SAND2018-7600PE

Sandia National Laboratories

An Overview

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525

Sandia's Governance Structure

Sandia Corporation
- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–present
- Honeywell: 2017 being negotiated

Government owned, contractor operated

research and development center

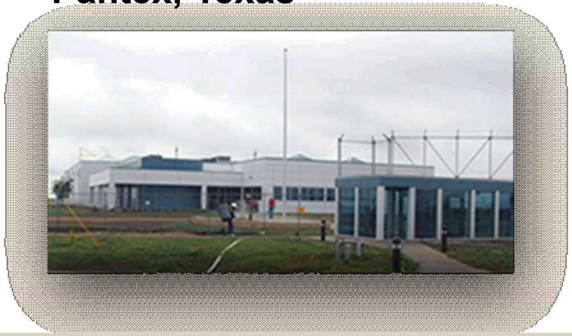
Sandia's Sites

Livermore,
California

Tonopah, Nevada

Waste Isolation Pilot Plant,
Carlsbad, New Mexico

Pantex, Texas



The Mission Has Evolved for Decades

1950s Production engineering & manufacturing engineering

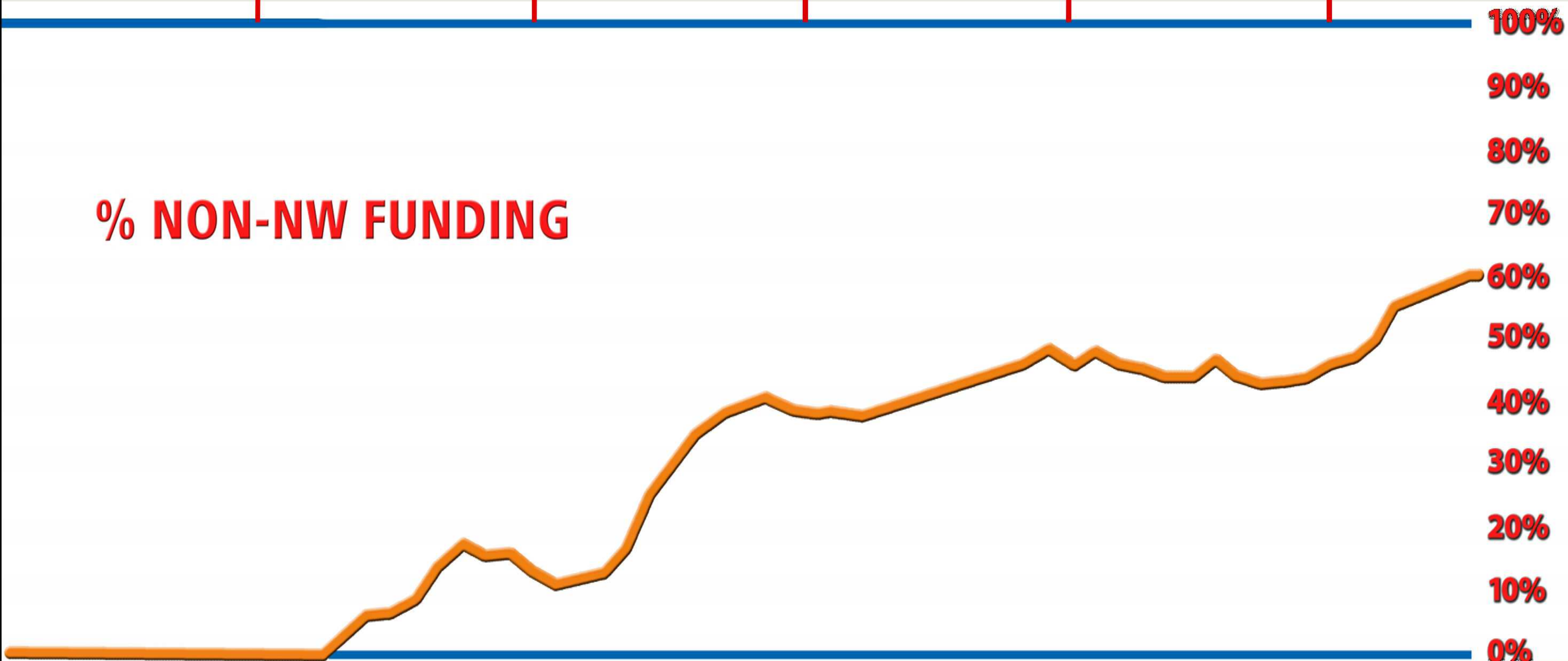
1960s Development engineering

1970s Multiprogram laboratory

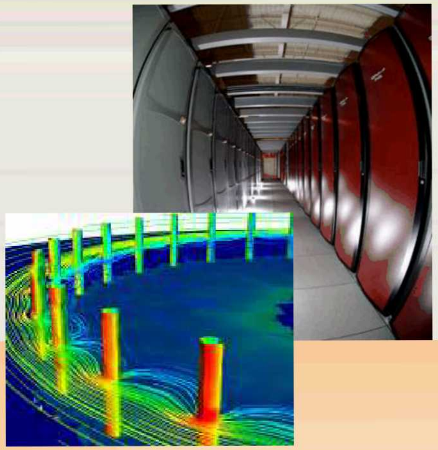
1980s Research, development and production

1990s Post-Cold War transition

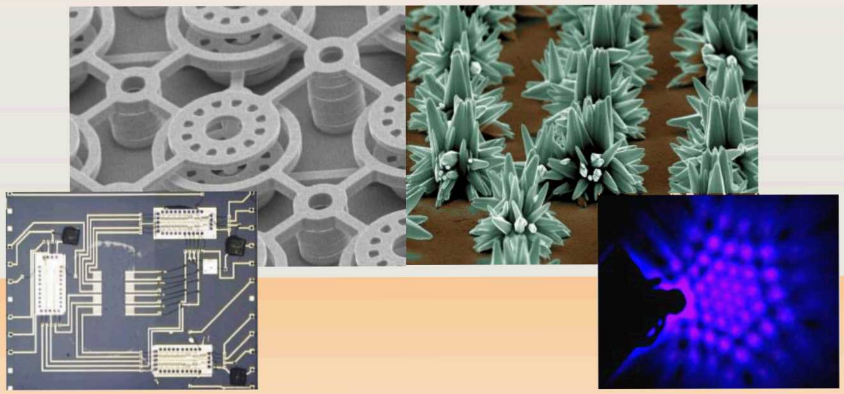
2000s Broader national security challenges



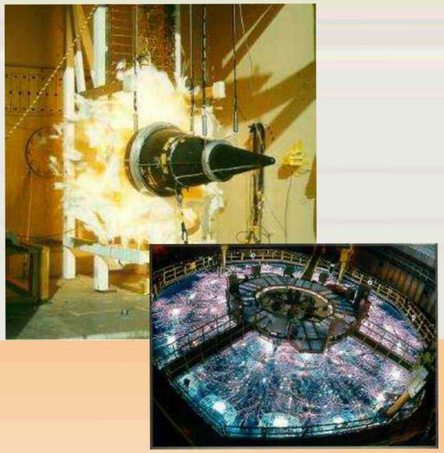
Research Disciplines Drive Capabilities



High Performance Computing

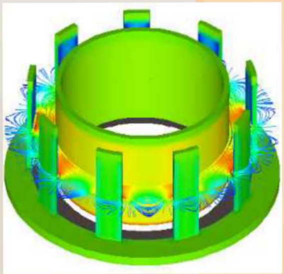


Nanotechnologies & Microsystems

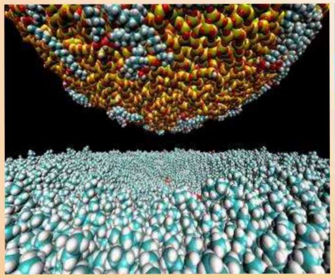


Extreme Environments

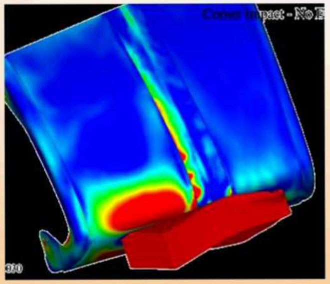
Computer Science



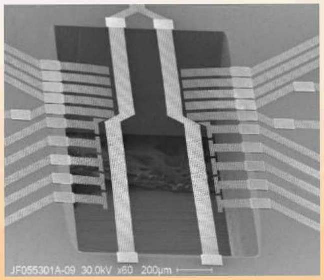
Materials



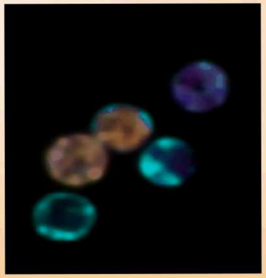
Engineering Sciences



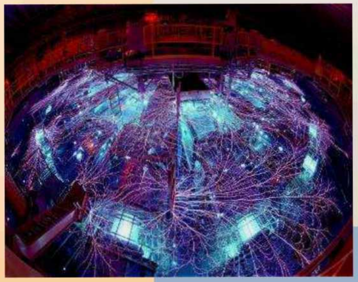
Micro Electronics



Bioscience



Pulsed Power



Research Disciplines

Advanced Materials Laboratory

Department 1815 Overview and Outlook

P. Randall Schunk, Manager

16 July 2018

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Advanced Materials Laboratory

Advanced Materials Laboratory (AML) – a Sandia-leased facility on the campus of the University of New Mexico

Original Vision: Foster substantive collaborative/partnering relationships in material science with UNM

Strategic Advantages:

- Access to students
- Greater opportunity for collaborations with UNM faculty
- Access to campus resources – equipment, library, computer resources
- Funding sources not readily available to Sandia (NSF)
- Technology transfer
- Joint purchase/maintenance of novel instrumentation

The Advanced Materials Laboratory, a part of Sandia National Labs since August, 1992
29,295 sq ft. (~14,000 sq ft lab space)

Developing materials science and engineering technology in the National Interest

AML Mission, Focus, and Vision

- The Advanced Materials Laboratory (AML) provides unique materials discovery solutions coupled with materials demonstration/deployment.

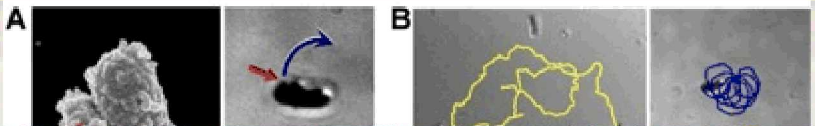
- AML's materials focus centers around synthetic chemistry routes with novel precursors and catalysts to explore new materials with solvo-thermal, solution-precipitation, and sol-gel routes.

- AML's rapidly advancing materials processing capability enables materials delivery ready for functional prototyping

  Integrated materials synthesis and materials processing breadth unique to the complex

The AML has a wide range of capabilities important to Sandia's missions

Synthetic Chemistry



embly

Characterization

- Diffractometry: XRD, XPS
- Thermal (TGA, DSC)
- Spectroscopy (mass, FTIR, ICP)
- Multispectral ellipsometer

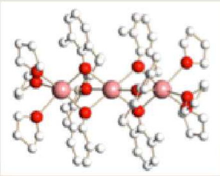
- Fibers (electrospinning)
- Bulk materials (sintering)
- Multiphoton lithography
- Direct/aerosol write, inkjet
- Gravure/flexography

1815 –Advanced Materials Laboratory Department

Inorganic and ceramics materials synthesis through chemistry, nano-materials synthesis and integration, electrochemistry for energy storage and conversion, catalytic materials, molecular structure and composition characterization, thermal processing

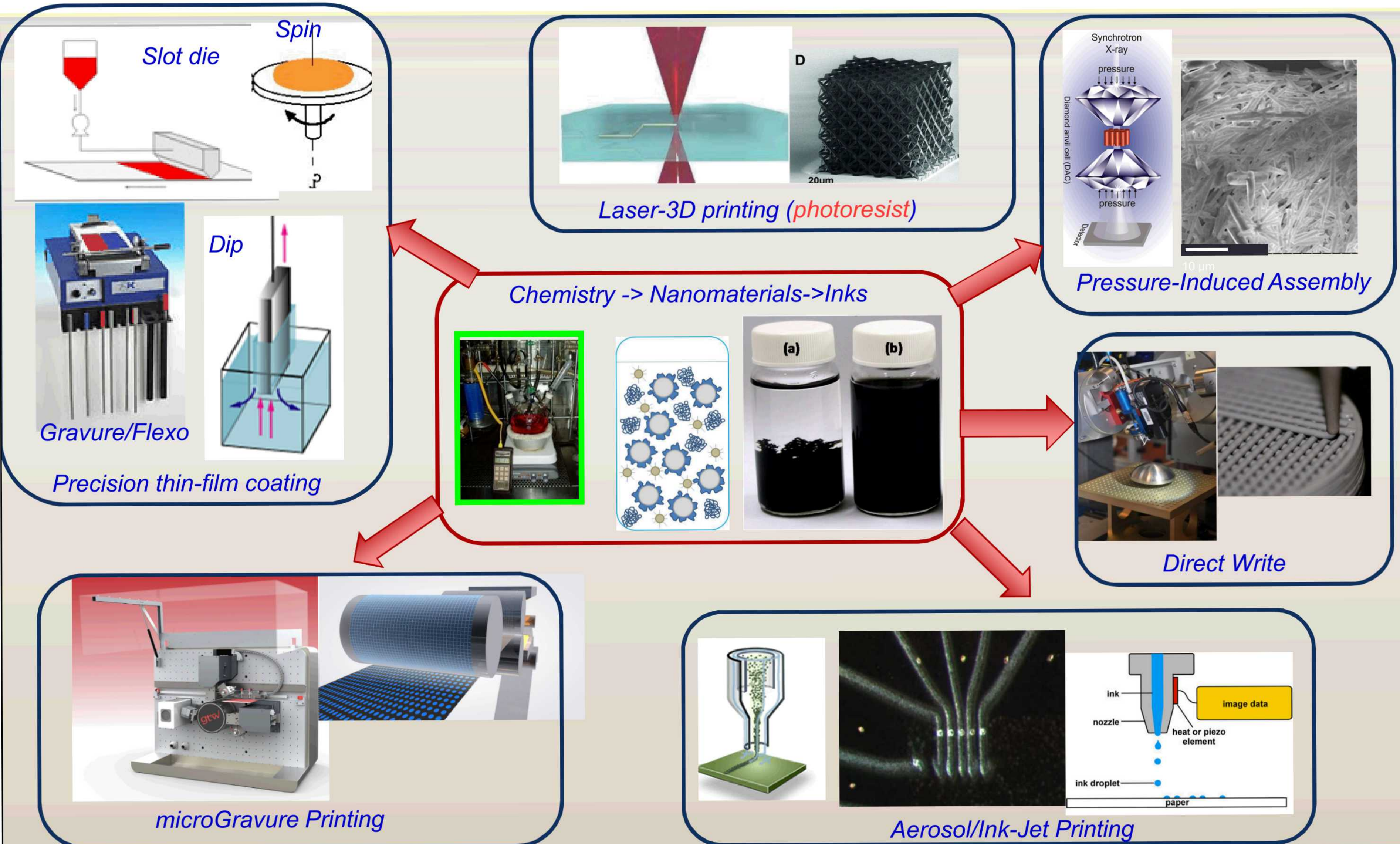
Randy Schunk, Manager

Joint UNM Appointments

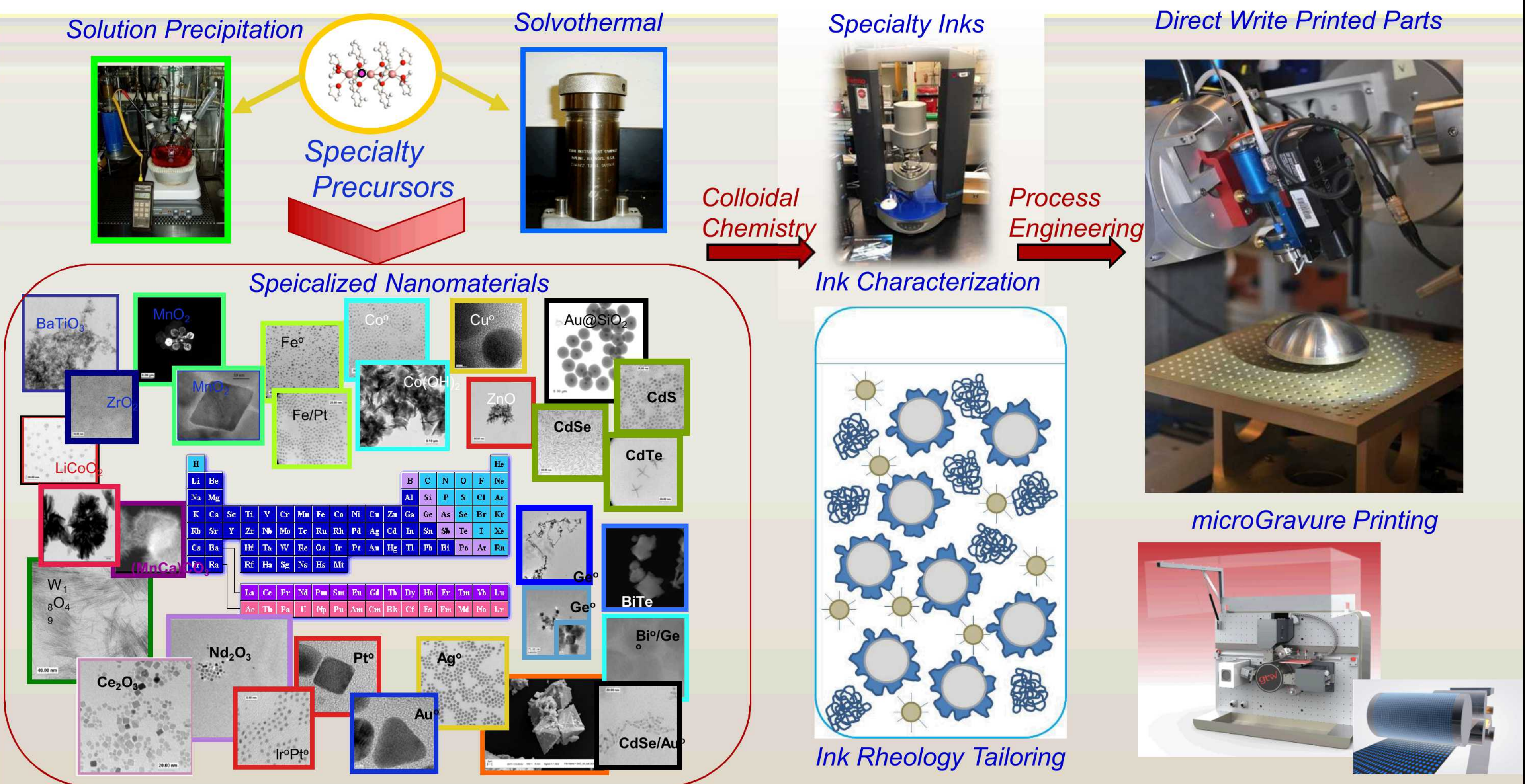


Tim Boyle	Technical staff	Inorganic chemistry and nanomaterial synthesis
Bernie Hernandez-Sanchez	Technical staff	Inorganic chemistry, nanomaterials, coatings
LaRico Treadwell	Technical staff	Inorganic chemistry, corrosion, microwave processing
Dave Keicher	Technical staff	Electrical engineering, additive manufacturing
Adam Cook	Technical Staff	Mechanical engineering, additive manufacturing
Nelson Bell	Technical staff	Materials science, colloidal dispersions
Jeremiah Sears	Technologist	Inorganic chemistry, rad chemistry, Crystallography
Derek Reinholtz	Technologist	Additive manufacturing
Amber Telles	Technologist	General chemistry, Rad materials
Hongyou Fan	Technical staff	Nanomaterials synthesis and assembly
Fernando Garzon	Technical staff	Materials science sensors, energy
Bryan Kaehr	Technical staff	Materials science, novel processing routes
Alexander Wirth	Technologist	Additive manufacturing
Lindsey Evans	Technologist	ChemE, pressure systems , safety
Ethan Secor	Truman Fellow	Materials science, additive manufacturing

AML Materials Processing Routes



From nano-materials to components at the AML

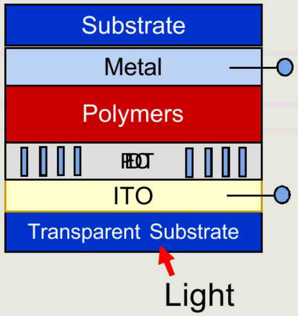


From specialized, tailored nano-materials to process-able inks requires chemical synthesis, colloidal chemistry, rheology/characterization, process engineering

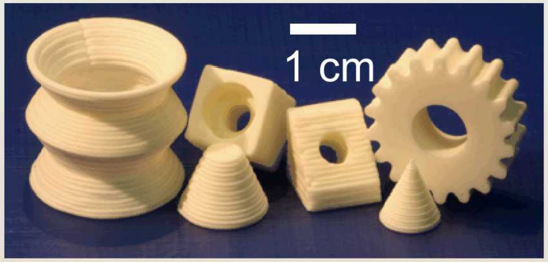
AM with Particulate Inks and Polymers at Sandia

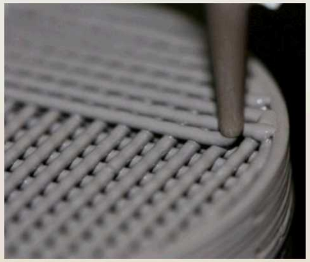
- Materials/devices for energy storage, generation, conversion, sensors needed in volume – *AM with physical template (viz.demands speed, materials flexibility, R2R)!*
- Ceramic piece parts, soft polymer parts, and other materials-by-design – *AM with digital template (e.g. demands design and materials flexibility - direct write)*
- Printed electronics – packaging and logic devices, power sources, passive antennas. *AM with digital and physical templates (demands materials flexibility and precision)*
- *Other at SNL: Energetic, Bio, photonics …*

Energy Storage/Generation Materials



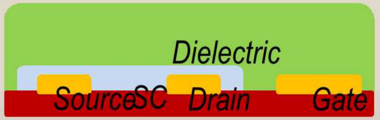
Ceramics and meta-materials





Flexible electronics

Mobile computing



Printable cables/connectors/electronics for advanced delivery platforms

Issue

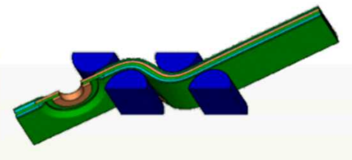
- Cables and connectors constrain system design options and drive significant costs*. Agility and modularity of future systems hinges on rapid prototyping of interconnects.
- Advanced delivery platforms will require components with new functionalities, more robust packaging and SWAP-agile integration methods not achievable with current commercial alternatives.
- Component agnostic electronic backbones for rapid technology insertion require agile connector and flexible cabling solutions.
- Material synthesis, rheology, and process science gaps inhibit timely development & adoption of electronic/cable/connector technologies.

Solution

- Established materials and process science basis for technology development and maturation contributing to an NW-qualified component insertion process to adapt to evolving mission environments.
- Fuller material selection palette to provide mission specific tailored functionality through engineered nanomaterials (semiconductors, conductors, dielectrics) with inherent hardening attributes.

Impact

- Reduced design cycles & development costs for electronic subsystems.
- Low-volume design capabilities with pathway to production.
- Enabled modularity & rapid response to threat environment shifts.
- Predictive capability for creating and introducing new materials and electronic components into the stockpile with an ability to quantify performance margins & loading response/resilience in mission use.

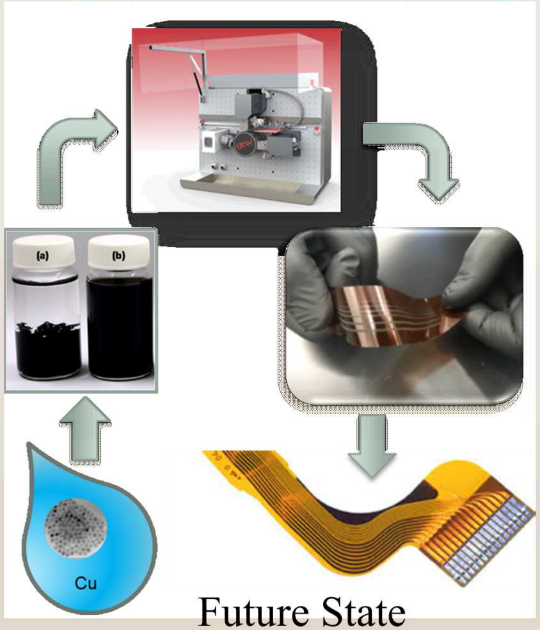


FEA model of deformed flex circuit

Circuit Failure

Current State

Components with demonstrated aging issues, limited resilience to insults, and constrained technology insertion agility for more extreme operating regimes.



Future State

Science guided materials synthesis & manufacturing routes for electronics, cables, and connectors with increased survivability margins.

Printing Inks Carry Functionality

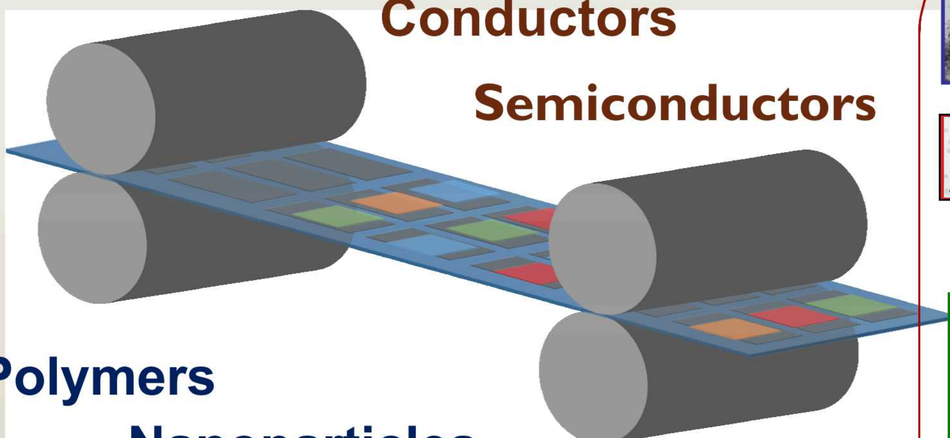
The strong suit of printed systems is the integration of diverse materials

But process design can depend on these material selections.

Dielectrics

Conductors

Semiconductors

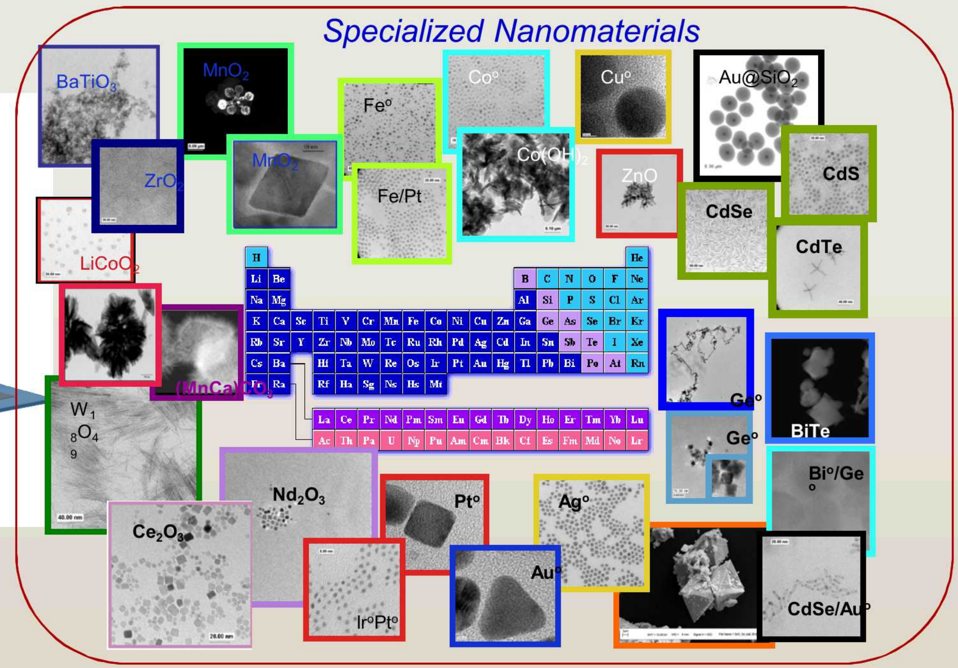


Polymers

Nanoparticles

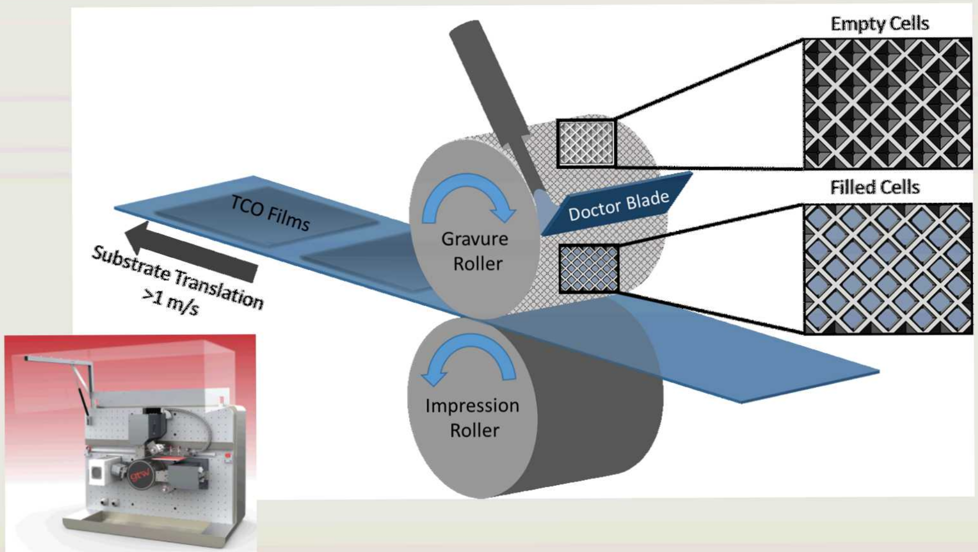
Composites

Sol-gels

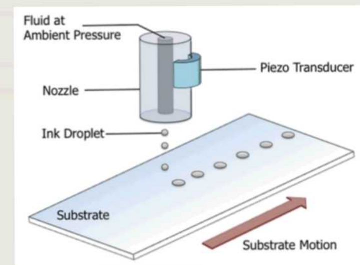


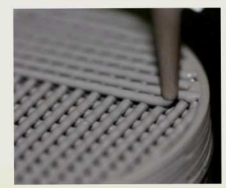
Ink-based printing routes

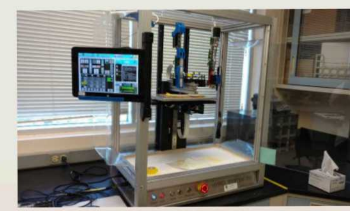
Gravure/Flexographic Printing



Direct Write (DoD, DW, Aerosol)



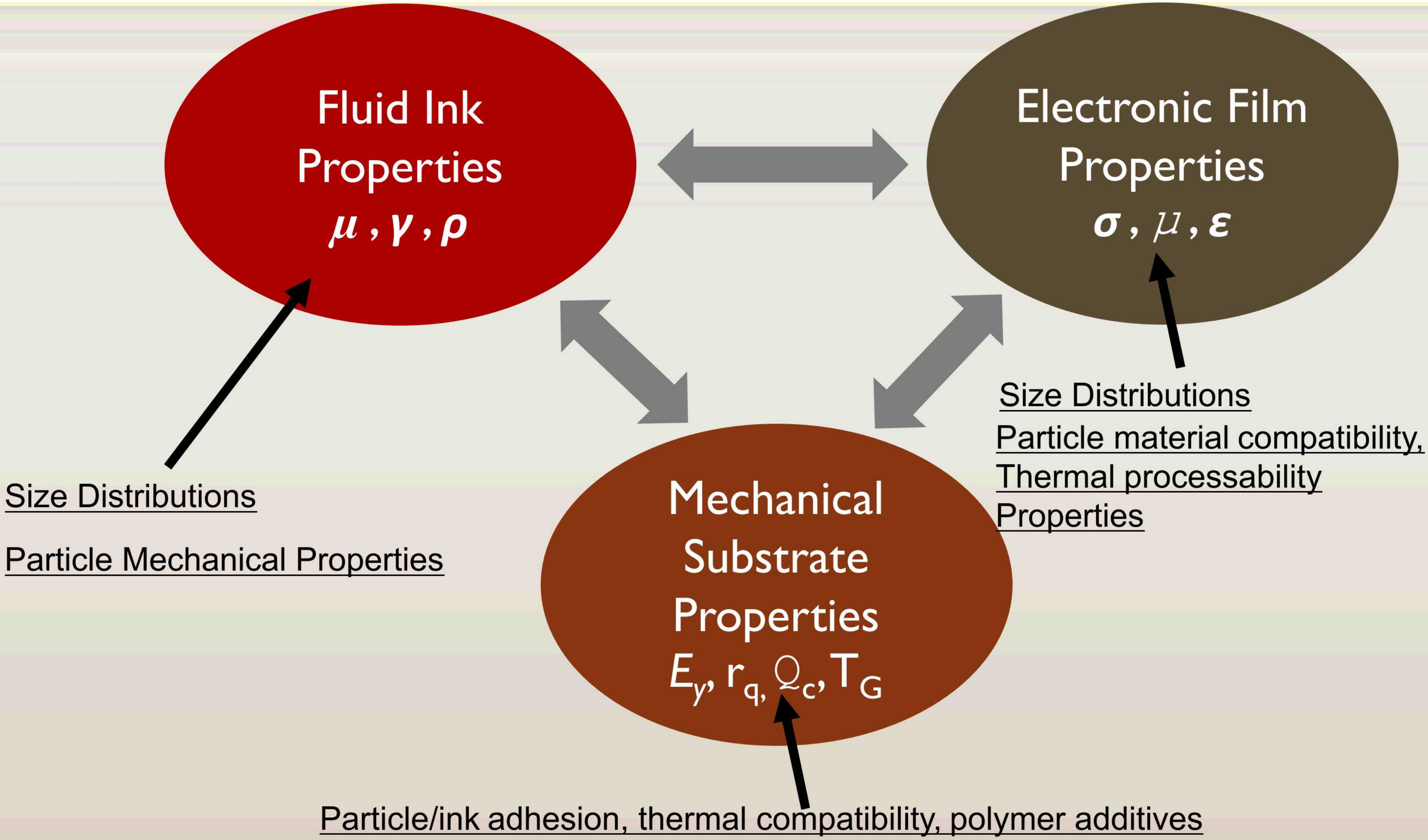




	Gravure	Direct write
Resolution	< 5 µm	< 30 µm
Speed	1 m^2/s	< 1m^2/hr
Ink Viscosity	1-500 cP	1 cP – 10^4 P
Method	Contact	Non-Contact

Inkjet and gravure are complementary methods for low-cost fabrication

Gravure/Ink-Jet Process science for ink-printing requires Co-Design

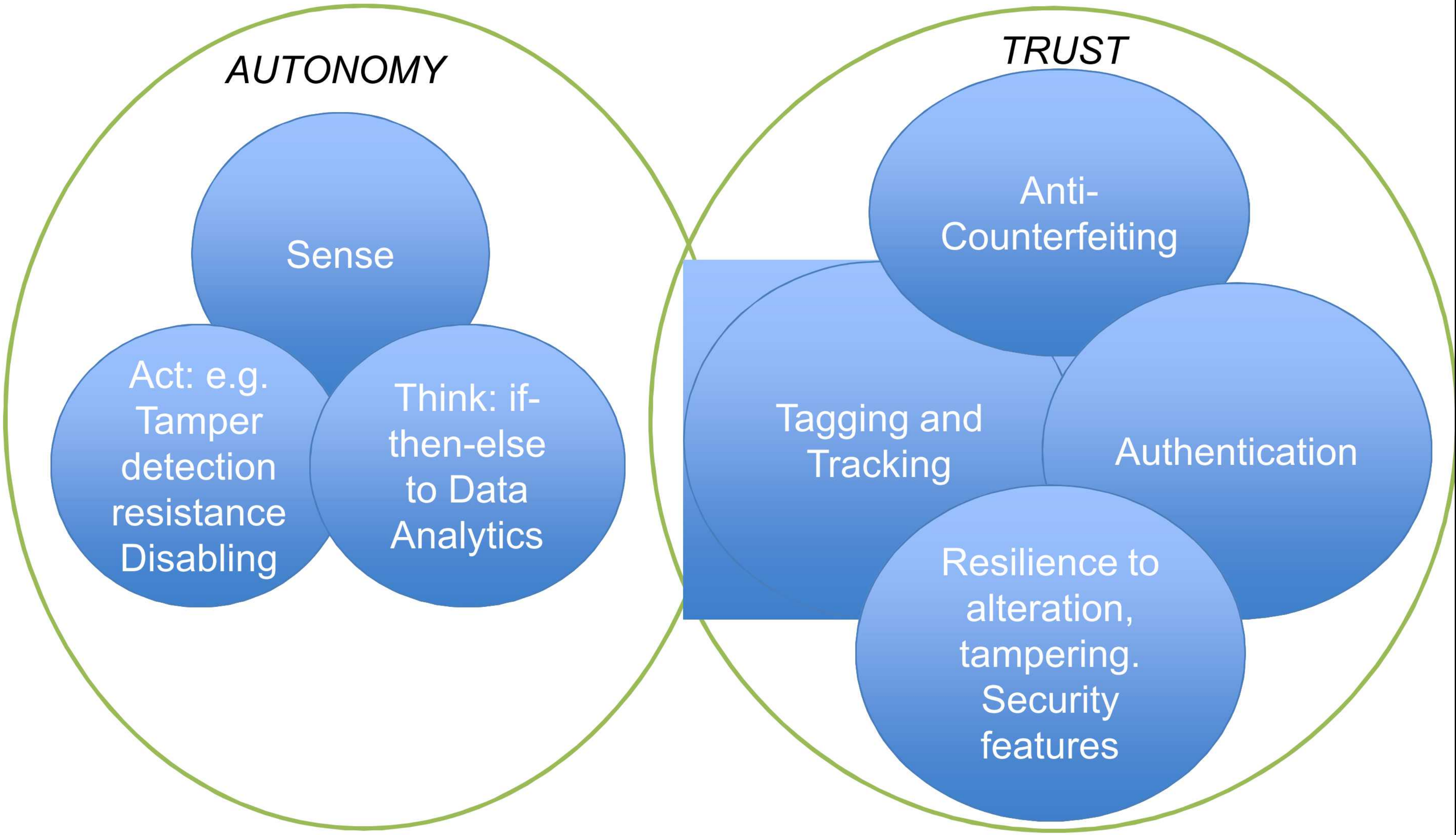


Inks, printing processes, and devices require iterative codesign

Relevant Partnerships at the AML

- Center for MicroEngineered Materials (UNM AML tenant)
  - Analytical equipment (microscopes – SEM, Raman, AFM)
  - XRAY Photoelectron Spectroscopy – Trace amounts of surface elements
  - Electrochemistry for advanced battery concepts, etc.
- NASCENT – NSF Engineering Research Center focused on nanomanufacturing systems (Kaehr – IAB, Schunk – Faculty)
- 3M, P&G, Corning, Avery Dennison
  - Modeling and simulation of manufacturing systems (including flexo/gravure)
- University of Akron
  - Printable sensory materials for trust and related
- Lockheed Martin
  - AM for active ceramics technology

Trust is but one Security Application for Materials



Many materials-based solutions in common, and all achievable in printed devices!

Achieve *Trust* through Materials, Chemistry, Advanced Manufacturing Science, and Metrology

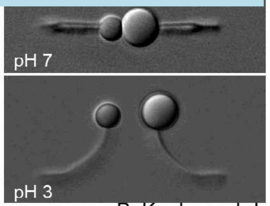
Materials and Chemistry

- Chemical/microstructure encoding (tagging and tracking, security features, counterfeit detection)
  - Nanomaterials (0d, 1D, 2D, core-shell, etc.)
  - Ion modification
  - Structural, phase change, or chemical release upon stimuli
  - Optical, electromagnetic emission upon stimuli

Thermochroic pigments

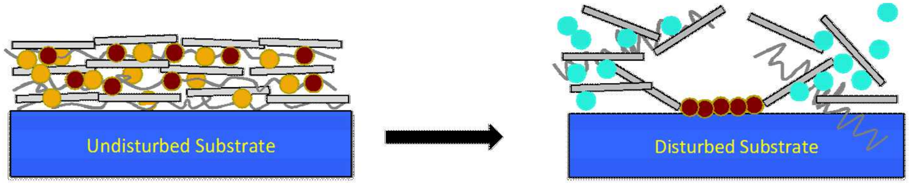
Piercetheorganist, wikipedia.o

Chemically responsive hydrogels



B. Kaehr and J. B. Shear, *PNAS*, 2008, 105, 8850-8854.

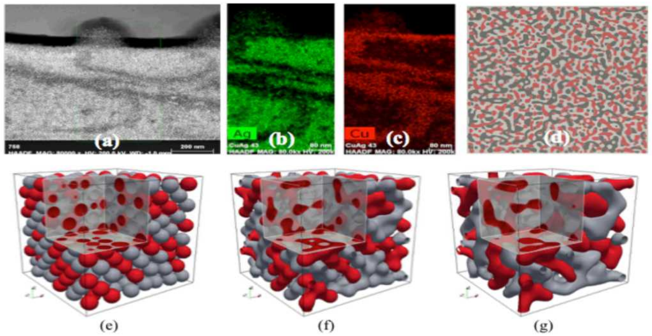
- Material resilience to alterations (Tamper resistant, Self-healing/self-destructing)
  - Polymers
  - Nanomaterial composites
  - Chemistry



Achieve *Trust* through Materials, Chemistry, Advanced Manufacturing Science, and Metrology

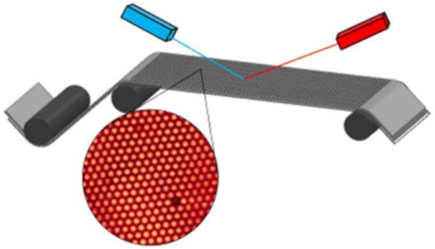
Advanced Manufacturing Science

- Adaptable, flexible processing of “encode-able” materials
  - Particulate inks and powders
  - Process-property control (polymer, metal/ceramic microstructure)
    - –Thermal
    - –electromagnetic processing
- Multi-material AM
- Substrate properties/response
- Device or printed packaging (disabling) – enables engineered trust in COTS.
- Process-property (polymer, metal microstructure)

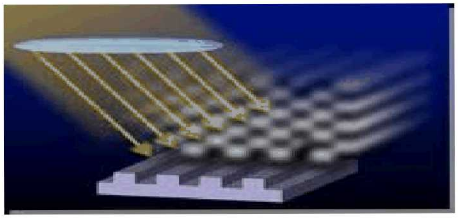


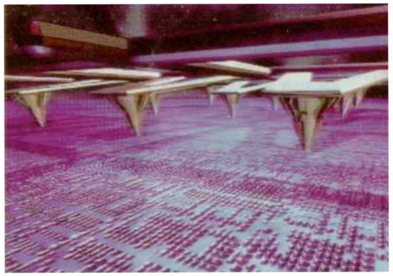
Achieve *Trust* through Materials, Chemistry, and Advanced Manufacturing Science, Metrology

Metrology (depends on the trust feature)



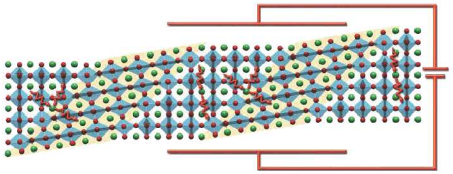
- Micro x-ray spectroscopy
- Electron, Raman, optical microscopy
- XRD – single crystal, powder, small-angle
- Orthogonal testing
- Optical inspection/metrology (spectroscopy on stimulated emissions, defect detection, scatterometry, interferometric, or related)

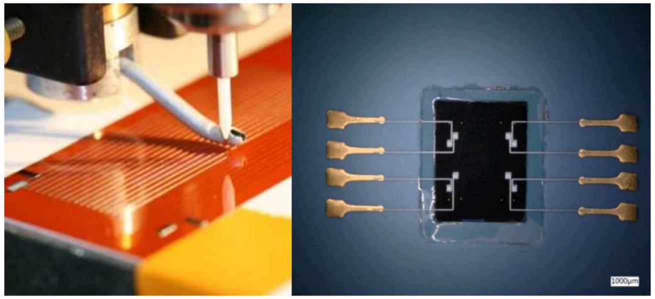


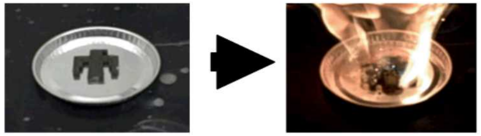


Why Sandia? Why Now? Why Partnership?

- **Applications (active and conceived)**
  - Wide area electronics.
  - Smart electronics packaging (wide area)
  - Unpowered power on/off devices in response to environmental conditions
  - War fighter technologies (wearables)
  - Materials with inherent trust features (chemical, structural) that are resilient to potential attacks throughout the lifecycle.
  - Beyond Moore Technologies (quantum computing, organic electronics)
  - Alter device functionality in presence of environmental stimulus including sensor automated functionality/response.
  - Self-healing materials.
  - Time-aware material performance to control functionality window.
  - Acoustic metamaterials for autonomous shock and vibration control
  - Reconfigurable memory
  - Smart sensors
  - Devices for non-proliferation
  - .....



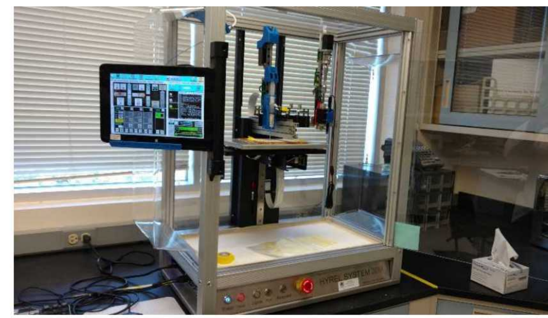




Sandia has the ability to create synergistic hybrid technologies

Why Sandia? Why Now? Why Partnership?

- **Manufacturing/Fabrication "Commons" at Sandia**
  - Silicon CMOS
  - III – IV Semi
  - Radiation hardened microelectronics
  - Reactive ion etching
  - Lithography of various forms (optical, imprint)
  - 3D printing (polymers, metal)
  - Advanced vacuum technologies
  - Advanced CVD technologies (viz. ALD)
  - Ionomeric polymers
  - Metal and polymer Additive manufacturing
  - *Polymer science and processing (Akron and others)*
  - ***2D printing, printed devices (AFRL, and others)***
  - ***Precision printing and liquid film coating***
  - ***Modeling and simulation at all scales***



Sandia's commons are complimentary…..

"Nano-Manufacturing" - Control of Structure in a "Practical" way

Functional Materials
- Nano-patterned materials
- Nano-patterned surfaces

Underpinning Science
- Bottom-up (self assembly, self organization*)
  - Exp.: Brinker, Fan, et al.
  - M/S: Schunk, Grest, et al.
- Top-Down: Nano Patterning
  - Exp: Talin, Bogart
  - M/S: Schunk, Reedy, Chandross et al.

Manufacturing "Science"
- Schunk, Kaehr, Boyle, Cook, et al. (AML)

Large Throughput Processing Fundamentals
-Coating, Molding, Embossing (AML, CRMPC, UT)

Nano-Particle Fundamentals
-Drying (NPFC, Schunk, Cook, Kaehr)
-Rheology (NPFC, Bell et al.)
-Phase and Thermo (all.)

Nano-Patterning Fu
-Imp
-Other Lithography

Nanoink development

Machine Design
-Summit V, MESA
(UT partner)

Template Fab.
-MESA
(UT partner)

NanoParticle Fab.
-Boyle et al., AML

Relevant, Ongoing Activities
-Fluctuating fluids
-Imprint, release
-Long range order
-filling at 30 nm

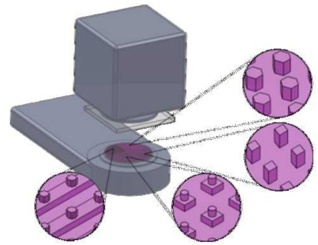
*Made practical by Pre-Processing to Concentrated form, before thermo takes over

Backups – and Partnerships

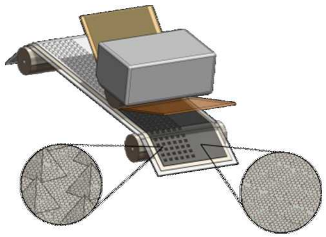
Sandia National Laboratories

NASCENT Enabling Technologies

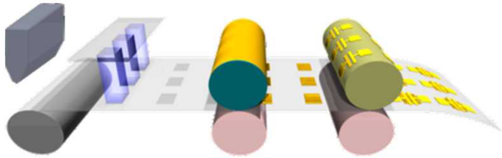
- 2D/3D Nanosculpting
  - Wafer Scale and R2R Substrates



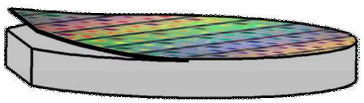
- Roll-to-roll (R2R) graphene transfer



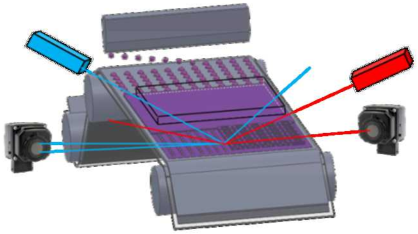
- R2R Printable Nanomaterials



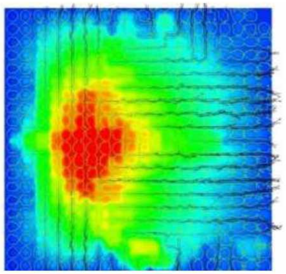
- Exfoliated crystalline materials



- In-line nanometrology



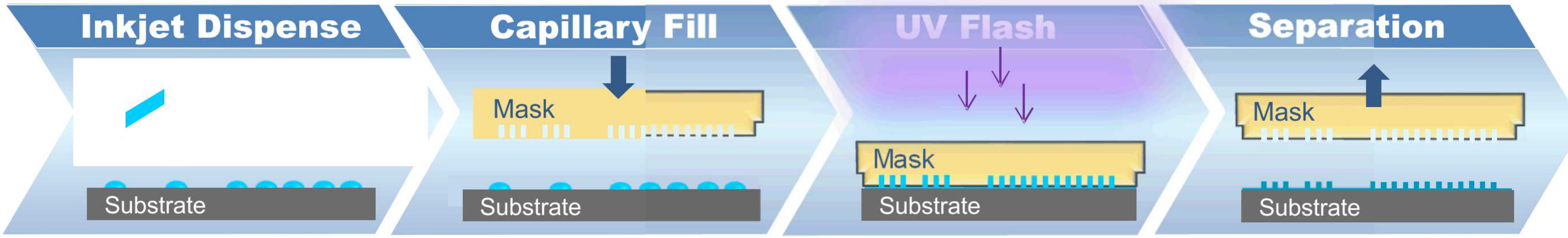
- Scale-Up and Reduced Order Model Simulators



Courtesy of Larry Dunn Ph.D.

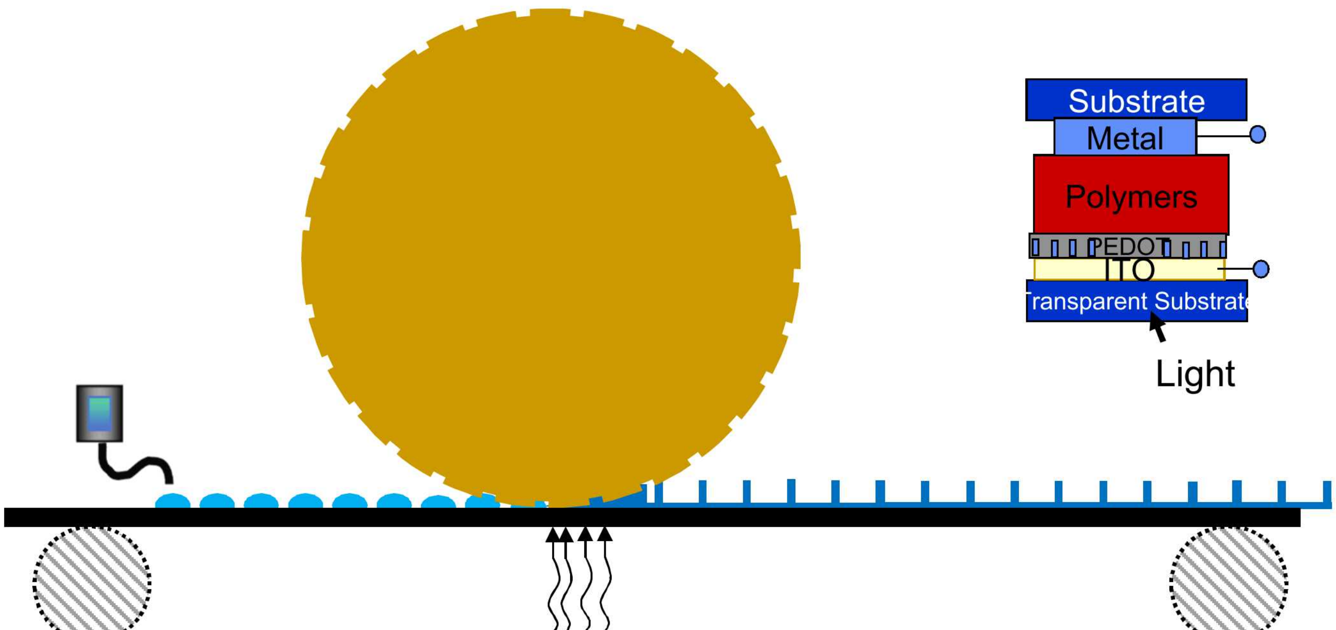
Nanosculpting: Nanoimprint Lithography

Jet Flash Imprint Lithography™ (J-FIL™)



Courtesy of MolecularImprints

Roll-to-Roll Nanoimprint Lithography (R2R_NIL)



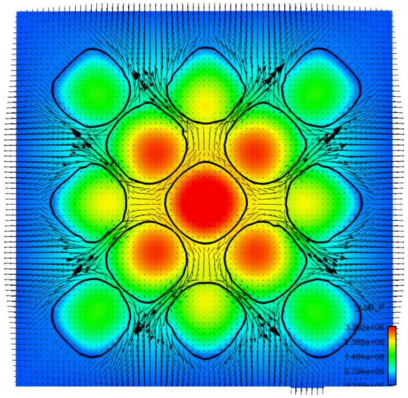
High density storage

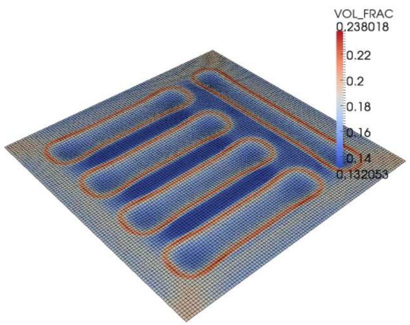
Courtesy of Akhilesh Jain

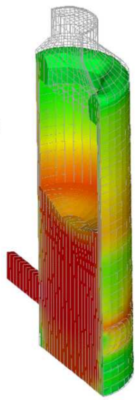
Sandia National Laboratories

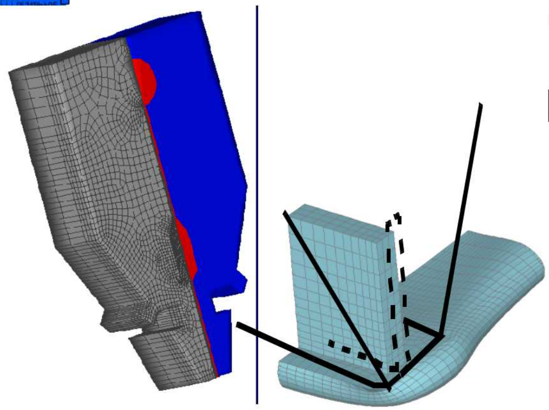
Research Group Capability: Goma 6.0

2014 R&D 100 Award Winner





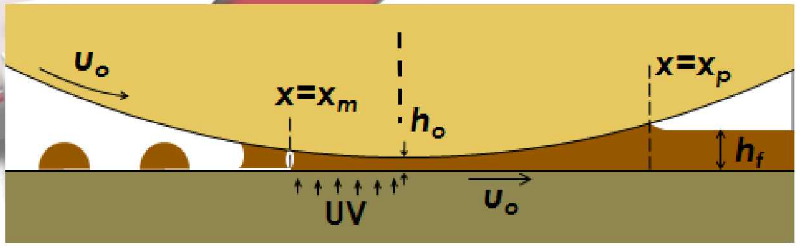




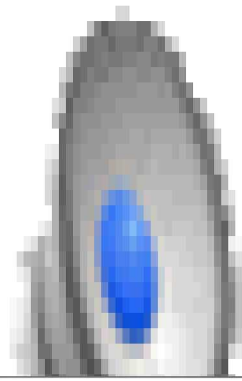
- Multiphysics ***finite element*** code, suitable for both ***research*** and ***production***
- Fully-coupled ***free*** and moving ***boundary*** parameterization – ALE, Level Set, etc.
- Modular code; ***easy to add equations*** – currently has 170+ differential equations
- ***Open source***! Available at **http://goma.github.io**
- ***Goma 6.0. training*** is available on regular basis

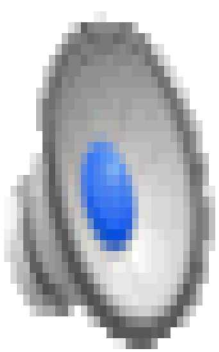
Goma has been used successfully in coating manufacturing for 2 decades!

…Also a competency in LAMMPS for colloidal rheology and self/directed assembly



Many Drops with Surface Tension





NASCENT Representative Application:
Wire Grid Polarizer

Photo-Polymer Pattern
Based on Volume analysis:
Final Uniform Layer of 75 nm

Drop Pattern

Radius:	20 μm
Initial Gap:	20 μm
Individual Volume:	25 pL
Pitch:	365 μm

Project goals, motivation

- Develop processes for printing of *0D and 1D materials*
- Develop tooling for high-speed functional materials printing (potential for submicron – transitors (Subramanium group)
- Develop underlying nanomaterials technology for high-speed printing
- System test-beds: Roll-to-roll nanofabrication system
- Our role: Use modeling and simulation to influence these developments

Applications:

- Printed electronics - use traditional printing techniques with specialized inks
- Flexible electronics
- Display layers, printed batteries, other nanomaterials processing

Other "options"

-Contact printing (flexographic, screen)
-Ink-jet/Aerosol printing
-Electrodydrodynamic printing
-Capillary printing (dip pen)
-Imprint lithography – but needs a subtractive step

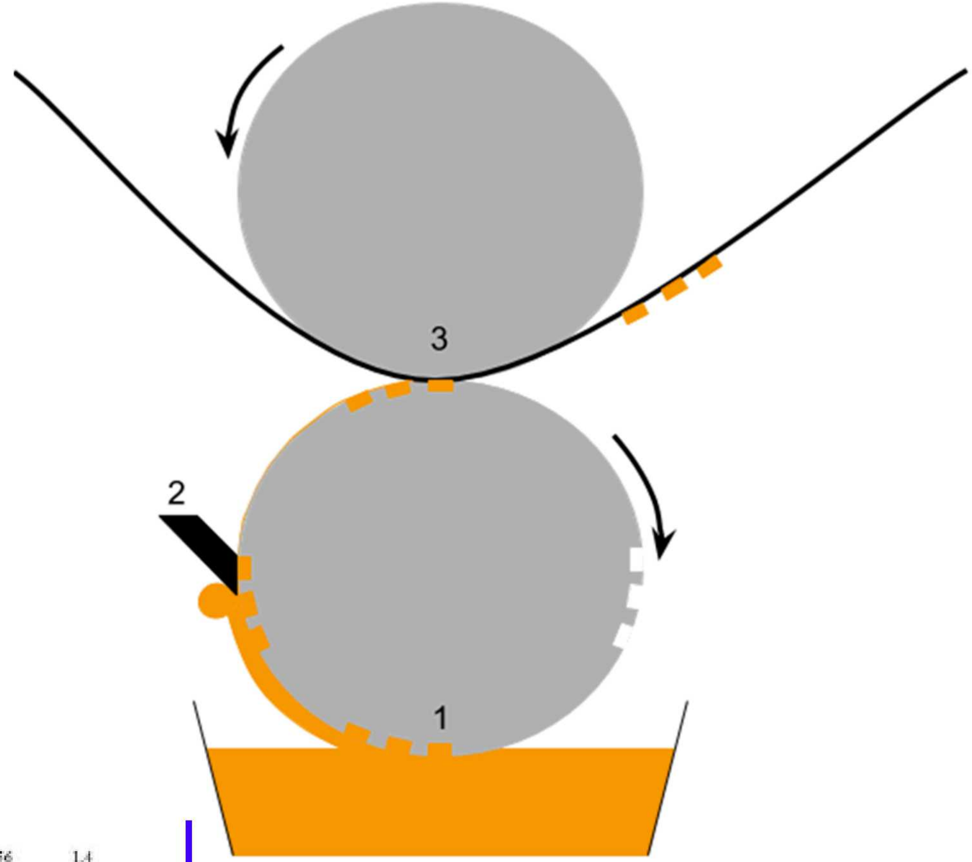
Gravure Printing Process

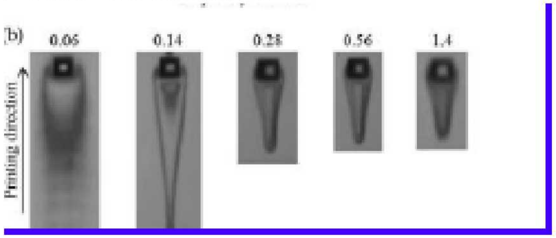
Gravure printing is a high throughput, high-fidelity, scalable printing technique

Involves three steps:

1. Filling - Fill template with fluid
2. Doctoring - Remove excess fluid
3. Transfer - Transfer fluid to substrate

Arguably, removing excess fluid is most important step for feature resolution

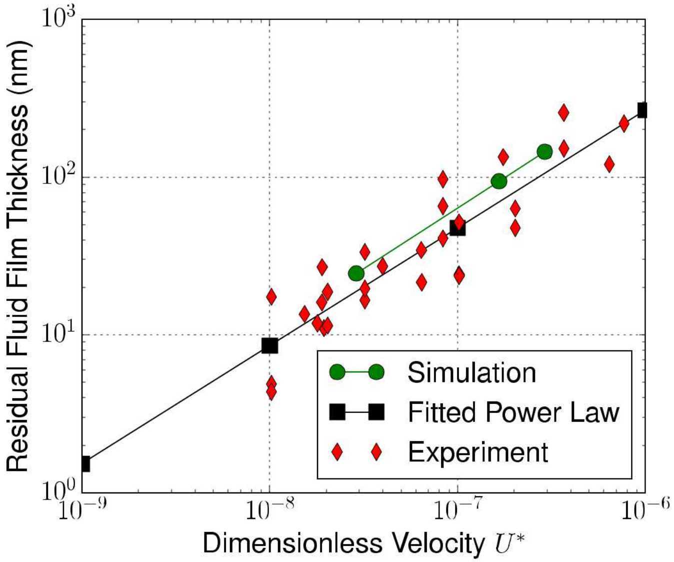


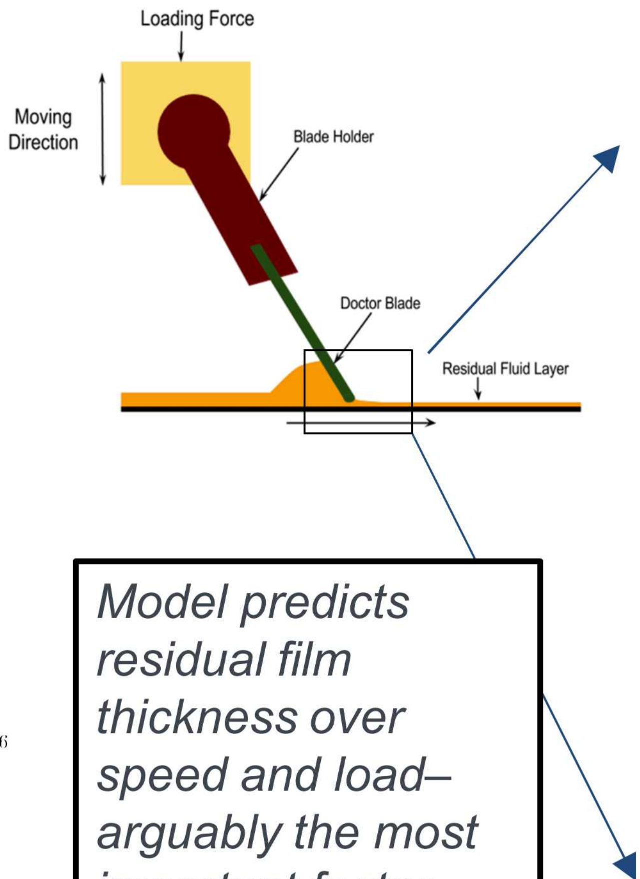


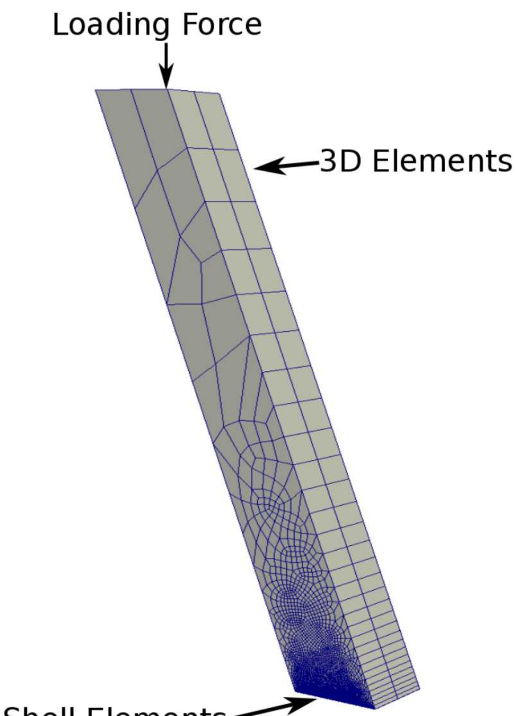
•Kitsomboonloha et al., *Langmuir* 30.12 (2014): 3612-3624.

Computational model of doctoring in gravure printing

Thrust: P-2C Reliable Processes for High-Speed Printing







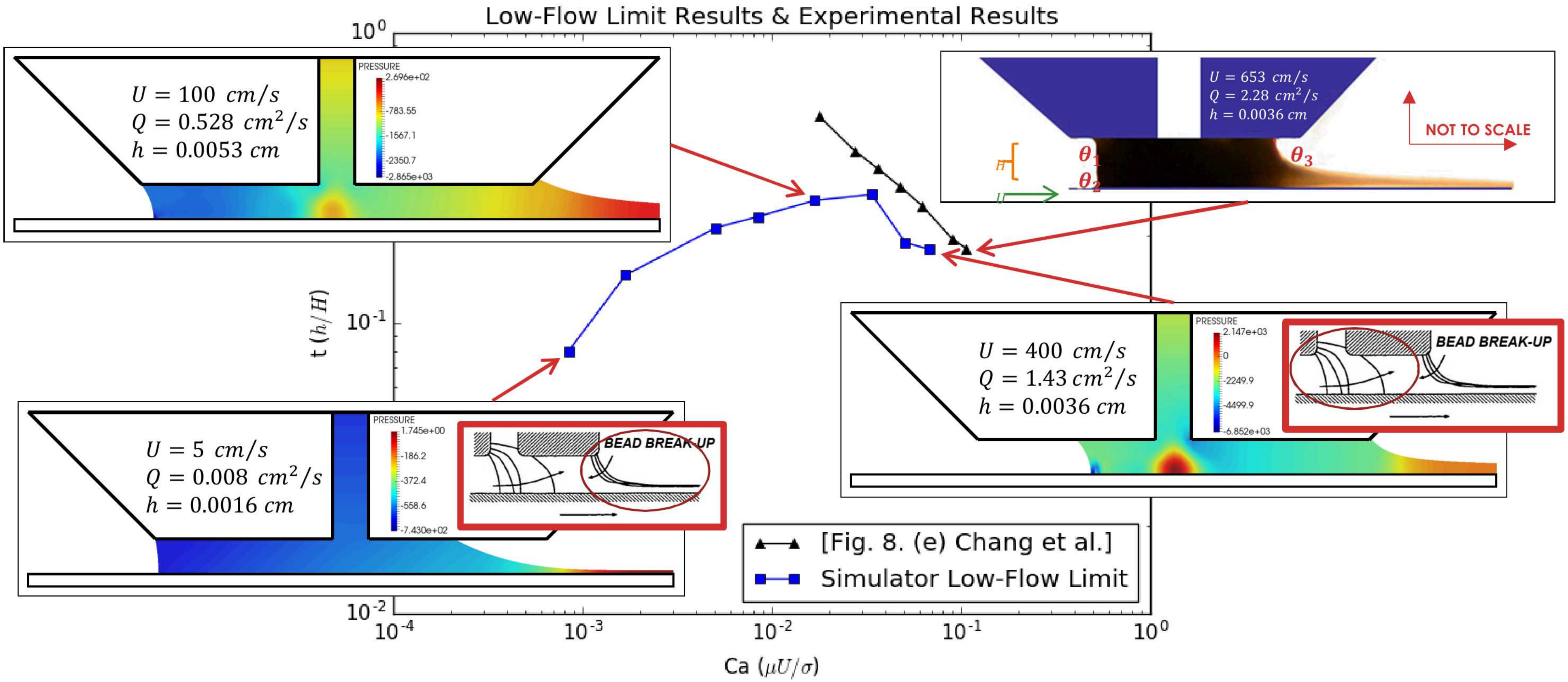
Model predicts residual film thickness over speed and load– arguably the most important factor affecting resolution limits

Hariprasad et al. 2016, J. Applied Physics, DOI: 10.1063/1.4945030

PRECISION SLOT-DIE COATING

Low-Flow limit comparison to experimental results

- Computational results reproduce experimental film thicknesses, meniscus topologies, and failure modes



Low-Flow limit three region coexistence analysis

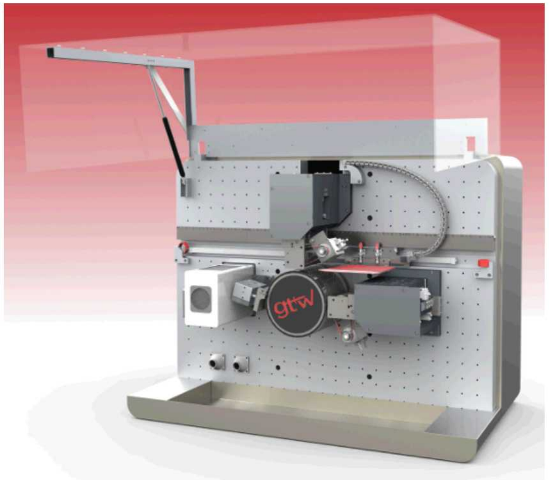
- Region 1 and 3 identified but region 2 not clear

Sandia/AML Resources and FRB's Tasks

Task 1: Adversarial Analysis
-Yes: Range of printing tools and breadth of ink capabilities you will see
Task 2: Overt Public Security Feature Research
-Yes: Many capabilities (ink, tools, process) to address novel routes and technologies
Task 3: Overt Public Device Assisted Security Features and Machine-readable
-Yes: Many ideas here but we feel better once we are under contract
Task 4: Ink Characteristics research
-Yes: Many capabilities (ink, tools, process) to address novel routes and technologies

Resources available for FY16, FY17 – We have bandwidth, especially in FY17.

Gravure/Flexo Platforms at the AML



Clip from movie

- Gravure, gravure offset, flexographic printing
- Low fluid consumption (1.5 ml)
- High printing speed (5 m/s)
- ***Multilayer alignment (<10 µm)***
- Printing hard/flexible substrates
- All parameters reproducibly adjustable

RK commercial printing tools

gravure

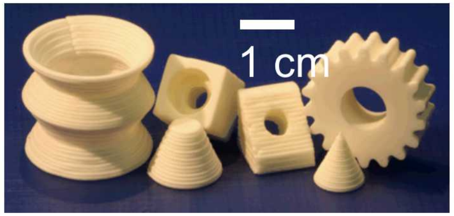
flexo

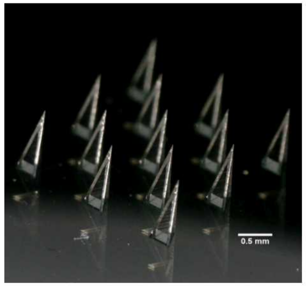
Meter Bar

QD System (Harper Technologies)
-Specs

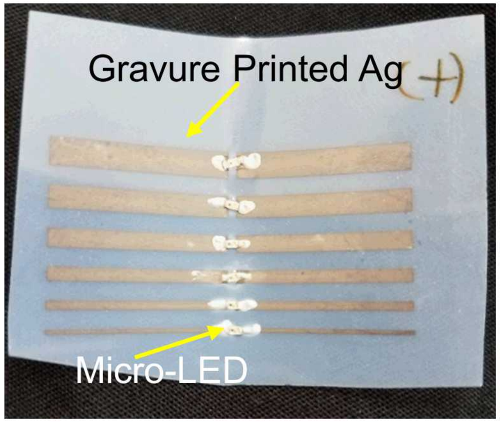
Current R&D and Applications of AML AM

Ceramic piece parts
Structural damping materials (DW)
Conformal barrier coatings (DW)
Printed electronics (Gravure, DW)
OPV, OLED, Antenna, memristors
Corrosion resistant electronic ink development/testing
Direct-laser printing of microneedles (LDW)
Photonic metamaterials (LDW)
Sensors (DW, Gravure, Flexography)
Radiation detectors
Trace gas sensors
Temperature
Humidity
Structural





Microneedle Array



Flexible Hybrid Electronic

Printed Photovoltaic device