CINT
  - Multiplex Detection of Pathogen-Biomarkers using Biosensor – Harshini Mukundan, C-PCS
  - Acoustically Engineered Materials using Acoustic Radiation Force – Dipen Sinha, MPA-11
  - Raman Spectroscopy of Chirality-Enriched Carbon Nanotubes – Steve Doorn, MPA-CINT
  - Epitaxial Nanotwinned Cu – Nan Li, MPA-CINT
  - Optical Switching with a Negative Index Metamaterial – Keshav Dani, MPA-CINT
  - Optical Spectroscopy of Individual "Giant" Quantum Dots – Han Htoon, C-PCS
  - Probing Properties and Dynamic Response at Nanoscale – Dzmitry Yarotski, MPA-CINT
  - Subwavelength Photonic, Plasmonic and Hybrid Waveguiding – Anatoly Efimov, MPA-CINT
  - A MaRIE first experiment: Nanostructured ferritic alloys – Nathan Mara, MPA-CINT
- **Gateway Tour**

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Novel Functional Semiconductor Nanocrystal Quantum Dots and Nanowires for Applications Involving Energy Conversion

J.A. Hollingsworth, H. Htoon (C-PCS/MPA-CINT)

To advance the state-of-the-art in the use of nanoparticles as functional building blocks for next-generation optoelectronic and photovoltaic devices, both new types of active nanomaterials and new synthesis/assembly approaches are needed. Here, we describe our efforts to address the former by (1) achieving an exciting leap forward in the field of semiconductor nanocrystal quantum dots (NQDs) and (2) developing new approaches for the fabrication and ordering of anisotropic semiconductor nanomaterials, known as quantum- or nanowires (NWs).

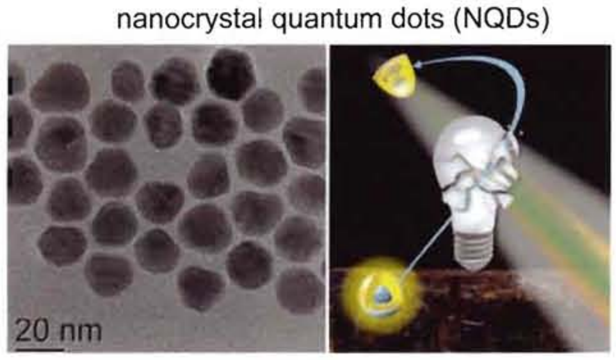
Specifically, we describe a functionally new class of NQD, the so-called "giant" NQD (g-NQD), which due to its unique physical and electronic nanoscale architecture, exhibits new and useful photophysics for light-emission applications. Similar to epitaxial QDs, our solution-grown g-NQDs possess a very thick, defect-free inorganic shell, and they are characterized by an altered NQD electronic structure. Together, these factors result in NQDs that do not photobleach, are insensitive to changes in surface chemistry and show markedly suppressed blinking (Chen, et al. *J. Am. Chem. Soc.* 2008), as well as suppressed nonradiative Auger recombination (Garcia-Santamaria et al. *Nano Lett.* 2009). Significantly, g-NQDs afford new exciton→photon conversion pathways for enhanced efficiencies and stabilities.

Secondly, we are addressing the opposite technological need – nanoparticles that convert light into electric energy. Here, we describe the first solution-phase synthesis of high-quality $CuInSe_2$ NWs (Wooten et al. *J. Am. Chem. Soc.* 2009). This has implications for photovoltaics, as NWs in general are considered important alternatives to isotropic nanocrystals as "building blocks" for light-harvesting devices, with key candidates including the structurally complex $CuInSe_2$. Furthermore, we advance the state-of-the-art in NW growth by establishing alternative solution-phase processing approaches that potentially provide unprecedented control over NW internal structure and ordering.

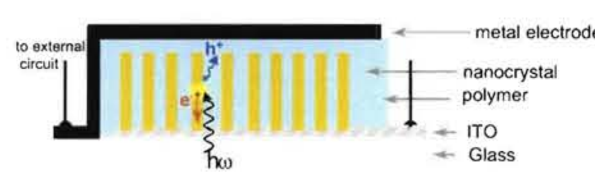
Novel Functional Semiconductor Nanocrystal Quantum Dots and Nanowires for Applications Involving Energy Conversion

J. A. Hollingsworth (C-PCS/MPA-CINT) and H. Htoon (C-PCS/MPA-CINT)

- **Exciting leap forward**
  - "Giant" thick-shell nanocrystal quantum dots (NQDs)



- **New synthesis capabilities**
  - Compositionally complex nanowires
  - "Flow" Solution-Liquid-Solid growth



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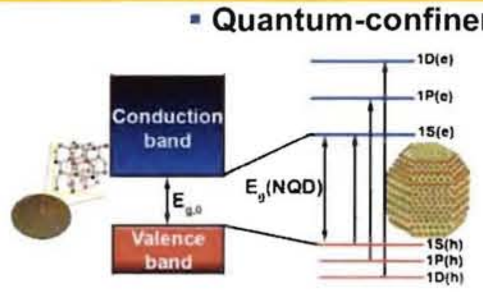
Nanocrystal Quantum Dots (NQDs): "Near-ideal" light emitters

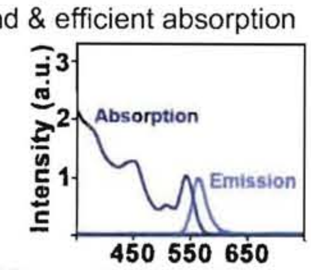
- **Quantum-confinement effects**



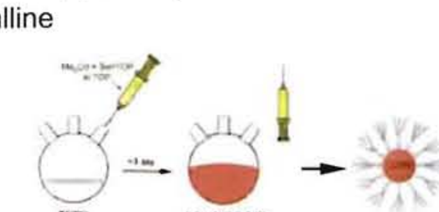
"Quantum box" model:

$$E_g(NQD) = E_{g,0} + \frac{\hbar^2\pi^2}{2m_{eh}R^2}$$

- Tunable bandgap
- Narrow & bright emission
- Broadband & efficient absorption



Chemically processible: "Low-tech" ⇒ "High-tech"
- Low polydispersity (+/- 4%)
- Single-crystalline



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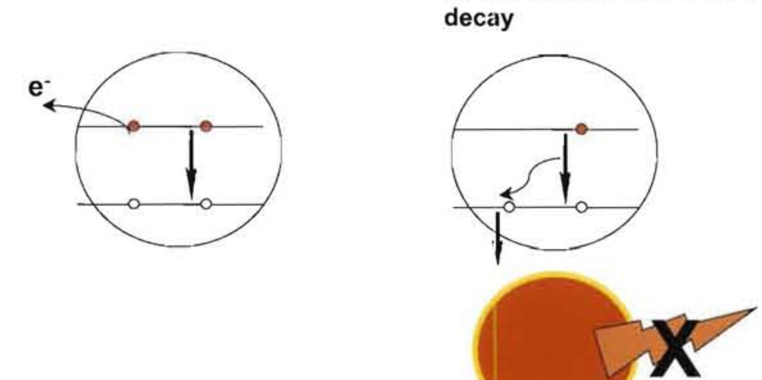
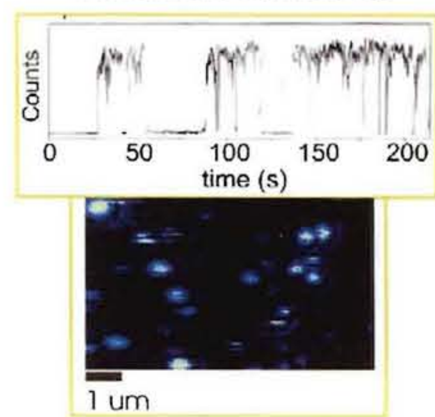
The darker side of NQDs: "Blinking" behavior and nonradiative Auger recombination

- **Quantum dot fluorescence intermittency**

(I) Continuous illumination or chemical red-ox stress leads to charged NQD → **(II) Photo-excited electron-hole recombination in charged NQDs dominated by efficient Auger non-radiative decay** → **(III) Random cycle of charging/ discharging events leads to blinking or fluorescence intermittency**



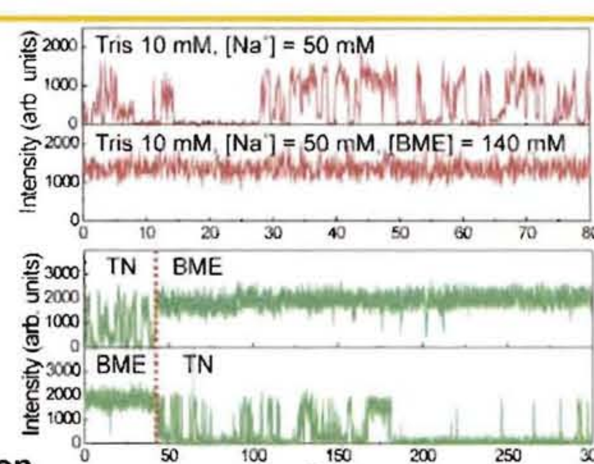


> Nirmal, Dabbousi, Bawendi, Macklin, Trautman, Harris & Brus *Nature* 1996, *383*, 802-804
> Efros *Nature Mater.* 2008, *7*, 612-613

Attempts to address the NQD blinking problem: 'Antiblinking reagents'

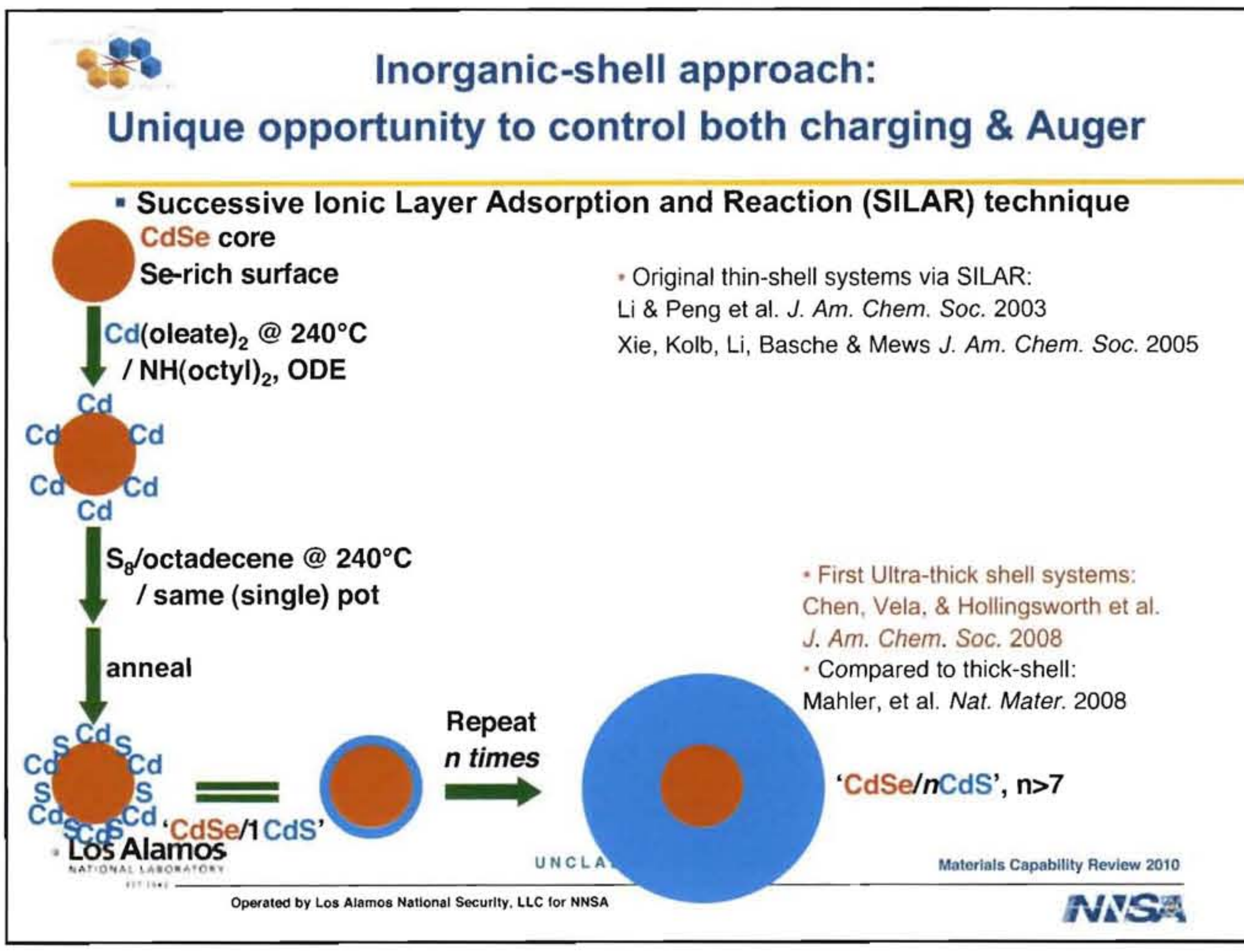
- **Charge mediators / compensators**
  - Short-chain thiols
  - Organic conjugated ligands
  - Propyl gallate ("antioxidant")

Hohng & Ha *J. Am. Chem. Soc.* 2004, *126*, 1324-1325
Hammer et al. *J. Phys. Chem. B* 2006, *110*, 14167-71
Fomenko & Nesbitt *Nano Lett.* 2008, *8*, 287-293



- **Organic approach: An incomplete solution**
  - Inherently short-term
  - Strongly concentration sensitive
  - pH dependent
  - Time / light conditions dependent
  - Incompatible **with applications**

Jeong & Hollingsworth et al. *J. Am. Chem. Soc.* 2005, *127*, 10126-10127


Inorganic-shell approach:
Unique opportunity to control both charging & Auger
▪ Successive Ionic Layer Adsorption and Reaction (SILAR) technique
CdSe core
Se-rich surface
Cd(oleate)$_2$ @ 240°C
/ NH(octyl)$_2$, ODE
S_8/octadecene @ 240°C
/ same (single) pot
anneal
Repeat
n times
'CdSe/1 CdS'
'CdSe/nCdS', n>7
▪ Original thin-shell systems via SILAR:
Li & Peng et al. J. Am. Chem. Soc. 2003
Xie, Kolb, Li, Basche & Mews J. Am. Chem. Soc. 2005
▪ First Ultra-thick shell systems:
Chen, Vela, & Hollingsworth et al.
J. Am. Chem. Soc. 2008
▪ Compared to thick-shell:
Mahler, et al. Nat. Mater. 2008
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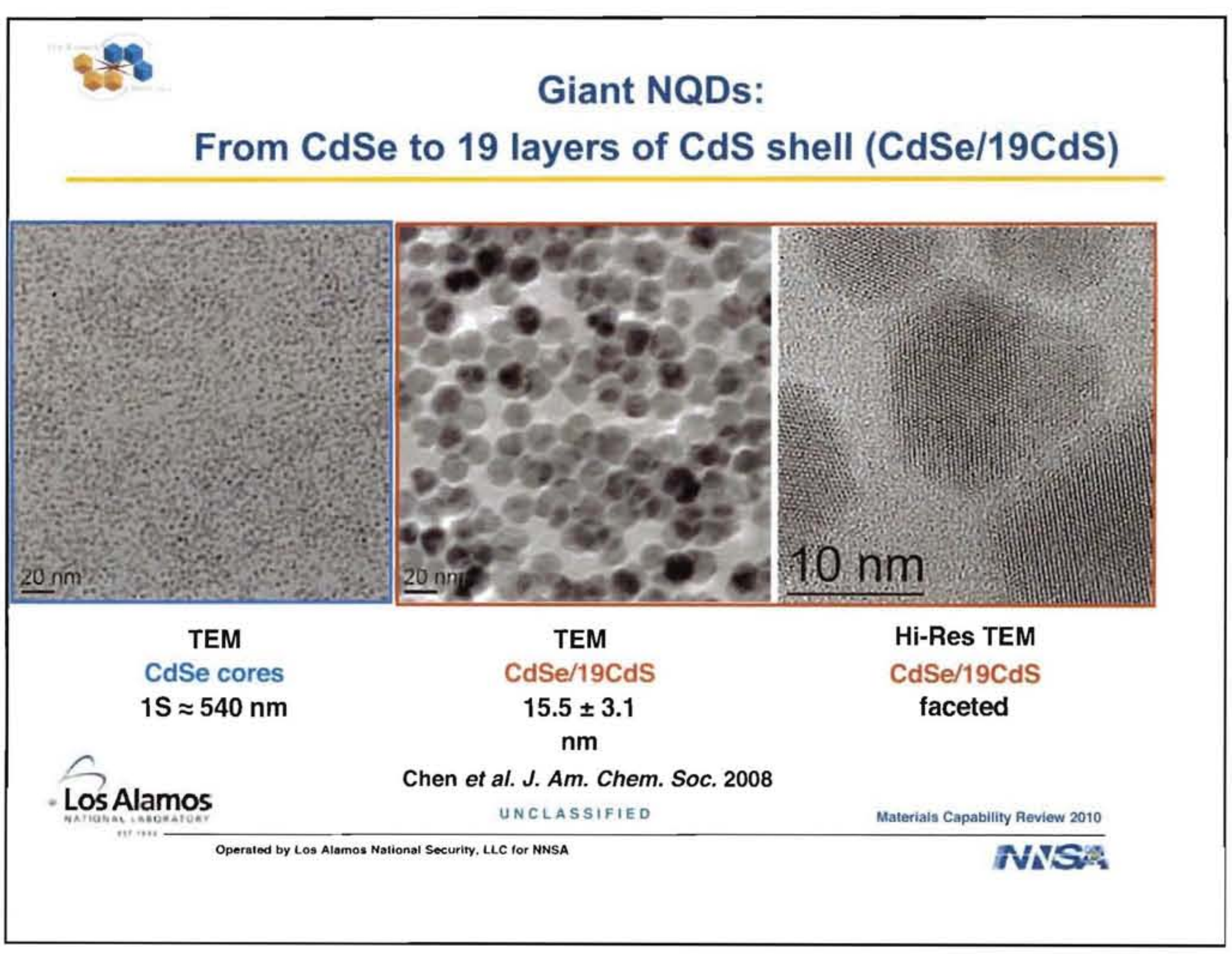
Giant NQDs:
From CdSe to 19 layers of CdS shell (CdSe/19CdS)
20 nm
20 nm
10 nm
TEM
CdSe cores
1S ≈ 540 nm
TEM
CdSe/19CdS
15.5 ± 3.1
nm
Hi-Res TEM
CdSe/19CdS
faceted
Chen et al. J. Am. Chem. Soc. 2008
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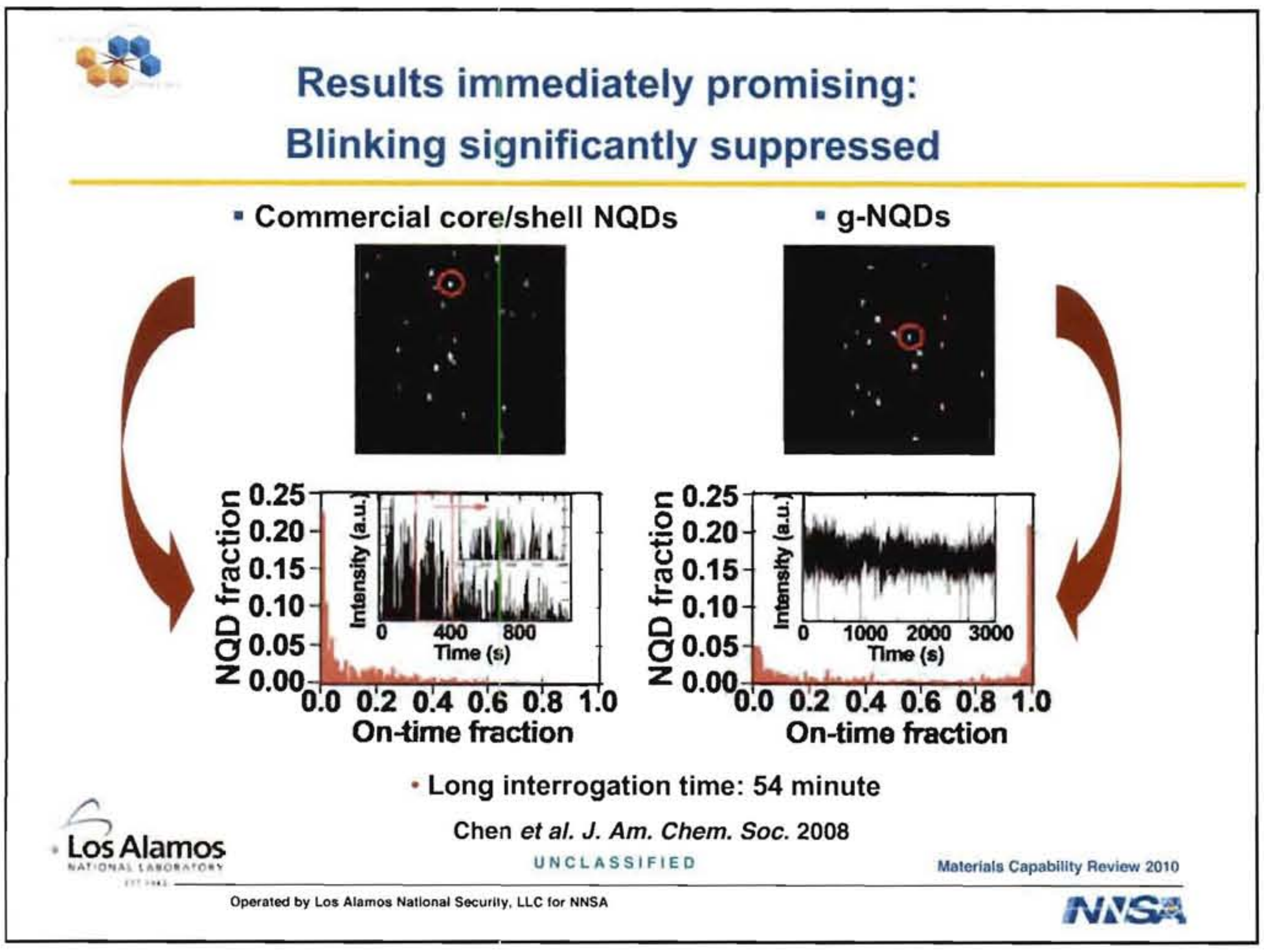
Results immediately promising:
Blinking significantly suppressed
Commercial core/shell NQDs
g-NQDs
NQD fraction
Intensity (a.u.)
Time (s)
On-time fraction
Long interrogation time: 54 minute
Chen et al. J. Am. Chem. Soc. 2008
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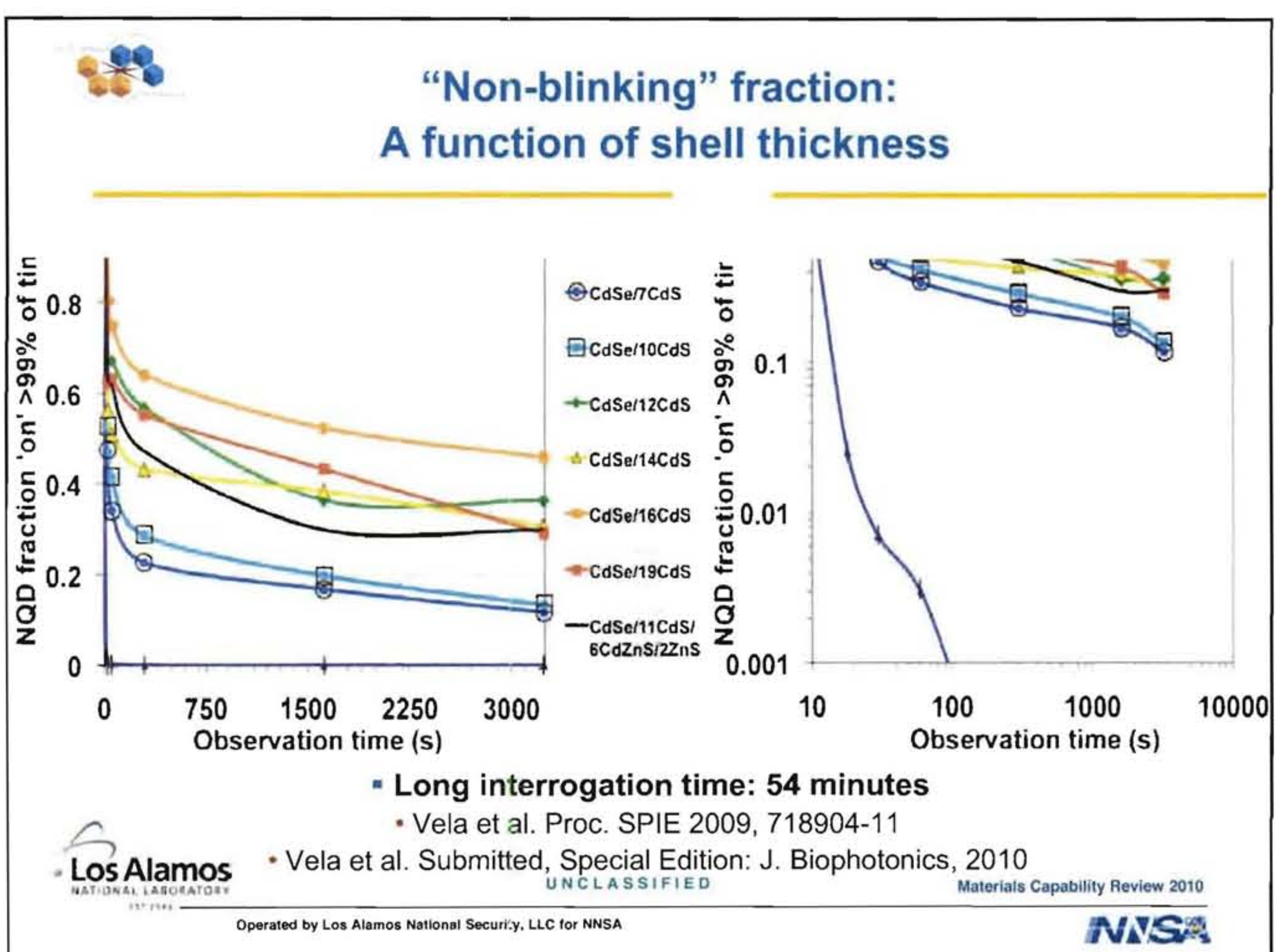
"Non-blinking" fraction:
A function of shell thickness
NQD fraction 'on' >99% of tin
CdSe/7CdS
CdSe/10CdS
CdSe/12CdS
CdSe/14CdS
CdSe/16CdS
CdSe/19CdS
CdSe/11CdS/6CdZnS/2ZnS
Observation time (s)
Long interrogation time: 54 minutes
Vela et al. Proc. SPIE 2009, 718904-11
Vela et al. Submitted, Special Edition: J. Biophotonics, 2010
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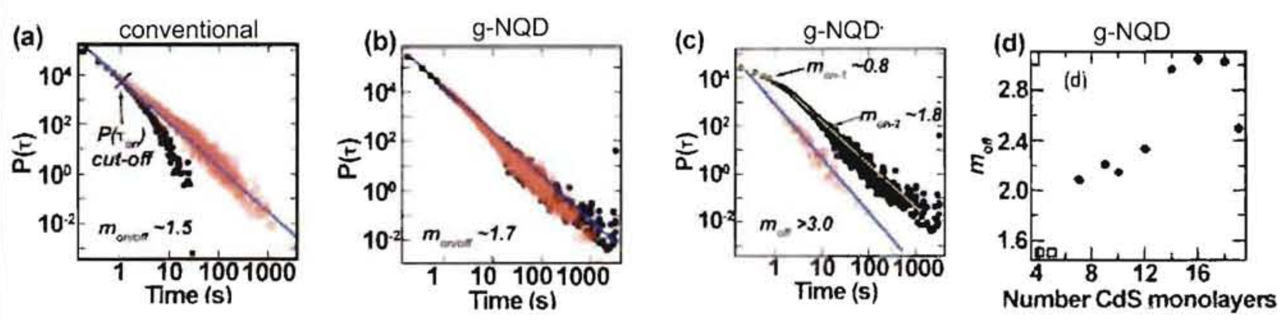
New statistical relationships in the probability densities of on- and off-time distributions

- **Giant NQDs deviate from power-law behavior: $P(\tau_{ON/OFF}) \propto (\tau_{ON/OFF})^{-m}$**



- **Conventional NQDs**
  - $m_{OFF} < m_{ON}$
    - Slow decay of τ_{OFF} distributions for infinite time average
  - On-times "cut-off"

- **Non-blinking Giant NQDs**
  - $m_{OFF} > m_{ON}$
    - τ_{OFF} converges to finite value
    - Different blinking mechanism
  - No on-time "cut-off"
  - m_{off} a facile predictor of shell-thickness-dependent blinking suppression

Poster: Dr. Han Htoon

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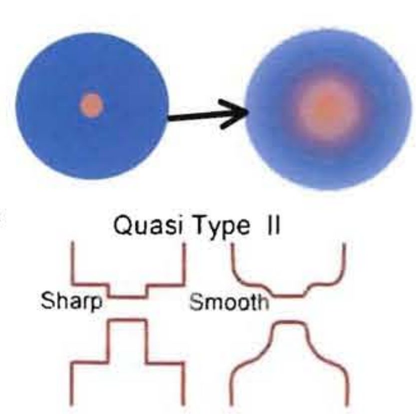
How is blinking suppressed?: A combination of suppressed charging and Auger recombination

- **Auger recombination is suppressed by:**
  - Decreasing exciton-exciton coupling
  - Separating electrons from holes
  - Smoothing the interfacial confinement potential

- **All modes active in giant NQDs:**
  - Volume effect
  - A Type-II or Quasi-Type-II electronic structure
  - Smooth interfacial confinement potential



- García-Santamaria et al. *Nano Lett.* 2009
- Htoon, Hollingsworth, & Klimov et al. *Phys. Rev. Lett.* 2003
- Supporting theory: Efros, A. L., in *Semiconductor Nanocrystals, 2003*

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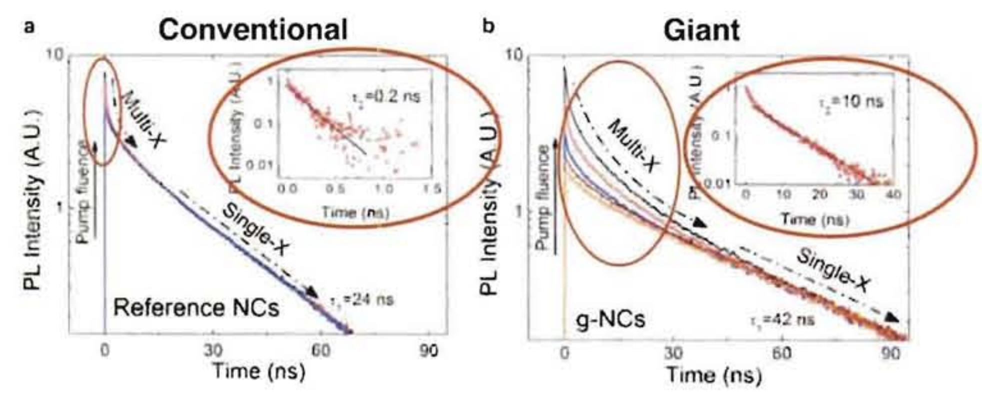
Direct evidence for suppressed Auger recombination: 50-fold increase in "biexciton" lifetime

- **Pump-intensity-dependent time-resolved photoluminescence**
  - Conventional – Multiexcitonic component is sub-ns due to Auger decay
  - Giant – Multiexcitonic component extends to 30 ns

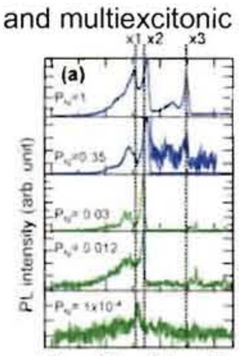


- **Insets: *50-fold increase* g-NQD derived biexciton lifetime**

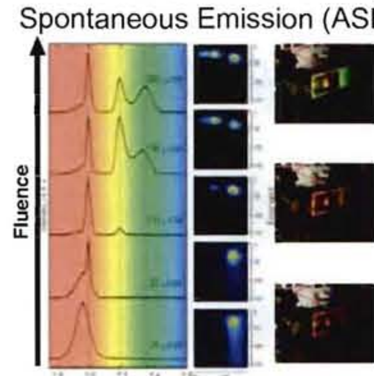
– Garcia-Santamaria et al. Nano Lett., 2009

Beyond suppressed blinking: Transformational new physics from novel chemistry

- **New pathways for electron→photon conversion**
  - Efficient emission from charged and multiexcitonic states
  - Low-threshold, multi-color Amplified Spontaneous Emission (ASE)



– Htoon et al., submitted 2010

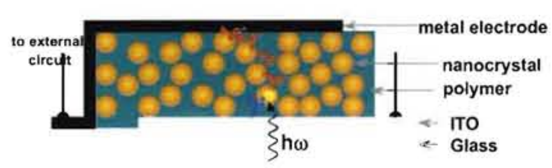


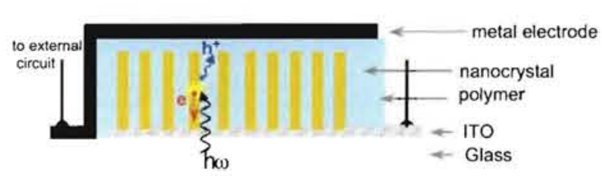
– Garcia-Santamaria et al., Nano Lett. 2009

- **g-NQD summary**
  - Our work: First inorganic-shell approach to blinking suppression
  - Mechanism: likely suppressed charging *and* Auger recombination
  - Our ultra-thick-shell g-NQDs (>12CdS shell monolayers) afford strongly suppressed Auger recombination and uniquely efficient radiative multiexciton recombination

Semiconductor nanowires for energy harvesting

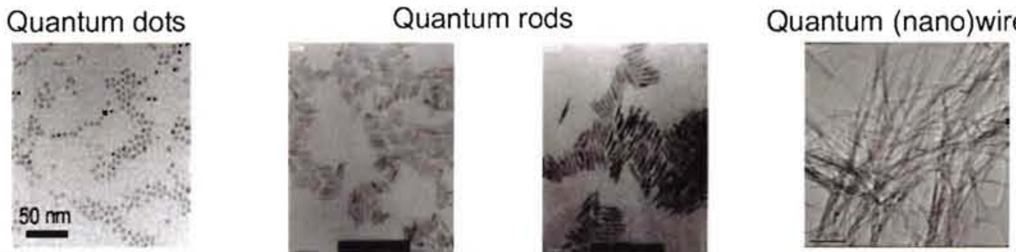
- "Random" NQD assemblies: Significant transport losses
- Quantum wire structures: Transport is greatly improved





- Solution synthesis provides facile control over the transition from 0D to 1D

Quantum dots | Quantum rods | Quantum (nano)wires



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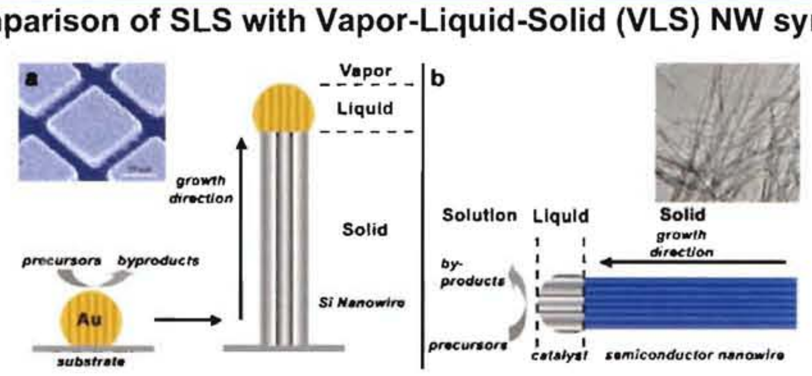
Our approach to nanowire synthesis: Solution-Liquid-Solid (SLS) growth

- Comparison of SLS with Vapor-Liquid-Solid (VLS) NW synthesis



- SLS differs from VLS:
  - Lower reaction temperatures
  - Solution-phase synthesis / processing
  - Fast growth rates in single-"pot" reaction,
  - "Free-standing" nanowires

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SLS provides facile access to range of materials systems ideally suited for solar energy conversion

- **e.g., PbSe NWs**

- Motivation:
  - Known near-infrared semiconductor
  - NQD photovoltaic comparisons available

- **e.g., CuIn(Ga)Se(S)$_2$ NWs**
- Motivation for CIGS:
  - "CIGS" solar cells hold world record in thin-film solar cell efficiency – 19.9% (2008)
  - Tunable bandgap: 730 - 1000 nm; high absorption coefficient; solar tolerant
- Motivation for CIGS *NWs*:
  - Test subjects for assessing if hole energy barrier at grain boundaries prevents electron-hole recombination
  - Vertically heterostructured NWs to make distributed p-n junctions

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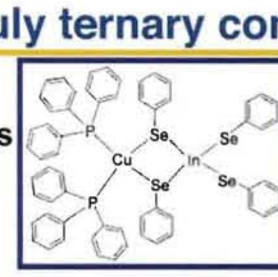
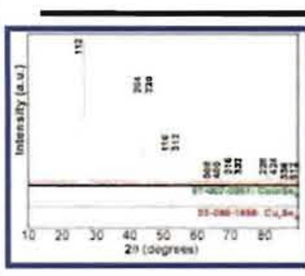
CuInSe$_2$ nanowires: Our work provided first demonstration of SLS synthesis of a truly ternary compound

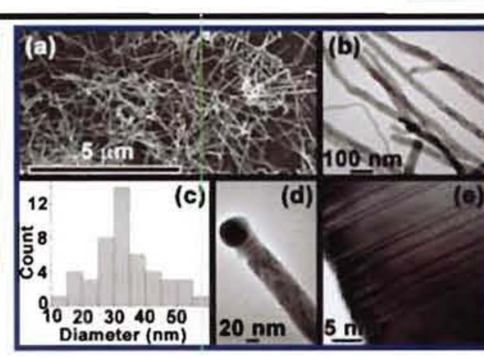
- **Single-source precursor: key to our success**
- **"Pre-assembled" Cu-Se-In bonds**

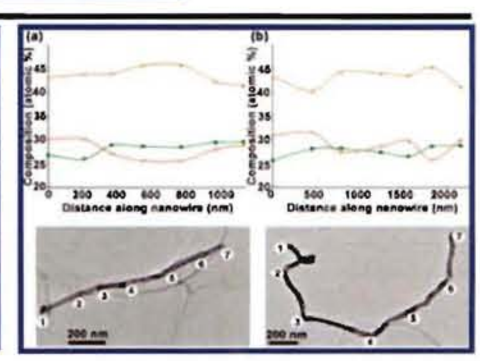


– Wooten et al. J. Am. Chem. Soc. 2009



- ~Phase-pure XRD





- Nearly stoichiometric CuInSe$_2$: $Cu_{1.1}In_{1.1}Se_{2.0}$
- Minimal between-NW variability
- Consistent incorporation of the 3 elements

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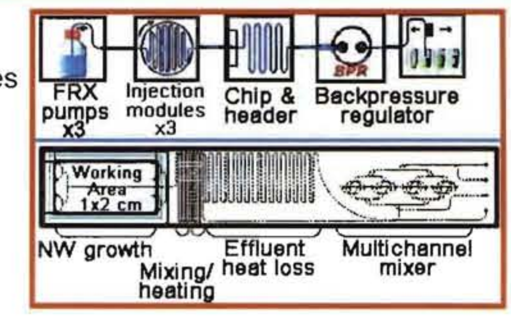
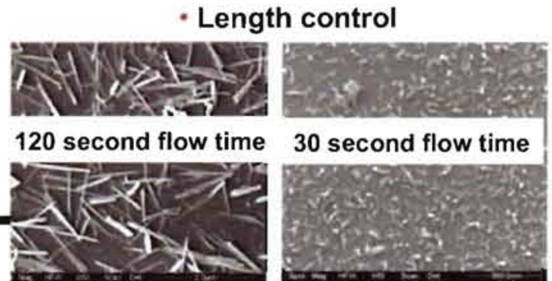
New capability development: "Flow" Solution-Liquid-Solid growth

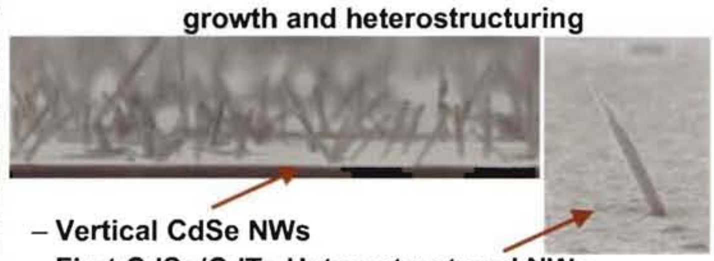
- **Transform static SLS into Flow SLS**
  - Address limitations of literature flask-based syntheses
    - Achieve controllable / tunable growth rates
    - Achieve nanoscale heterostructuring
    - Achieve device-friendly vertical growth
  - Target applications in PV and thermoelectrics



- **Length control**



- **Unprecedented, controlled vertical NW growth and heterostructuring**



- Vertical CdSe NWs
- First CdSe/CdTe Heterostructured NWs

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Transformational materials chemistry approaches: New compositions and new methods

- **Nanowire summary**
  - Our work in new nanowire materials development
    - Demonstrated and reported first truly ternary system synthesized by SLS
    - $CuInSe_2$ targeted: ideal system for testing photovoltaic concepts
  - Our work in new-capability development for nanowire synthesis
    - Established "Flow" SLS for advancing control over solution-phase nanowire growth
    - Recently provided first demonstration of controlled vertical-nanowire growth by SLS and proof-of-concept for nanoscale (i.e., sharp-interface) vertical heterostructuring

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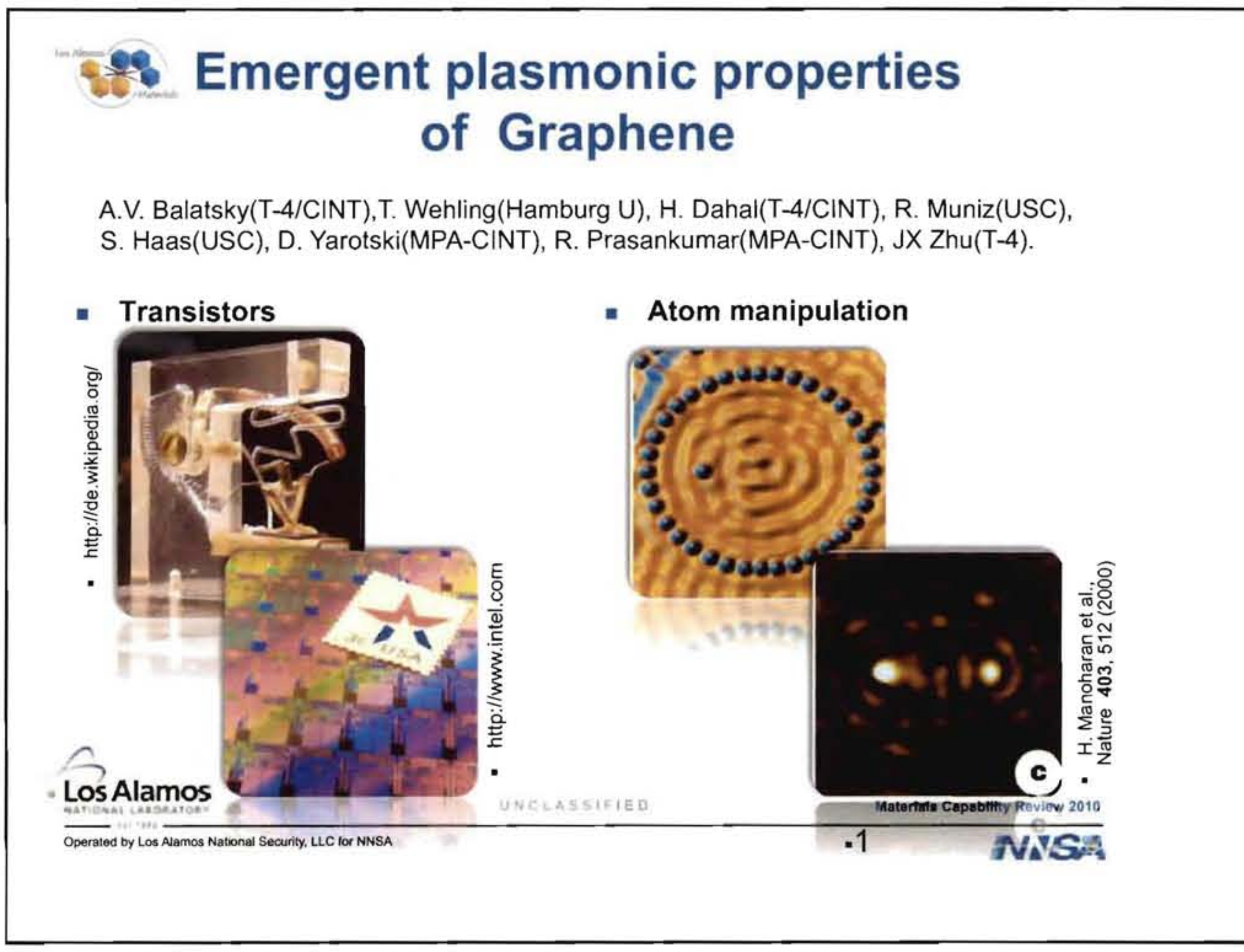
Emergent Plasmonic Properties of Graphene

A. V. Balatsky (T-4/CINT)

Recently a new single-layer material—graphene—has been discovered. This is a material where Dirac points in the fermionic spectrum lead to very unusual properties, including transport and impurity states. Highlights will be presented of recent experimental and theoretical efforts to directly probe the nanoscale electronic and optical properties of graphene and possible routes to functionalization.



Emergent plasmonic properties of Graphene
A.V. Balatsky(T-4/CINT),T. Wehling(Hamburg U), H. Dahal(T-4/CINT), R. Muniz(USC), S. Haas(USC), D. Yarotski(MPA-CINT), R. Prasankumar(MPA-CINT), JX Zhu(T-4).
Transistors
http://de.wikipedia.org/
http://www.intel.com
Atom manipulation
H. Manoharan et al., Nature 403, 512 (2000)
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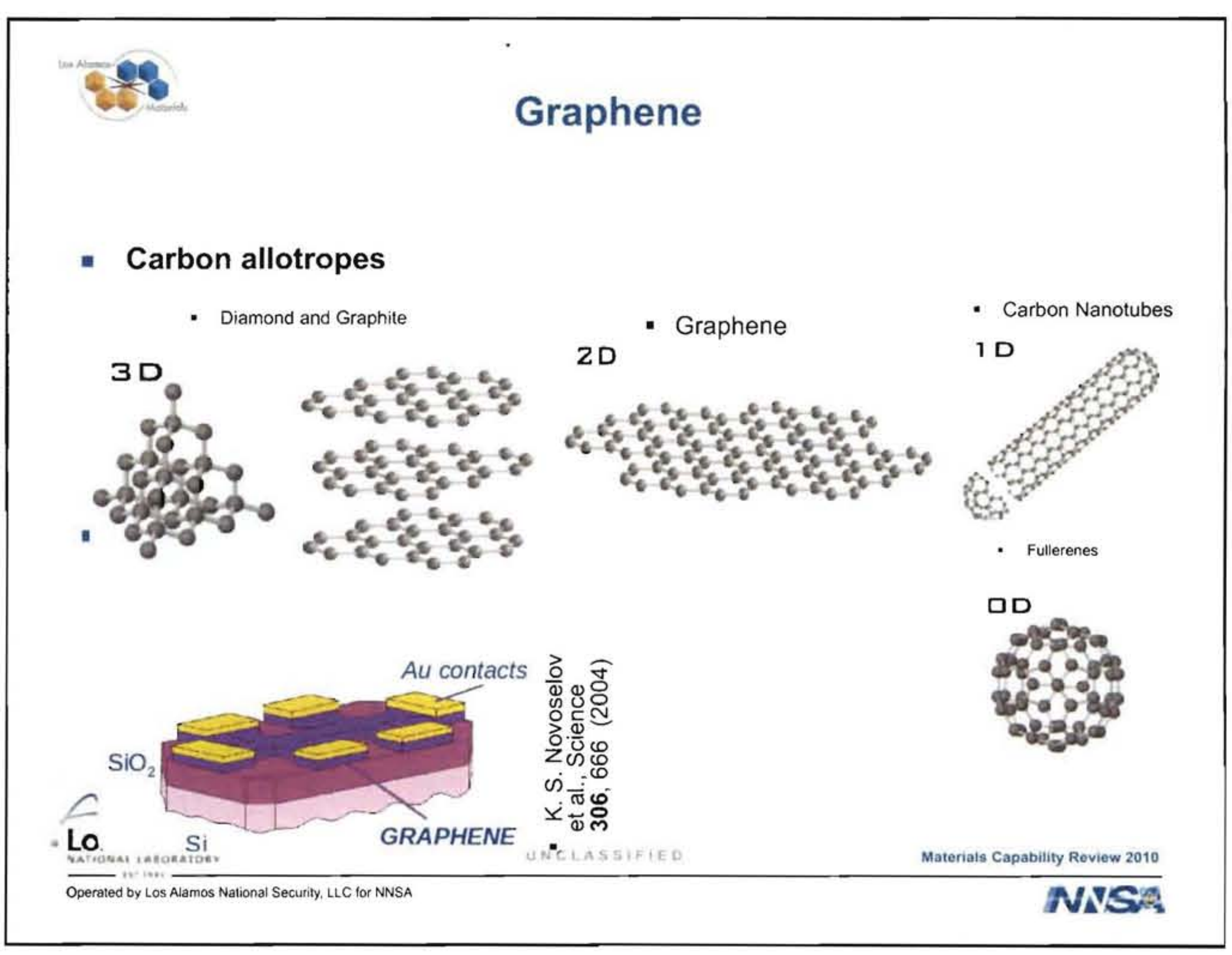

Graphene
Carbon allotropes
Diamond and Graphite
3D
Graphene
2D
Carbon Nanotubes
1D
Fullerenes
0D
Au contacts
SiO2
Si
GRAPHENE
K. S. Novoselov et al., Science 306, 666 (2004)
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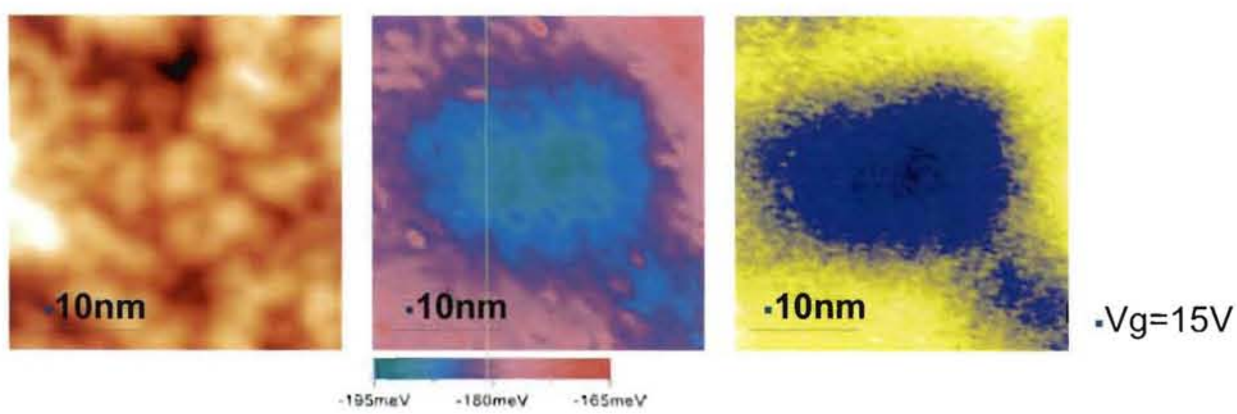
Localized plasmons in graphene

•Graphene Topography •Map of Dirac Point Energy •dI/dV Map (@ 50meV below E_D)



•Charge puddles in graphene due to charge impurities (Zhang et. al., Nature Physics 5, 722)

•What are the consequences of the charged impurity on the dielectric response of graphene?

•(Plasmonic excitation in graphene)

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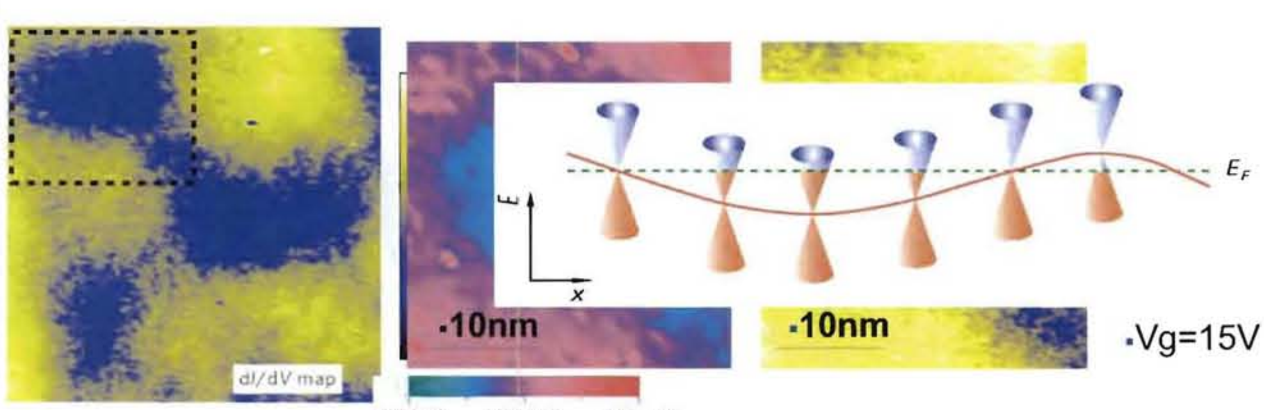
Localized plasmons in graphene



•Charge puddles in graphene due to charge impurities

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•Zhang et. al., Nature Physics 5, 722

•(Plasmonic excitation in graphene)

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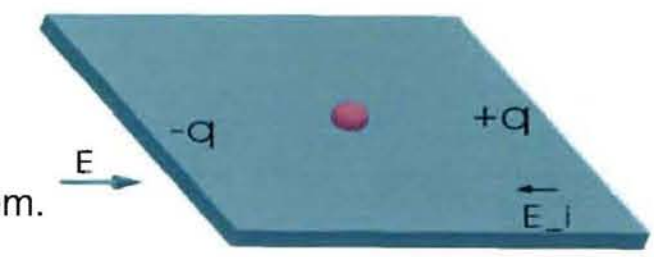
Plasmonic excitation



- External field E polarizes the system.
- The induced field E_i acts as a restoring force leading to collective oscillation of charges.
- A quantum of oscillating charges is called plasmon.
- In the absence of disorder plane waves are created.
- How does the response changes in the presence of a charged impurity?

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Model

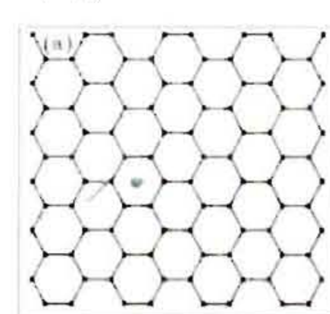
$$H = -t \sum_{<a,b>} \left(c_a^\dagger c_b + c_b^\dagger c_a\right) + \sum_a U_a c_a^\dagger c_a - \mu \sum_a c_a^\dagger c_a + \sum_{a \neq b} V_{ab} \rho_a \rho_b$$

- Kinetic energy Impurity chemical potential Interaction

$$\Pi(\omega) = \Pi^0(\omega)\left(1 - V\Pi^0(\omega)\right)^{-1}$$

- polarization operator:

- **<u>Plasmonic excitation is obtained from</u>**
- **<u>the pole of the polarization operator.</u>**
- **<u>Spatial distribution of induced charges on the lattice is calculated.</u>**



- Geometry used in numerical calculation

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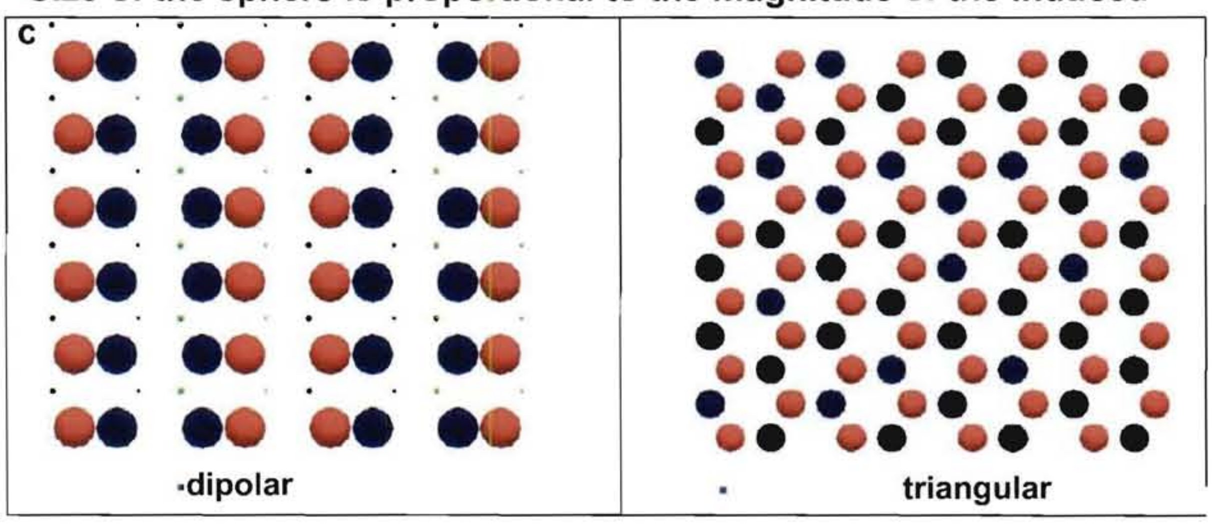
Non localized plasmonic excitation in pristine graphene

Positive induced charge · Negative induced charge

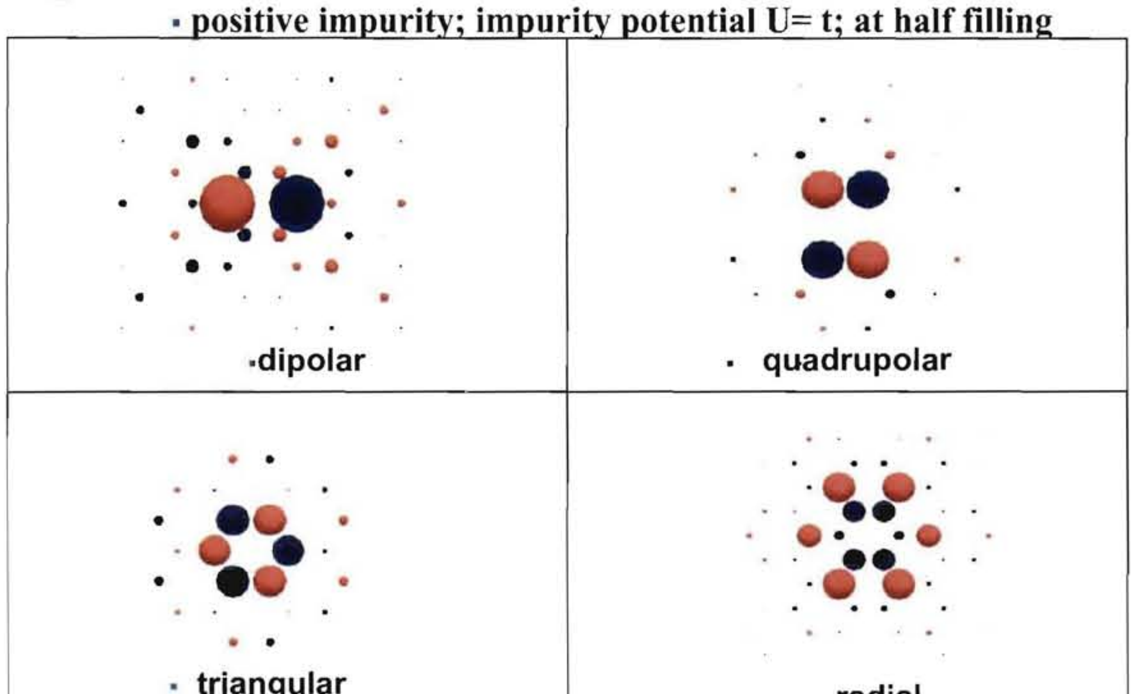
- Size of the sphere is proportional to the magnitude of the induced



- Observation: 1)Non localized excitation 2) locally charge conserving, 3) periodic

Localized plasmonic excitation in impure graphene

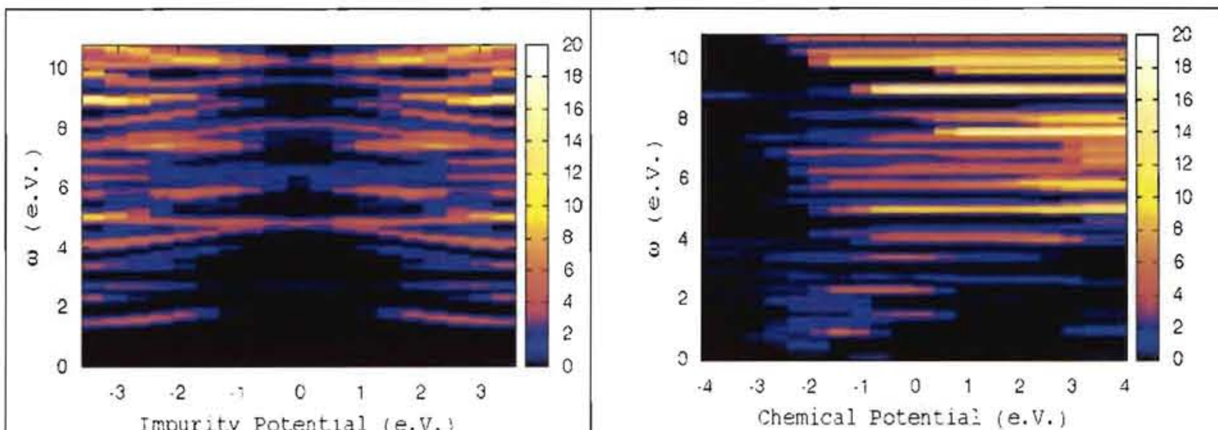
- positive impurity; impurity potential U= t; at half filling



- These are some of the Localized excitations.

Spectral density

$$A(\omega) = -\frac{1}{\pi} Im \Pi^R(\omega)$$



- Excitations are particle-hole symmetric
- Excitations are particle-hole asymmetric

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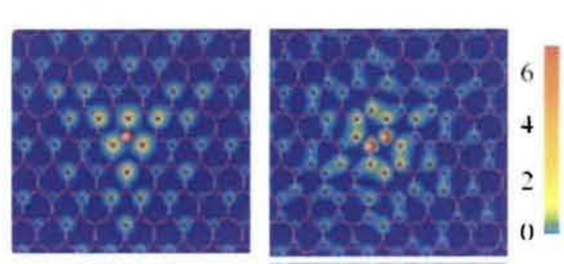
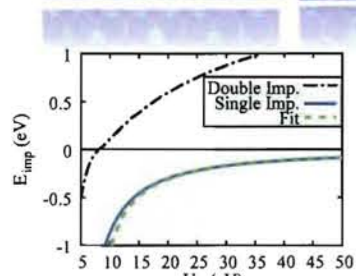
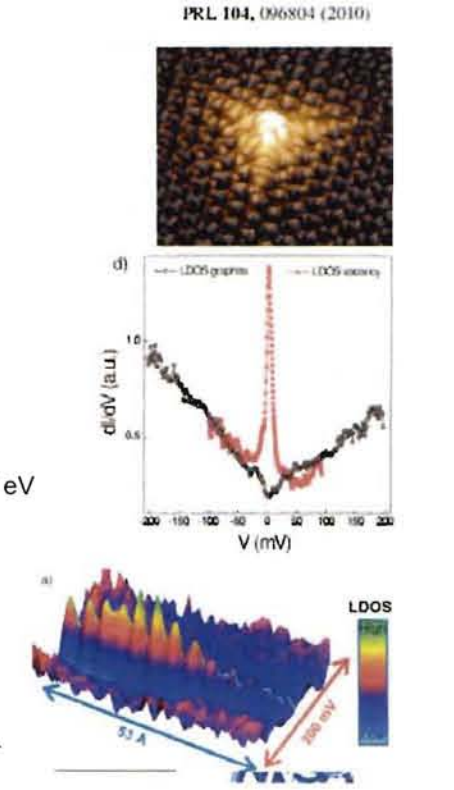
Old theory predictions and new data

PRL 104, 096804 (2010)





LDOS at E=−0.1 eV for a single impurity with U_0=45 eV and a double impurity with U_0=6.9 eV



Wehling, Balatsky et al, PRB 75, 125425 (2007)

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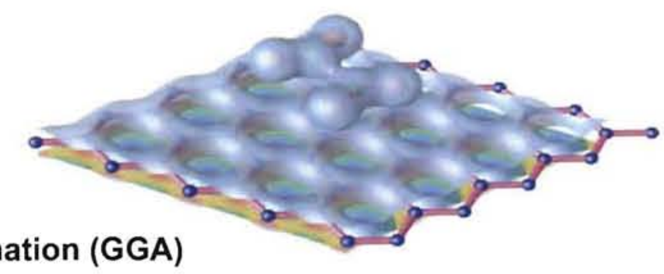
Simulations of realistic impurities for plasmonics functionalization



- Density functional theory
- Generalized gradient approximation (GGA)
- Vienna ab-initio simulation package (VASP)
- Projector augmented wave (PAW) basis sets
- Fully relaxed adsorption geometries

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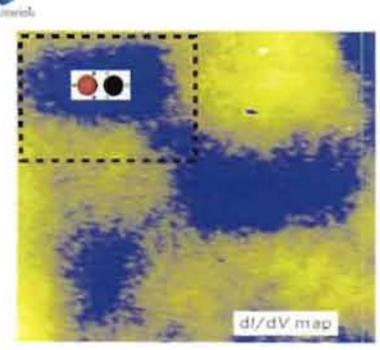
Conclusion



•Graphene is an intrinsic nano-plasmonic material. Emergent properties for pasmon at nanoscale

•Going beyond simplified models (beyond spherical cow models) ab initio

•Relaistic localized plasmon polariton response,

•Plan to elucidate the role of defects and and patterned substrate on the plasmonic response.

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Optimizing the Behavior of Supported Lipid Membranes on Nanoporous Metals

G. Gupta, A. Misra, A.M. Dattelbaum (MPA-CINT); P. Sekhar (MPA-11)

Supported lipid bilayers are used to mimic biological cell membranes and are useful for elucidating membrane function in a controlled laboratory environment. Organization of lipids into membrane architectures can lead to emergent and cooperative behavior of lipids that strongly affects the ion transport and fluidity of the membrane. In addition, incorporation of intact transmembrane proteins/peptides into supported lipid bilayers is possible and allows one to controllably study transmembrane protein function. However, interactions between the extra-membrane piece of the protein with the substrate can cause the protein to lose functionality. To minimize protein-surface interactions, we use nanoporous metal films that provide a water-filled pocket at the surface for the extra-membrane piece of a transmembrane protein. Because the nanoporous metal is inherently conductive, one can also readily measure ion transport through the supported membranes.

For this work, we take advantage of fabrication techniques, which were recently developed at LANL, to make ordered nanoporous metal structures with controllable pore size and structure to support lipid bilayers. We show for the first time that lipid membranes on nanoporous noble metal films can be both fluid and electrochemically resistive. We make use of several techniques, including ellipsometry, imaging fluorescence microscopy and impedance electrochemical spectroscopy, to characterize the supported lipid membrane architectures. The development of fluid lipid bilayers on conducting supports is broadly applicable for studying transmembrane protein function and may potentially be useful for new energy harvesting devices.

Fluorescent Gold and Silver Nanoclusters for Detection of Biological Materials

H.-C. Yeh, J. Sharma (MPA-CINT); Y. Bao, D.M. Vu (C-PCS); A.P. Shreve, J.H. Werner, J.S. Martinez (MPA-CINT)

Biological molecular imaging and sensing requires fluorophores that are not only stable and bright, but also small enough to allow the unencumbered observation of the movement of biological molecules. Toward this goal, we have studied the formation of fluorescent metallic gold nanoclusters stabilized by small molecule ligands. These clusters are found to be subnanometer sized, with nanosecond fluorescence lifetimes and as bright, or brighter, than the commercial dye norharmane. Toward production of nanoclusters directly in biological molecules, we have produced silver nanoclusters in DNA and studied their photophysical properties. These bright clusters are produced in a single reaction condition and are tuned to common laser excitation wavelengths. Additionally, taking advantage of both salt- and ligand-induced effects, we have used these DNA templated nanoclusters for detection of proteins (salt-induced) and for the enhancement of DNA detection (liquid-induced).

Multiplex Detection of Pathogen-Biomarkers using Quantum Dots on a Waveguide-based Biosensor

H. Mukundan (C-PCS); H. Xie (Idexx Inc.); D. Price (C-PCS); J. Kubicek-Sutherland (UCSB); K. Grace, A. Anderson (C-PCS); J.S. Martinez (MPA-CINT); N. Hartman (nGiMat Ltd.); B.I. Swanson (C-DO)

Accurate diagnosis of disease is quintessential to proper intervention. One approach is to detect biomarkers specific to the pathogen in the infected host. If successful, this approach can allow for the rapid, sensitive, early and specific detection of disease. However, application of this strategy has two primary limitations: 1) most conventional platforms lack the sensitivity to detect the very low concentrations of biomarkers in complex biological samples such as serum and 2) since no single biomarker is an accurate indicator of disease, such a platform should be able of detection of a limited suite of such molecules.

The sensor team at LANL is an interdisciplinary group of researchers attempting to tackle this problem. We have developed a waveguide-based optical biosensor platform for the rapid and accurate detection of biomarkers with exquisite sensitivity. Most recently, we have developed multichannel waveguides capable of the detection of a limited suite of biomarkers. This approach uses specific antibodies conjugated with photostable and tunable quantum dots as the fluorescence reporter. We have successfully demonstrated the simultaneous quantitative detection of protective antigen and lethal factor of *Bacillus anthracis*, in serum, within 15 minutes, with sensitivities that are much better than those achieved by traditional immunaossays for each antigen. One of the major reasons for the assay efficiency is the development of robust silane-based self-assembled monolayers for waveguide-functionalization. These surfaces are robust, easy to make and highly efficient in resisting non-specific binding in complex biological samples.

The design, fabrication and development of the multichannel system, antibody-quantum dot conjugation and assay development and chemistry of functional surfaces will be demonstrated.

Acoustically Engineered Materials using Acoustic Radiation Force

D.N. Sinha, B. Raeymaekers, F. Mitri (MPA-11)

Acoustic radiation force in a fluid-filled resonator cavity can be used to manipulate particles in a host fluid. The magnitude of the force depends on the sound pressure, the size of the particle and the acoustic contrast factor. Depending on the sign of the acoustic contrast factor, the particles either move to the pressure nodes or to the antinodes. The particles collect in that area to create a periodic pattern that follows the standing wave pattern in the resonator cavity. We have used this type of acoustic manipulation and bulk wave to create both two-dimensional and three-dimensional patterns of various types of particles including nano-particles and hollow microspheres in a host fluid (e.g., epoxy or gel) and freeze the pattern creating novel materials, such as sonic crystals or acoustic metamaterials. These artificially created materials can have many interesting properties, such as negative refractive index, negative bulk modulus, or existence of band gaps and this is currently being studied. The majority of the materials built so far by researchers elsewhere are in the cm length-scale and include mm-size spheres, cavity resonators or other inclusions. Because of the mechanical fabrication techniques used in these studies, scaling to smaller length scales is both problematic and difficult. In contrast, the acoustic approach allows fabrication of novel materials that extends the length scale by orders of magnitude, from a few nanometers to 100s of microns. Possible applications of these new materials can vary in a wide-ranging.

Raman Spectroscopy of Chirality-Enriched Single Walled Carbon Nanotubes

S.K. Doorn, J. Duque (C-PCS); E. Haroz, J. Kono (Rice University); A. Swan (Boston University); X. Tu, M. Zheng (DuPont Central Research and Development Experimental Station)

Recent advances in carbon nanotube separations are providing samples highly enriched by metallicity and in single chiralities. We present Raman measurements that reveal new behaviors that would be difficult to probe at the single-tube level and may be masked in mixed-chirality ensembles. Density gradient ultracentrifugation of nanotubes suspended in cosurfactant systems provide fractions enriched in armchair metallic chiralities. We present Raman characterization of the enrichment process. G-band data for spectroscopically isolated armchair chiralities show that the low frequency LO mode is absent for these structures, in contrast with recent theoretical results. We also present resonance window behavior of G-band spectra for single chirality semiconducting species. The Raman excitation profiles allow testing of different models for the Raman scattering process and reveal new evidence for the importance of non-Condon effects in the Raman response.

Epitaxial Nanotwinned Cu with High Strength and High Electrical Conductivity

N. Li, O. Anderoglu, A. Misra (MPA-CINT)

We show synthesis via sputter deposition of single-crystal-like nanotwinned Cu with average twin lamellae thickness in the 7-16 nm range. These epitaxial nanotwinned Cu films exhibit much higher ratio of strength to electrical resistivity as compared to bulk Cu. Due to island growth in sputtering, the regions where a matrix lamellae in one island joins a twin lamellae in the adjoining island form incoherent twin boundaries. Although coherent twin boundaries are weak scattering sites for electrons, the periodic array of dislocations in the incoherent twin boundaries and occasional stacking faults observed in the columns contribute to the electron scattering, and result in resistivity that is slightly higher than oxygen-free, high-conductivity (OFHC) Cu. The room temperature resistivity of epitaxial nanotwinned Cu films with an average twin spacing of 16 nm is only ‰10% higher than the resistivity of 1.58 μ‡ocm for OFHC Cu. The flow strength of nanotwinned Cu approaches 1 GPa, over an order of magnitude higher than bulk Cu. We developed models to interpret the formation of nanotwinned structures in terms of synthesis parameters and to correlate the nanotwinned structure to mechanical and electrical properties.

Subpicosecond Optical Switching with a Negative Index Metamaterial

K.M. Dani (MPA-CINT); Z. Ku (University of New Mexico); P.C. Upadhya, R.P. Prasankumar (MPA-CINT); S.R.J. Brueck (University of New Mexico); A.J. Taylor (MPA-CINT)

Metamaterials are a new class of nano-engineered materials that exhibit novel optical properties like negative index of refraction, optical cloaking and imaging beyond the diffraction limit. Here, we demonstrate a nanoscale, subpicosecond metamaterial device capable of terabit per second all-optical communication in the near-IR. The subpicosecond (600 fs) response of the device is two orders of magnitude faster than previously reported, thus taking a significant step towards high-speed all-optical communication. The nanoscale size (~100 nm thickness) of the device allows for easy integration into other photonic devices and applications. Lastly, by simply adjusting the device-geometry, we can tune the response over the near-IR range (1-2 μm).

Our metamaterial device consists of alternating layers of Ag, α-Si and Ag perforated by a two-dimensional square periodic array of holes – a fishnet structure. The geometry of the device (hole size, layer thicknesses) is tuned to provide two negative resonances in the near-IR. Then by photoexciting carriers in the α-Si layer of the device, we alter the material properties from a negative index resonance to a plasmonic one. We thereby modulate the intensity of a near-IR optical beam transmitted through the device in 600 fs. This fast response is achieved by accessing a previously unused regime of high-injection level, subpicosecond carrier dynamics in a-Si. The high non-linearities inherent in metamaterial structures allow for a device that is nanoscale is size, while still providing 70% modulation of the near-IR optical beam. The device also provides a roadmap towards other ultrafast, nanoscale, tunable photonic device.

Optical Spectroscopy of Individual "Giant" Nanocrystal Quantum Dots: A Study on Radiative and Nonradiative Recombination Pathways of Multi-exciton States

H. Htoon (C-PCS); A.V. Malko (University of Dallas); Y.S. Park (C-PCS); D. Bussian (Life Technologies); S. Sampat (University of Dallas); J. Vela-Becerra (Iowa State University); Y. Chen (Life Technologies); J.A. Hollingsworth, V. I. Klimov (C-PCS)

Recently, we have developed "giant" nanocrystal quantum dots (g-NQDs), in which a small emitting core of CdSe is overcoated with a thick shell of a wider-gap CdS. Preliminary studies of these g-NQDs revealed a dramatic suppression of photoluminescence (PL) intermittency (blinking) and non-radiative auger recombination. Since these two issues are the major road blocks in successful utilization of NQDs in light emitting applications, our g-NQD present a tremendous opportunity for a transformational breakthrough in this area. In this poster, we will present our single g-NQD optical spectroscopy studies aimed toward understanding and ultimately controlling the competition between radiative and nonradiative recombination pathways of multi-exciton states. Specifically, we will present our low temperature steady state PL studies, which reveal the sequential emergence of multiple multi-exciotnic PL peaks with the increase of pump power. These multi-excitonic PL peaks are not possible to be observed in case of standard NQD because their PL is quenched due to efficient non-radiative Auger processes. This observation, therefore, provides clear evidence on strong suppression of non-radiative Auger process. Furthermore, we will also present systematic time resolved PL studies on g-NQDs of different shell thickness that allow us to understand how the competition of radiative and non-radiative recombination pathways of multi-excitons evolve as the function of g-NQDs' shell thickness. These studies provide the fundamental understandings essential for effective utilization of multi-excitonic PL emission in improving the efficiency of NQD based light emitting diodes.

Probing Material Properties and Dynamic Response at Nanoscale

D. Yarotski (MPA-CINT); S. Kilina, S. Tretiak (T-1); A. Balatsky (T-4); A. Taylor (MPA-DO)

Controlling functionality of the materials is essential to address the everlasting need for advanced materials. A key prerequisite to predicting and manipulating material functionality is the understanding of the relationship between material structure and its properties. Since many next-generation materials involve atomic-scale inhomogeneity and complexity, an experimental means for probing the structure and ensuing function at atomic length and time scales are essential to unveiling the fundamental relationship and development of novel predictive theoretical frameworks.

Here, we present our ongoing efforts to combine ultrafast optical techniques with scanning tunneling microscopy (STM) into a single instrument, an ultrafast STM (USTM), which is capable of characterization of dynamical events occurring at the nanoscale. In this technique, a femtosecond laser pulses initiate ultrafast electronic processes in the materials, and ensuing transients in the tunneling current are monitored as a function of time and position. When applied to study InAs/GaAs self-assembled quantum dots, USTM has demonstrated the ability to probe photo-induced carrier dynamics with simultaneous picosecond (temporal) and nanometer (spatial) resolutions.

The ability to visualize the nanoscale structure also holds great promise in the rapidly growing field of nano-bio interfaces. For instance, practical implementation of carbon nanotube (CNT)-based devices has long been prevented by the absence of reliable methods for CNT separation by the structural and electronic properties. Recently, an unexpected breakthrough in separation technology was achieved by attaching the DNA molecules to the nanotubes surface. In the pursuit of deeper understanding of DNA-CNT interactions pertinent to the subsequent technology development, we used STM to observe the structure of the CNT-DNA hybrids with unprecedented morphological details. Besides optimization of DNA-assisted CNT separation, the results should be relevant to electronic DNA sequencing, bio-sensing and drug delivery.

Subwavelength Photonic, Plasmonic and Hybrid Waveguiding

A. Efimov (MPA-CINT)

This research is focused on studying the fundamental properties of subwavelength and otherwise highly confining complex waveguides for electromagnetic fields. Subwavelength photonic, plasmonic and hybrid waveguides can be used in future high-density integration technologies, novel instrumentation, laser sources, and sensors where both linear and nonlinear operational regimes are involved. We study dielectric, metallic, photonic crystal and hybrid systems for dispersive linear and solitonic nonlinear propagation regimes, accompanied by intricate interaction between solitons and dispersive waves, including supercontinuum generation, Raman frequency shifting, and harmonic generation. We designed a novel axially non-uniform photonic fiber structure for improved soliton self-frequency shifting, which allows access to mid-infrared optical region with ultrashort solitons generated by a standard 1550 nm fiber laser. Further, a novel scheme was designed to use ultrashort solitons for the generation of an octave-spanning fully coherent supercontinuum via resonant generation of a dispersive wave in a short length of a dispersion zero-sliding waveguide. In addition, an optimal subwavelength hybrid metal-dielectric waveguide was designed for future Terahertz integrated components. This waveguide simultaneously shows both good confinement properties and low loss. Pure plasmonic (metallic) waveguides are studied for optimal confinement of broadband and ultrashort pulses for precise routing and delivery in future chip-scale integrated optical devices.

A MaRIE First Experiment: Process Aware Materials Performance Approach to Nanostructured Ferritic Alloys

N.A. Mara (MPA-CINT, MST-6); P. Hosemann, M.J. Demkowicz (Massachusetts Institute of Technology); R.E. Hackenberg (MST-6); I.J. Beyerlein (T-3)

Currently, lead candidate materials for application in extreme irradiation environments include oxide dispersion strengthened (ODS)/nanostructured ferritic alloy (NFA) steels, chosen for their ability to mitigate damage caused by irradiation-induced defects, and high strength and microstructural stability over a range of elevated temperatures. These favorable characteristics are attributed to the high density of (1-5nm diameter) nanoparticulate oxides distributed through the matrix, providing interfacial content for recombination and annihilation of radiation-induced point defects, He trapping, as well as impedance of dislocation motion. Despite their promise in nuclear applications (especially as cladding), a lack of fundamental understanding of key atomic-level processes encountered during synthesis and service such as defect-interface interactions, nucleation and growth of nanodispersed oxides in a metallic matrix, and corrosion phenomena have limited the development of this class of materials from widespread application and certification for use in nuclear reactors. Through a series of proposed experiments at MaRIE, direct observation of these phenomena will facilitate the mechanistic understanding necessary to develop and validate physics-based, multi-scale predictive models, forming the scientific foundation for a process-aware materials performance approach to design radiation-resistant structural materials.

Tab 8

Materials Review Committee

GARY S. WAS (Chair)
Department of Materials Science and Engineering
Department of Nuclear Engineering and Radiological Sciences
Michigan Memorial Phoenix Energy Institute
University of Michigan

Gary S. Was received his ScD from MIT in 1980. He is the Walter J. Weber, Jr. Professor of Sustainable Energy, Environmental and Earth Systems Engineering, and holds appointments in nuclear engineering and radiological sciences, and materials science and engineering at the University of Michigan. He is currently the director of the Michigan Memorial Phoenix Energy Institute and has held positions as associate dean of the College of Engineering and chair of the Nuclear Engineering and Radiological Sciences Department. Professor Was' research is focused on materials for advanced nuclear energy systems and radiation materials science, including environmental effects on materials, radiation effects, ion beam surface modification of materials and nuclear fuels. He has worked extensively in experiments and modeling of the effects of irradiation, corrosion, stress corrosion cracking and hydrogen embrittlement on iron- and nickel-base austenitic alloys. He has led the refinement of models for radiation induced segregation to account for composition dependent processes, and developed the first comprehensive thermodynamic and kinetic model for chromium carbide formation and chromium depletion in nickel-base alloys. Most recently his group has led the development of proton irradiation as a technique for emulating neutron irradiation effects in reactor structural materials and has conducted some of the first stress corrosion cracking experiments of austenitic and ferritic alloys in supercritical water.

THOMAS BRILL
Chemistry & Biochemistry
University of Delaware

Thomas Brill is a professor of chemical engineering at the University of Delaware. He received his BS (1966) with high honors in chemistry from the University of Montana and his PhD (1970) in inorganic chemistry from the University of Minnesota. He has taught at the University of Montana, the University of Minnesota, and North Carolina State University. He has been an assistant, associate, and full professor at the University of Delaware. He spent two years as a visiting professor at the University of Oregon and at Zhongshan University in the Peoples' Republic of China.

Professor Brill has lectured at numerous universities and conferences in the United States and abroad dealing with such topics as energetic materials, molecular processes in condensed matter, advanced oxidation technologies, and emerging technologies in hazardous waste management. He has been a consultant to business, industry, and national laboratories. His current research topics are structure and decomposition mechanisms of energy-rich compounds; chemistry of a burning surface; reactions in supercritical water; solid-state chemical processes; Fourier-transform infrared spectroscopy; laser Raman spectroscopy; synthesis, structure, and bonding of inorganic and organometallic complexes; and the Arbuzov reaction.

He has published 248 research papers and 3 books and has given 212 conference presentations. He is a member of several professional organizations, including the American Chemical Society and the Materials Research Society and was named Fellow of the Center for Advanced Studies. He is listed in such publications as *Who's Who in Science and Technology* and *Who's Who in the United States*.

MICHAEL FLUSS
Chemistry & Materials Science
Lawrence Livermore National Laboratory

Michael J. Fluss has been a senior scientist in the Chemistry Materials and Life Science Directorate at LLNL since 1984. He has recently performed research with plutonium alloys, focusing on radiation damage materials aging, alloy phase stability, and solid-state properties. Additionally, he is interested in the materials physics of highly correlated electron systems. Fluss received his BS degree in chemistry from Rutgers University (1964) and his PhD degree in chemical physics from Columbia University (1968). Fluss has served as group leader and division leader in the Chemistry and Materials Division at LLNL and has successfully led projects in a variety of materials research areas. Prior to 1984, Fluss worked as a senior scientist at Argonne National Laboratory in the Chemistry, Chemical Engineering, and Materials Science Divisions.

M. BRIAN MAPLE
Department of Physics
University of California, San Diego

M. Brian Maple is a professor in the Department of Physics at the University of California, San Diego. He received his PhD from UC, San Diego in Physics in 1969. He is the director for the Institute for Pure and Applied Physical Sciences and the Center for Interface and Materials Science, both at the university. Maple is presently the Bernd T. Matthias Endowed Chair in Physics. He has served on several national laboratory committees, is a National Academy of Sciences member, an American Physical Society Fellow, an American Association for the Advancement of Science Fellow, a Materials Research Society member, and serves on many other committees for the materials community.

I. CEVDET NOYAN
Department of Applied Physics & Applied Mathematics
Columbia University

I. Cevdet Noyan is a professor in materials science and engineering at Columbia University. He received his PhD from Northwestern University in materials science and engineering in 1984. Dr. Noyan is a Fellow in the American Physical Society, is the US representative to the International Residual Stress Analysis Conferences, a member of ASM, TMS-AIME, ACA, APS, Sigma Xi, and IEEE. He holds 23 patents. Noyan's research interests lie in mechanical response of crystalline materials over various length scales. He was one of the first researchers to combine the theory of micromechanics with that of x-ray and neutron diffraction. From 2005 on, he was a co-principal investigator on the new X13B microbeam diffraction line, whih was built at NSLS and commission in 2008.

RALPH NUZZO

Department of Chemistry
University of Illinois at Urbana-Champaign

Ralph G. Nuzzo is the William H. and Janet G. Lycan Professor of Chemistry at the University of Illinois at Urbana-Champaign, a faculty he joined in 1991 and where he also holds an appointment as a professor of materials science and engineering. He received an AB degree with high honors and highest distinction in chemistry from Rutgers College in 1976, where he was also recognized as a Henry Rutgers Scholar, awarded the Merck Prize for undergraduate research, and elected to Phi Beta Kappa. He earned a PhD in organic chemistry from the Massachusetts Institute of Technology in 1980. He accepted the position of member of technical staff in materials research at Bell Laboratories in Murray Hill, NJ in 1980, where he was named a distinguished member of the staff in research in 1987—a title held until he left to join the Illinois faculty in 1991.

Professor Nuzzo is a Fellow of the American Academy of Arts and Sciences and Fellow of the World Innovation Foundation. In 2006 he was awarded the *Wall Street Journal* Innovators Award for Semiconductors. He received the Adamson Award of the American Chemical Society in 2003 for original discoveries leading to the development of self-assembled monolayers. Nuzzo has been recognized three times by ISI for citations in chemistry and the American Chemical Society—*Journal of the American Chemical Society*—for his co-authorship of one of the 12 most highly cited papers published in the journal during its 125 year history.

Nuzzo is the senior editor of *Langmuir* and serves on the advisory, review, and executive boards of numerous entities—ones both public and private. He is a senior advisor to the Dreyfus Foundation and the Petroleum Research Fund, and a member of the scientific advisory boards of Surface Logix Inc. and the Intermolecular Corporation. He more recently co-founded and serves as a member of the board of directors of the Semprius Corporation. Nuzzo holds 16 U.S. patents and is the author of more than 200 research publications.

CHRISTINE ORME

Chemistry & Materials Science
Lawrence Livermore National Laboratory

Christine Orme is a senior scientist at Lawrence Livermore National Laboratory working in the Physical and Life Sciences Directorate. She received her PhD in physics from the University of Michigan. Orme is a Fellow of the American Physical Society and won the Presidential Early Career Award for Science and Engineering and the Office of Science Early Career Scientist and Engineer Award. She was elected to the Materials Research

Society board of directors and is involved in planning and organizing many programs and conferences. Her research interests are in shape control in metal and metal-oxide nanostructures, biomineralization, biomimetic synthesis, physics of assembly, corrosion, and in situ methods for investigating interfacial dynamics.

ANTHONY ROLLETT

Department of Materials Science & Engineering
Carnegie Mellon University

Tony Rollett has been a professor in materials science and engineering at Carnegie Mellon University since 1995 and was department head from 1995 to 2000.

Before coming to Carnegie Mellon, Rollett was a staff member at Los Alamos National Laboratory in the Materials Science & Technology Division. In 1991, he became the group leader of LANL's Metallurgy group. In 1994, he became LANL's deputy division director for the MST Division.

At Carnegie Mellon, Rollett's research program emphasizes quantification of microstructure, especially in three dimensions, and its impact on properties and processing using both computational and experimental techniques. Important recent results include relating the optimization of magnetic properties in electrical steels to grain growth stimulated by variable stored energy in electrical steels; investigation of nucleation mechanisms in low-carbon steels; measurement of anisotropic grain boundary mobility (in Al); development of methods for generating statistically representative three dimensional microstructures; measurement and modeling of texture development during processing (recrystallization) in aluminum alloys; dependence of fatigue crack initiation on microstructure. The ultimate aim is to put microstructure-properties relationships on a quantitative basis for the prediction and optimization of materials processing and application.

Rollett is a member of the NSF-supported Materials Research Science and Engineering Center. He is also the focal area point of contact for computational chemistry and materials for the DoD's high performance computing program.

Rollett has authored more than 60 publications and two book chapters. He is a Fellow of ASM-International and of the Institute of Physics (UK). In 2005, he was a recipient of the Howe Medal for the Best Paper in *Metallurgical & Materials Transactions.*

JAMES WILLIAMS

Honda Professor of Materials
Ohio State University

James Williams is a professor of materials science and engineering and Honda Chair at Ohio State University, where he is engaged in teaching and research activities in structural materials including their application and the manufacturing of high value components. Williams earned his PhD from the University of Washington and is a member of the

National Academy of Engineering, a Fellow of ASM International, a Fellow of TMS-AIME, and a member of the Air Force Scientific Advisory Board. He is involved in several externally funded projects dealing with various aspects of the behavior of Ni-base and Ti-base structural alloys. He is also regularly invited as a speaker at conferences that deal with these subjects. From July 2001-June 2004 he was also dean of engineering at OSU. In 2003, he and Prof. Lütjering completed a book *Titanium*, published by Springer-Verlag. A second edition of the book was released in spring 2007.

While at General Electric Aircraft Engines, Williams was the general manager of the materials and process engineering department . In his general manager capacity, he had overall responsibility for the materials effort at GE Aircraft Engines. This included all research, development and the qualification of new materials and processes, including process developmental efforts with an extensive base of outside suppliers that manufacture a wide range of high value components. These business relationships included casting, forging, metal powder, wrought product and polymer composite materials and component suppliers. The internal GE program encompassed ceramic, metal and polymer matrix composites including fibers; the full range of metallic materials, intermetallic compounds, coatings and lubricants. It also included process development. In addition to materials research, development and qualification activities, Williams' department had the responsibility for generating, collecting, analyzing and presenting material property data for use in component design and life prediction.

Williams began his time at Rockwell International as a research staff member and then became the program manger for an inter-divisional technology program that supported technology transfer between the aircraft, space, rocket engine, nuclear power and electronics divisions. The period he was doing this coincided with the start-up phases of the B-1, the space shuttle and the space shuttle main engine programs. Each of these programs encountered their own materials manufacturing challenges and this became a major focus of the inter-divisional technology program.

LANS Science and Technology Committee Representatives

ALEXANDRA NAVROTSKY
Department of Chemical Engineering & Materials Science
University of California, Davis

Alexandra Navrotsky is the interdisciplinary professor of ceramic, earth, and environmental materials chemistry at the University of California, Davis. She holds an interdisciplinary appointment in the Departments of Chemical Engineering and Materials Science; Chemistry; Land, Air, and Water Resources; and Geology. Her areas of specialization are physics and chemistry of minerals, geochemistry, solid-state chemistry, and materials science.

Before joining UC Davis, Dr. Navrotsky was a professor in the Department of Geological and Geophysical Sciences at Princeton University and held the Albert G. Blanke Jr. Professorship in the Department of Chemistry. Earlier, she was a research associate at

Technische Hochschule, Clausthal, Germany, Institut fur Theoretische Huttenkunde; a research associate in the Department of Mineralogy and Geochemistry at Pennsylvania State University; and then a faculty member in the Department of Chemistry at Arizona State University.

Professor Navrotsky was named Fellow of the Mineralogical Society of America, the American Geophysical Union, and the Geochemical Society and was elected to the National Academy of Sciences. She has received the Mineralogical Society of America Award and the Arizona State University Graduate College Distinguished Research Award. She has also served as president of the Mineralogical Society. She was named Doctor Honoris Causa of Uppsala University in Sweden.

ROCHUS (ROBBIE) VOGT

California Institute of Technology
Department of Physics, Mathematics & Astronomy

Rochus (Robbie) E. Vogt is the R. Stanton Avery Distinguished Service Professor and Professor of Physics, Emeritus at the California Institute of Technology (Caltech), where he began his service in1962. Dr. Vogt has served as chairman of the faculty, as chairman of the Physics, Mathematics, and Astronomy Division, and as vice president and provost at Caltech.

A recipient of the NASA Exceptional Scientific Achievement Medal, Vogt was the chief scientist at Caltech's Jet Propulsion Laboratory in 1977-78 and was acting-director of Caltech's Owens Valley Radio Observatory in 1980-81. He served as the director and principal investigator of the Caltech-MIT Laser Interferometer Gravitational-Wave Observatory (LIGO) Project from 1987-1994. He is a U.S. citizen, born near Heidelberg, Germany in 1929, studied as a Fulbright Fellow, and earned his doctorate in 1961 at the University of Chicago, which has honored him with the Alumni Association's Professional Achievement Award. Before coming to Caltech, he worked at the Enrico Fermi Institute for Nuclear Studies at the University of Chicago. His research career has focused on astrophysical aspects of cosmic radiation, gamma-ray astronomy, and gravitational-wave astronomy. Vogt has done extensive consulting work with government and industry. He has been a member of NASA's Physical Sciences Committee, and of the University of California (UC) Scientific & Academic Advisory Committee for the Los Alamos and Lawrence Livermore National Laboratories. He currently serves on the UC President's Council on the National Laboratories and chairs its Science and Technology Panel. He also serves on the LANS LLC Science and Technology Committee. He has served as vice chairman of the board of directors of the California Association for Research in Astronomy; he also serves on the board of directors of International Rectifier Corporation, a semiconductor company. In 1982, Vogt was honored as Caltech's first R. Stanton Avery Distinguished Service Professor.

Tab 9

Materials Capability Review Presenters and Theme Leaders

ALEXANDER V. BALATSKY

Center for Integrated Nanotechnologies (MPA-CINT) and
Physics of Condensed Matter and Complex Systems (T-4)
Laboratory Fellow

Alexander Balatsky is a staff member of the theory and simulation of nanoscale phenomena science thrust at Center for Integrated Nanotechnologies and a staff member at the Physics of Condensed Matter and Complex Systems group (T-4). His long-term interests are in the theory of strongly correlated materials, superconductivity, and local electronic properties at nanoscale. He is an author of 197 papers. He is a Los Alamos Fellow and an American Physical Society Fellow.

JOHN BINGERT

Structure/Property Relations Group (MST-8)
Dynamic Materials Properties: Testing and Modeling
Team Leader

John Bingert serves as research and development manager for the Dynamic Materials Properties team in MST-8 and as a project leader within the DoD/DOE Joint Munitions program. He received his MS in metallurgical engineering from Colorado School of Mines in 1990. Bingert's research activities have included deformation processing, high-temperature superconductor (HTSC) fabrication, ferrous metallurgy, hydrostatic extrusion, and P/M processing. His current efforts involve texture characterization, plastic anisotropy, and microstructural damage quantification, concentrating on large strain and high strain-rate deformation conditions. Bingert completed a two-year external change-of-station to the Naval Research Laboratory in 2003 focused on image-based modeling and friction-stir welding research and he continues to remain active in DoD-related programmatic work. He is the co-author of more than 85 publications (65 peer-reviewed, 3 publication awards) and 2 book chapters, and the recipient of 6 patents related to advanced materials processing. Bingert is also nearing completion of an Executive MBA at UNM's Anderson School of Business.

WENDY R. CIESLAK

Materials Science & Technology (MST-DO)
Division Leader

Wendy R. Cieslak is the leader of the Materials Science & Technology (MST) Division at Los Alamos National Laboratory. MST Division, an organization of ~300 people and $90M, performs materials research and engineering for diverse national security challenges from nuclear weapons to energy security. The Division has specialized capabilities in processing of actinides, primarily plutonium and uranium, as well as precision machining for target fabrication, and a full spectrum of materials analysis and microscopy. Prior to joining Los Alamos in January 2009, Cieslak was deputy to the vice president for Science, Technology and Engineering (ST&E) at Sandia National Laboratories, where she led the Laboratory Directed R&D program, the University

Partnerships program, and operations of the ST&E Strategic Management Unit. Her technical staff career started at Sandia in 1983 with basic and applied corrosion research of metals in liquid and atmospheric environments. She spent about a decade stewarding power sources from early R&D through to prototype production, specifically lithium/thionyl-chloride battery development and lithium-ion battery research programs. Cieslak earned her PhD and BS in materials engineering from Rensselaer Polytechnic Institute. A graduate Hertz Fellow, she was inducted to the Hertz Foundation board of directors in October 2008. She is a Fellow of ASM, International.

DAVID L. CLARK

National Security Science Education Center
Institutes Office (INST-OFF)
Plutonium Strategy Leader

David L. Clark received a BS in chemistry in 1982 from the University of Washington, and a PhD in inorganic chemistry in 1986 from Indiana University. His thesis work was recognized by the American Chemical Society with the Nobel Laureate Signature Award for the best chemistry PhD thesis in the United States. Clark was a postdoctoral fellow at the University of Oxford before joining Los Alamos National Laboratory as a J. Robert Oppenheimer Fellow in 1988. He became a technical staff member in the Isotope and Nuclear Chemistry Division in 1989. He has held various leadership positions at the Laboratory, including program management for nuclear weapon's and Office of Science programs, and director of the Glenn T. Seaborg Institute for Transactinium Science between 1997-2009. He is a Fellow of the American Association for the Advancement of Science, a Laboratory Fellow, and leader of the plutonium science strategy for Los Alamos National Laboratory. His research interests are in the structure and bonding of actinide materials, applications of synchrotron radiation to actinide science, behavior of actinides in the environment, and in the aging effects of nuclear weapons materials.

SCOTT A. CROOKER

National High Magnetic Field Laboratory (MPA-CMMS)
Scientist

Scott Crooker is a staff member in the National High Magnetic Field Laboratory (NHMFL) of the Materials Physics and Applications Division. Crooker received his BA in physics from Cornell University in 1992 and his PhD in physics from the University of California, Santa Barbara in 1997. He was a Los Alamos Director's Postdoctoral Fellow (1998-2000) at the NHMFL in Los Alamos and has been working there as a staff member since 2000. Crooker directs a research laboratory concerned generally with the development of ultra-sensitive magneto-optical spectroscopies to probe the static and dynamic behavior of electron spins and magnetic moments in semiconductor materials, in high magnetic fields to 90 tesla. He received the 2007 Los Alamos Fellow's Award for Outstanding Research. The results of his research have been reported in more than 90 journal publications (including high-impact journals *Science*, *Nature*, *Physical Review Letters*, *Nature Physics*, and *Nature Materials*) with more than 1,700 citations to date, and he has presented more than 40 invited talks on his work at domestic and international conferences and seminars.

DIEGO DALVIT

Physics of Condensed Matter and Complex Systems (T-4)
Scientist

Diego Dalvit is a technical staff member in the Theoretical Division at Los Alamos. He was previously a Director's Funded Postdoctoral Fellow at LANL. His research interests include the physics of Casimir quantum fluctuations in nanostructures and atom-surface interactions, quantum and atom optics, and fundamental issues of decoherence and quantum information processing. He has published more than 60 papers in these areas, written a book on statistical physics published by Institute of Physics in 1999, and is editing a book on Casimir physics to be published in the spring of 2010. He is a member of the American Physical Society. In 2009 he won a LANL Merit Award for leadership in basic and applied Casimir science. Dalvit is the theory team leader of two multidisciplinary DARPA programs on controlling Casimir forces with metamaterials (a LANL/Sandia project) and with deformable nanostructures (a LANL/ANL/NIST/Indiana project).

JENNIFER HOLLINGSWORTH

Physical Chemistry and Applied Spectroscopy (C-PCS)
and Center for Integrated Nanotechnologies (MPA-CINT)
Scientist

Jennifer Hollingsworth is a technical staff member, scientist 4, in the Physical Chemistry and Applied Spectroscopy and Center for Integrated Nanotechnologies groups of the Chemistry and Materials Physics and Applications Divisions, respectively, at Los Alamos. She joined Los Alamos as a Director's Funded Postdoctoral Fellow and subsequently was awarded a LANL Postdoctoral Small Team Award. As a staff member, she has received several LANL awards for outstanding scientific achievement, a LANL Associate Directorate for Chemistry, Life, and Earth Sciences Achievement Award for Program Development, and a Women's Career Development Mentoring Award. She leads numerous research efforts in the development of novel optical nanomaterials, including an NIH-R01 (PI) and a DOE SISGR (co-PI) program. Her research interests include establishing "materials-by-design" principles for solution-phase synthesis (and assembly) of functional semiconductor nanomaterials. She endeavors to understand and exploit structure-function relationships (effects of dimension, nanoscale hetero-structuring and surface chemistry) in different systems toward optimizing optical and electronic properties. She has published more than 40 papers, submitted 4 patents, and written 3 book chapters in these areas.

GORDON D. JARVINEN

Stockpile Manufacturing and Support (ADSMS)
Seaborg Institute Deputy Director

Gordon D. Jarvinen is deputy director of the Glenn T. Seaborg Institute for Transactinium Science at Los Alamos National Laboratory. He received a BS in chemistry from the Massachusetts Institute of Technology in 1973 and a PhD in inorganic chemistry from the University of California, Los Angeles in 1979. He was a resident research fellow at the

Central Research Department of E. I. Du Pont de Nemours & Company in Wilmington, Delaware during the summer 1973. He came to LANL in 1979 to do postdoctoral research in the Chemistry and Nuclear Chemistry Division and has worked at the Laboratory since then. Jarvinen was a staff member from 1981-1989 in the Isotope and Nuclear Chemistry Division and moved to the Nuclear Materials Technology Division in 1989 where he worked as process chemistry team leader 1991-1994 in the Nuclear Materials Process Technology Group and development team leader 1994-1996 in the Advanced Technology Group. Jarvinen received the R.D. Baker Award in Science & Technology from the Nuclear Materials Technology Division in 1999. In 2000, he served as chair of the separation science and technology subdivision of the Division of Industrial & Engineering Chemistry of the American Chemical Society. In 2008 he received the G.T. Seaborg Actinide Separations Award. Jarvinen has authored more than 50 publications in refereed journals, book, and encyclopedia chapters, has received 5 patents with 1 patent pending. His research interests include actinide and lanthanide coordination chemistry and development of systems for improved separation and analysis of actinides, including chelating and ion exchange materials, and membrane separation systems.

RICHARD L. MARTIN

Physics and Chemistry of Materials (T-1)
Staff Member

Richard L. Martin is a staff member for the Physics and Chemistry of Materials group (T-1) in the Theoretical Division. He received the PhD in chemistry from the University of California, Berkeley, and spent two years as a Chaim Weizmann Fellow at the University of Washington before joining the Theoretical Division at Los Alamos National Laboratory in 1978. His research interests lie in the electronic structure theory of molecules and solids, especially transition metal and actinide chemistry, charge and energy localization and transport in molecularly engineered electronic materials and devices, strongly correlated materials, and homogeneous catalysis. He has published over 175 papers in refereed journals, which have been cited some 6000 times, with an h-index of 46. Richard is a Fellow of the AAAS, has served on numerous national panels and boards for the NSF and DOE, and received a DOE Award of Excellence as a member of the Pit Lifetime Assessment Team. He is past editor of the *Wiley Series on Theoretical Chemistry* and a member of the board of the International Association of Scientists in Interdisciplinary Areas.

RICK MARTINEAU

Weapons Directorate (ADW)
Program Manager

Rick Martineau is the program manager for Campaign 2, which resides in the Weapons Directorate at Los Alamos National Laboratory. Campaign 2 is a subset of the science campaigns, the principle responsibility of which is to obtain thermodynamic and constitutive data for materials of interest to the nuclear weapons program. Martineau has a broad experience base in the weapons program from his background in the Dynamic Experiments Division and Applied Physics Division. His area of research includes the dynamic response and failure of thin ductile shells subjected to internal high explosive detonations. Most recently Martineau has been contributing to the modern reassessment of underground test anomalies and working to establish related performance metrics and thresholds.

EDWARD A. MCKIGNEY

Safeguards Science and Technology (N-1)
Scientist

Edward McKigney has led the nanocomposite scintillator development project at Los Alamos National Laboratory for the last several years. This is an effort to develop composite materials with performance characteristics similar to single crystalline materials for radiation detection. McKigney received his PhD in physics from the University of London in 1998. He received the Carey Foster Prize from University College London for his research and work on the OPAL experiment on the Large Electron Positron accelerator at the European Organization for Nuclear Research (CERN). This was a study of virtual photon-photon scattering using lead-scintillator sandwich calorimeters. In addition, he has worked with organic and inorganic scintillators in a number of contexts; the BaF3 calorimeter for the Galactic Emission Mapping experiment at Superconducting Super Collider, the sampling Central Electromagnetic Calorimeter of the collider detector experiment at Fermilab, and two plastic scintillator fiber tracking detectors for muon measurements. He was responsible for the design, fabrication, testing and running of the scintillating fiber muon tracker for the MuScat experiment at TRIUMF in Canada and for the conceptual design, scoping and preliminary design of the scintillating fiber muon tracker for the Muon Ionization Cooling Experiment at the Research Applications Laboratory. He has more than 230 publications.

DAVID MORRIS

Center for Integrated Nanotechnologies (MPA-CINT)
Center Leader/Co-director

David Morris is the co-director and center leader for the Center for Integrated Nanotechnologies (CINT), one of five DOE Office of Science Nanoscale Science Research Centers. Morris received his PhD in analytical chemistry from North Carolina State University, specializing in electrochemical and spectroscopic studies of transition-metal complexes. He was a Robert A. Welch Foundation Postdoctoral Fellow at the University of Texas at Austin and a Director's Funded Postdoctoral Fellow at Los Alamos. He has been a technical staff member at Los Alamos National Laboratory since 1986 and has led projects for a variety of DOE and intelligence community sponsors. His research interests include the application of laser-based and conventional spectroscopic methods and electrochemical techniques; problems in transition-metal, actinide, and materials chemistry. He has more than 100 peer-reviewed publications and three book chapters with a citation count of more than 2,000 and an h-index of 26 on topics in transition-metal and f-element chemistry.

JOHN O'HARA
Center for Integrated Nanotechnologies (MPA-CINT)
Scientist

John O'Hara is a technical staff member in the Center for Integrated Nanotechnologies. He began work at Los Alamos National Laboratory as a postdoctoral research associate in MST-10 (2003-2004) and an IC Postdoctoral Research Fellow in MPA-CINT (2005-2006). His research interests are in the field of electromagnetic science and technology, with particular emphasis on ultrafast terahertz and optoelectronics technology. Most recently, he has engaged in numerous basic scientific studies of engineered materials for terahertz technology development via the plasmonics and metamaterials approaches. He is the principle investigator and leads a team of staff scientists and postdoctoral researchers on five metamaterials and terahertz research programs (two internal to LANL and three external) as well as serving as a key member in other ongoing research projects and CINT user programs. O'Hara's terahertz and metamaterials research has garnered several invited journal and conference publications, invited talks, and three patents in addition to more than 20 regular publications in numerous journals, including *Nature Photonics*, *Optics Letters*, *Optics Express*, *Applied Physics Letters*, and several others. He is also a frequent scientific reviewer for seven physics, optics, and electromagnetics journals.

WILLIAM REES, JR.
Global Security (PADGS)
Principal Associate Director

William Rees, Jr. is the principal associate director for Global Security at Los Alamos. He plays a key role in integrating strategy for non-nuclear weapons national security programs across the Laboratory.

Coming to Los Alamos from key leadership positions that include the Office of the Secretary of Defense, Department of Homeland Security, and Georgia Institute of Technology, Rees's credentials are broad and deep in both scientific research and national security. At the Pentagon, as Deputy Under Secretary of Defense for Laboratories and Basic Sciences, Rees was responsible for providing scientific leadership, management oversight, policy guidance, and coordination of the more than $1.8 billion annual Basic Research (6.1) programs of the Military Services and Defense Agencies.

In addition, at OSD Rees was responsible for defense laboratories policy for a workforce of more than 45,000 scientists and engineers, international S&T programs, DoD science, technology, engineering, and mathematics (STEM) education and workforce issues and grants policy. He was the U.S. S&T lead to NATO and the US principal on the NATO Research and Technology Board. Prior to his service in DoD, he was with the DHS S&T Directorate.

Rees has earned BS (Texas Tech University) and PhD (UCLA) degrees in chemistry and is a Fellow of several national and international professional societies. He held a postdoctoral fellowship at MIT and was a Humboldt Research Fellow at Technische Universitaet in Germany. He has chaired and served on numerous national and international scientific committees, panels, commissions, and task forces. He has been a professional journal editor, and he served on the international advisory boards of six technical journals—including as a founding board member for *Advanced Materials*, the most cited journal in the profession.

Rees has more than140 publications, has edited 1 book, holds 7 patents, and has delivered invited technical lectures at more than 20 international meetings, more than 75 universities and more than 200 other locations.

Rees is widely recognized internationally as a chemist and as leader in national security, basic research and national laboratory policy. He has been an external PhD examiner at several international universities. For more than a decade prior to entering federal service, Rees was a full professor and director of the Molecular Design Institute at Georgia Tech, where he mentored 23 undergraduate research students, 19 graduate research students, and 20 postdoctoral fellows.

JOHN L. SARRAO

Science Program Office-Office of Science (SPO-SC)
Program Director

John Sarrao is the program director for Los Alamos National Laboratory's Office of Science Programs, a $100-million-a-year portfolio, and for MaRIE (Matter-Radiation Interactions in Extremes), LANL's signature facility concept that will provide transformational materials solutions for national security challenges. Since 2002, Sarrao has held leadership positions of increasing responsibility within LANL's materials community. He has also served on numerous U.S. Department of Energy Basic Energy Sciences Advisory Committee (BESAC) Subcommittees, helping to set strategic directions for materials research. Sarrao received his PhD in physics from the University of California, Los Angeles in 1993 based on thesis work performed at LANL. He returned to LANL as a technical staff member in 1997 following postdoctoral research with Zachary Fisk at the University of California, San Diego and the National High Magnetic Field Laboratory in Tallahassee, Florida. Sarrao's primary research interest is in the synthesis and characterization of correlated electron systems, especially actinide materials. He is the coauthor of more than 520 publications, including 56 papers in *Physical Review Letters*, *Nature*, and *Science*. These publications have been cited more than 9,000 times. He was the 2004 winner of the LANL Fellows Prize for Research, in part for his discovery of the first plutonium superconductor and is a Fellow of the American Association for the Advancement of Science and the American Physical Society.

ALEXANDER SAUNDERS

Subatomic Physics (P-25)
Team Leader

Alexander Saunders has been a member of Physics Division at LANL since 1998, where he also received his PhD in nuclear physics from the University of Colorado in that year. Saunders is the P-25 team leader for proton radiography and also the run coordinator for the experimental effort at LANSCE. In Physics Division he has worked on two main projects: proton radiography and ultracold neutrons. The proton radiography project uses high energy protons from the LANSCE accelerator to produce multi-frame radiographs of dynamically driven objects, such as dynamic material failure and equation of state and high explosive burn, in support of the weapons program. The ultracold neutron project is a fundamental science effort to measure the parameters of the weak nuclear force through neutron beta decay, using the unique properties of ultracold neutrons to achieve smaller systematic uncertainties than any other technique. The ultracold neutron project is also based at LANSCE, using the high energy protons to produce the needed neutrons. Saunders is co-spokesperson and onsite lead investigator of this multi-institutional effort.

SUSAN SEESTROM

Experimental Physical Sciences (ADEPS)
Associate Director

Susan Seestrom brings to this position a combination of strong science credentials and management skills developed during her 20-year tenure at LANL.

In her recent role as associate director of Weapons Physics, Seestrom led six LANL divisions that executed program work in experimental, simulation, and weapons physics assessment. She directed the major line organization responsible for carrying out research and development for the weapons program and technical work in support of stockpile certification and assessment. She oversaw the operation of complex facilities, including the Dual-Axis Radiographic Hydrodynamic Test Facility, the Los Alamos Neutron Science Center, and the U1a laboratory at the Nevada Test Site.

Previously, Seestrom led the Physics Division at LANL for three years after serving as a deputy group leader in the Neutron Science and Technology group. Seestrom's personal research efforts focused on nuclear structure with medium energy probes and fundamental physics with neutrons. Together with Laboratory scientist Tom Bowles, Seestrom led the effort to develop an ultracold neutron source that culminated in demonstration of the world's most intense source of such neutrons. She received a Distinguished Performance Award for this work in 2001.

Seestrom holds PhD and BS degrees in physics from the University of Minnesota. She has published 135 papers and has had 1,663 career citations. She is a Fellow of the American Physical Society.

DARRYL SMITH
Physics of Condensed Matter and Complex Systems (T-4)
Laboratory Fellow

Darryl Smith works in the Physics of Condensed Matter and Complex Systems group (T-4) at Los Alamos. He received a BS degree in physics from St. Mary's College Winona, MN in 1968, served in the United States Marine Corps from 1969-1970, and received a PhD in physics from the University of Illinois in 1974. He was at California Institute of Technology from 1974-1980, Honeywell from 1980-1983, and joined LANL in 1983. His research interests are in condensed matter physics and electronic/photonic materials including III-V semiconductor heterostructures and nanostructures; the electronic and optical properties of conjugated organic materials, and electrical and electro-optic devices fabricated from these materials. He was a member of the Defense Sciences Research Council 1998-2005. His awards include A. P. Sloan Foundation Fellow (1977); W. H. Sweatt Award (1982); Los Alamos Fellow's Prize (1988); Los Alamos National Laboratory Fellow (1996); American Physical Society Fellow (2000); AAAS Fellow (2009).

ANTOINETTE (TONI) TAYLOR
Materials Physics and Applications (MPA-DO)
Division Leader

Antoinette (Toni) Taylor is the leader of the Materials Physics and Applications Division at Los Alamos. Prior to this position she was director of the Center for Integrated Nanotechnologies (CINT), a joint Sandia/LANL nanoscience research center funded through BES. Her research interests include the investigation of ultrafast dynamical nanoscale processes in materials and the development of novel optics-based measurement techniques for the understanding of new phenomena. She has published more than 250 papers in these areas, written 2 book chapters and edited 3 books. She is a former director-at-large of the Optical Society of America, topical editor of *Journal of the Optical Society B: Optical Physics*, and member of the Solid State Science Committee, Board of Physics and Astronomy, the National Academies, and chaired the National Academies' Committee on Nanophotonics Applicability and Accessibility. She is a member-at large, Division of Laser Science of the American Physical Society and OSA's representative to the Joint Council of Quantum Electronics. She is a Los Alamos National Laboratory Fellow and a Fellow of the American Physical Society, the Optical Society of America, and American Association for the Advancement of Science. In 2003, Taylor won the inaugural Los Alamos Fellow's Prize for Outstanding Leadership in Science and Engineering.

DAN THOMA
Institutes Office (INST-OFF)
Research and Development Manager

Dan Thoma is a research and development manager at LANL and director of the Materials Design Institute, a collaborative educational research program with the University of California, Davis. He received his bachelor's degree in metallurgical engineering from the University of Cincinnati and his master's degree and PhD in metallurgical engineering from the University of Wisconsin at Madison. Thoma's research interests include physical metallurgy, with a particular focus on microstructural development during materials processing. He has over 120 publications and 200 presentations, and his technical efforts have been devoted to alloying theory, the thermodynamics and kinetics of phase transformations (both liquid/solid and solid/solid transitions), and property response as a function of microstructural evolution. Thoma has been active within The Minerals, Metals, Materials Society (TMS), having served as 2003 TMS President, on the board of directors as programming director, and as chair and member of multiple committees. He is also active within the American Institute of Mining, Metallurgical, and Petroleum Engineers (AIME), where he is the past president. Thoma is also president of the Federation of Materials Societies, and a newly elected member to the board of trustees for the United Engineering Foundation. He received the 2007 Distinguished Service Award from TMS, LANL's 2007 Fellow's Prize for Leadership, and was US Chair for a Joint Working Group on Nuclear Materials with the United Kingdom. His materials expertise was recognized in 2008 by being elected as a Fellow of ASM International.

TERRY WALLACE

Science, Technology & Engineering (PADSTE)
Principal Associate Director

Terry Wallace is the principal associate director of Science, Technology, and Engineering, which is responsible for all basic science programs at Los Alamos, and coordinates the activities of the four science and engineering directorates. During the period of 2005 to June 2006, Wallace was the associate director of the Strategic Research Directorate, which encompassed LANL's science program offices and the five line divisions that implemented those programs and supported LANL's nuclear weapons, threat reduction, and energy security missions. He was also responsible for LANL's non-National Nuclear Security Administration Department of Energy programs, including basic science, energy technology, and environmental technology. Before becoming the associate director for Strategic Research, Wallace was the division leader of the Earth and Environmental Sciences Division.

Raised in Los Alamos, Wallace returned in 2003 after 20 years as a professor of geosciences and an associate in the applied mathematics program at the University of Arizona. In addition to teaching, he carried out research on global threat reduction, nonproliferation verification, and computational geophysics. During his academic career, he worked with LANL on nuclear test monitoring and threat reduction, in particular on interpreting the indications of nuclear testing by a foreign government. He has an international reputation in geosciences as applied to national security issues.

Wallace holds PhD and MS degrees in geophysics (California Institute of Technology) and BS degrees in geophysics and mathematics (New Mexico Institute of Mining and Technology). He is the author or coauthor of more than 80 peer-reviewed publications on seismology and tectonics, including ground-based nuclear explosion monitoring and forensic seismology. He also wrote a widely used textbook on seismology. Wallace is a Fellow of the American Geophysical Union (AGU), and in 1992 he received the AGU's Macelwane Medal. Wallace has served as president of the Seismological Society of America, chairman of the Incorporated Institutions for Research in Seismology, and authored the position paper for the American Geophysical Union on the verifiability of a comprehensive test ban treaty. He has testified before Congress on the comprehensive test ban and participated in numerous National Academy panels, including ones on research in support of comprehensive test ban monitoring. From 2000-2006, Wallace was the chair on the National Research Council's Committee on Seismology and Geodynamics.

ANNA ZUREK

Structure/Property Relations (MST-8)
Group Leader

Anna Zurek is the group leader of MST-8. Zurek joined the Laboratory in 1985 as a staff member in MST-5 where she studied damage and fracture of materials under dynamic loading conditions. Prior to joining Los Alamos she was employed at Rockwell Science Center as a research scientist studying fatigue fracture in aerospace materials, hydrogen embitterment and properties of metallic vapor deposited circuits on silicon and gallium-arsenate wafers.

Since 2002, Zurek has been with the management team at Los Alamos National Laboratory in several different capacities: deputy group leader, group leader of MST-8, and from August 2006–October 2007 as acting deputy principal director for Science, Technology and Engineering.

Her professional interests include physical metallurgy, high strain rate deformation, fracture characterization and modeling, structure-property relationship, and general materials science. As a staff member, she was devoted to hard-core science, programs development, mentoring postdoctoral researchers, undergraduate and graduate students, junior staff, and technicians. During 1993-1996 she was a member, vice-chair, and chair of the postdoctoral committee, two-term panelist advisory for National Science Foundation (1996). In 2002 she served on the Fellows Selection Committee. In 1998 she received the prestigious Maria Sklodowska-Curie International Fund II Award funded for three years. In 1997 and 2002 she received Los Alamos National Laboratory Achievement Awards. Zurek holds a master's degree form The University of Mining and Metallurgy in her native Krakow, Poland and a PhD from the University of Texas at Austin. She is a member of ASM and DYMAT. Zurek is an author and co-author of more than 120 publications and delivered more than 70 presentations many of which were invited.

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2010 May 3-6

Los Alamos Materials

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Materials
Capability
Review
May 3 - 6

Los Alamos
NATIONAL LABORATORY
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National Academy of Engineering, a Fellow of ASM International, a Fellow of TMS-AIME, and a member of the Air Force Scientific Advisory Board. He is involved in several externally funded projects dealing with various aspects of the behavior of Ni-base and Ti-base structural alloys. He is also regularly invited as a speaker at conferences that deal with these subjects. From July 2001-June 2004 he was also dean of engineering at OSU. In 2003, he and Prof. Lütjering completed a book *Titanium*, published by Springer-Verlag. A second edition of the book was released in spring 2007.

While at General Electric Aircraft Engines, Williams was the general manager of the materials and process engineering department . In his general manager capacity, he had overall responsibility for the materials effort at GE Aircraft Engines. This included all research, development and the qualification of new materials and processes, including process developmental efforts with an extensive base of outside suppliers that manufacture a wide range of high value components. These business relationships included casting, forging, metal powder, wrought product and polymer composite materials and component suppliers. The internal GE program encompassed ceramic, metal and polymer matrix composites including fibers; the full range of metallic materials, intermetallic compounds, coatings and lubricants. It also included process development. In addition to materials research, development and qualification activities, Williams' department had the responsibility for generating, collecting, analyzing and presenting material property data for use in component design and life prediction.

Williams began his time at Rockwell International as a research staff member and then became the program manger for an inter-divisional technology program that supported technology transfer between the aircraft, space, rocket engine, nuclear power and electronics divisions. The period he was doing this coincided with the start-up phases of the B-1, the space shuttle and the space shuttle main engine programs. Each of these programs encountered their own materials manufacturing challenges and this became a major focus of the inter-divisional technology program.

LANS Science and Technology Committee Representatives

JOHN BERCAW
Department of Chemistry
California Institute of Technology

John Bercaw received his BS degree from North Carolina State University in 1967, his PhD from the University of Michigan in 1971, and undertook postdoctoral University of Chicago for one year. He joined the faculty at the California Institute of Technology as an Arthur Amos Noyes Research Fellow in 1972, and in 1974 he joined the professorial ranks, becoming professor of vChemistry in 1979. From 1985 to 1990 he was the Shell Distinguished Professor of Chemistry, and in 1993 he was named Centennial Professor of Chemistry. Bercaw has been a Seaborg Scholar at Los Alamos National Laboratory (2004), the Robert Burns Woodward Visiting Professor at Harvard University (1999), Visiting Miller Professor at University of California, Berkeley (1990), and in 1989-90 a Royal Society of Chemistry Guest Research Fellow at Oxford University. Bercaw

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consulted with Exxon for more than 20 years and is now a consultant with Dow. He has served on numerous panels for the Department of Energy and the National Research Council, has been a member of the University of California, Office of the President's Panel on Science and Technology for Lawrence Livermore, Lawrence Berkeley and Los Alamos National Laboratories since 1999, and is a member of the LANS Science and Technology Committee. His research interests are in synthetic, structural and mechanistic organotransition metal chemistry. Recent studies include metallocene catalysts for Ziegler Natta polymerization of olefins and investigations of hydrocarbon hydroxylation with transition metal complexes.

ROCHUS (ROBBIE) VOGT
California Institute of Technology
Department of Physics, Mathematics & Astronomy

Rochus (Robbie) E. Vogt is the R. Stanton Avery Distinguished Service Professor and Professor of Physics, Emeritus at the California Institute of Technology (Caltech), where he began his service in1962. Dr. Vogt has served as chairman of the faculty, as chairman of the Physics, Mathematics, and Astronomy Division, and as vice president and provost at Caltech.

A recipient of the NASA Exceptional Scientific Achievement Medal, Vogt was the chief scientist at Caltech's Jet Propulsion Laboratory in 1977-78 and was acting-director of Caltech's Owens Valley Radio Observatory in 1980-81. He served as the director and principal investigator of the Caltech-MIT Laser Interferometer Gravitational-Wave Observatory (LIGO) Project from 1987-1994. He is a U.S. citizen, born near Heidelberg, Germany in 1929, studied as a Fulbright Fellow, and earned his doctorate in 1961 at the University of Chicago, which has honored him with the Alumni Association's Professional Achievement Award. Before coming to Caltech, he worked at the Enrico Fermi Institute for Nuclear Studies at the University of Chicago. His research career has focused on astrophysical aspects of cosmic radiation, gamma-ray astronomy, and gravitational-wave astronomy. Vogt has done extensive consulting work with government and industry. He has been a member of NASA's Physical Sciences Committee, and of the University of California (UC) Scientific & Academic Advisory Committee for the Los Alamos and Lawrence Livermore National Laboratories. He currently serves on the UC President's Council on the National Laboratories and chairs its Science and Technology Panel. He also serves on the LANS LLC Science and Technology Committee. He has served as vice chairman of the board of directors of the California Association for Research in Astronomy; he also serves on the board of directors of International Rectifier Corporation, a semiconductor company. In 1982, Vogt was honored as Caltech's first R. Stanton Avery Distinguished Service Professor.

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Emergent Phenomena – CINT Overview

David E. Morris

Co-Director and Center Leader

Center for Integrated Nanotechnologies

Overview

- **Introduction to the Center for Integrated Nanotechnologies**
  - Distinguishing Characteristics
  - Some Performance Statistics and Comparisons
- **Scientific Structure and Focus of CINT**
  - The CINT Thrusts
  - Mapping to the Materials Strategy
  - Examples of Emergent Phenomena from the Thrusts
  - CINT Signature Initiatives
- **The Role of CINT in the NNSA Mission**
  - CINT / LANL Relationship
  - Mission-specific Research
- **Summary of the Emergent Phenomena Session**

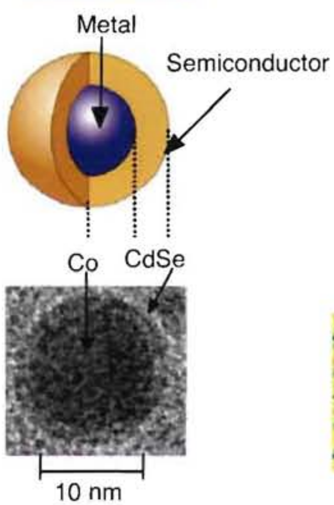
CINT: Distinctive Among the Five DOE Nanoscale Science Research Centers

- **A joint venture between Los Alamos National Laboratory and Sandia National Laboratories**
  - Two Laboratory – Single Center Model
- **Only NSRC associated with NNSA – all others at Office of Science labs**

CINT Signature: Focus on Nanoscience Integration

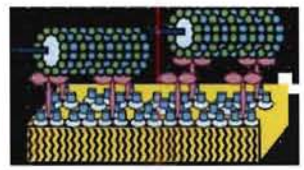
Assembling diverse nanoscale materials across length scales to design and achieve new properties and functionality – intrinsically emergent

Bifunctional Materials



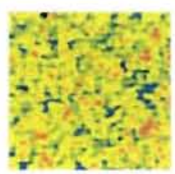
Combining ferromagnetic & semiconducting behavior

Directed Assembly

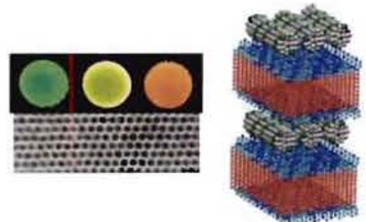


Microtubules + Motor Proteins

Nanocomposite materials

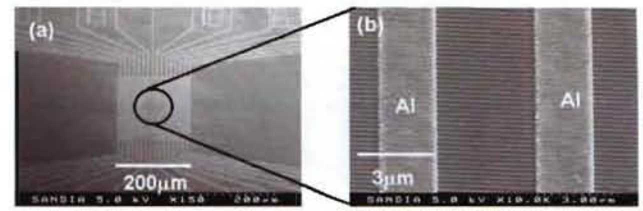


Nanoscale inhomgeneities



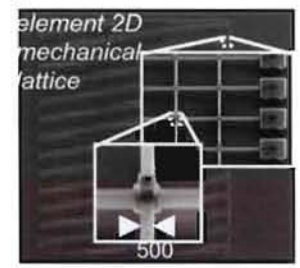
Engineered nanocomposites

Active Nanosystems



Nanowire arrays

Switchable metamaterials



Nanomechanical arrays

Nano → Micro

The Five DOE NSRCs and Co-located DOE User Facilities

Advanced Photon Source

Center for Nanoscale Materials
Argonne National Laboratory

Advanced Light Source

Molecular Foundry
Lawrence Berkeley National Laboratory

Center for Functional Nanomaterials
Brookhaven National Laboratory

National Synchrotron Light Source

LANSCE Lujan Center + NHMFL and MESA

Center for Integrated Nanotechnologies
Los Alamos National Laboratory & Sandia National Laboratory

Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

Spallation Neutron Source

CINT Technical Staffing (LANL & SNL)

- Scientists – 36 (all 0.5 FTE or higher *)
- Postdoctoral Researchers – 66 total
  - ✓ CINT supported – 17
  - ✓ Distinguished Fellowship – 12
  - ✓ Lab leveraged & CINT mentored – 37
- Graduate Students – 7
- Technologists – 14

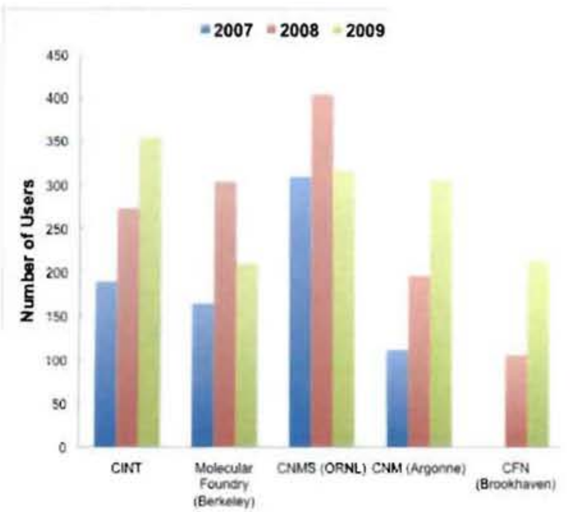
Recent CINT Scientist Hires:
Quanxi Jia, Stephen Doorn, Nathan Mara

** Other support from BES Core, LDRD, programmatic, etc*

NSRC Comparison: Key Statistical Areas

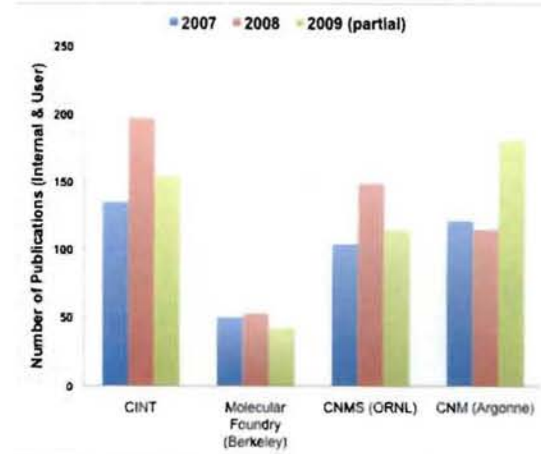
(individual NSRC web sites)

Users

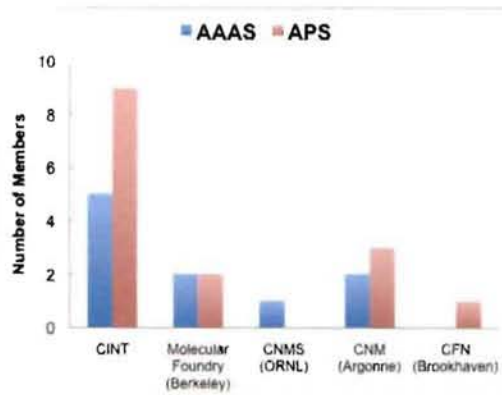


(http://www.sc.doe.gov/bes/users.htm)

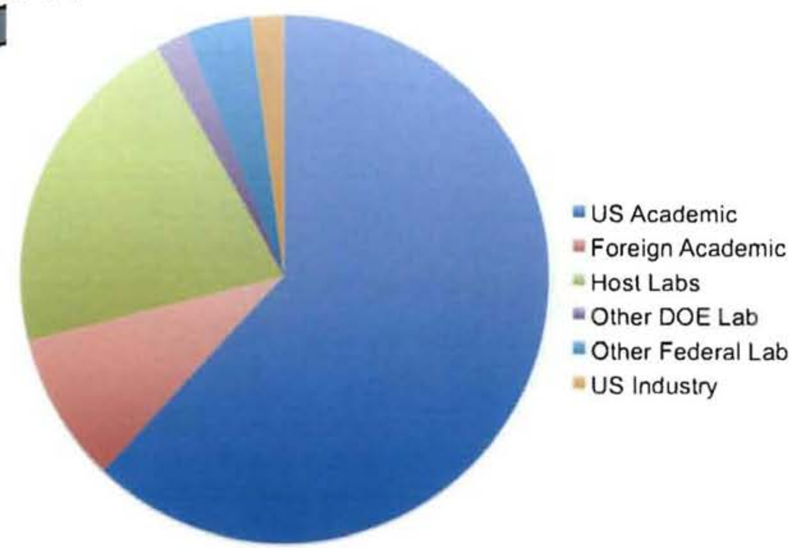
Publications



Society Recognition



CINT: User Facility Demographics

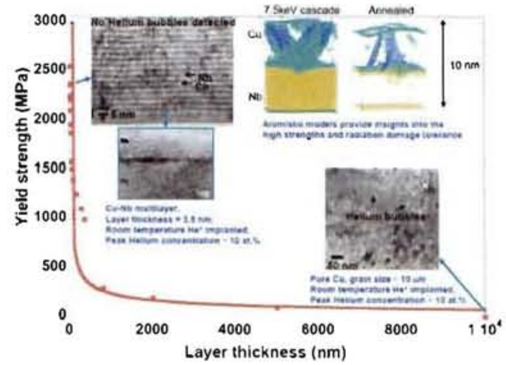


CINT: International Gateway to Nanoscience

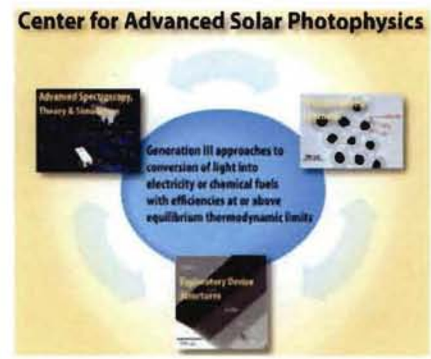
- *User Program and Postdoctoral / Student Staffing give CINT a true international flavor*
- *NNSA foreign national requirements are not a limiting factor*

CINT: A Key Role in the EFRC Initiative

- **CINT-led EFRCs**
  - Center for Materials at Irradiation and Mechanical Extremes (MIME)
    - PI: Mike Nastasi (w/ LLNL, UIUC, MIT)
  - Center for Advanced Solar Photophysics
    - PI: Victor Klimov (w/ NREL, Rice, UC…)



- **CINT Partnering Roles**
  - Science of Precision Multifunctional Nanostructures for Electrical Energy Storage
    - PI: Rubloff, U. Maryland (Hwang, Picraux)
  - EFRC for Solid State Lighting Science
    - PI: Simmons, Sandia (Prasankumar)
  - Photosynthetic Antenna Research Center
    - PI: Blankenship, Wash. Univ. (Montano)



CINT Science Structure: Four Thrusts

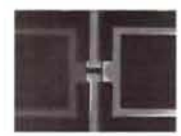
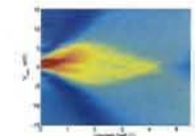
Nanophotonics & Optical Nanomaterials (NPON)

Synthesis, excitation and energy transformations of optically active nanomaterials and collective or emergent electromagnetic phenomena (plas -monics, metamaterials, photonic lattices)



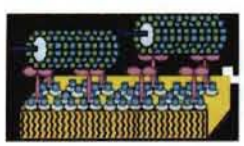
Nanoscale Electronics & Mechanics (NEM)

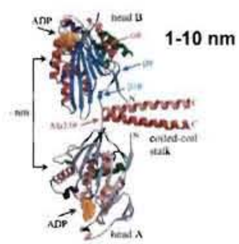
Control of electronic transport and wavefunctions, and mechanical coupling and properties using nanomaterials and integrated nanosystems


Soft, Biological, & Composite Nanomaterials (SBCN)

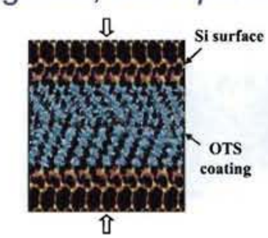
Solution-based materials synthesis and assembly of soft, composite and artificial bio-mimetic nano -systems

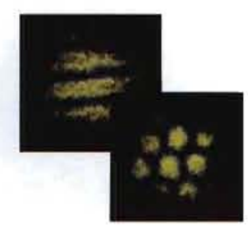




Theory & Simulation of Nanoscale Phenomena (TSNP)

Assembly, interfacial interactions, and emergent properties of nanoscale systems, including their electronic, magnetic, and optical properties



CINT Science – Mapping to the Materials Strategy

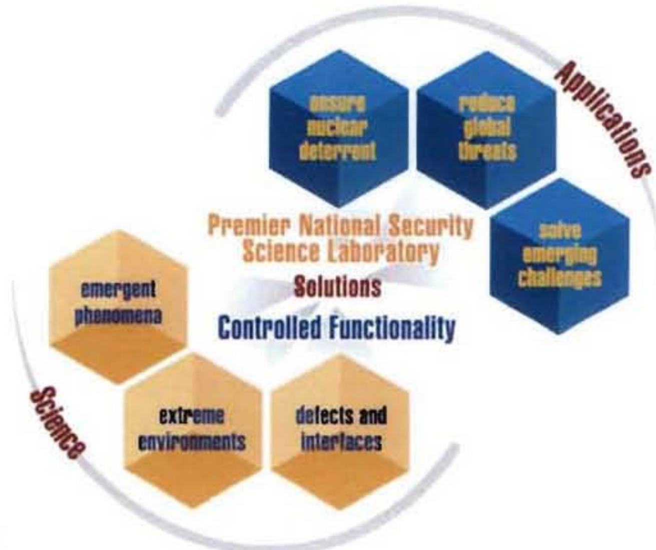
CINT Thrusts

NEM — Semiconductor heterostructures, Radiation-tolerant thin films

NPON — Photonic crystals, Metamaterials, Plasmonic structures

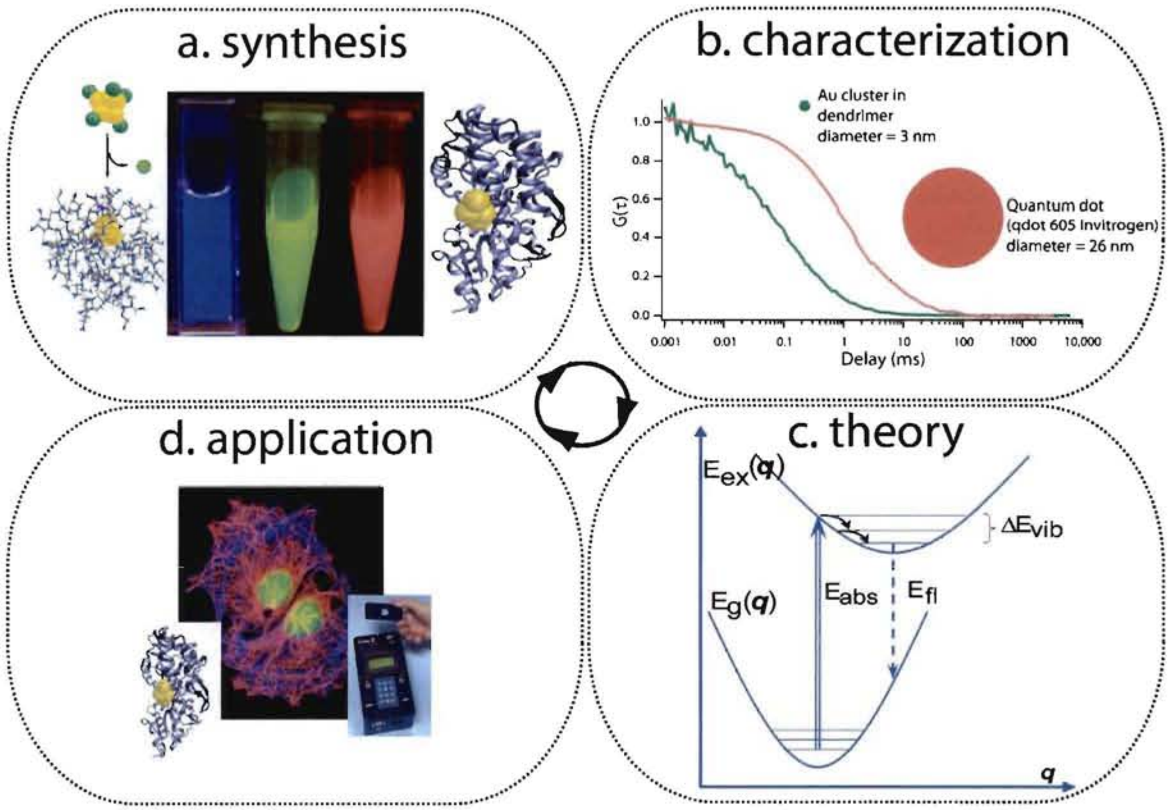
SBCN — Membrane nanocomposites, Biologically templated nano-structures

TSNP — Nanodomain / nanostructure interactions, Excitation / transport in nanostructures



Emergent Phenomena – SBCN Thrust Example

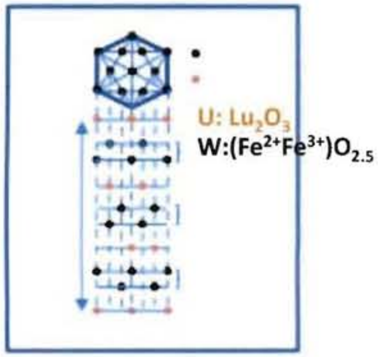
Predictive Design of Noble Metal Nanoclusters – Jen Martinez, PI



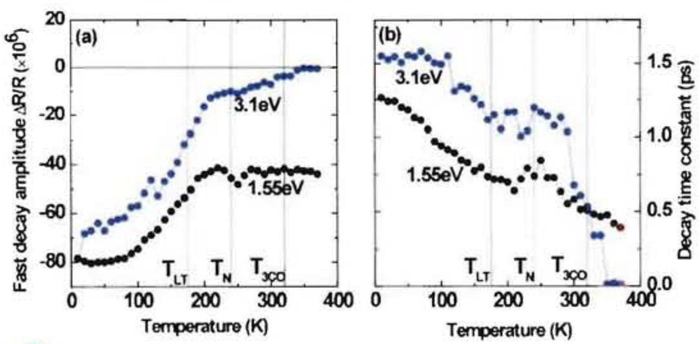
Emergent Phenomena – NPON Thrust Example

Ultrafast Polaron Dynamics in Multiferroic $LuFe_2O_4$ – R. Prasankumar, PI

Crystal structure of $LuFe_2O_4$ (unit cell)

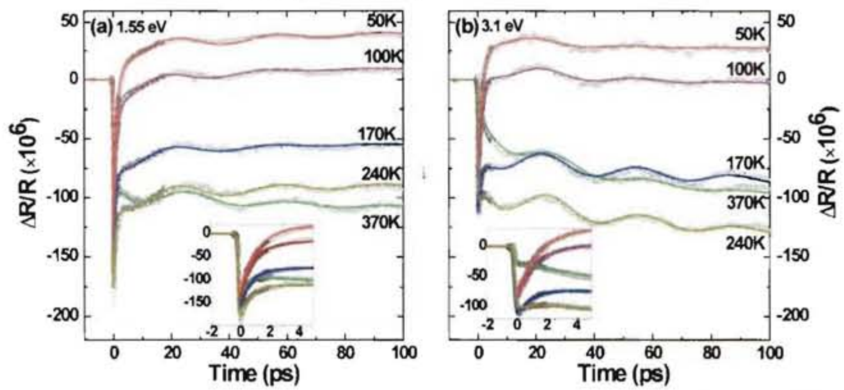


- First ultrafast optical experiments on this intensely studied multiferroic system reveal influence of charge and spin order on polaron dynamics
- $LuFe_2O_4$ is a frustrated multiferroic material with strong magnetoelectric coupling, even at room temperature
- ~100 fs difference in the initial decrease in $\Delta R/R$ between site-to-site and on-site excitation
- Frustrated triangular lattice leads to longer polaron redressing time (~1 ps compared to 500 fs in cubic systems)
- Strong spin-charge coupling influences the fast decay amplitude of the on-site excitation below T_N=240 K



Site-to-site excitation ($Fe^{2+} \rightarrow Fe^{3+}$ charge transfer)

Fe^{2+} on-site excitation

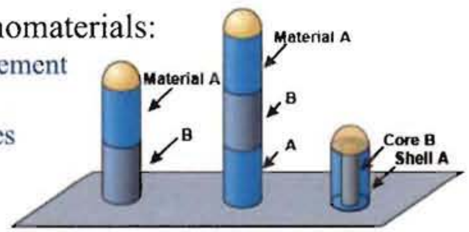


Emergent Phenomena – NEM Thrust Example

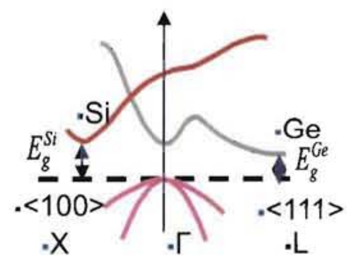
Si-Ge Nanowire Heterostructures – Tom Picraux, PI

Bandgap engineering

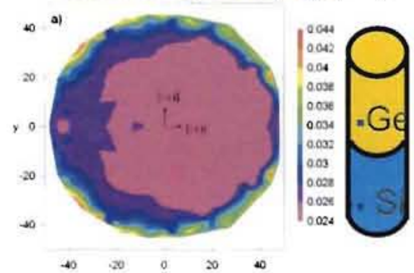
- Tailored nanomaterials:
  - carrier confinement
  - band offsets
  - doping profiles
  - strain



Properties

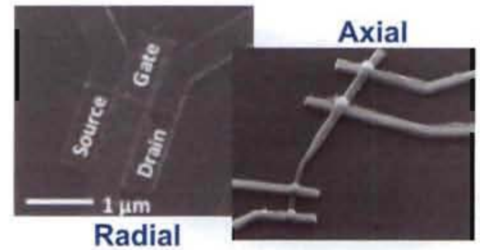


Strain Ge interface, ε_{xx}, (MD)

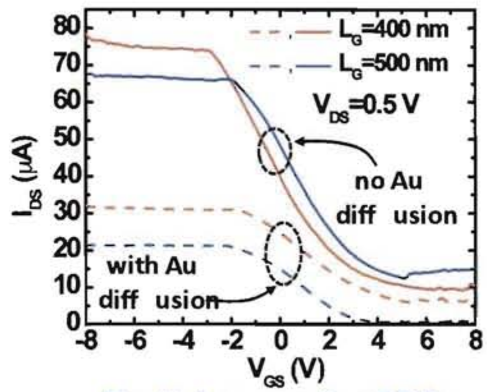


Prototype Devices

Axial



Radial

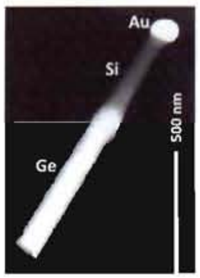


Radial nanowire FETs

Transfer curves: highest drive currents ever achieved in p-type materials.

Syntheses

Axial heterostructure



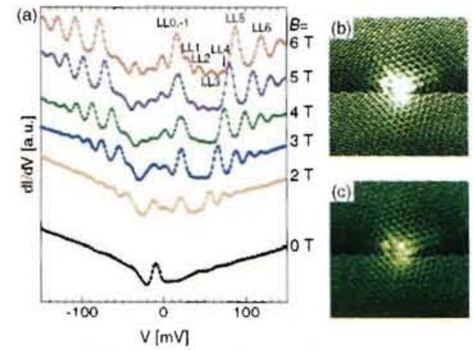
Radial Heterostructure

Nanowire Arrays

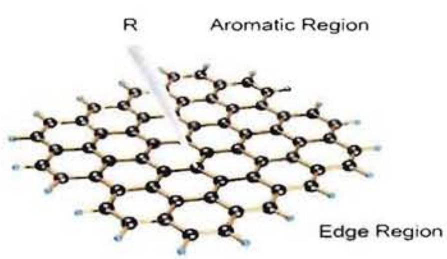
Emergent Phenomena – TSNP Thrust Example

Emergent Properties of Graphene (G) – Sasha Balatsky, PI

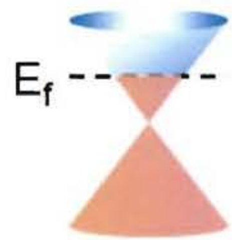
- **G - single atomic layer of carbon atoms**
  Discovered in 2004
- **Unusual electronic properties: Dirac point in the spectrum-> electronic control**
- **Novel states due to functionalization**
- **Goal: control and functionalization of electronics and optics of G**



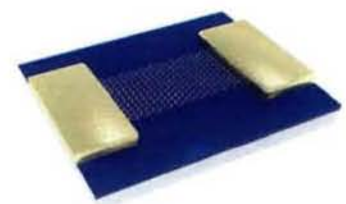
Modification of graphene states by dopants



functionalize →



change properties →

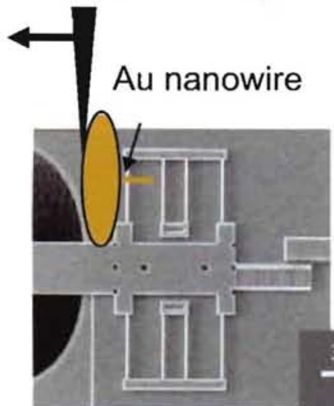


Graphene-based Device for Targeted Sensing

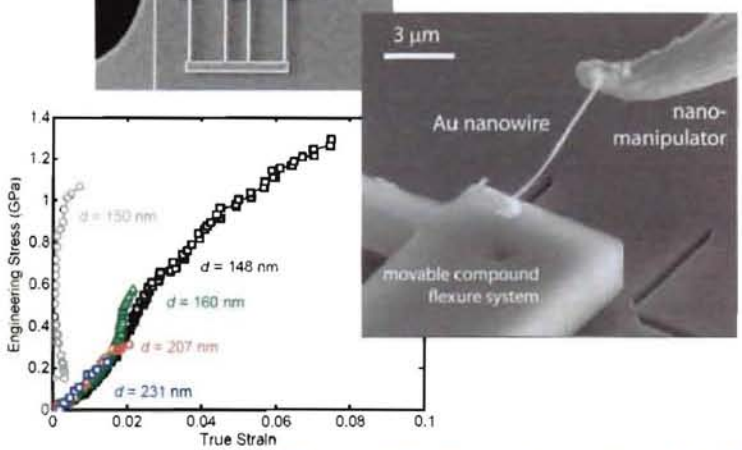
new materials, sensors

CINT Signature Initiatives – Discovery Platforms

Cantilever Array Discovery Platform™

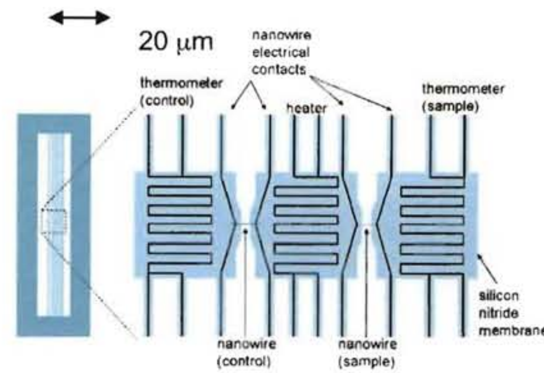


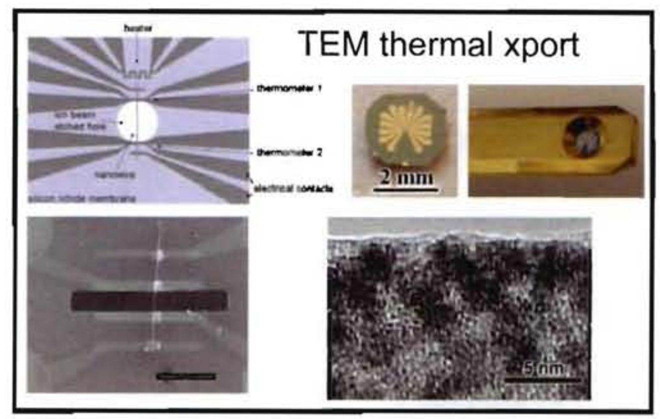
Rapid nanowire calibrated tensile testing



Quantitative tensile studies of of Au nanowires

Thermal Transport Discovery Platform



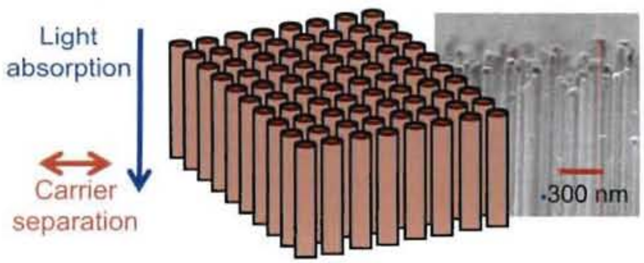


CINT Signature Initiatives – Integrated Focus Activities

Nanowires for New Energy Concepts

Photovoltaics ⟵ Energy Harvesting ⟶ Thermoelectrics

Discovery new ways to decouple and enhance light absorption and carrier collection



Discover new ways to independently control thermal and electrical energy flow

Integration Science Issues:

- Electrical transport in wires and at interfaces
- Optical & optoelectronic excitation of nanowires
- Thermal transport in wires and at interfaces

50 related user projects

The Symbiotic CINT / LANL Relationship

- **Value of CINT to LANL**
  - Outstanding people, expertise, capabilities
  - LANL access to CINT facilities and expertise
  - Enabling new programs (BES, Energy, TR)
  - Partnership with Sandia
  - Strong connections to LANL Materials Strategy and MaRIE

- **Value of LANL to CINT**
  - Access to LANL capabilities and facilities including Lujan and NHMFL
  - Connections to LANL Institutes and Centers for outreach and science enhancement
  - Competitive engagement in LDRD process
  - Programmatic opportunities to extend CINT science

CINT: A Valued Enabler of Mission Relevant Research

Examples of Recent CINT User Projects led by LANL PIs

- **Nuclear Deterrence**
  - Quantum control of initiation in nanoenergetics [Dave Moore DE-9]
  - Nanoscale plasticity within energetic single crystals [Kyle Ramos, DE-9]
  - Physical and optical characterization of thin-films for laser-driven shock compression experiments [Dan Eakins, DE-9]
  - Mechanical properties of nanocrystalline substructures in regions of shear localization [Ellen Cerreta, MST-8]
  - Nanomechanics of irradiated materials [Peter Hosemann, MST-8]
- **Global Threat Reduction**
  - A versatile protein-based nanobio sensor [Dung Vu, C-PCS]
  - Agile plasmon filters [Amy Ross, MST-16]
  - Visualization applied to molecular scintillator design [Rich Martin, T-1]
  - Morphology and composition of gamma-ray glass scintillators [Markus Hehlen, C-CDE]

Emergent Phenomena

- **Oral Presentations**
  - Novel Functional Semiconductor Nanocrystal Quantum Dots and Nanowires for Applications Involving Energy Conversion – Jennifer Hollingsworth, C-PCS
  - Nanoscale Features in Graphene – Sasha Balatsky, T-4
- **Poster Presentations**
  - Supported Lipid Membranes on Nanoporous Metals – Andrew Dattelbaum, MPA-CINT
  - Gold and Silver Nanoclusters for Detection of Biological Materials – Tim Yeh, MPA-CINT
  - Multiplex Detection of Pathogen-Biomarkers using Biosensor – Harshini Mukundan, C-PCS
  - Acoustically Engineered Materials using Acoustic Radiation Force – Dipen Sinha, MPA-11
  - Raman Spectroscopy of Chirality-Enriched Carbon Nanotubes – Steve Doorn, MPA-CINT
  - Epitaxial Nanotwinned Cu – Nan Li, MPA-CINT
  - Optical Switching with a Negative Index Metamaterial – Keshav Dani, MPA-CINT
  - Optical Spectroscopy of Individual "Giant" Quantum Dots – Han Htoon, C-PCS
  - Probing Properties and Dynamic Response at Nanoscale – Dzmitry Yarotski, MPA-CINT
  - Subwavelength Photonic, Plasmonic and Hybrid Waveguiding – Anatoly Efimov, MPA-CINT
  - A MaRIE first experiment: Nanostructured ferritic alloys – Nathan Mara, MPA-CINT
- **Gateway Tour**

Pages 51 - 60

MaRIE Update

John Sarrao

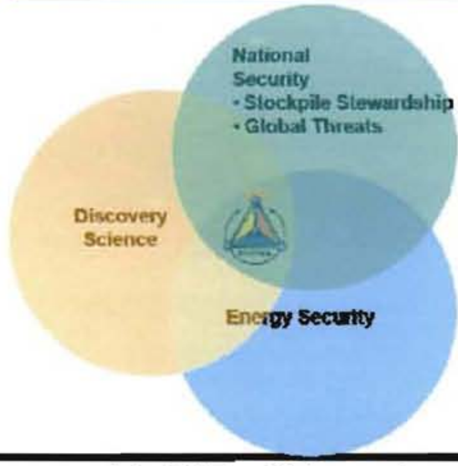
Objectives

- Current Definition: The Why/What/How of MaRIE
  - You've heard about MaRIE in past years
  - Is the story better?

- MaRIE FY10 Status & Plans
  - Defining a path to CD-0; LANSCE-R and beyond
  - Are we making progress on a credible plan?

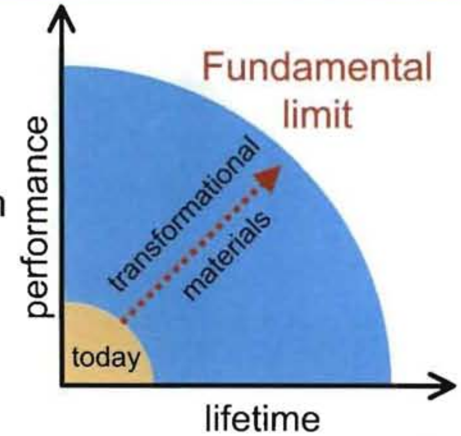
- Your Advice/feedback
  - How can you help (advocacy and promoting partnerships)?
  - Last Year:
    - " vastly more understandable this year with better differentiation of the LANL strengths. **Need to build support from the other Labs (Sandia and LLNL and non-DP Labs,) and industry.** "

MaRIE: Revolutionizing Materials in Extremes



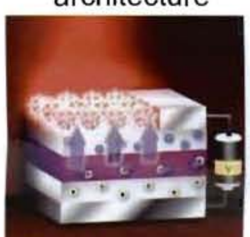
MaRIE addresses materials challenges across missions

MaRIE enables the transition from "observation" to "control"



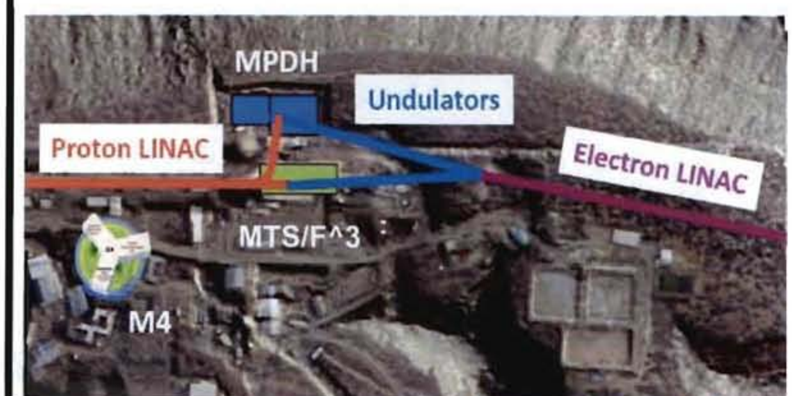
MaRIE will transform the science of microstructure, interfaces, and defects

Next-generation solar cell architecture



Radiation-induced swelling

MaRIE provides tools for transformational materials performance in extremes



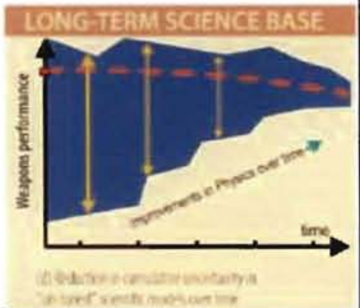
MaRIE Will Provide Dynamic Observations of Microstructure that Yield Control of Materials Needed to Reduce Costs & Increase Confidence for the Stockpile

Mission Need: Beyond the Predictive Capability Framework

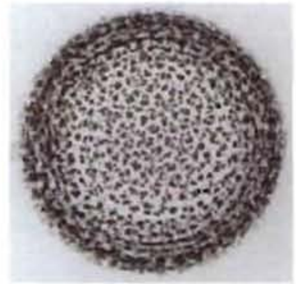
Enables complex transformation and the science base

Process Aware Models
- Enhanced Surety or Safety
- Confidence against aging

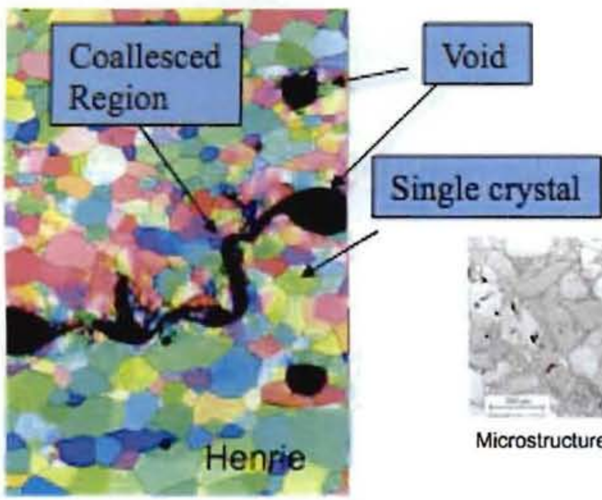
MATERIALS MATTER

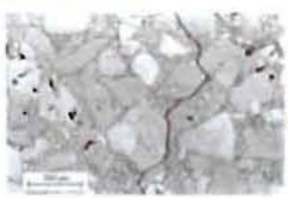


Process-based certification towards Product-based certification



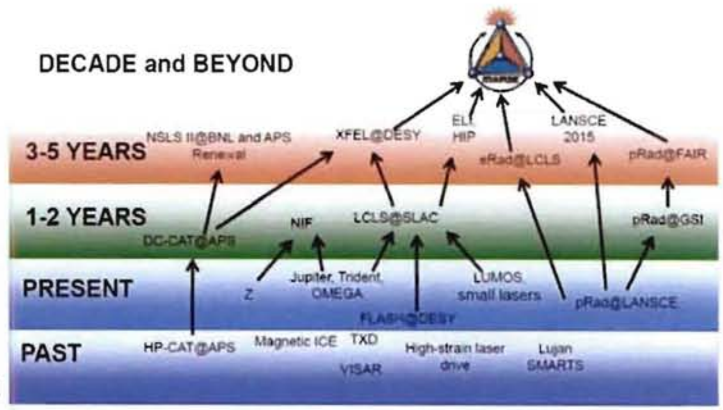
Micron-scale materials properties are key to uncertainties in many current knobs





Microstructure of PBX 9501

We are executing with DP the DC-CAT to MaRIE Roadmap



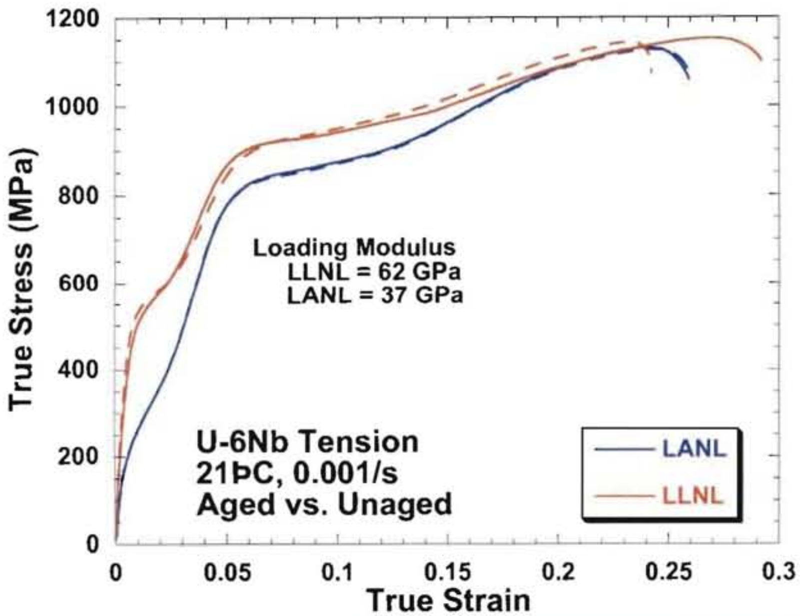
LASSIFIEI

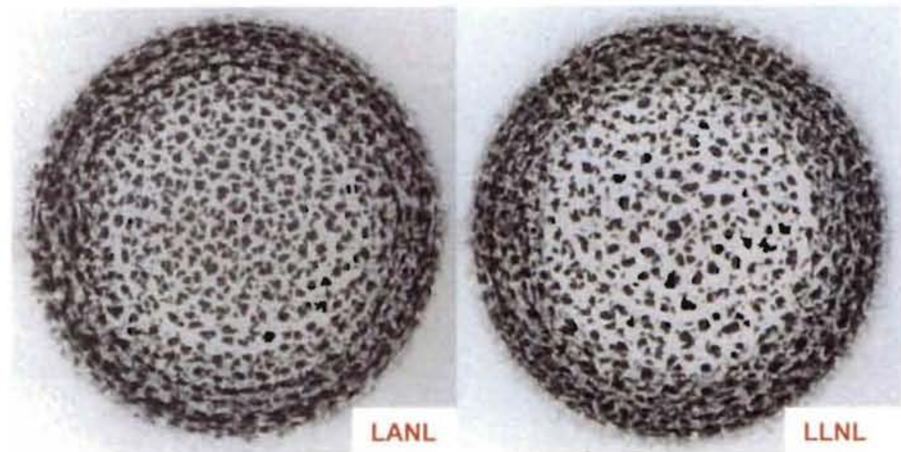
NNSA

Mechanical behavior and HE-driven fragmentation of U-6Nb show strong influence of metallurgical state

LANL = Solution treated / Quenched

LLNL = Solution treated / Quenched + Aged



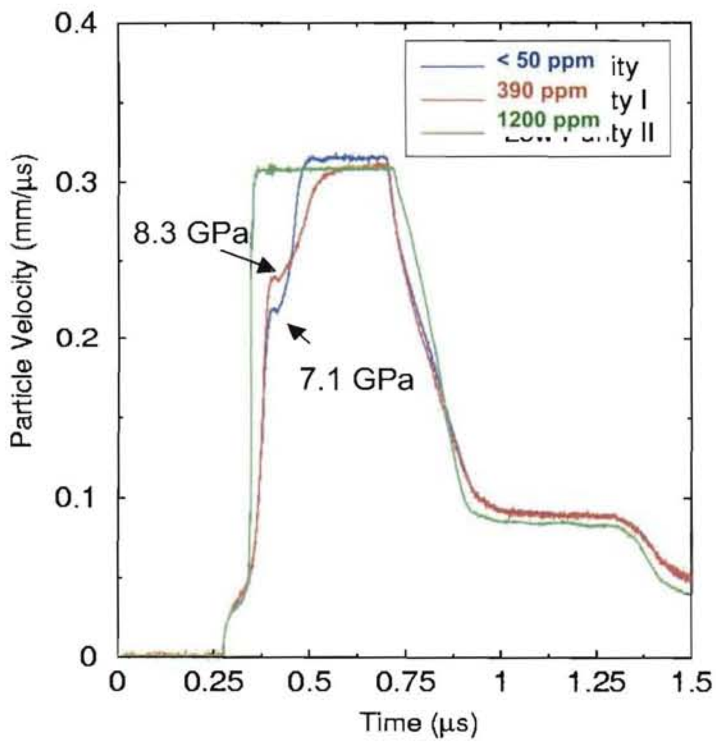


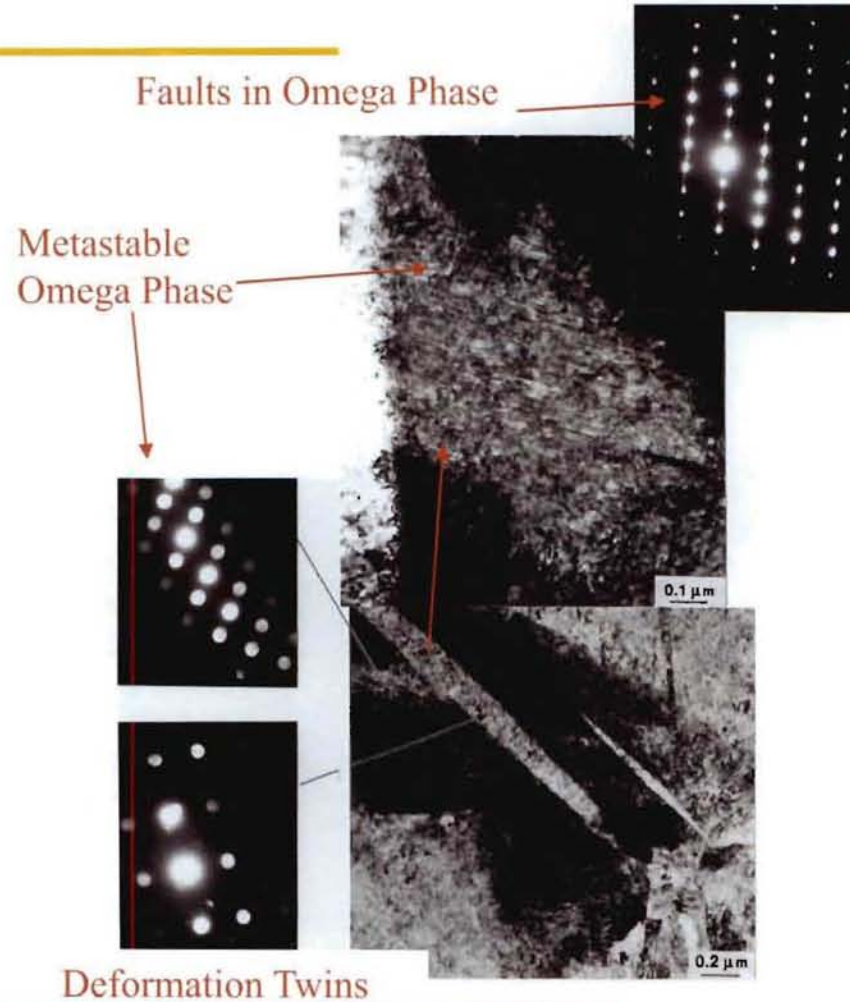
Quantitative analysis reveals 6σ difference in open area between images

Process-aware understanding of materials performance is lacking

Shock-induced phase transitions reveal spatially complex processes with strong materials sensitivities

Oxygen content suppresses the $\alpha - \omega$ phase transition in Zr

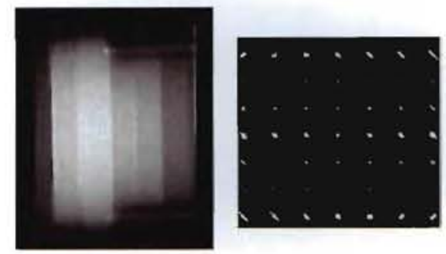




Predictive models must acknowledge that solids are an assembly of crystals that deform according to their local state of stress

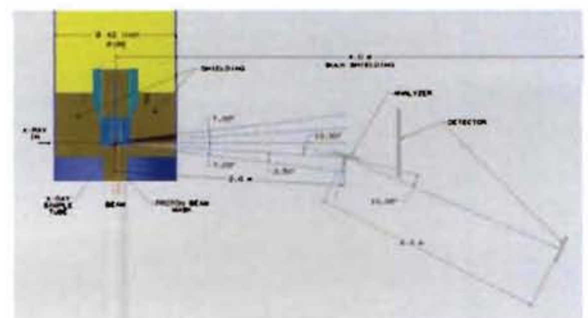
MaRIE : What does success look like?

- **Predicting materials performance, including failure, in extremes of pressure and strain for multi-phase materials**
- **Developing radiation resistant structural materials and fuels by design**
- **Exploiting complex materials and architectures for next generation electronics**



Simultaneous diffraction & dynamic density imaging

Defect manipulation in multiphase materials

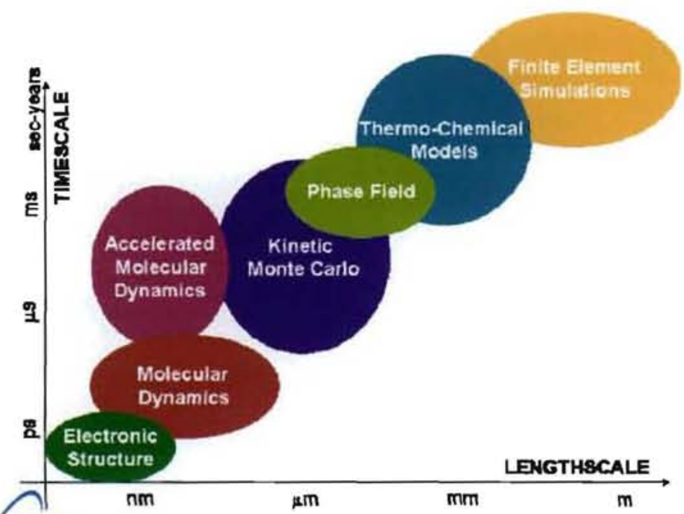


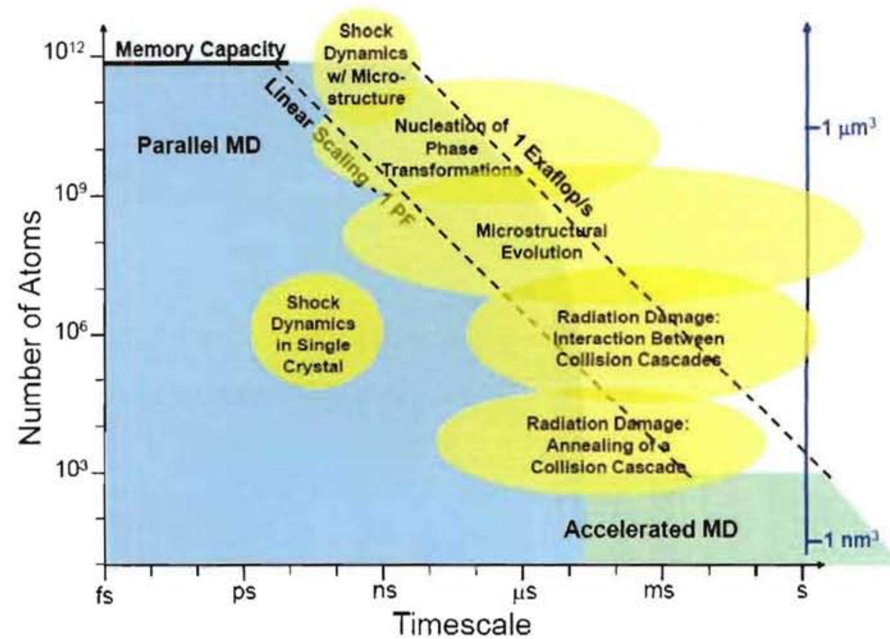
In situ characterization in extreme environments

In-situ, transient measurements on real materials in extremes

Experimental tools with unprecedented resolution are needed to validate and test the limits of modeling and simulation

One of the greatest challenges in multi-scale modeling is the physically-based treatment of defects and interfaces



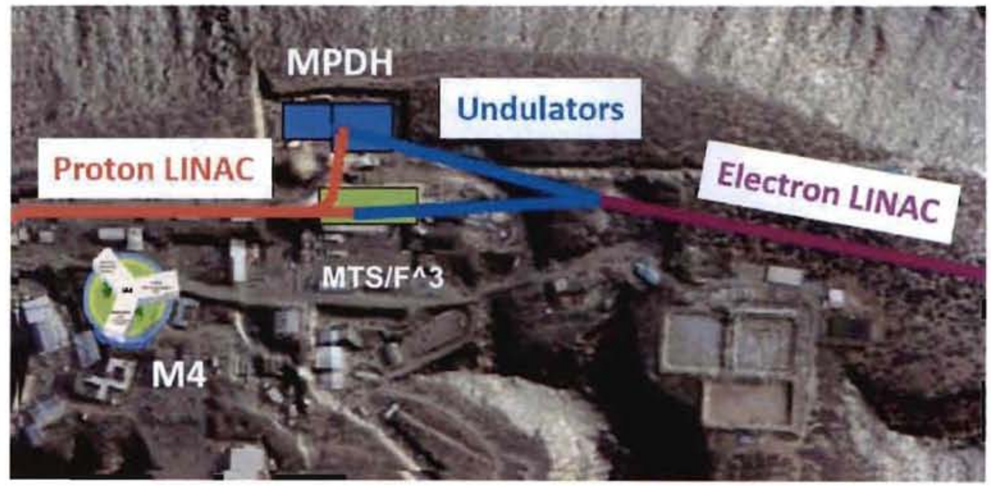


Anticipated advances in petaflop/s and exaflop/s computing – with advanced models - put us on the verge of accessing new phenomena on the micron scale

MaRIE provides the first comprehensive set of co-located tools to realize transformational advances in materials performance in extremes

First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

(MPDH: Multi-Probe Diagnostic Hall)



Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(F^3: Fission and Fusion Materials Facility)

Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(M4: Making, Measuring & Modeling Materials Facility)

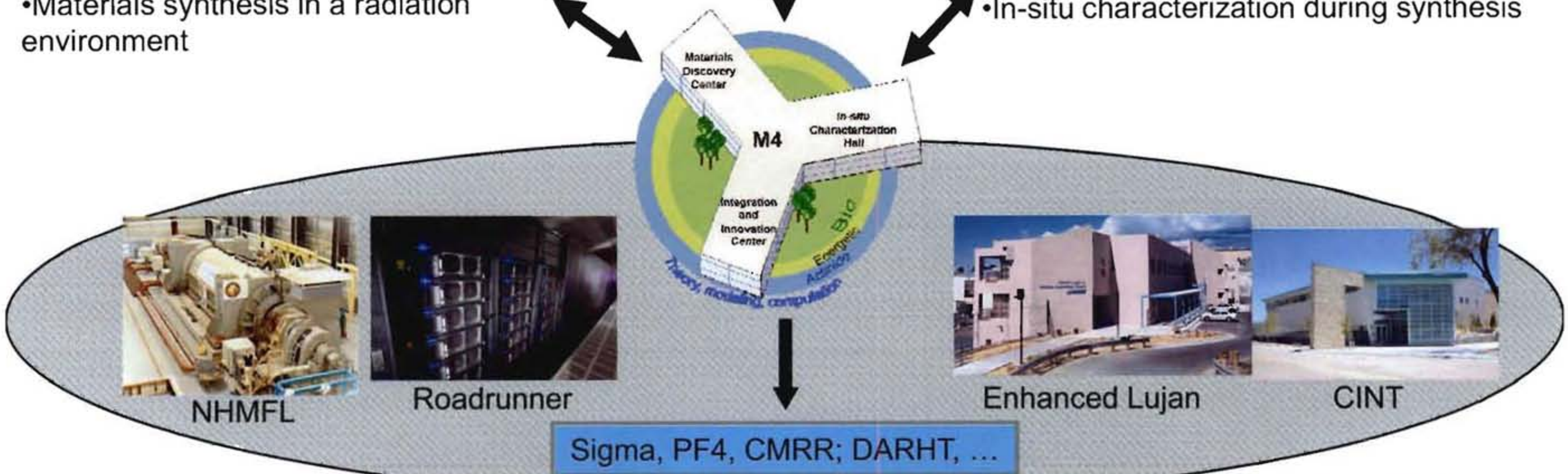
MaRIE will provide unprecedented international user resources

MaRIE: Integration is key – integrated facility capabilities and gateway to broader LANL

F^3
- Pre and post irradiation characterization
- Radiation hard materials
- Materials synthesis in a radiation environment

Portal to the External User Community

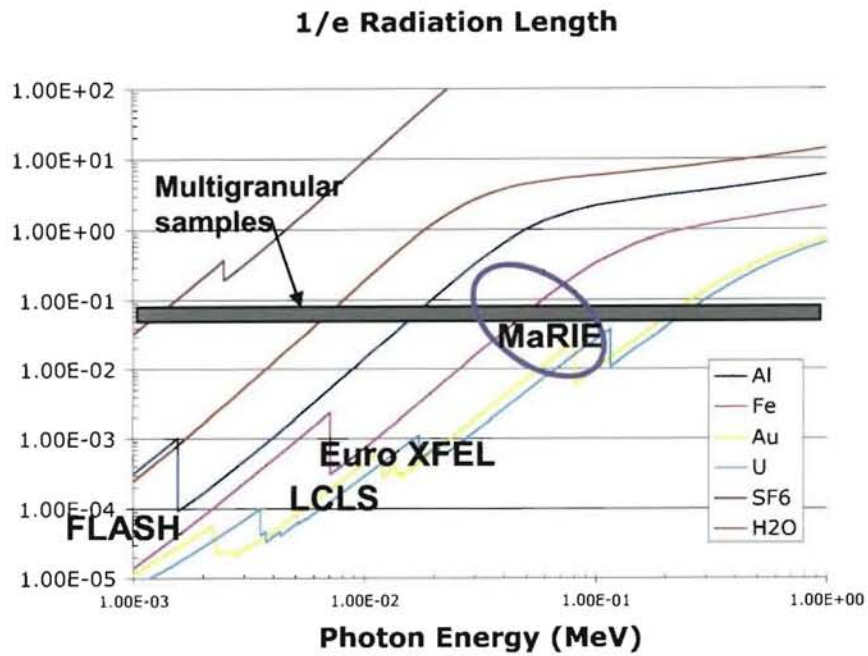
MPDH
- Samples with controlled microstructure
- Complimentary ultrafast characterization
- In-situ characterization during synthesis

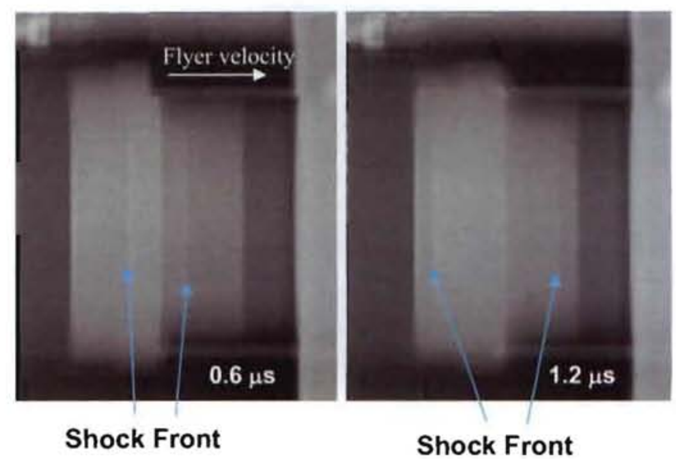


Integrated Solid State Solutions
- Materials with process-aware controlled microstructure
- New radiation hard materials (self healing materials)
- Next generation photovoltaics/Advanced radiation detectors

Through Multi-Probe Diagnostic Hall, MaRIE provides unique scattering and imaging capabilities to bridge the micron gap in extreme environments

A high-energy-photon (50-115 keV) XFEL allows multigranular sample penetration and multipulse dynamics without significant sample perturbation



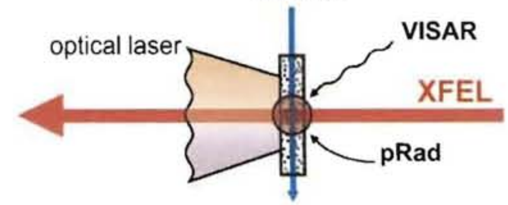


pRad absolute Density:
$\rho = 3.07 \pm 0.03$ g/cm^3 (1.1%)

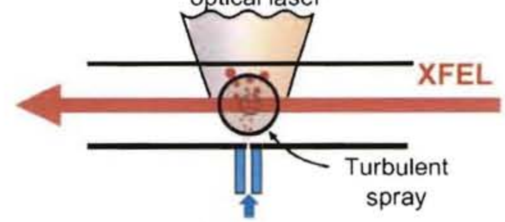
Meanwhile, proton microscopy can provide absolute density and velocities through the sample volume

Frontier experiments identify performance gaps that form the basis of MaRIE's functional requirements

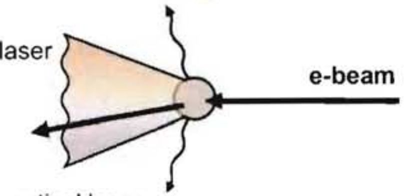
- **Meso-scale Material Dynamics**
  - Response of multi-granular material to dynamic deformation
  - Evolution of radiation-damage cascade
  - Micron-scale insights towards predicting high explosives
  - Includes key earth science materials



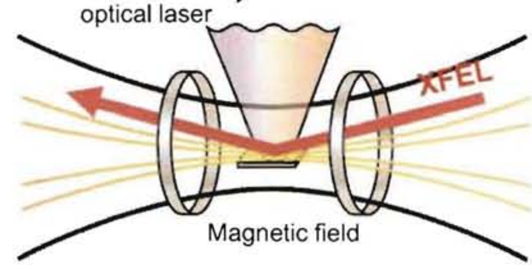
- **Multi-scale Fluid Dynamics**
  - Measure 3D multi-scale mean flow and turbulence
  - Variable material turbulent flows for diverse applications
  - Ability to measure *all* relevant scales for validation



- **Extreme Field Interactions with Matter**
  - Light intensities $>10^{24}$W/cm^2
  - 10–200 MeV gamma-ray nuclear physics



- **Emergent Phenomena in Complex Materials**
  - Ultrafast (10–100 fs) measurements in Extreme Environments



Facility Definition Process

Science-driven Requirements Lead to Integrated Facility Needs Fulfilled by MaRIE

User Driven Science → Materiel Needs → **Functional Requirements** → Alternatives Analyses → **Performance Gaps** → Preferred Alternative & Roadmap → **Facility Concept**

Decadal Challenges Report (01/10)

MaRIE 1st Expts (03/10)

MaRIE Technical Alternatives (06/10)

MaRIE Pre-Conceptual Definition (06/10)

Radiation Extremes

Thermal Transport

Phase Stability

Strength & Structural Integrity

Corrosion

Swelling

Control of Complex Materials & Processes

Superconductivity

High Explosives

Energy Conversion & Storage

Radiation Extremes

ironments

treme p, T, strain rat

gh-flux fast n irradiat

ecial nuclear & hazar

terials

ctronic state excitati

B extremes

surements

Microstructure

Crystallography, composition, phase, defect density

Imaging

Density, ejecta, particles, strain, cracks, corrosion layers, & interface control

Phys & Chem properties

Synthesis with Characterization

Ability to predict new mat'ls

Defect/interface control

-2s-1 fast n w/ relevant m, trans- n, He & H tion

keV coherent, t x-ray source

c charged imaging

Intense ion source for isochoric heating of solid matter to 10-100 eV

Extremely short optical photon pulses for pumping & probing

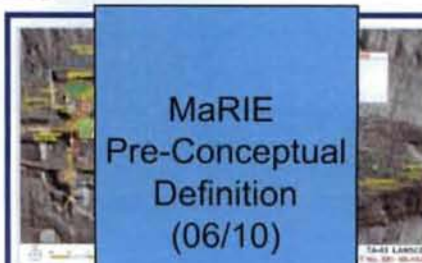
Synthesis capability

Single crystal growth

Metastable phases

Flexible fabrication & processing

10-nm control of 2D & 3D structures



Mar existing $B investments at LANSCE with the addition of the:

- XFEL
- Multiprobe Diagnostic Hall
- Fission-Fusion Materials Facility
- Making, Measuring, & Modeling Material Facility

We are actively engaging the scientific community through research needs workshops

Decadal Challenges for Predicting and Controlling Materials Performance in Extremes

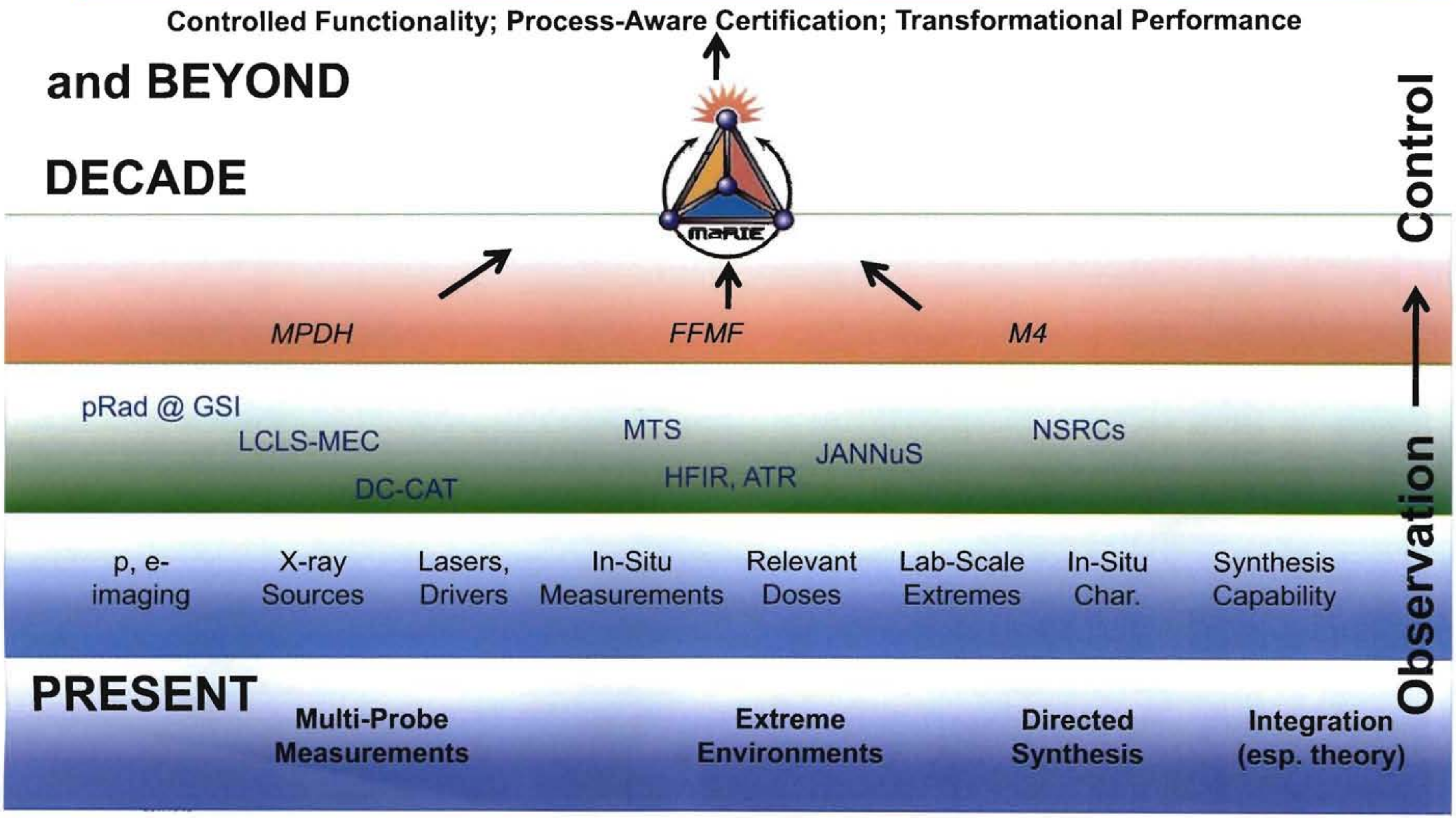
December 6 - 10, 2009 • Santa Fe, New Mexico

- **Jan 20-22, 2009** — **"Research Frontiers and Capability Gaps for Controlling and Designing Functional Materials**
- **July 29-31, 2009** — **"Structural Materials Under Extreme Conditions"**
- **Sept 21-23, 2009** — **"Opportunities for Studies of Activated Samples at National User Facilities"**
- **Sept 23-25, 2009** — **"21 st Century Needs in Compression Science"**

"...purpose is to identify the scientific challenges and research directions to achieve predictive materials performance in extreme environments...the workshop will focus specifically on needed capabilities and tools to seize this opportunity...Outcomes will be documented in a publicly available workshop report..."

External Workshop Leadership: Todd Allen, Steve Zinkle; Paul Follansbee, George Crabtree; Roger Falcone, Bob Cauble, Rus Hemley, Malcolm McMahon; Tony Rollett, Tomas Diaz de la Rubia, Richard Lesar

We have developed a Roadmap that identifies capabilities on the road to MaRIE and partnering opportunities



Consistent with our roadmap, we are fostering strategic partnerships

- National Laboratories

  -LLNL & SNL: nuclear weapons

  -ORNL & INL: nuclear energy

  -ANL & LBNL & SLAC, and FNAL: photon and proton accelerator development

  -SRNL, PPPL, BNL, PNNL, JLAB: ongoing outreach

  -Ames, NREL, NETL: initial interactions

- Universities

  -Key partners in community outreach/first experiments teams

    -typically not stewards of large-scale facilities

- Industry

  -Focus on consortia advocacy

    -pillar specific; lead with F^3

LANSCE remains a key step on the road to MaRIE AND an important institutional priority

- **LANSCE-R reached CD-1, Oct. 2009**
- **President's FY11 Budget request put LANSCE-R on the "to be terminated" list**
- **Actions being pursued:**
  - Convert existing project funding to operating/maintenance funding
  - Support ongoing operational funding to allow responsible stewardship/future reliability of LANSCE
  - Communicate importance of continuing LANSCE operations to weapons program within NNSA and to DOE (SC, NE)
  - Champion importance of experimental capabilities for materials in extremes for current and future weapons program needs

Department of Energy
Washington DC 20585

March 24, 2010

Dear Dr. Anastasio:

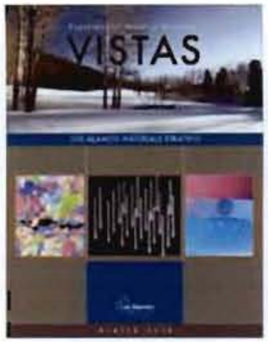
We are writing to clarify the Department's expectations for the future of the Los Alamos Neutron Science Center (LANSCE). LANSCE is currently performing programmatic research of importance to the National Nuclear Security Administration as well as fundamental science for the Office of Science (including the Lujan Center Neutron Scattering Facility for Basic Energy Sciences and the Isotope Production Facility for Nuclear Physics) and materials research and testing relevant to nuclear energy. We

Department of Energy missions. The Department's focus on materials under extreme conditions relevant to fission, fusion and nuclear weapon systems could provide a focal point for your consideration of the longer term science facility development at LANL. We encourage you to continue the process of engaging the broader community in order to frame the key scientific challenges in this area for the next decade. We look forward to hearing of your continued progress in defining the path forward.

Sincerely,

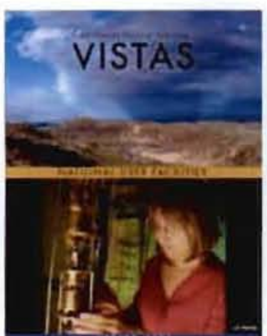
Thomas P. D'Agostino	Kristina M. Johnson	Steven E. Koonin
Under Secretary for Nuclear Security	Under Secretary for Energy	Under Secretary for Science

Following our materials strategy, we are doing MaRIE science now



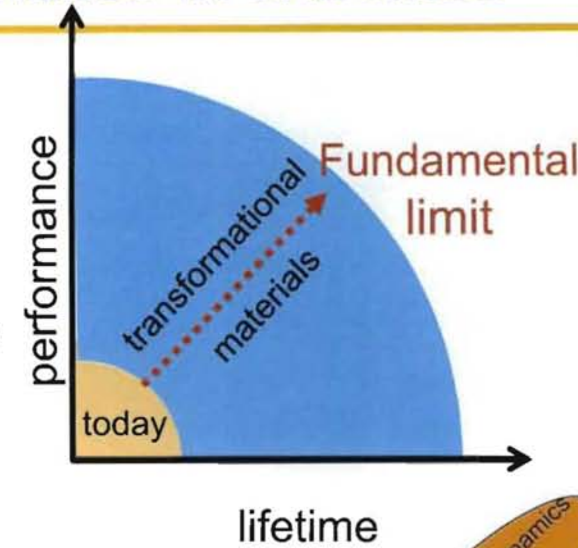
Current and *pending* MaRIE-relevant LDRD-DR investments

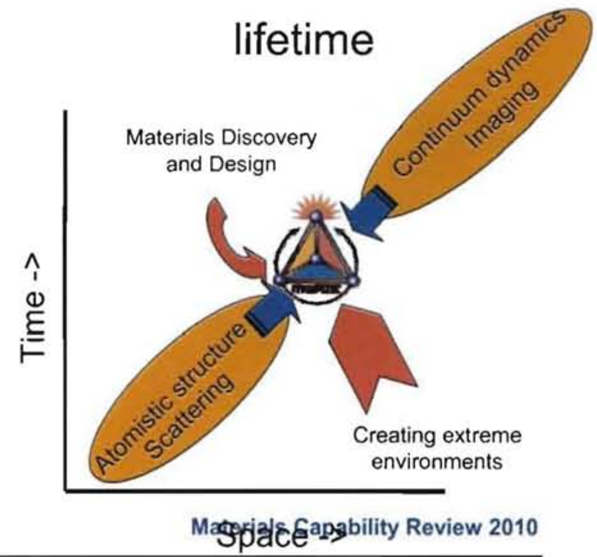
Kurt Sickafus	Advanced Fuel Forms with Microstructures Tailored to Naturally Induce Fission Product Separation During Service
Dana Dattelbaum	Hot Spot Physics and Chemistry in Energetic Materials Initiation
Rico Del Sesto	Design, Synthesis, and Theory of Molecular Scintillators
George Rodriguez	Ultrafast Nanoscale XUV Photoelectron Spectroscopy
Mike Nastasi	Enhance Radiation Damage Resistance via Manipulation of the Properties of Nanoscale Materials
Jen Martinez	Predictive Design of Noble Metal Nanoclusters
Filip Ronning	Understanding Anisotropy to Develop Superconductors by Design
Tim Germann	Spatial-temporal frontiers of atomistic simulations in the petaflop computational world
Darcie Dennis-Koller	Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage Evolution
Ivar Martin	Understanding and Controlling Complex States Emerging from Frustration
Quanxi Jia	Understanding, Exploiting, and Controlling Competing Interactions in Complex Oxides
Chris Stanek	*Radioparagenesis: Robust Nuclear Waste Form Design and Novel Materials Discovery*
Dana Dattelbaum	*First Reactions: Simple Molecule Chemistry Behind the Shock Front*
Robert Scharff	*Tunable explosive materials with on demand performance*
Irene Beyerlein	*Innovative and validated sub-micron to meso-scale modeling of the evolution of interface structure and properties under extreme strains*
Yongqiang Wang	*Characterization of Radiation Effects in Refractory Alloys using the Isotope Production Facility at LANSCE*
Bruce Carlsten	*Exploiting Hamiltonian Properties of Beams to Revolutionize X-Ray Free-Electron Laser Architectures*



MaRIE will be the first capability with unique co-located tools necessary to realize transformational advances in materials performance in extremes

- **"The micron frontier" is key to solving transformational materials grand challenges**
- **MaRIE will provide unique capabilities**
  - Accessing materials irradiation/damage extremes
  - Simultaneous *in situ* imaging & scattering measurements
  - Accelerating materials discovery and solutions through control of defects and interfaces
- **MaRIE provides unprecedented international user resources for the transition from observation to control**
- **Facility definition being driven by community-validated performance gaps & functional requirements**
- **LANSCE is essential for MaRIE's success**





First Principles Predictive Capabilities for Transuranic Materials: Mott insulators to metals

LDRD/DR: October 1, 2009

Eve Bauer, A. K. Burrell, Quanxi Jia, M. McCleskey, B. L. Scott

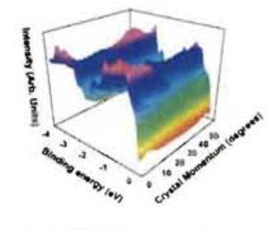
Tomasz Durakiewicz, Kevin Graham, John Joyce
Steve Conradson, Patrick Kennedy, Stosh Kozimor

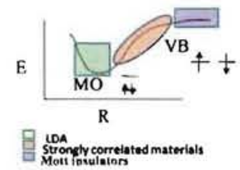
Enrique Batista, **Richard L. Martin,** Jianmin Tao, Tony Rappe (CSU)
Jason Ellis, Miguel Morales, Takeshi Tsuchimochi, Gustavo Scuseria (Rice)
Alberto Ambrosetti, Shi Guo, Kevin Rasch, Lubos Mitas (NCSU)

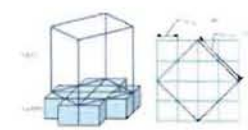
Los Alamos

What do we want to do and why?

We wish to develop a first principles predictive tool to describe the electronic structure and behaviour of strongly correlated actinide metals







Why do this?

none now exists: 'f-electron grand challenge'

actinide materials at core of LANL mission

Pu Center of Excellence

general tool needed

threat reduction (scintillators)

environmental contexts ($PuO_{2.25}$)

nuclear fuel cycles (UC, UN, UO_2),

weapons contexts (PuO_2, Pu_2O_3, δ-Pu)

radiation resistant materials

Why now?

transuranic capability in PAD

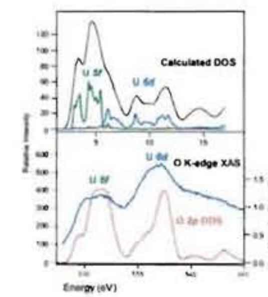
transuranic capability in ARPES

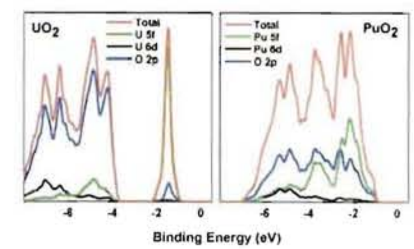
transuranic capability in XAS

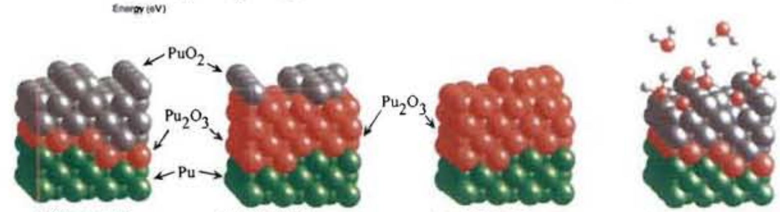
conceptual breakthroughs in theory

Why us?

capabilities unique to LANL







(a)Room T (b) 25 °C/Vacuum (c) 150 °C/Vacuum (d) Ambient, H_2O

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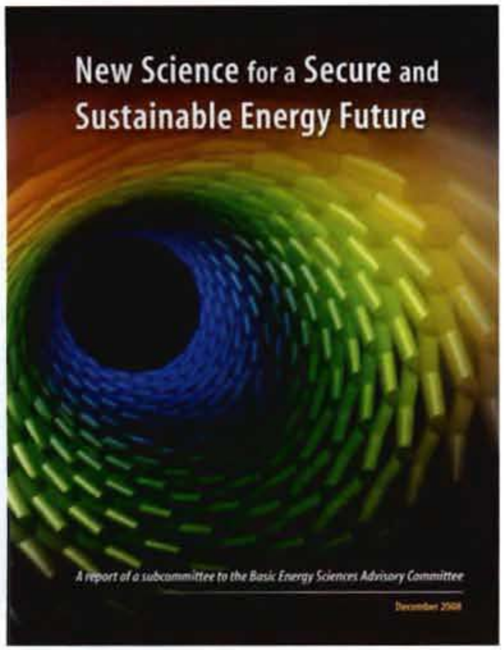
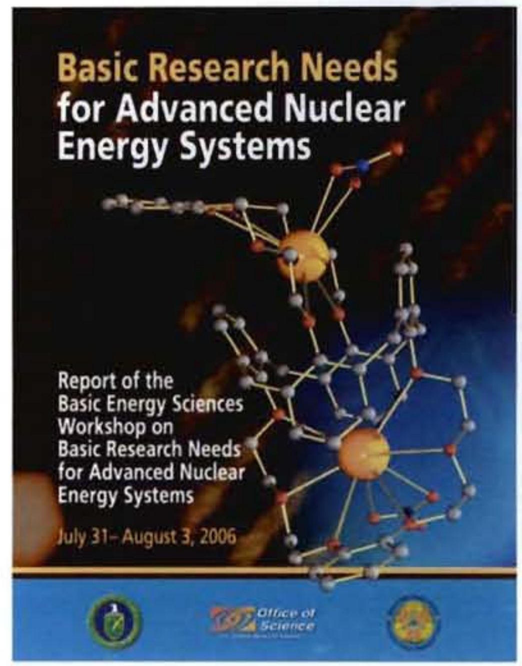
Significance



"The scientific challenge is to develop a well-formulated and predictive **first-principle theory** for relativisitic correlated *f*-electron materials and complexes" (p. 88, ANES)



"It will take 'dream teams' of highly educated talent, equipped with forefront tools, and focused on the most pressing challenges to increase the rate of discovery. To make progress most rapidly, these teams must work to close gaps between needs and **capabilities in synthesis, measurement, theory, and computation**" (New Science for a Secure and Sustainable Energy Future).

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The problem

Bristol (1937) : electrical conduction mechanisms

deBoer and Verwey : conductivity data
NiO, CoO, MnO, Fe_2O_3, Mn_2O_3, Mn_3O_4, Co_3O_4
all insulators – very surprising!
in ionic picture, all have partially filled d bands,
Bloch-Wilson band theory implies they should be metals

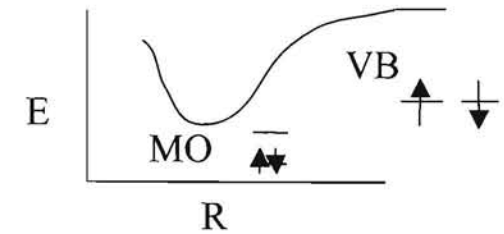
they suggested that when the barrier for tunneling between sites is large, there may be a critical range in which conductivity varies rapidly as a function of the barrier height

Wilson : noted the similarity with the sharp energy levels of the 4f electrons in rare earth compounds;

Peierls: suggested the Coulomb interaction between electrons caused them to localize on the cation sites, implying a drastic breakdown of band theory

Mott: chaired the conference, summarized these remarks for the published proceedings

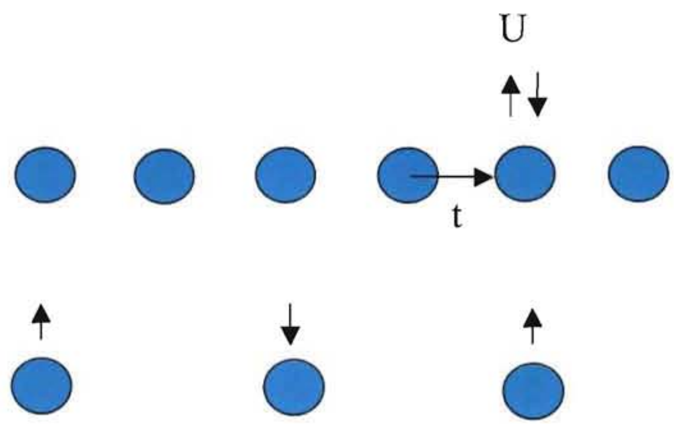
Mott insulators



Mott (1949); Hubbard (1955)
on-site electron–electron repulsion

molecular orbital vs. valence bond limit:
competition between delocalization and Coulomb repulsion
hopping (t) vs. on-site U

H_n



t/U large;
delocalized (metal)

t/U small;
localized (insulator)
Gap ~ U

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Mott insulators and conventional DFT

	Δ_{LDA}	Δ_{exp}	m_{LDA}	m_{exp}
$CaCuO_2$ (d^9)	0.0	1.5	0.0	0.65
CuO(d^9)	0.0	1.4	0.0	0.65
NiO(d^8)	0.2	4.0,4.3	1.0	1.7,1.9
CoO(d^7)	0.0	2.4	2.3	3.4,3.8
FeO(d^6)	0.0	2.4	2.3	3.3
MnO(d^5)	0.8	3.6-3.8	4.4	4.6,4.8
La_2CuO_4(d^9)	0.0	2.0	0.0	0.5
$LaTiO_3$(d^1)	0.0	0.2	0.0	--
UO_2(f^2)	0.0	2.0	0.0	1.7

LDA: yields metals as opposed to insulators;
when it supports a gap it's usually too small
same holds for GGA, meta-GGA

Alternatives:

- SIC — Perdew and Zunger, PRB **23,** 58(1981).
- LDA+U — Anisomov, et al., PRB **44**, 943(1991).
- GWA — Hybertsen and Louie, PRL **55**, 1418 (1985).

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Progress and problems with density functional theory (DFT)

Hybrid DFT: Becke (1993)

4th generation functional

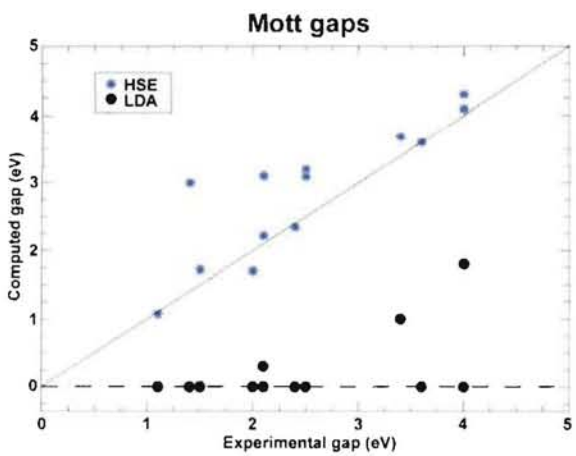
includes component of full, nonlocal HF exchange

PBE0, HSE:

$$E_{xc} = [\ \tfrac{1}{4}\ E_x^{HF} + \tfrac{3}{4}\ E_x^{PBE}] + E_c^{PBE}$$

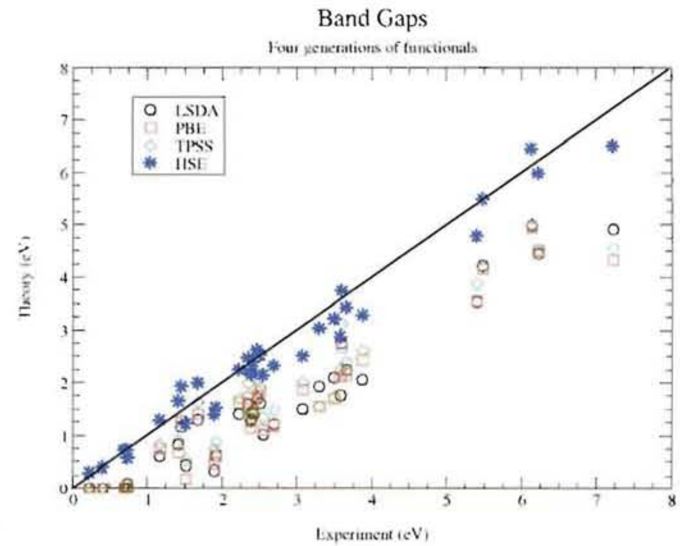
revolutionized molecular quantum chemistry

solids: improved gaps, lattice constants, magnetic properties, densities-of-states, optical spectra, dielectric constants



L. E. Roy, R. L. Martin, and G.E. Scuseria (2008):

MnO, FeO, CoO, NiO, CuO $CaCuO_2$, La_2CuO_4, $LaCrO_3$, $LaMnO_3$, $LaFeO_3$, $CeBr_3$, Ce_2O_3, UO_2.



Heyd, Peralta, Scuseria, and Martin, JCP **123**, 174101 (2005).

SC-40 bandgaps(eV)

	LSDA	PBE	TPSS	HSE
Mean absolute error:	1.136	1.127	0.977	0.263

hybrid DFT suggests UO_2 quite ionic; PuO_2 covalent
appears to have problems with correlated metals;
I-M in MnO; PES of UPt_3, UN

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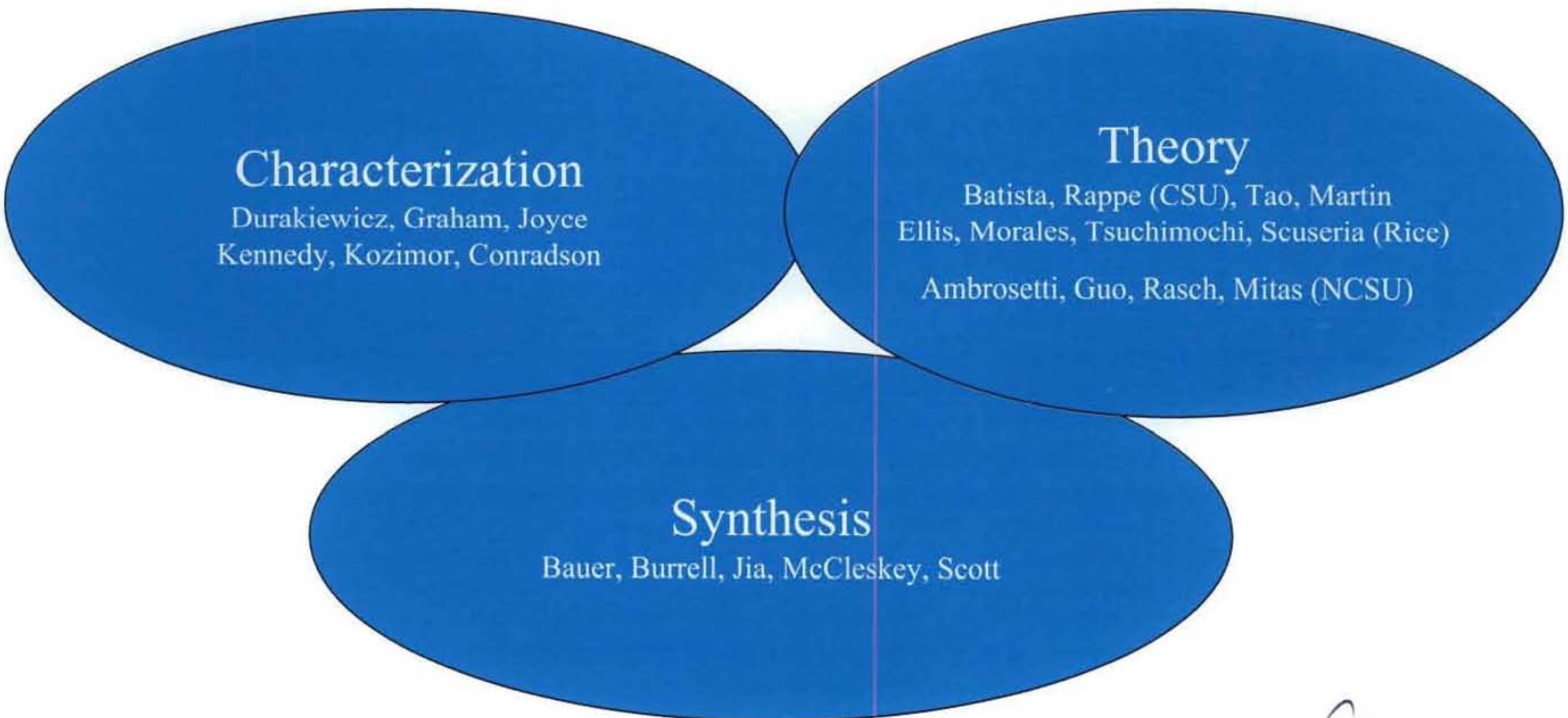
The team

We propose to synthesize and characterize AnC, AnN, AnO_2 (An=U, Np,Pu) thin films, a series which spans correlated metals -> Mott insulator, and to develop a fifth generation "functional" capable of treating the correlated metal



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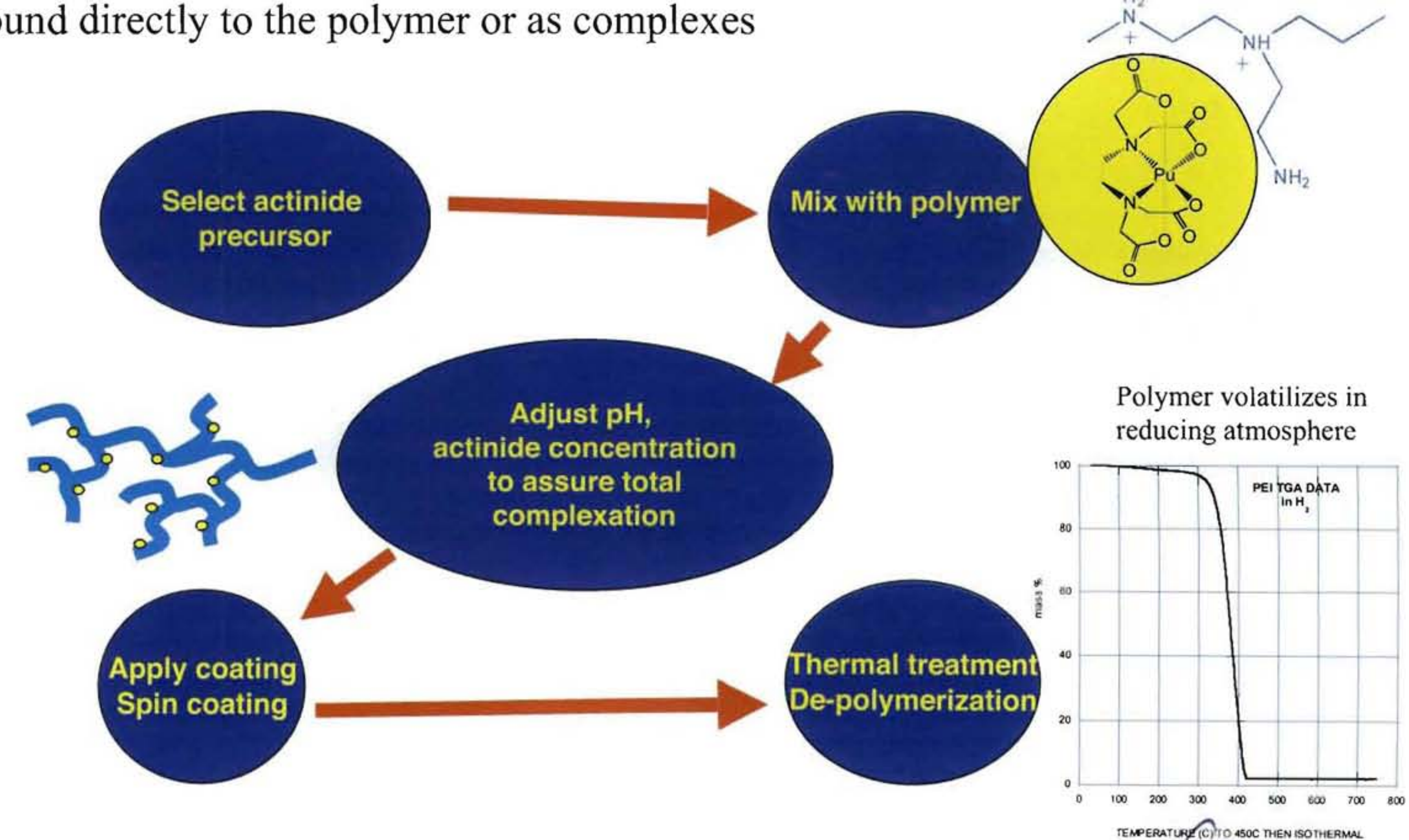
Polymer Assisted Deposition (PAD)

Eve Bauer, Tony Burrell, Quanxi Jia, Mark McCleskey

- Water-based process
- Non-volatile precursors for actinides
- Metals bound directly to the polymer or as complexes



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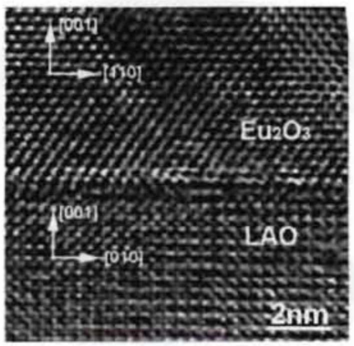
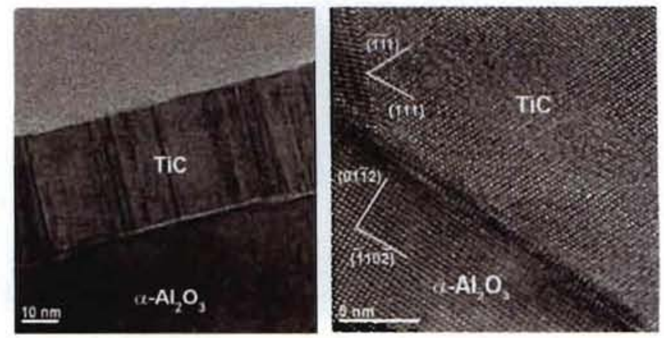
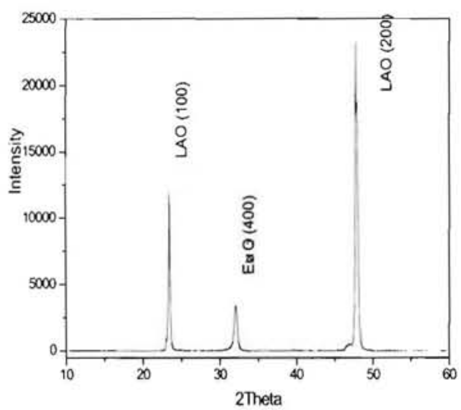
Epitaxial Films by PAD

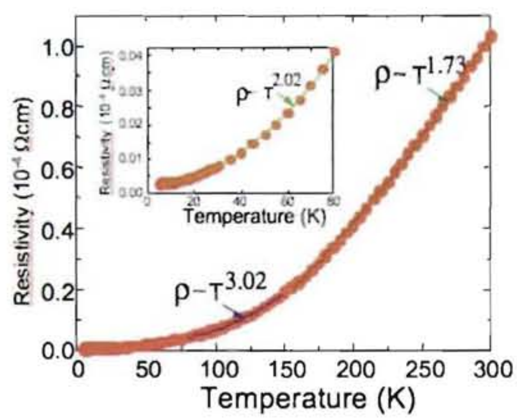
Versatile solution route with control of stoichiometry

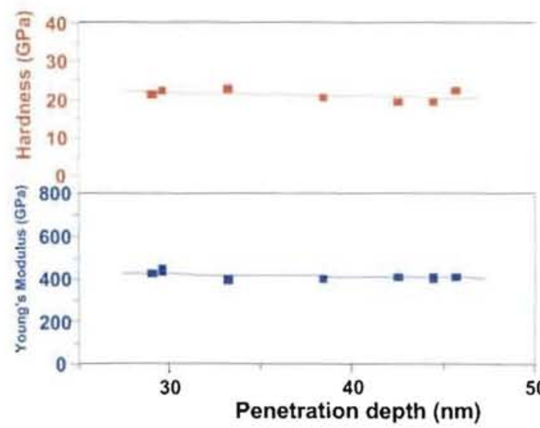
Oxides	Nitrides	Carbides











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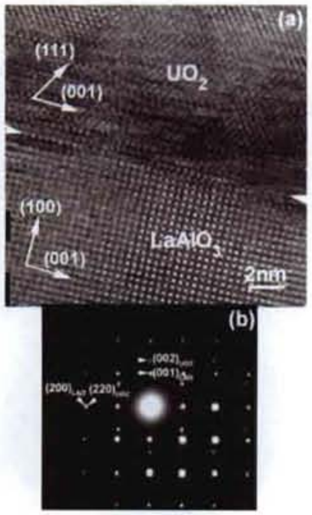
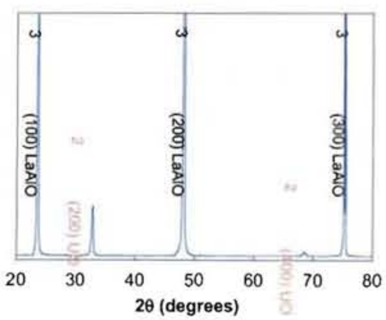
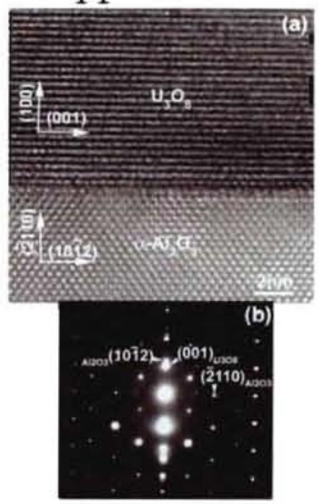
Control of Valence State

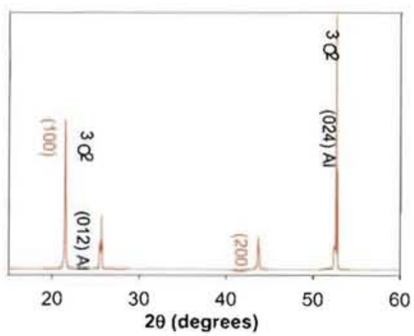
UO_2 on LAO lattice



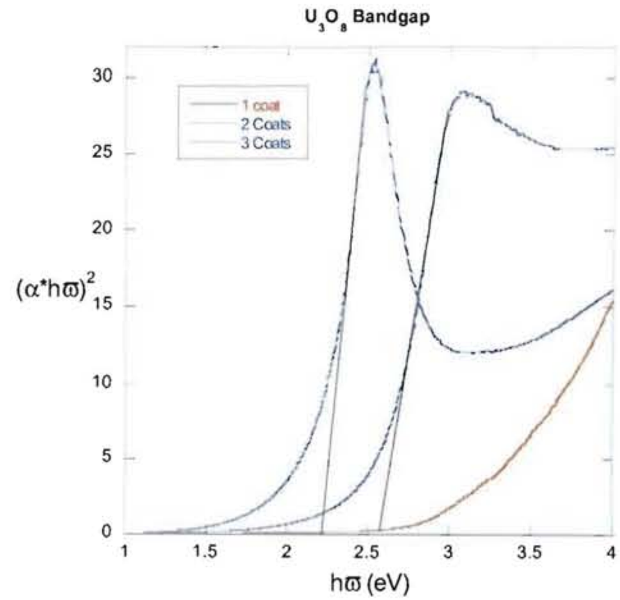


U_3O_8 on hexagonal sapphire lattice





First single crystal quality samples of U_3O_8 allow for measurement of band gap



2 coats 2.55 eV

3 coats 2.21 eV

Thy (HSE): $\Delta = 2.2$eV

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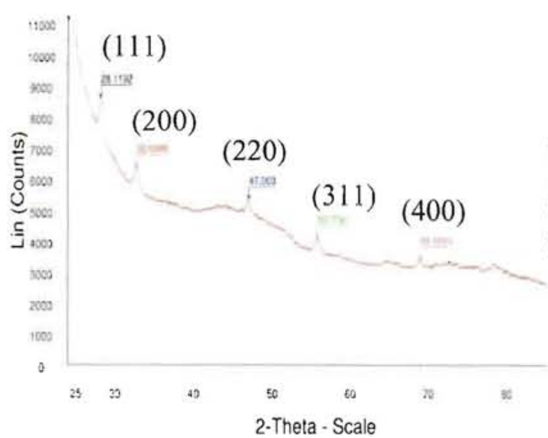
Substrate Influence on Epitaxy of NpO_2 Films

Buffer layers deposited by PAD can help

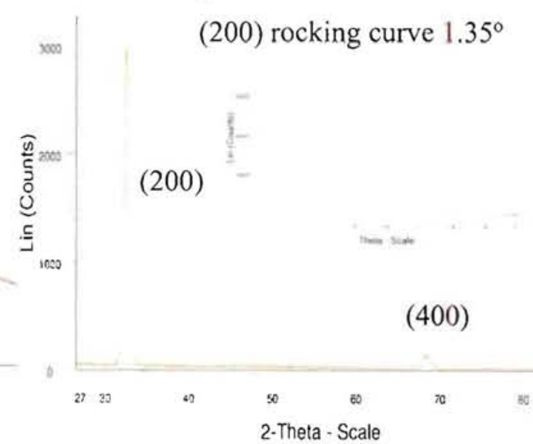
Lattice match and surface termination are important

Best films obtained on YSZ

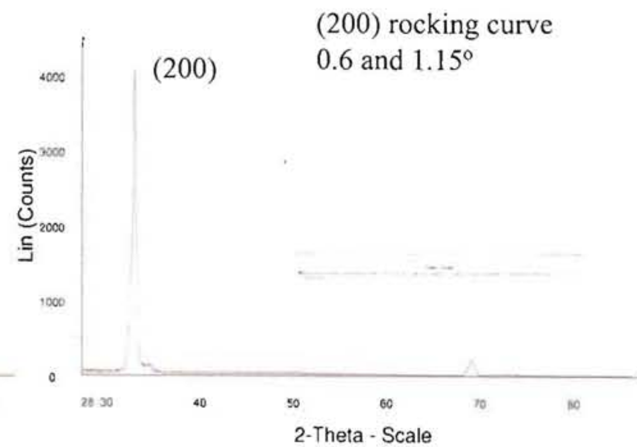
Polycrystalline NpO_2 on LAO



Aligned NpO_2 on LAO with UO_2 buffer layer



Aligned NpO_2 on YSZ



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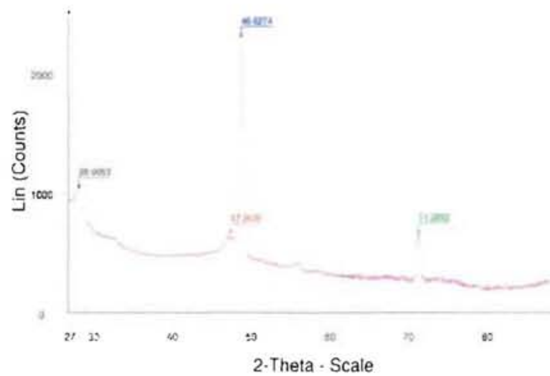
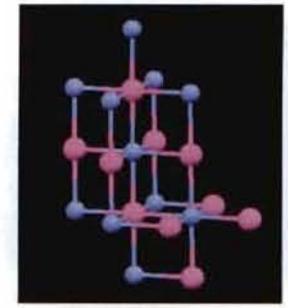
Approach to Nitrides

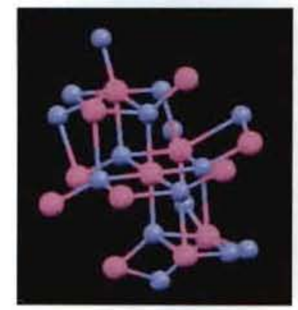
UN_2 obtained on LAO, N appears to come from EDTA



UN_2 on LAO (400)



UN_2



U_2N_3

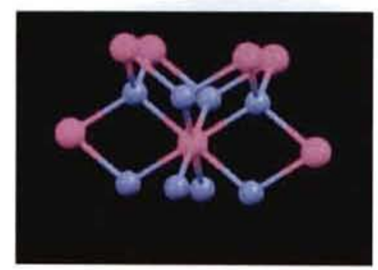
	Lattice
UN_2	5.30
UN	4.89
LAO (45°)	5.37
YSZ	5.13

Can UN_2 -> UN in the thin films?

Typically as one heats UN_2 -> U_2N_3 -> UN

UN_2 and UN lattices are both cubic

- contraction of the unit cell
- nitrogen moves from O_h to T_d sites



UN

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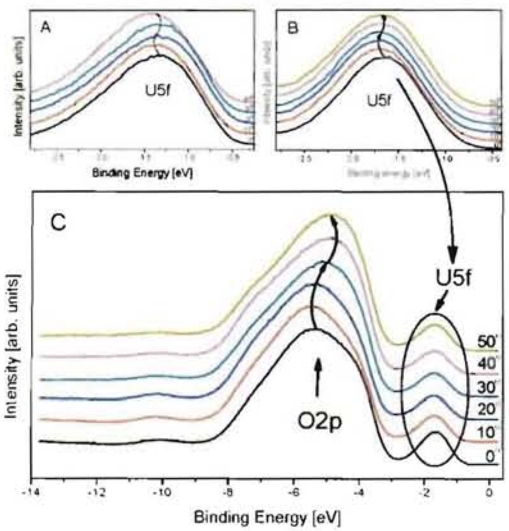
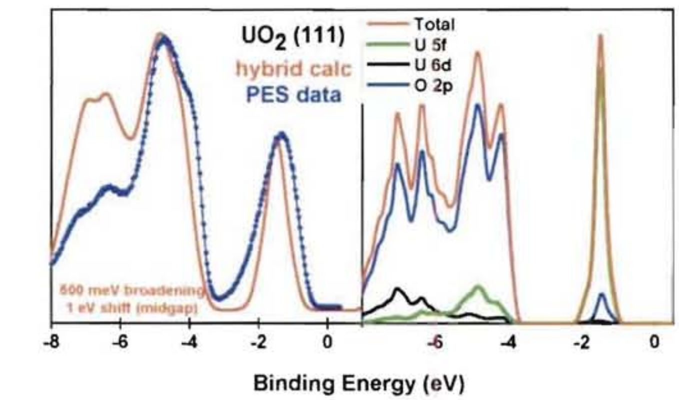
Photoemission

Tomasz Durakiewicz, John Joyce

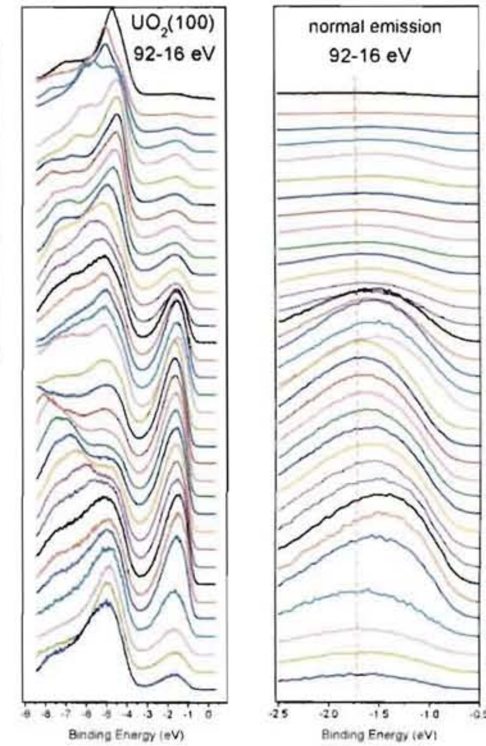


A.K. Burrell, *et al.*, *Adv. Mater.*, ***19***, *3559–3563 (2007)*



L.E. Roy, *et. al*, J. of Computational Chemistry **29**, 2288(2008)

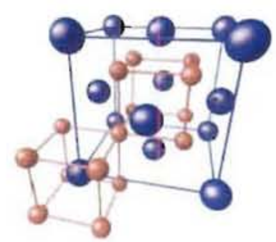
Hybrid DFT in excellent agreement with experiment



J.J. Joyce, *et. al*, Mat. Res. Soc. Symp. Proc. **986**, 35–40 (2007).

UO_2 single crystal ARPES equivalent to PAD sample

ionic solid;
small, but measureable dispersion



$R_{U\text{-}U} = 3.87A$

resonant PES:
- peak near E_f : *f* character
- normal emission => probing bulk

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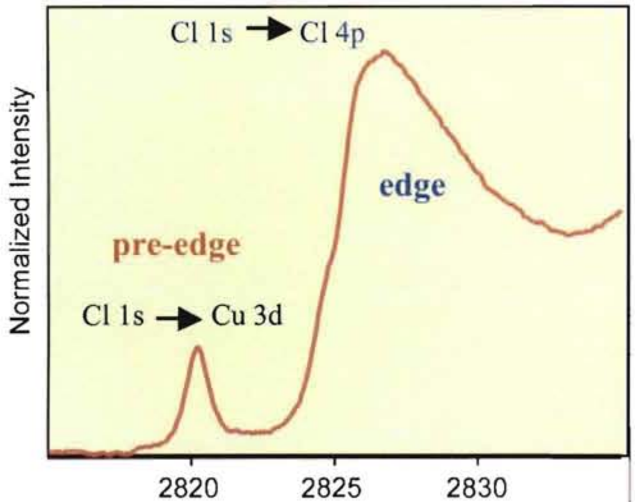
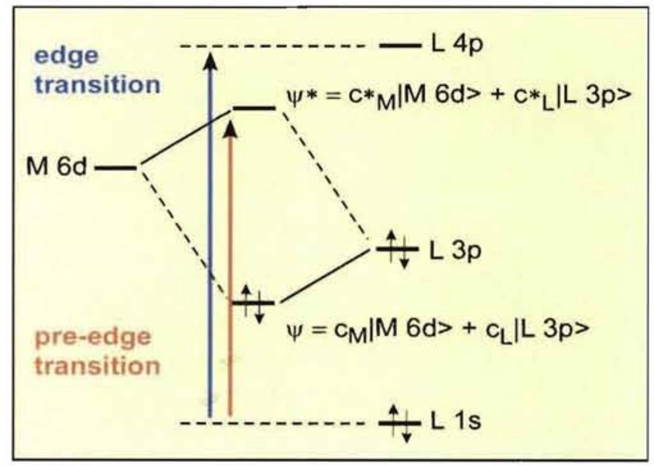
X-ray absorption measurements

Steve Conradson, Stosh Kozimor

Ligand K-edge XAS is a well-defined, quantitative probe of covalency in M-L bond



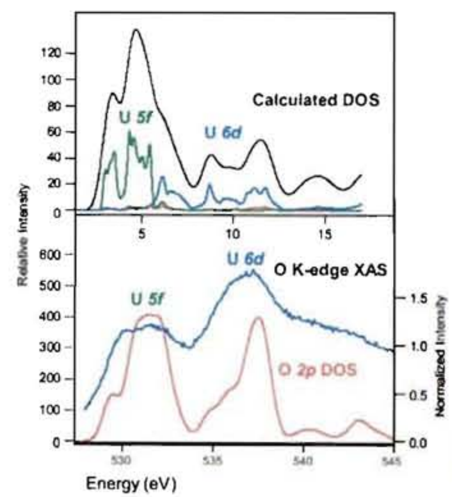
Cl K-edge XAS: $CuCl_4^{2-}$



$$\sigma_{1s,\psi^*} \sim |\langle Cl_{1s} | \boldsymbol{r} | \psi^* \rangle|^2 \sim c_L^{*2} \, |\langle Cl_{1s} | \boldsymbol{r} | Cl_{3p} \rangle|^2$$

Good agreement for UO_2

-- will provide details of bonding interactions in AnC, AnN, AnO_2



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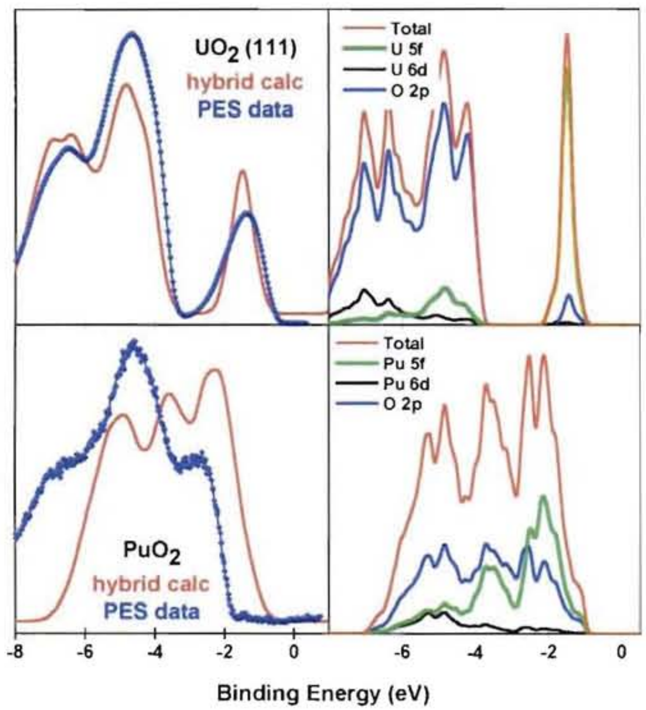
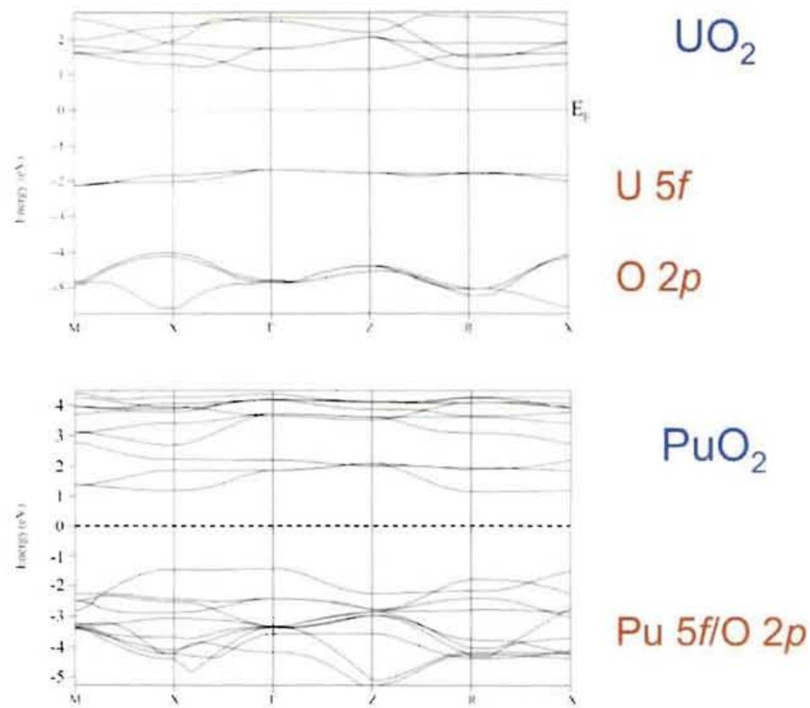
Goal 1: Test ionic vs. covalent behavior predicted in AnO_2





UO_2 looks like typical ionic solid; very little dispersion

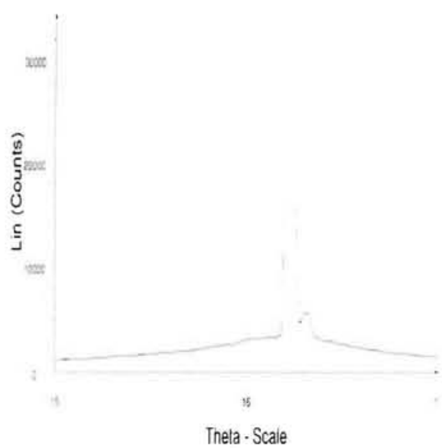
Γ -> X; 190meV calculated; 130meV measured

PuO_2 shows much more hybridization; stronger band dispersion

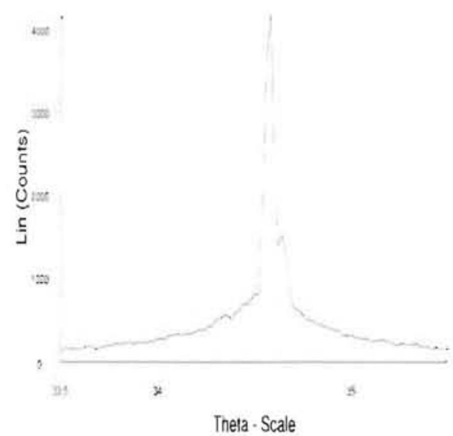
Goal 1: Epitaxial PuO_2 Films on YSZ

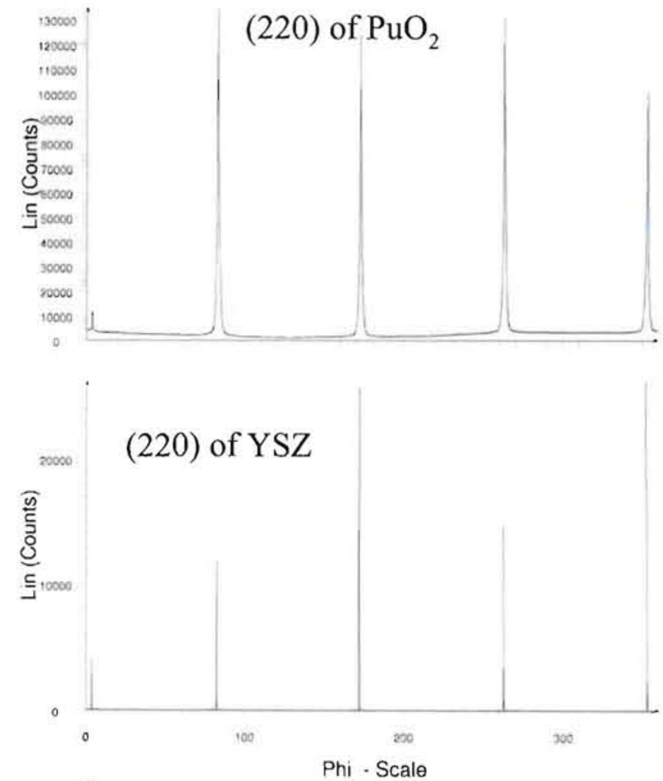
- c-axis oriented - only 200 and 400 peaks
- extremely high quality epitaxy - rocking curves 0.05°
- in plane orientation shown by Phi scan

(200) rocking curve 0.05°
shoulder – YSZ substrate



(400) rocking curve 0.05°
shoulder – Kα_2 line





Phi Scan for in plane orientation

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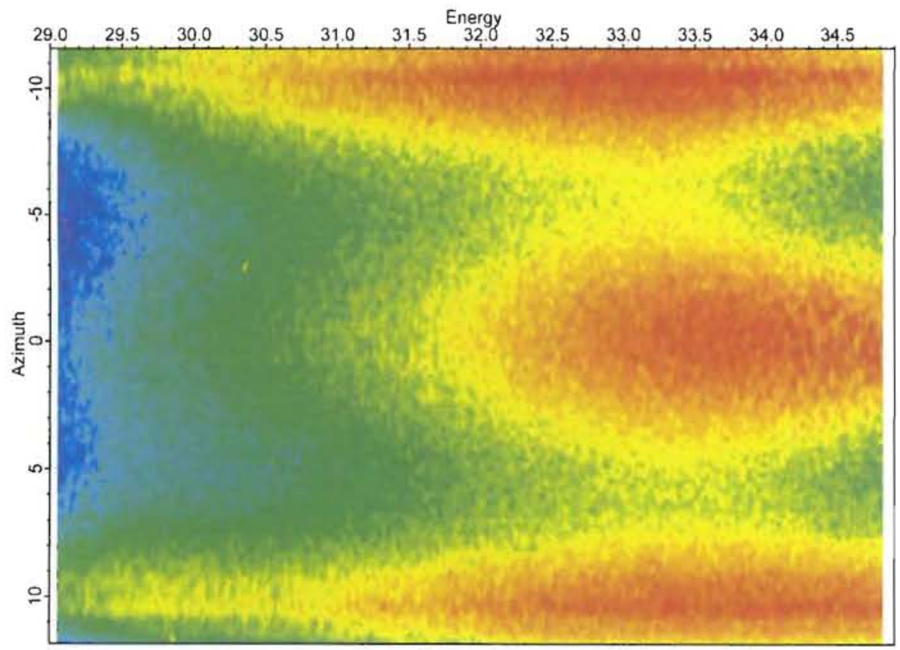
Goal 1: Photoelectron Spectroscopy for PuO_2

preliminary measurements



- Model predicts strong hybridization in Pu
  - merging of O 2p and Pu 5f
  - significant dispersion
- 1st ARPES shows **k**-dep. and hybridization

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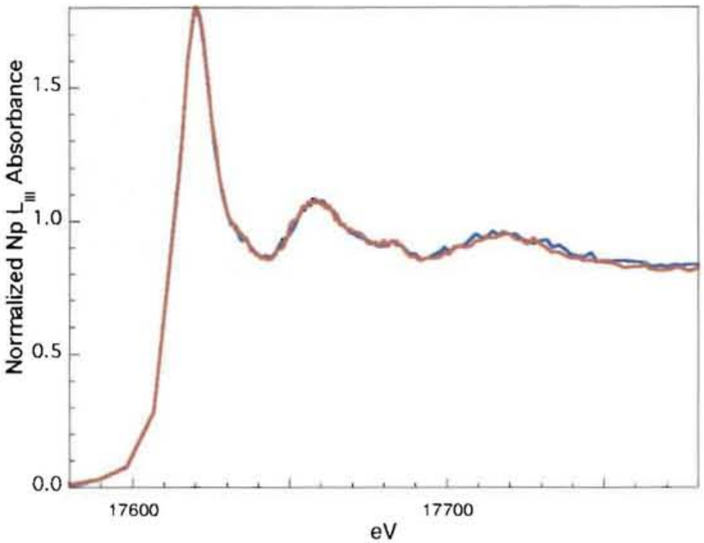
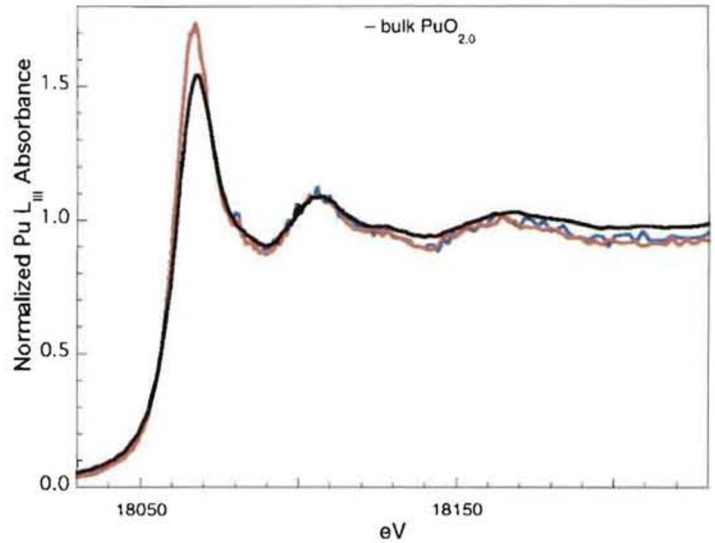
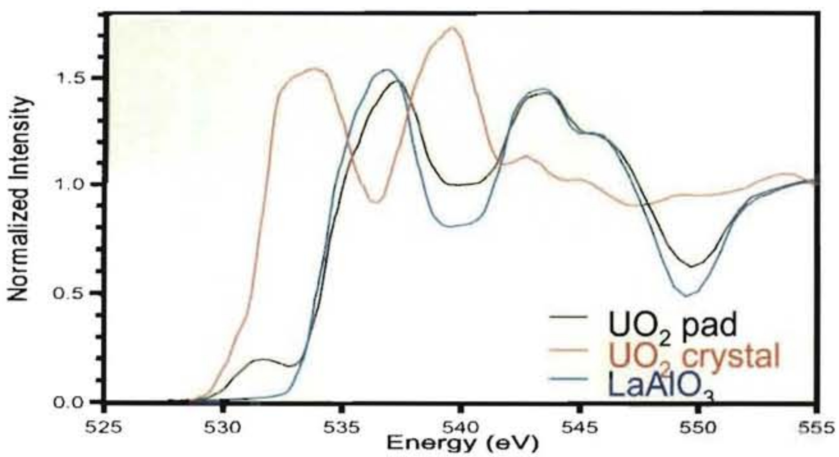
Goal 1: XAS for PuO_2

M $L_{2,3}$ edge: Good agreement between bulk sample and films for NpO_2, PuO_2 (YSZ)







O K-edge: UO_2 films (LAO):

substrate visible

(go to grazing incidence)

PuO_2 scheduled for June

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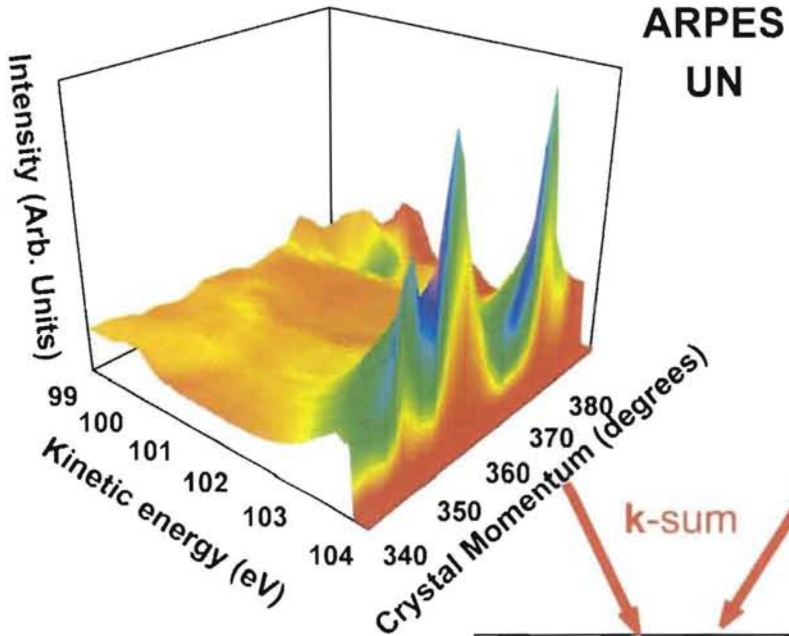
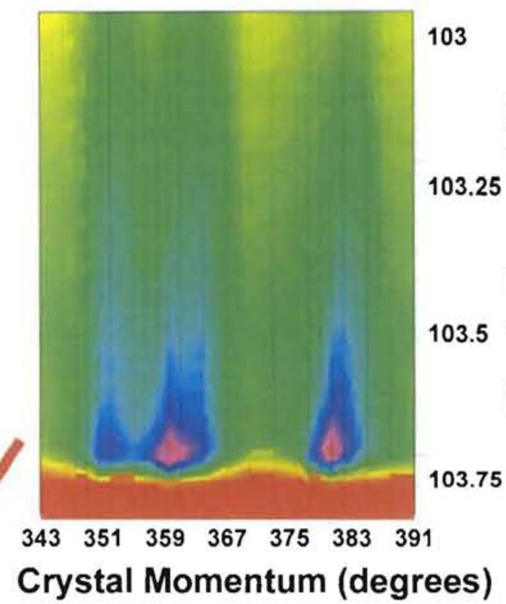
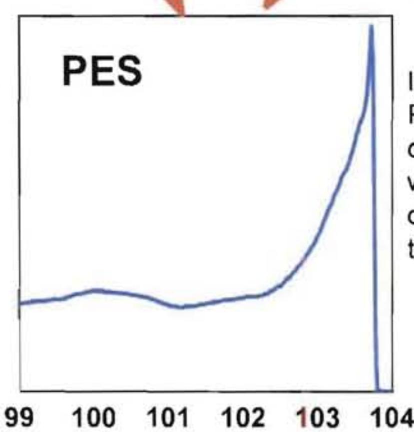
Goal 2: Correlated Metals



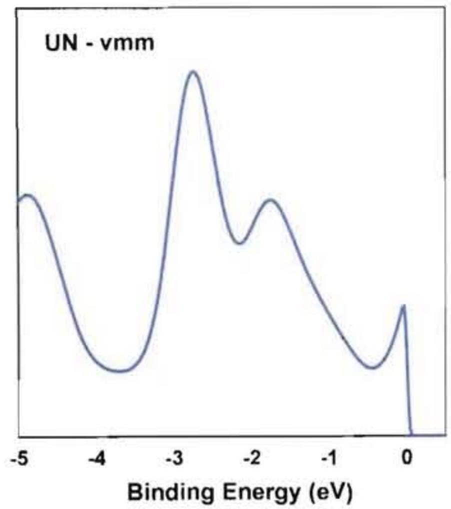


Basically, the PES spectrum (right) is the sum of the 25 independent E vs. **k** spectra in the ARPES data set (above).

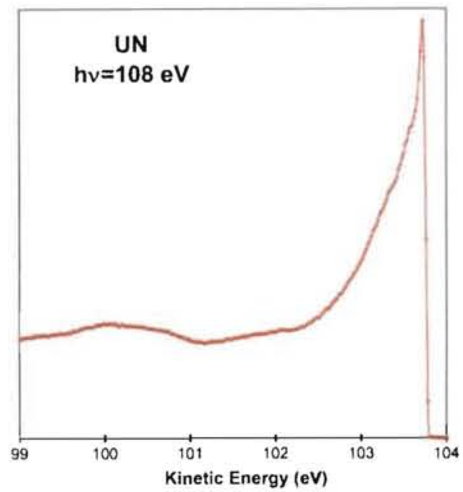


In a one-electron picture, conventional PES relates the energy distribution curves to a density-of-states (DOS) while ARPES, which includes the crystal mometum (**k**) compares with the full band structure (E vs. **k**).

Goal 2: Correlated Metals

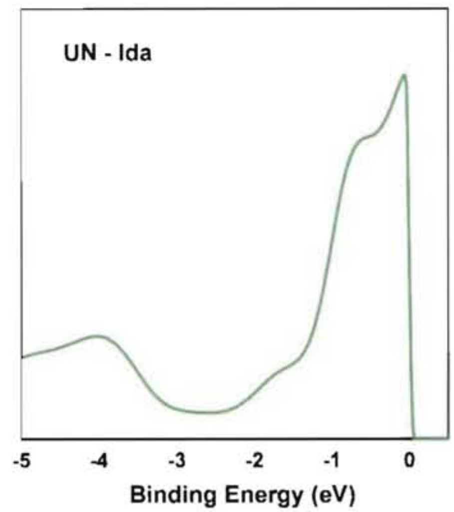


HSE (occupied DOS)

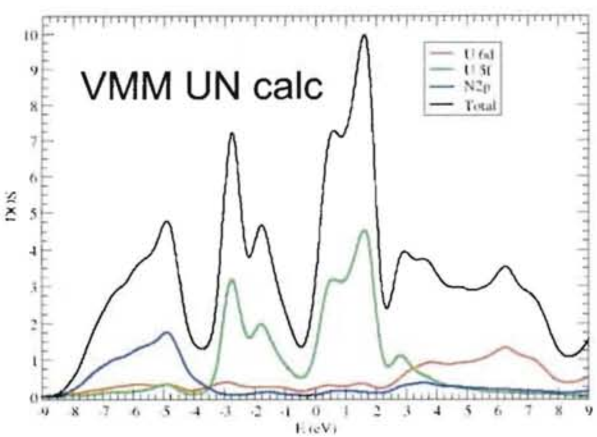


PES

U 5*f* component enhanced at 108eV



LDA(total DOS)



HSE (partial DOS)

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Theory efforts

Correlated metals

Functional development (Rice)

DQMC extension (NCSU)

Applications (LANL)

Rice: investigating DFT/RPA in molecules; extending to solids
developing Hartree-Fock-Bogliubov / DFT method (**coupled pair mean field theory**)

NCSU: Diffusion Quantum Monte Carlo (DQMC): our gold standard;
extension to actinides completed;
in progress:
- calculations on Cp_2AnL_2 (L=Cl, OH, NH_2, CH_3)
- **developing spin-orbit capability**

LANL: accumulating experience with HSE for correlated metals:
- in progress: AnN, AnN_2, An_2N_3; An = U, Np, Pu

HSE investigation of IM transition in VO_2
hybrid DFT calculations on Cp_2AnL_2 (L=Cl, OH, NH_2, CH_3)
developing pair/multiplet/DFT approaches

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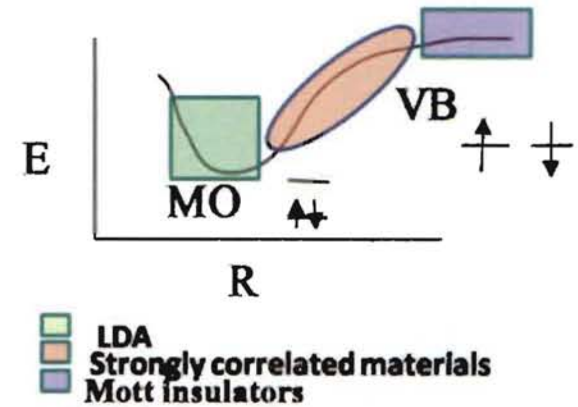
What is hybrid DFT missing?

DFT is a one-electron, **single determinant** approximation.
it cannot account for
proper magnetic correlations
Kondo singlets
multiplet states
Cooper pairs



Magnetic correlations:

$\Psi = \sigma^2 - \lambda \sigma^{*2}$

@ R_e $\lambda \sim 0$

@ large R $\lambda \sim 1$

Another problem DFT cannot do:
Van derWaals interaction:
He_2 at long distance;
arises from simultaneous dipole-dipole fluctuation
double excitations

$\Psi =$ $He_A(1s^2)$ x $He_B(1s^2)$ repulsive

$+ \alpha\, He_A(1s2p)$ x $He_B(1s2p)$ attractive

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How do we put these correlations in?

DFT/RPA (Rice)

Adiabatic connection fluctuation-dissipation theorem:
  yields formally exact expression for E_c
    depends on **frequency dependent density-density response $\chi_\lambda(\omega, x_1, x_2)$**
      approximate χ in the RPA

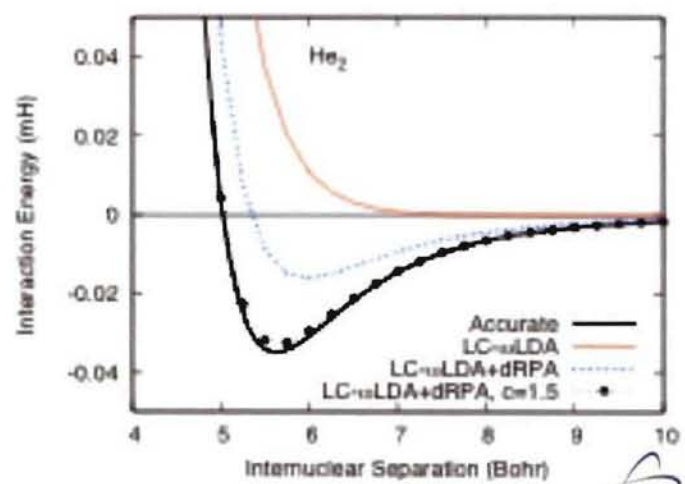
Langreth and Perdew, Solid State Comm. **17**, 1475 (1975) N^6
Furche, JCP **129**, 114105 (2008) N^5
Scuseria, et al, JCP **129**, 231101 (2008) N^4
  equivalence of RPA with coupled cluster doubles (CCD) approach
  continues theme of coupling DFT with wavefunction techniques

A path for hierarchical improvements to DFT now seems practical

THE JOURNAL OF CH EMICAL PHYSICS 130, 081105 2009
Long-range-corrected hybrids including random phase approximation correlation
Benjamin G. Janesko, Thomas M. Henderson, and Gustavo E. Scuseria

$$E_{xc} = E_{xc}^{\text{SR-LSDA}} + E_x^{\text{LR-HF}} + c_{\text{RPA}} E_c^{\text{LR-RPA}}. \quad (6)$$

Will screen HF exchange dynamically



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How do we put these correlations in?

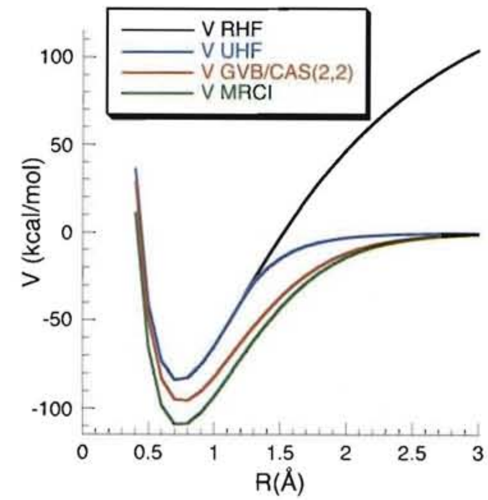
GVB / DFT (CSU, LANL): preliminary

Generalized Valence Bond Theory:

include magnetic correlations through **multi-determinant reference state**

Ensemble DFT: Kait and Hoffmann, JCP **120**, 5005 (2004).

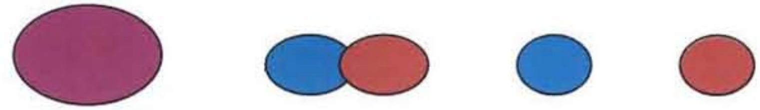
multi-determinantal reference allows us to treat multiplets



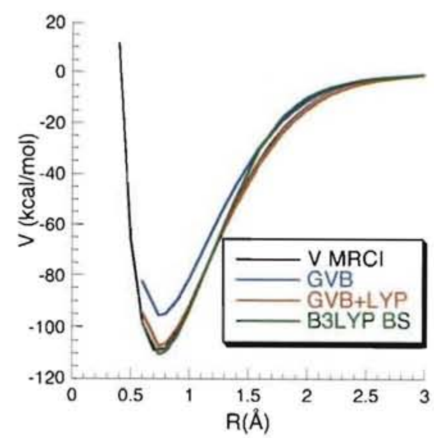
Magnetic correlations: $\Psi_{GVB} = (\phi_g\phi_g - \lambda\,\phi_u\phi_u) \quad (\alpha\beta-\beta\alpha)$

$= (\phi_g + \lambda_i^{1/2}\phi_u)(\phi_g - \lambda_i^{1/2}\phi_u)(\alpha\beta-\beta\alpha)$

$= \phi_1' \quad \phi_2' \quad (\alpha\beta-\beta\alpha)$



$\lambda = 0$ $\lambda \sim 1/2$ $\lambda = 1$



GVB:

$\Psi_{GVB} = A\,[\text{core}]\,\Pi_{i\,\varepsilon\,\text{active}}(\phi^2_i - \lambda_i\phi^{2\,*}_i)(\alpha\beta-\beta\alpha)$

antisymmetrized product of geminals

simple "one-electron" energy expression

GVB/DFT

add E_c and correct for overcounting

$$E = 2\sum_{i=1}^{nocc} f_i h_{ii} + \sum_{i,j=1}^{nocc}\left(a_{ij}J_{ij} + b_{ij}K_{ij}\right) + E_c(\rho) + \sum_{k=1}^{nactive} f_k\left[E_k^{self}(\rho_k) - E_k^{field}(\rho_k)\right]$$

$$a_{ij}, b_{ij} = f(\lambda)$$

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How do we put these correlations in?

GVB / DFT : preliminary

Multiplets: Carbon atom (s^2p^2)

$$^3P: \frac{1}{\sqrt{2}}(x\bar{y}+\bar{x}y)$$
$$\frac{1}{\sqrt{2}}(x\bar{z}+\bar{x}z)$$
$$\frac{1}{\sqrt{2}}(y\bar{z}+\bar{y}z)$$

$$^1D: \frac{1}{\sqrt{2}}(x\bar{y}-\bar{x}y)$$
$$\frac{1}{\sqrt{2}}(x\bar{z}-\bar{x}z)$$
$$\frac{1}{\sqrt{2}}(y\bar{z}-\bar{y}z)$$
$$\frac{1}{\sqrt{2}}(x\bar{x}-\bar{y}y)$$
$$\frac{1}{\sqrt{6}}(x\bar{x}+\bar{y}y-2z\bar{z})$$

$$^1S: \frac{1}{\sqrt{3}}(x^2+y^2+z^2)$$

$$E = 2\sum_{i=1}^{nocc} f_i h_{ii} + \sum_{i,j=1}^{nocc}\left(a_{ij}J_{ij}+b_{ij}K_{ij}\right) + E_c(\rho) + \sum_{k=1}^{nactive} f_k\left[E_k^{self}(\rho_k) - E_k^{field}(\rho_k)\right]$$

Slater: tabulates atomic couplings: F^k, G^k
others easily derived

O: s^2p^4

Method	ΔE (ev) ^1D	ΔE (ev) ^1S	$\langle S^2\rangle$ $M_s=1$	$\langle S^2\rangle$ $M_s=0$
UHF	1.02		2.006	1.007
UBLYP	0.69		2.003	1.002
UB3LYP	0.73		2.002	1.002
ROHF	2.17	4.39	2.0	0.0
ROHF+LDA	1.84	3.34	2.0	0.0
ROHF+LYP	1.95	4.17	2.0	0.0
ROHF+TPSS	1.97	4.20	2.0	0.0
Exp. (J_{ave})	1.97	4.19	2.0	0.0

Summary

Synthesis:

PuO_2 synthesized; structure determined;
U_3O_8 synthesized and gap measured; excellent agreement with theory

PES:

UN ARPES completed;
PuO_2 measurement in progress;

XAS:

UO_2, NpO_2, PuO_2 (An $L_{2,3}$-edge) XAS in films compared to bulk (SSRL);
UO_2 (O K-edge); will go to grazing incidence (June, LBNL)

Theory:

AnN calculations progressing; GVB/DFT pair/multiplet approximations promising
progress at Rice with DFT/RPA and Bogliubov/DFT pair approximations;
DQMC for actinides in place; will begin with molecular bond energy benchmarks

Follow-ons:

NNSA Pu Science Strategy (Dave Clark)
BES (John Sarrao)
Nuclear Energy programs (Sara Scott)

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Nuclear Detection Materials

Bryan Bennett[1], Michael Blair[2], Leif Brown[3], Jon Cook[4], Rico Del Sesto[5], Rob Gilbertson[1], Andy Li*[4], Edward McKigney@[4], Ross Muenchausen[1], Nick Smith[1], Sy Stange*[4], Mark Wallace[6], Debra Wrobleski[1]

@ presenter *graduate student

[1] MST-7 [2] EES-14 [3] C-CDE [4] N-1 [5] MPA-MC [6] ISR-1

May 5, 2010

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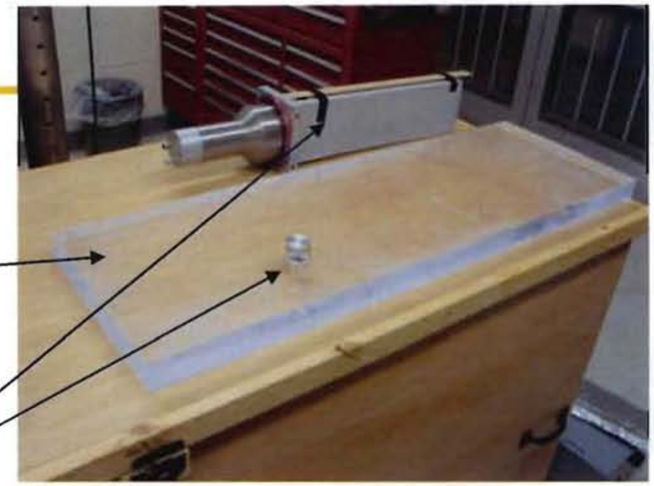
Outline

- Context – relevant mission needs and gap
- Approach – technical approach
- Results – highlight of one of the optical results
- Conclusions – current status and next challenges

Conceptual Overview

- Nanocomposite scintillators will combine the performance of inorganic crystalline scintillators with the cost and processing of organic plastic scintillators.

- This will be accomplished by eliminating the need for crystal growth and synthesizing the materials using bulk chemical processing.



Plastic Scintillator
- Low Cost
- Large Volume
- Poor Energy Resolution
- Poor Stopping Power

Inorganic Crystalline
Scintillator
- Medium-High Cost
- Small-Medium Volume
- Good Energy Resolution
- Good Stopping Power

- Straddle Carrier instrumented for scanning cargo containers

- Portal monitors for scanning vehicular or pedestrian traffic

- Hand-held radioisotope identifier for secondary inspection and search

Optical Transparency

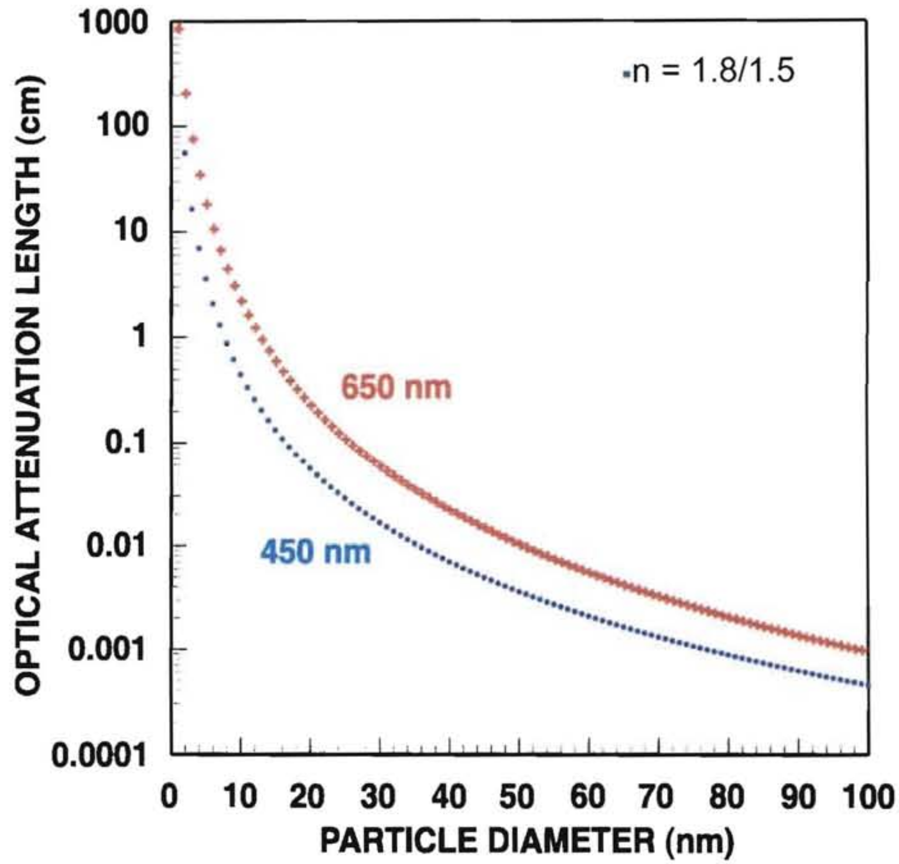
- Rayleigh scattering is an important source of opacity for composites, due to mismatch of indices of refraction between particle and matrix.

$$T = \frac{I}{I_0} = e^{-N\sigma x}$$

$$\sigma = \frac{2\pi^5}{3}\frac{d^6}{\lambda^4}\left(\frac{n^2-1}{n^2+2}\right)^2$$

$$N = \frac{v_{fraction}}{\frac{\pi}{6}d^3}$$

$$n = \frac{n_{particle}}{n_{matrix}}$$

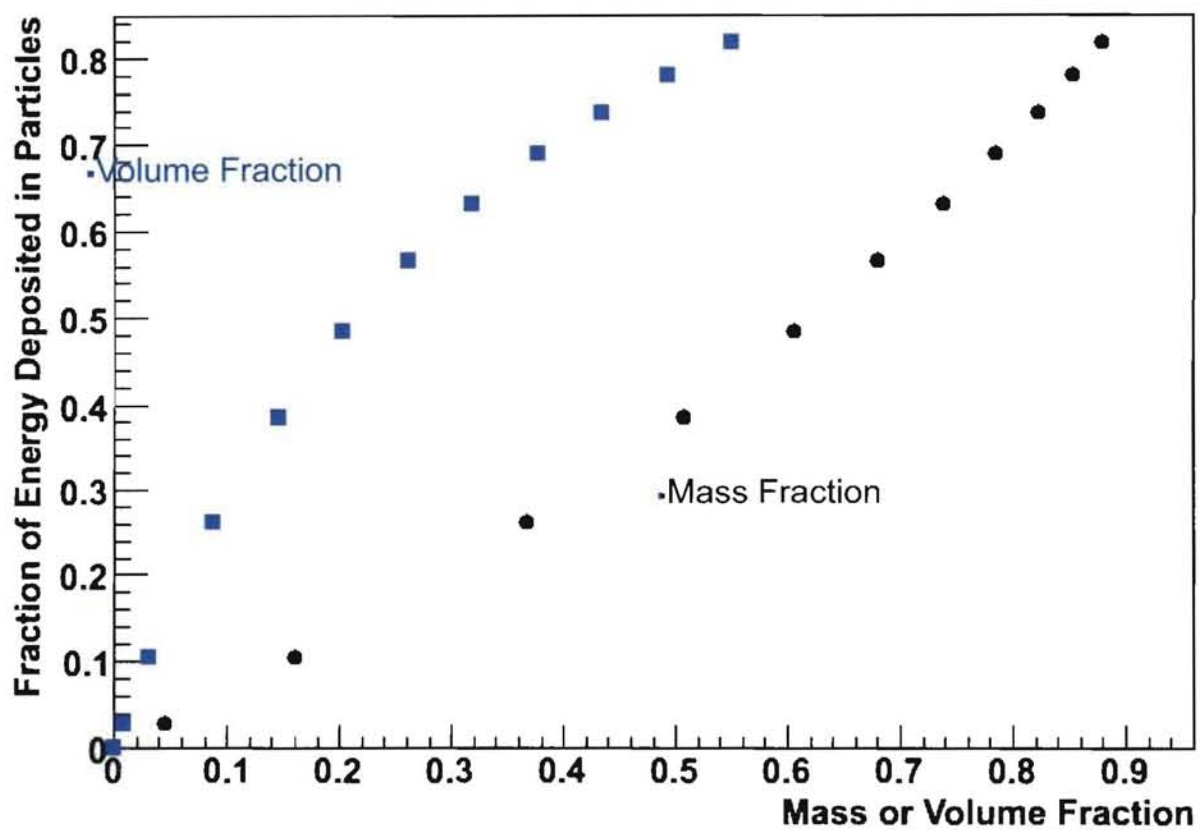


Energy Deposition Model

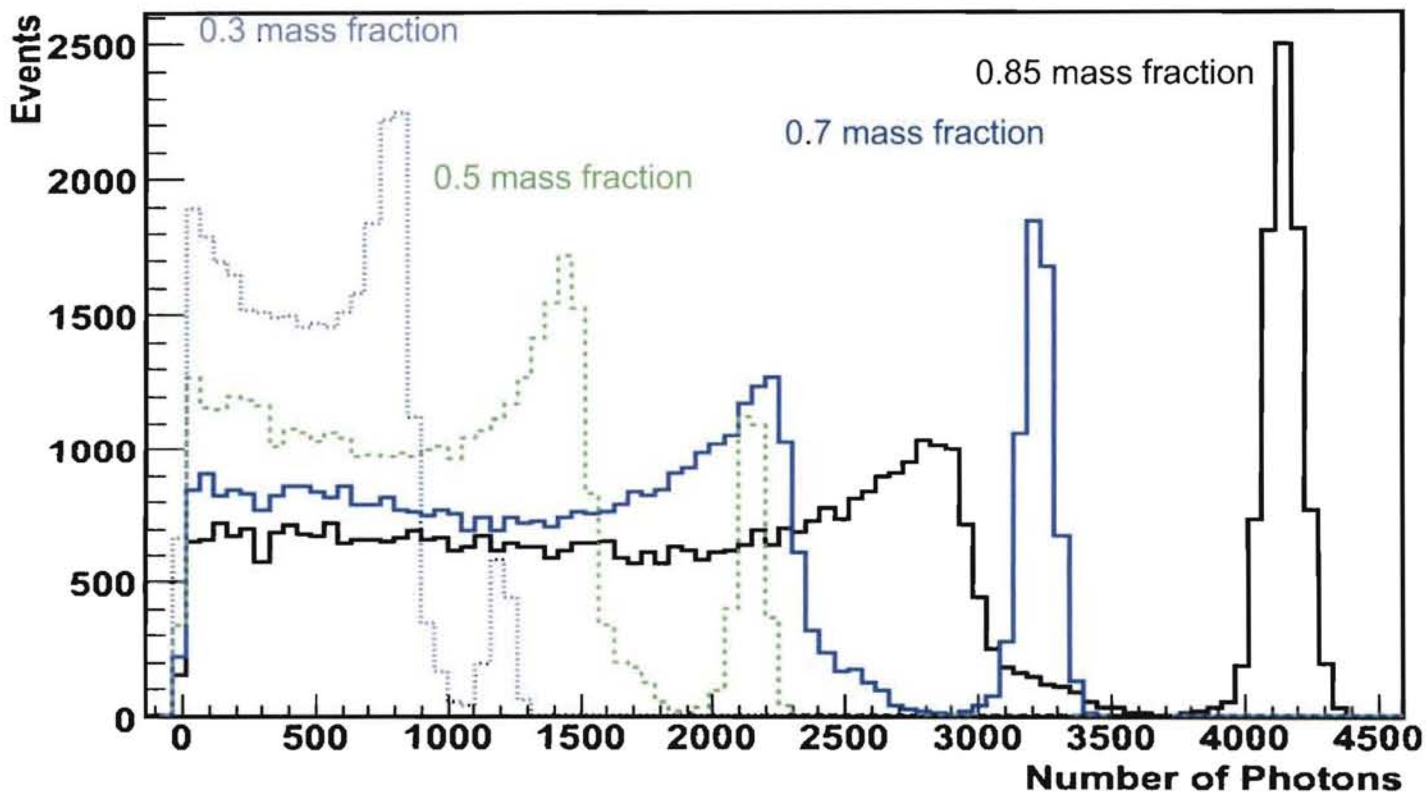
- Uses NIST estar database for dE/dx and range tables
- Incorporates binomial statistics for particle sampling at each step
- Provides calculation of energy deposition in particles, ligand and matrix
- Assumes no interaction between constituents

$$E_p = \int_{range} f_v^p \frac{dE_p(E)}{dx} dx$$

Calculated Energy Deposition

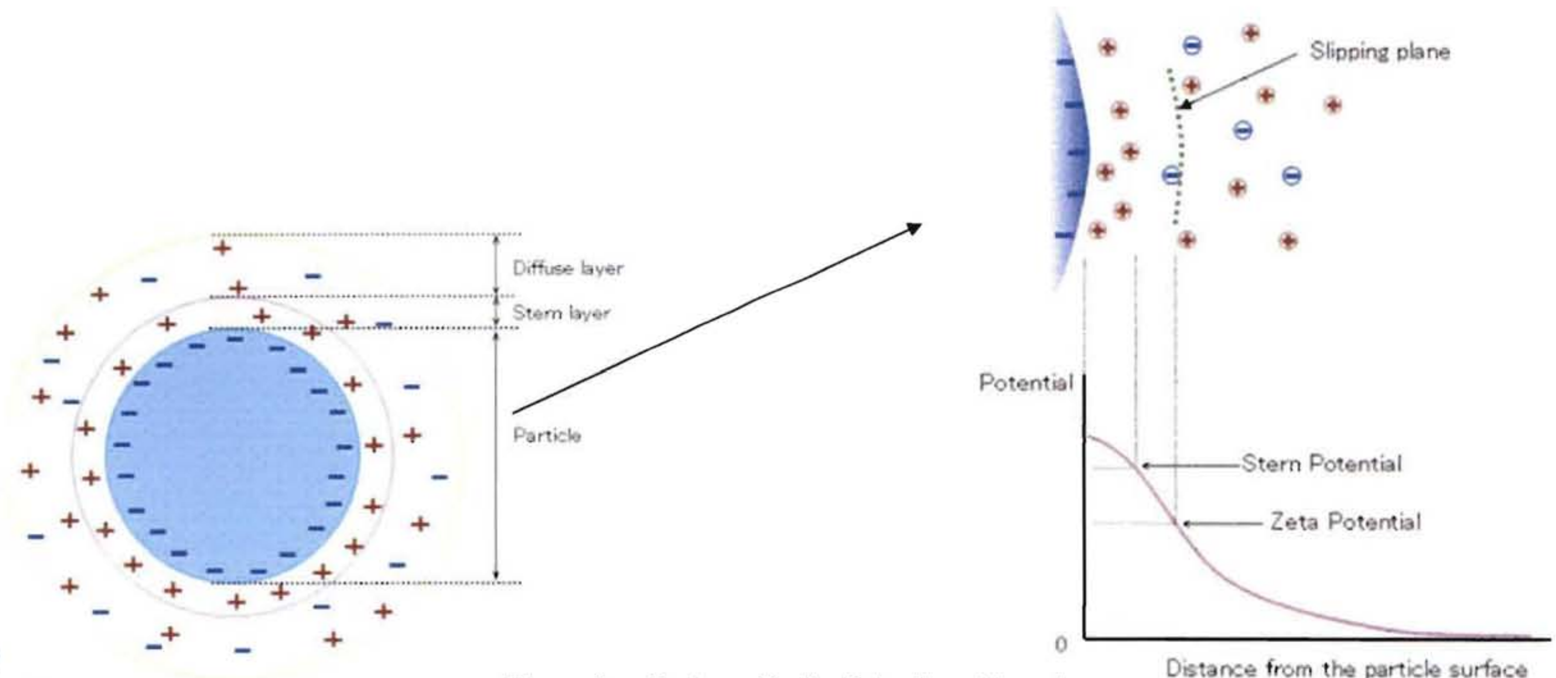


Simulated ^{137}Cs Energy Spectra



Zeta Potential

- **The zeta potential is the potential at the interface of charges that move with the particle and charges that do not**
  - This quantity is strongly correlated with the stability of dispersions



•Figures from Beckman Coulter Delsa Nano Manual

Industrial Scale Dispersion

•Mini-Cer

•150 ml grinding chamber

Mini-Cer is smallest practical bead mill, larger mills are also standard items

•Zeta RS

•4 liter grinding chamber

•Factor of 25 scale-up

•LMZ 25

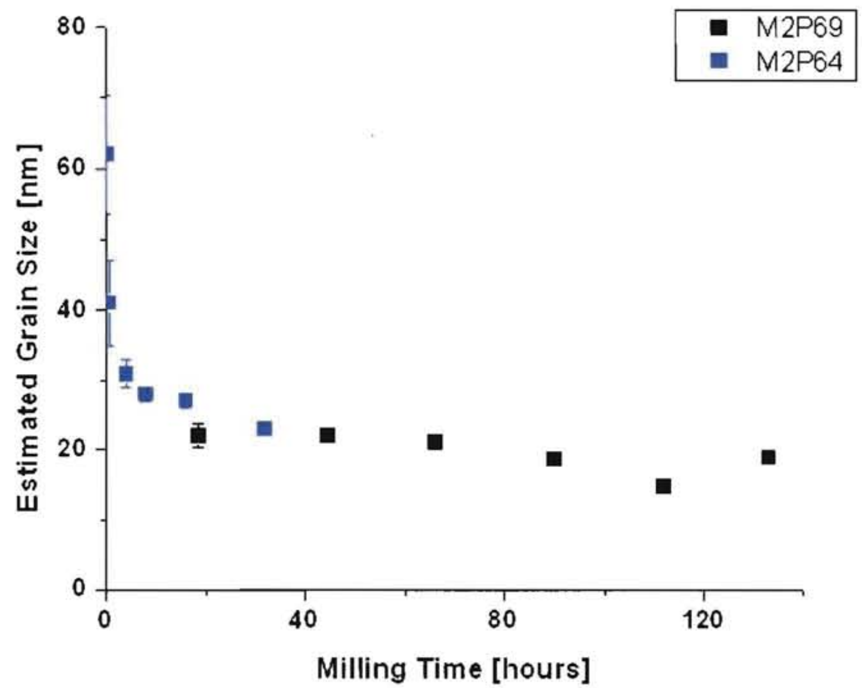
•25 liter grinding chamber

•Factor of 165 scale-up

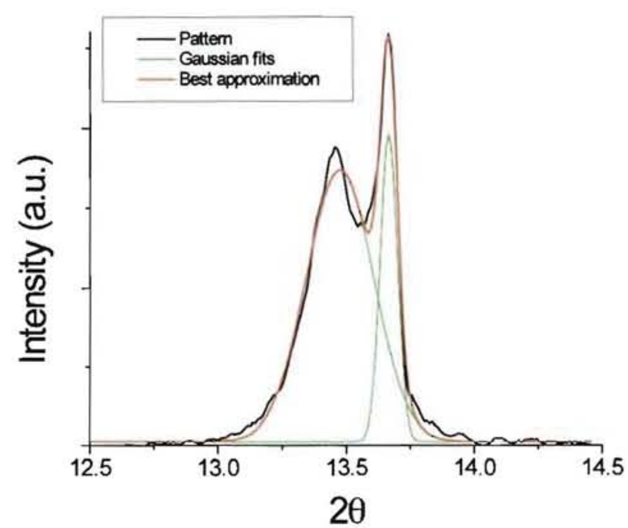
•LMZ 150

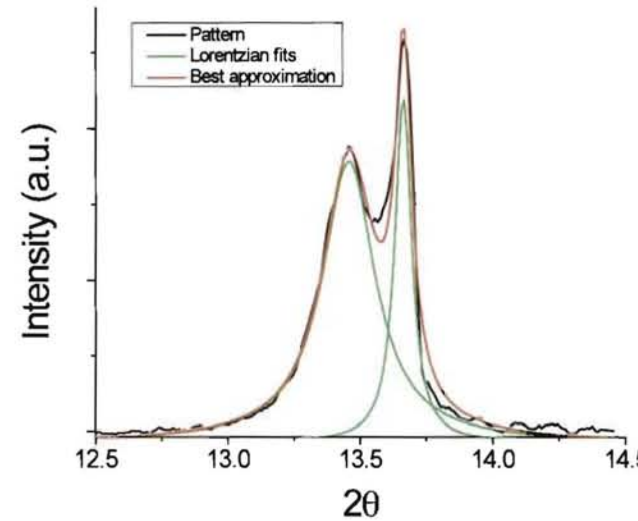
•150 liter grinding chamber

•Factor of 1000 scale-up



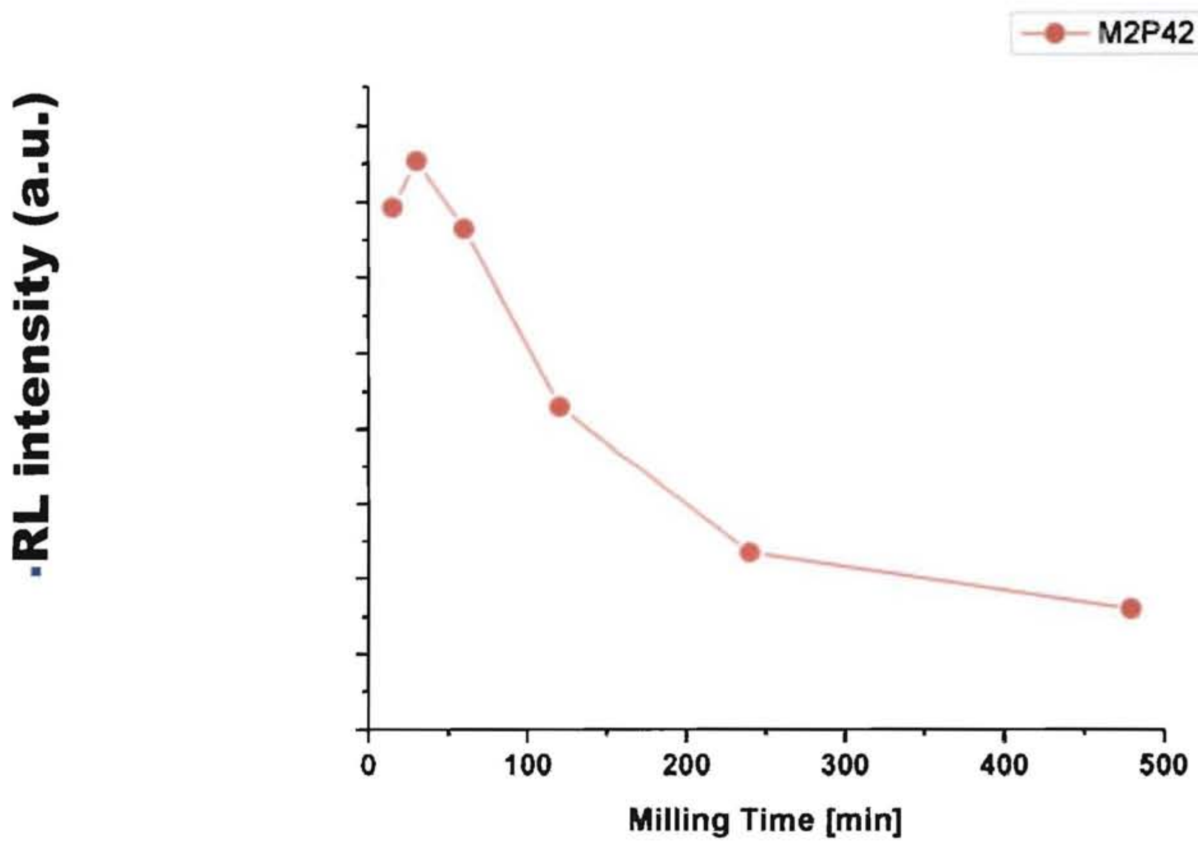
- Grain size as a function of milling time. Two independent milling



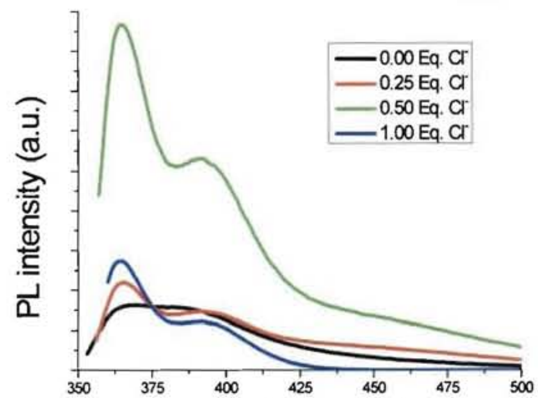


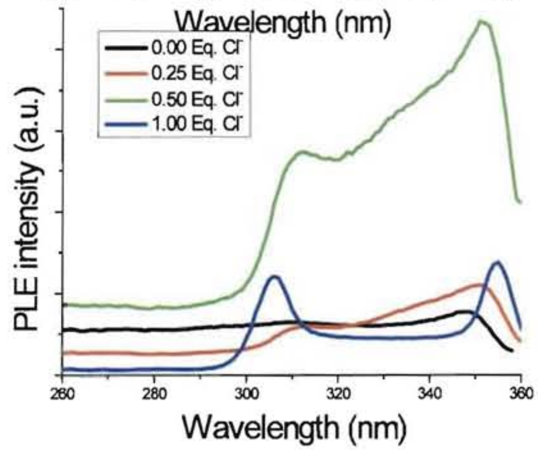
- Typically, XRD peaks are a mix of Gaussian and Lorentzian

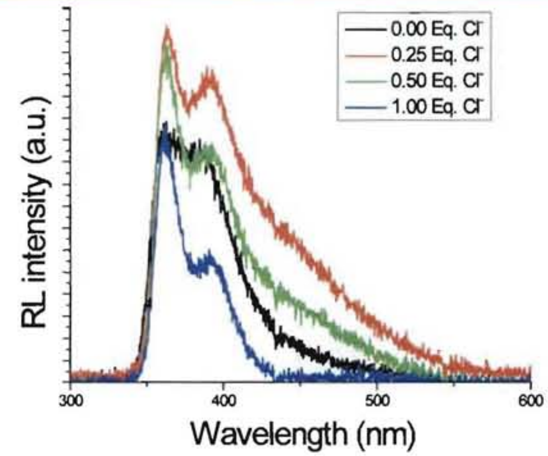
	Peak A (Bulk)	Peak B (nano)
d-spacing:	0.6472 nm	0.6563 nm
Grain size:	> 100 nm	~30 nm



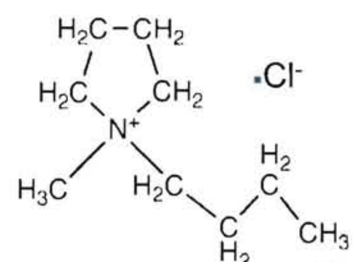
M2P42
RL intensity (a.u.)
0
100
200
300
400
500
Milling Time [min]

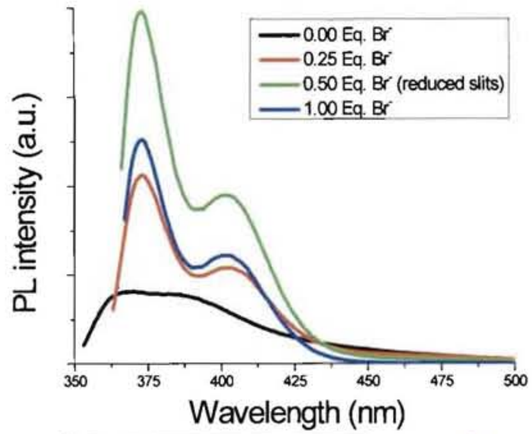


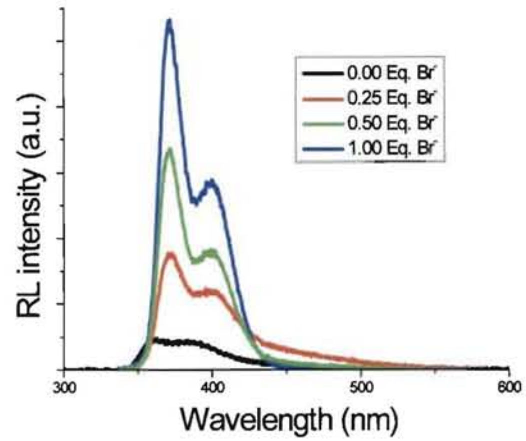


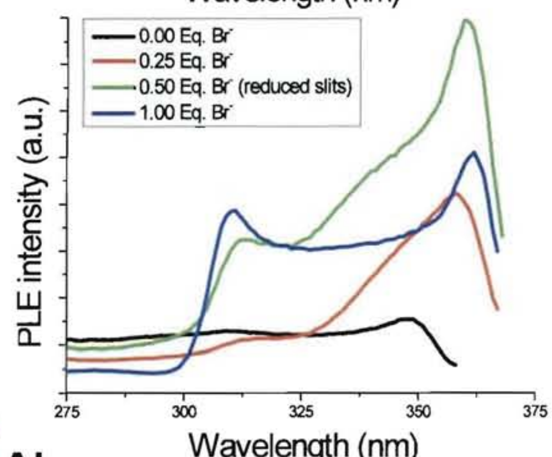


- Chloride salt addition to $CeCl_3$

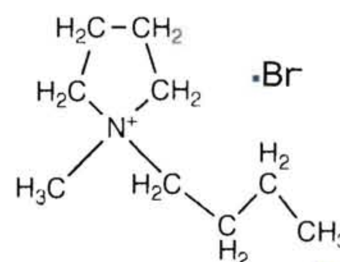


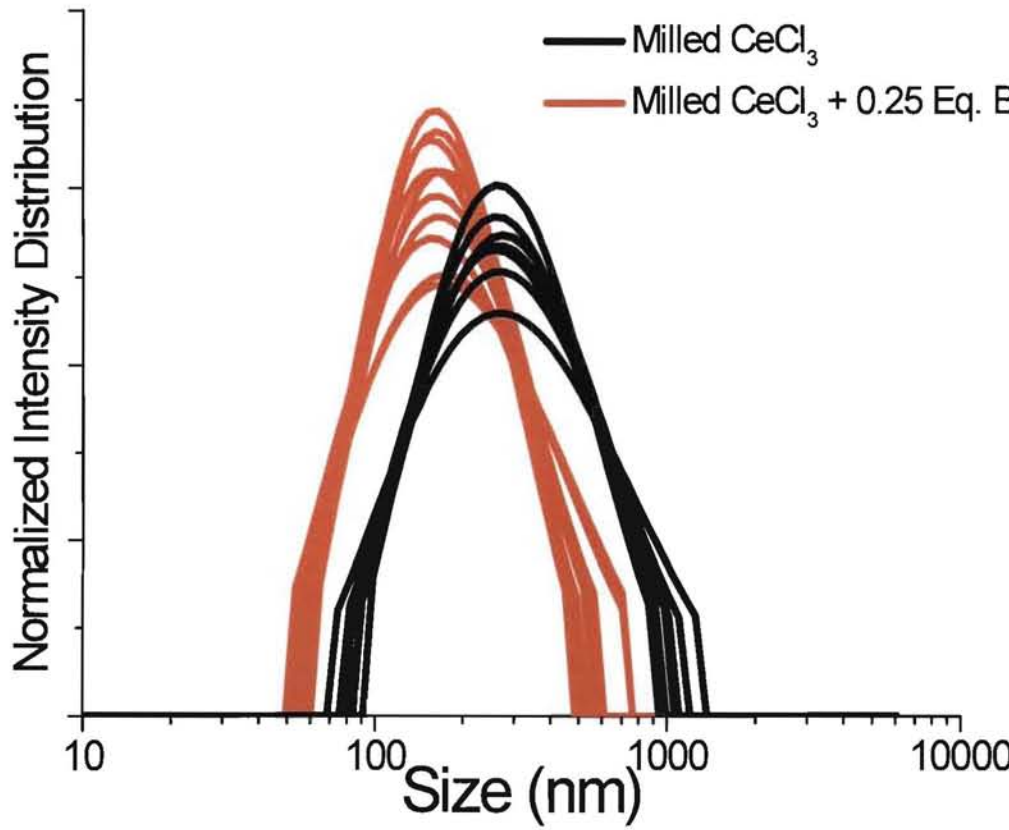


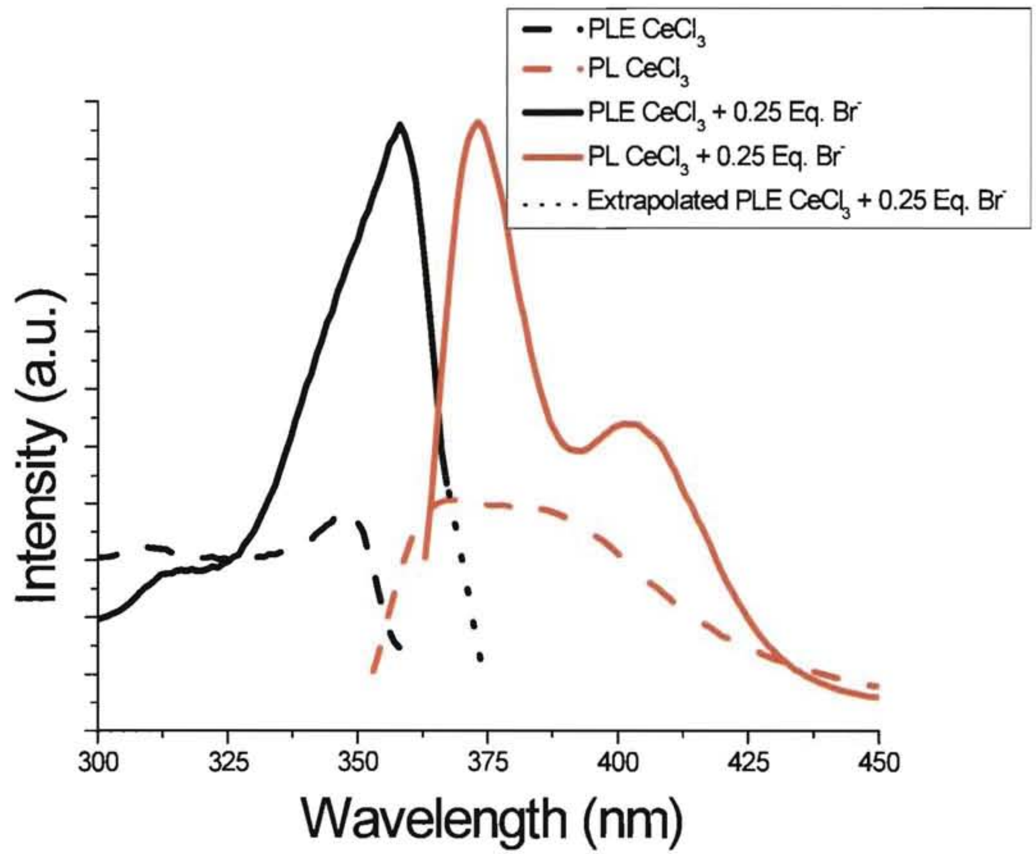




- Bromide salt addition to $CeCl_3$

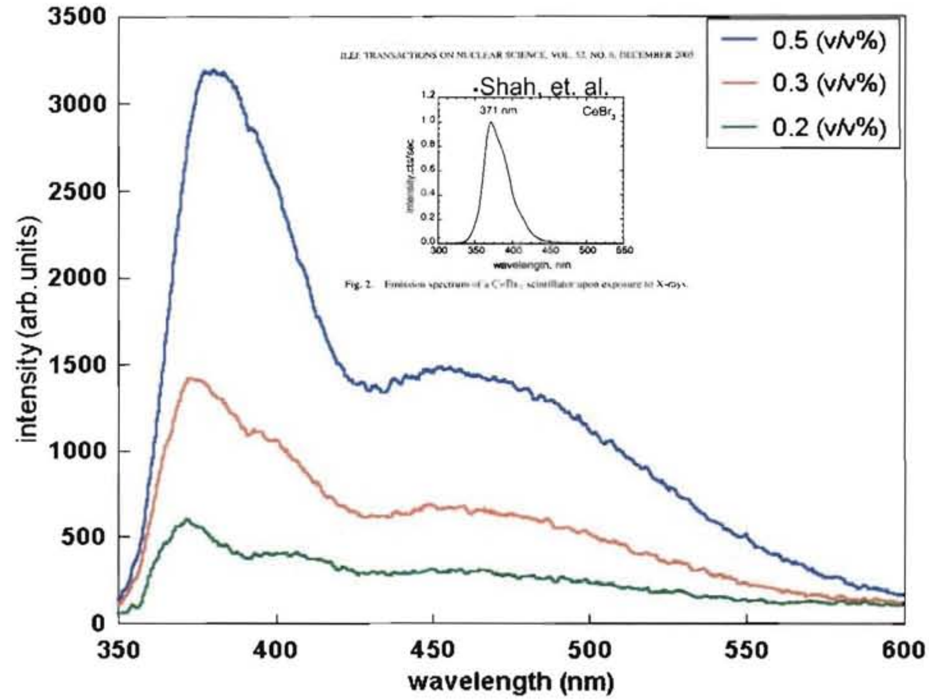



Milled $CeCl_3$
Milled $CeCl_3$ + 0.25 Eq. Br^-
Normalized Intensity Distribution
10
100
1000
10000
Size (nm)



PLE $CeCl_3$
PL $CeCl_3$
PLE $CeCl_3$ + 0.25 Eq. Br^-
PL $CeCl_3$ + 0.25 Eq. Br^-
Extrapolated PLE $CeCl_3$ + 0.25 Eq. Br^-
Intensity (a.u.)
300
325
350
375
400
425
450
Wavelength (nm)

$CeBr_3$ Nanomaterial



- Optical Response to Ionizing Radiation is consistent with that for single crystal material

Publication and Patents

- **Patent applications**
  - US 20090302195, 20080191168, 20080128624, 20080093557
- **Publications**
  - **Nanocomposite scintillators for radiation detection and nuclear spectroscopy McKigney, EA ; Del Sesto, RE ; Jacobsohn, LG ; Santi, PA ; Muenchausen, RE ; et al. NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT (AUG 21 2007) Vol.579, iss.1, p.15-18**
  - **LaF3 : Ce nanocomposite scintillator for gamma-ray detection - art. no. 67061A McKigney, EA ; Muenchausen, RE ; Cooke, DW ; Del Sesto, RE ; Gilbertson, RD ; et al. PROCEEDINGS OF THE SOCIETY OF PHOTO-OPTICAL INSTRUMENTATION ENGINEERS (SPIE) (2007) Vol.6706, p.A7061 -A7061**

Casimir Interactions

Diego Dalvit, Peter Milonni, Felipe da Rosa (T)

John O'Hara, Toni Taylor, Jianfeng Zhou (MPA)

in collaboration with I. Brener, P. Davids, M. de Boer, and S. Howell (Sandia)

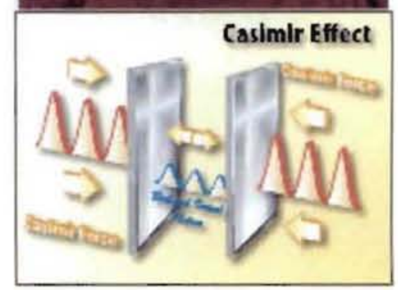
The Casimir force

- **Macroscopic manifestation of the quantum vacuum**
  - Originates from changes in quantum vacuum fluctuations imposed by material boundaries.
  - Predicted by the Dutch physicist Hendrik Casimir in 1948.
  - Typically an attractive force.
  - Related to van der Waals force.

$$E = \frac{1}{2} \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \Rightarrow \boxed{\frac{F}{A} = \frac{\pi^2}{240} \frac{\hbar c}{d^4}}$$

$$(130\text{nN}/\text{cm}^2 \ @ \ d = 1\mu\text{m})$$

  - Not small, nN is a large force on the microscale $\approx 10^{13} F_{\text{grav}}$

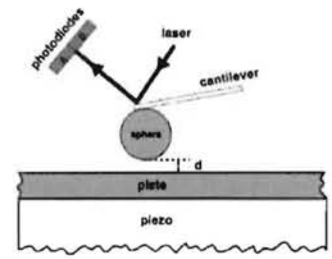


- **Magnitude and sign depend on geometry and composition of materials**

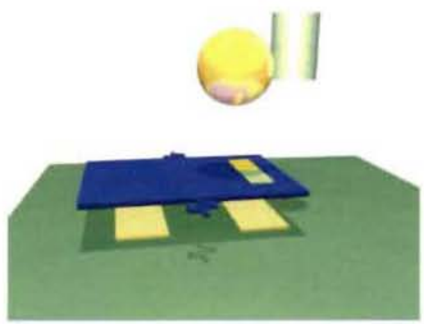
Modern Casimir force experiments

- **Torsion pendulum**

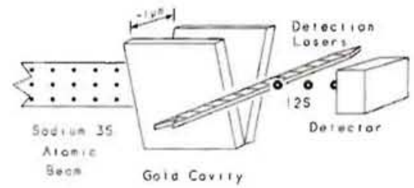
- **AFM**

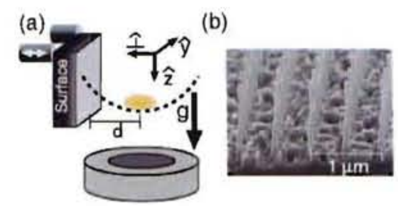


- **MEMS and NEMS**



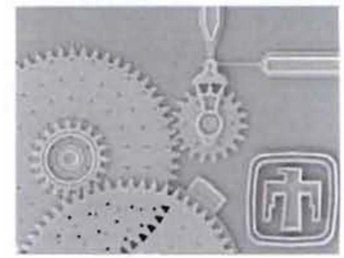
- **Atom deflection/reflection**



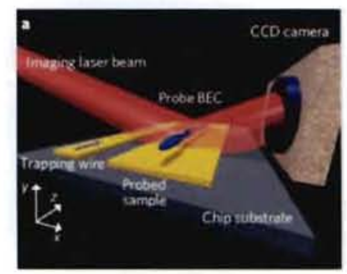


Examples of relevant applications

- **Nanotechnology**
  - MEMS and NEMS
    - Casimir force limiting factor to stiction in nanomachines
    - Quantum levitation via repulsive Casimir
  - Casimir actuation
    - Contactless force transmission via lateral Casimir
    - Quantum friction between materials in relative motion



- **Quantum science and technology**
  - Casimir atom-surface interactions
    - Precision measurements with ions, neutral atoms
    - Quantum technologies: e.g. atom chips



Materials aspects of Casimir force

- **Casimir force manipulation requires the ability to tailor the electric and magnetic properties of a material over the electromagnetic spectrum**
  - Material properties included via reflection matrices in Lifshitz formula

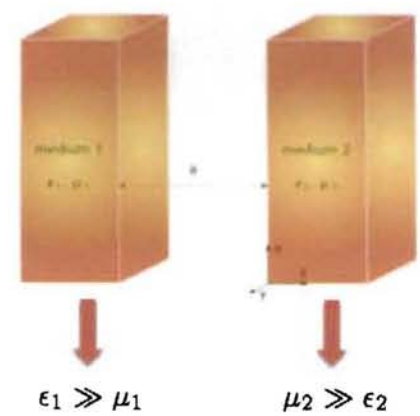
$$\frac{F}{A} = 2\hbar\,\mathrm{Im}\int_0^\infty \frac{d\omega}{2\pi}\int \frac{d^2\mathbf{k}_\parallel}{(2\pi)^2} K_3 \mathrm{Tr}\frac{\mathbf{R}_1\cdot\mathbf{R}_2 e^{2iK_3 d}}{1-\mathbf{R}_1\cdot\mathbf{R}_2 e^{2iK_3 d}}$$

$$\mathbf{R}_i[\epsilon(\omega),\mu(\omega),\ldots]$$

$$K_3 = \sqrt{\omega^2/c^2 - k_\parallel^2}$$

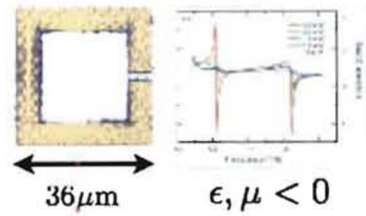
  - Sum over all possible quantum fluctuations: broad-band, all angles of incidence, all polarizations.

- **Goal of this project: Casimir force engineering with metamaterials**
  - Measurement
  - Neutralization
  - Dynamical control

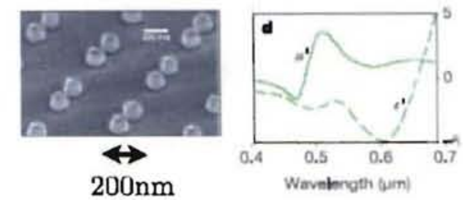


Why metamaterials?

- **Artificial structured composites with designer EM response**
- **Novel material properties:**
  - Independent tuning of $\epsilon(\omega)$ and $\mu(\omega)$
  - High frequency magnetism
  - Chirality



THz MM: SRR



Optical MM: nanopilars

- **Largely unexplored design space**
- **Dynamic (electronic/photonic) control of material response**

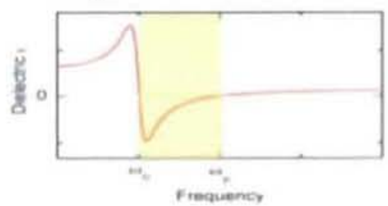
- **Requirements for MM approach for Casimir force control are challenging:**
  - High $\mu(\omega)$, low $\epsilon(\omega)$ (for neutralization/repulsion)
  - Isotropy: scalar $\epsilon(\omega)$, $\mu(\omega)$
  - Role of E-B coupling (chiral MMs)
  - Homogeneity (eff. medium)
  - Broadband

$$\begin{bmatrix} \mathbf{D} \\ \mathbf{B} \end{bmatrix} = \begin{bmatrix} \varepsilon & \xi \\ \zeta & \mu \end{bmatrix} \begin{bmatrix} \mathbf{E} \\ \mathbf{H} \end{bmatrix}$$

Effective EM response of MMs

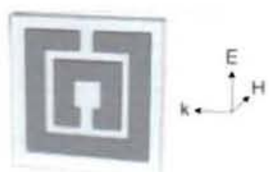
- **Effective medium approximation**
  - MM is probed with EM wavelengths much larger than unit cell
  - MM describable by effective homogeneous optical parameters

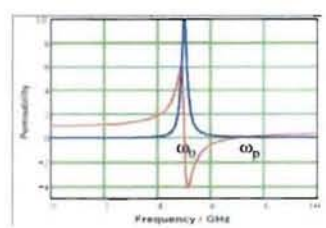
- **Effective electric response**



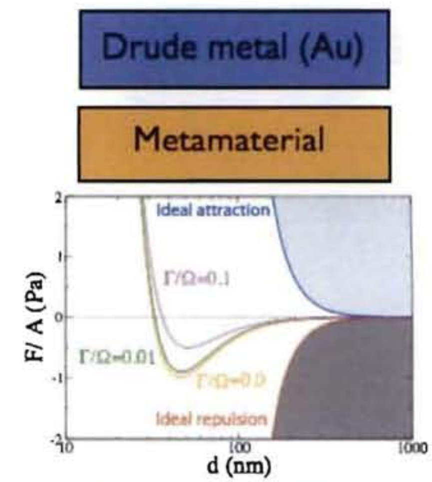
$$\varepsilon(\omega) = 1 - \frac{\omega_p^2 - \omega_0^2}{\omega^2 - \omega_0^2 + i\omega\Gamma}$$

- **Effective magnetic response**





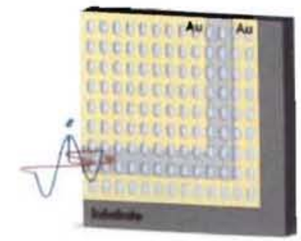
$$\mu_{eff} = 1 - \frac{\frac{\pi r^2}{a^2}}{1 + \frac{2\sigma}{\omega r \mu_0} - \frac{3}{\pi^2 \mu_0 \omega^2 C r^3}}$$

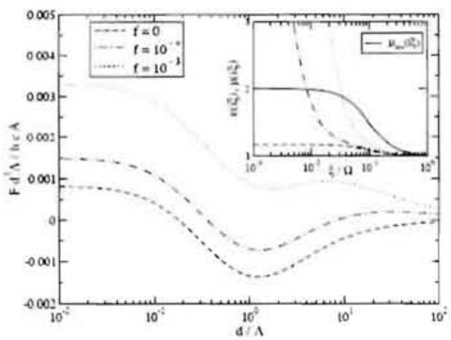


Repulsion-attraction

Casimir force with metallic-based MMs

- **Fishnet designs**
  - Demonstrated magnetic response at optical frequencies
  - Continuous Drude metal good for dynamic switching
  - Deleterious for Casimir neutralization/repulsion





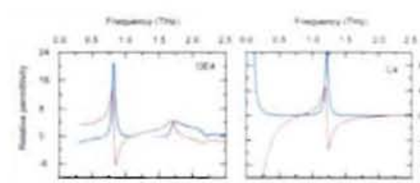
$$\epsilon(\omega) = 1 - f\frac{\Omega_D^2}{\omega^2 - i\omega\gamma_D} - (1-f)\frac{\Omega_e^2}{\omega^2 - \omega_e^2 + i\gamma_e\omega}$$

f : filling factor

$$\mu(\omega) = 1 - \frac{\Omega_m^2}{\omega^2 - \omega_m^2 + i\gamma_m\omega}$$

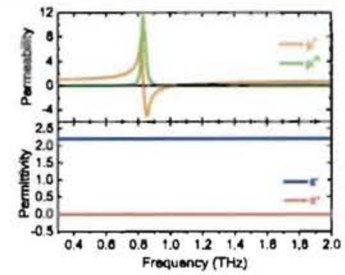
Phys. Rev, Lett. **100**, 183602 (2008); Phys. Rev. A **78**, 032117 (2008)

- **MMs with diminished permittivity**



Other MM possibilities for Casimir control

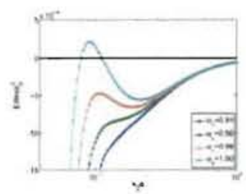
- **All-dielectric metamaterials**
  - Path to magnetism without metals
  - No Drude background, low permittivity
  - Requires high index contrast

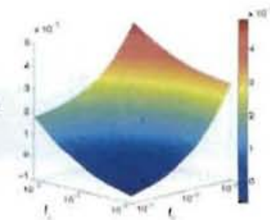


- **Chiral metamaterials**
  - Mixing of E-H fields

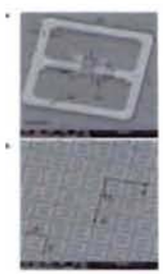
$$D(r,\omega) = \epsilon(\omega)E(r,\omega) - i\kappa(\omega)H(r,\omega)$$
$$B(r,\omega) = i\kappa(\omega)E(r,\omega) + \mu(\omega)H(r,\omega)$$

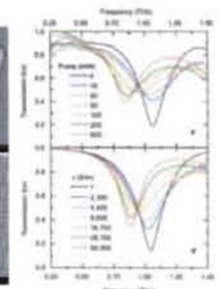
  - Path to neutralization w/ strong chirality
  - Anisotropy: generalization of Lifshitz





- **Active control**
  - Dynamics MMs made of metals and semiconductors
  - Photonic or electronic dynamic control of EM response: frequency, amplitude, phase





EMA approach to Casimir enhancement using MM

- **Calculation of force-displacement curves**
  - Inclusion of real optical data

$$\varepsilon(i\xi) = 1 + \frac{2}{\pi}\int_0^\infty \frac{\omega\,\varepsilon''(\omega)\,d\omega}{\omega^2+\xi^2}, \quad \mu(i\xi) = 1 + \frac{2}{\pi}\int_0^\infty \frac{\omega\,\mu''(\omega)\,d\omega}{\omega^2+\xi^2}$$

  - Casimir-Lifshitz force between two slabs

$$F(a) = -\frac{1}{\pi\beta}\sum_{p=te}^{tm}\sum_{n=0}^{\infty}{}' \int_0^\infty dk\,k\,(k^2+\xi_n^2/c^2)^{1/2} \times \frac{r_p^{(1)}(\xi_n,\mathbf{k})r_p^{(2)}(\xi_n,\mathbf{k})e^{-2a(k^2+\xi^2/c^2)^{1/2}}}{1-r_p^{(1)}(\xi_n,\mathbf{k})r_p^{(2)}(\xi_n,\mathbf{k})\,e^{-2a(k^2+\xi^2/c^2)^{1/2}}}$$

  - Reflection coefficients

$$r_{tm}^{(i)} = \frac{\epsilon_i\sqrt{k^2+\frac{\xi^2}{c^2}} - \sqrt{k^2+\epsilon_i\mu_i\frac{\xi^2}{c^2}}}{\epsilon_i\sqrt{k^2+\frac{\xi^2}{c^2}} + \sqrt{k^2+\epsilon_i\mu_i\frac{\xi^2}{c^2}}}$$

$$r_{te}^{(i)} = r_{tm}^{(i)}, \quad \epsilon \leftrightarrow \mu$$

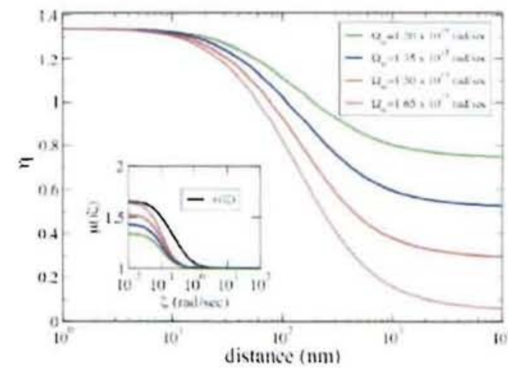


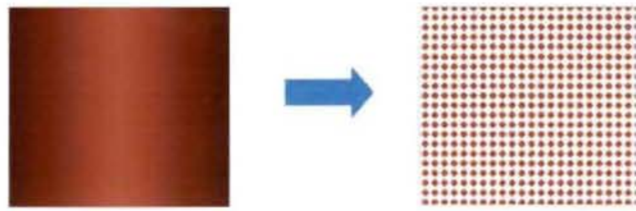
Fig. III.7: Normalized Casimir force between a Au plate and a Au-based non-connected MM for different magnetic resonance frequencies. Parameters are $\Omega_D = 1.36\times10^{16}$ rad/sec, $\gamma_D = 5.17\times10^{13}$ rad/sec, $f = 0.1$, $\varepsilon_S(\omega) = 1$, $\omega_e = 2.25\times10^{15}$ rad/sec, $\Omega_e = 1.36\times10^{15}$ rad/sec, $\gamma_e = 1.36\times10^{14}$ rad/sec, $\omega_m = 2.04\times10^{15}$ rad/sec, and $\gamma_m = 1.36\times10^{14}$ rad/sec. The inset shows the corresponding permittivity and permeabilities as a function of imaginary frequency.

Beyond effective medium approximation

- **For Casimir EMA not enough: feature sizes comparable to wavelengths**

Homogeneous medium

$\epsilon_{\text{eff}}(\omega)$
$\mu_{\text{eff}}(\omega)$



Non homogeneous medium

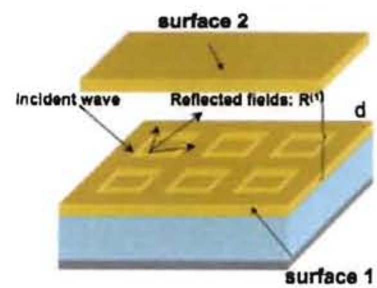
$\epsilon(\mathbf{r},\omega)$
$\mu(\mathbf{r},\omega)$

- **Exact numerical methods for Casimir force in complex material structures**
  - Green function approach: computation of Casimir stress tensor (FDTD)
  - Scattering approach: computation of Casimir energy (RWCA)

$$\frac{E(d)}{A} = \hbar \int_0^\infty \frac{d\xi}{2\pi} \log\det\left[1 - \mathcal{R}_1 e^{-\mathcal{K}d}\mathcal{R}_2 e^{-\mathcal{K}d}\right]$$

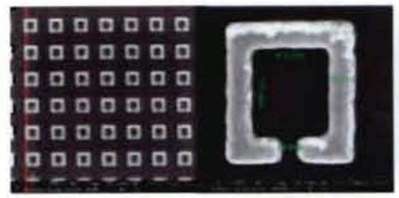
$$-ik\frac{\partial \mathrm{E}_t}{\partial z} = \nabla_t[\chi\hat{e}_3\cdot\nabla\times \mathrm{H}_t] - k^2\mu\hat{e}_3\times \mathrm{H}_t$$
$$-ik\frac{\partial \mathrm{H}_t}{\partial z} = -\nabla_t[\zeta\hat{e}_3\cdot\nabla\times \mathrm{E}_t] + k^2\epsilon\hat{e}_3\times \mathrm{E}_t$$

$$-ik\frac{\partial\Psi_{m'n'}}{\partial z} = \sum_{mn} H_{m'n',mn}\Psi_{mn}$$

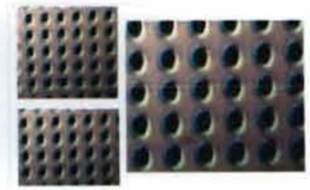


Fabrication, characterization, and measurement

- **Nanofabrication at CINT-LANL with state-of-the-art electron-beam writer**



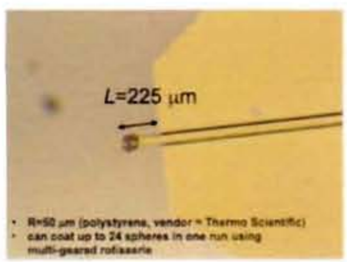
SRR: Au on InSb (3-12 um)

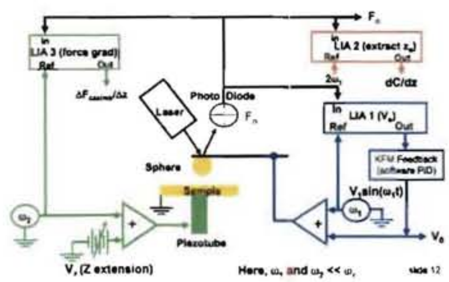


Fishnets: Al on BaF2 (7-12 um)

- **Complex T&R (angle resolved) and n&k (ellipsometry)**

- **Casimir force measurement with AFM**





Calibration via Coulomb forces

Measurement of contact potentials

Measurement of Casimir force

Relevance to LANL & materials strategy – Key points

- **Impact to LANL missions on basic science and technology**
  - Applications to nanotechnology and quantum: stiction, actuation, atom chips
- **Contribution to LANL materials strategy**
  - Emergent phenomena at interfaces : materials controlled functionality for Casimir force manipulation.
- **Key points of our project**
  - Casimir force engineering with metamaterials.
  - High profile publications (PRL, Nature) and media coverage (New Scientist, IEEE).
  - Partnership between LANL and Sandia: leverages CINT, cross-disciplinary.
  - Initial work funded by LDRD-ER. Transitioned to external DARPA funding. A program development success.
  - >20 white papers, only 5 funded proposals nationwide.
  - Organized international conference on Casimir force control.
  - Book on Casimir physics, to be published by Springer.