SAND2013-8591P

*Exceptional service in the national interest*

Tensile Direction

Sandia National Laboratories

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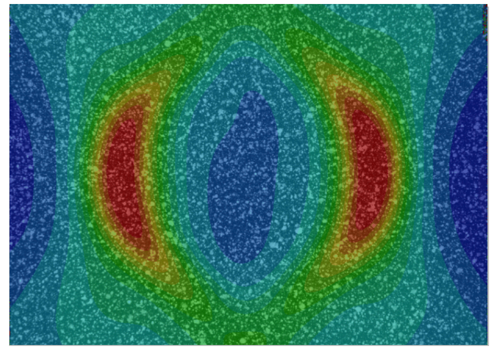
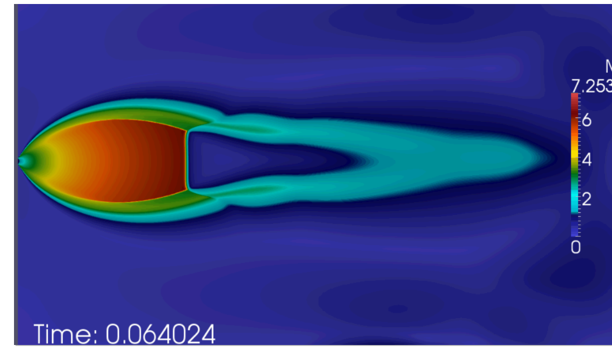
Photos placed in horizontal position with even amount of white space between photos and header






# Examples of Research at Sandia National Laboratories and My Experience

Bryan R. Loyola[1]

[1]Sandia National Laboratories, Livermore, CA, USA

U.S. DEPARTMENT OF ENERGY

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NNSA National Nuclear Security Administration

# Myra Blaylock, Ph.D.

- BS Astrophysics:
  - University of Oklahoma
  - Supernova Spectroscopy Simulations
- MS Physics:
  - University of Arizona
  - Geophysics of the San Pedro River Valley
- PhD Aeronautical Engineering: UC Davis
  - Advisor: Case van Dam
  - Computational Fluid Dynamics (CFD) for active load control of wind turbines
    - Microjets at trailing edge of airfoil to reduce the change in lift during a wind gust

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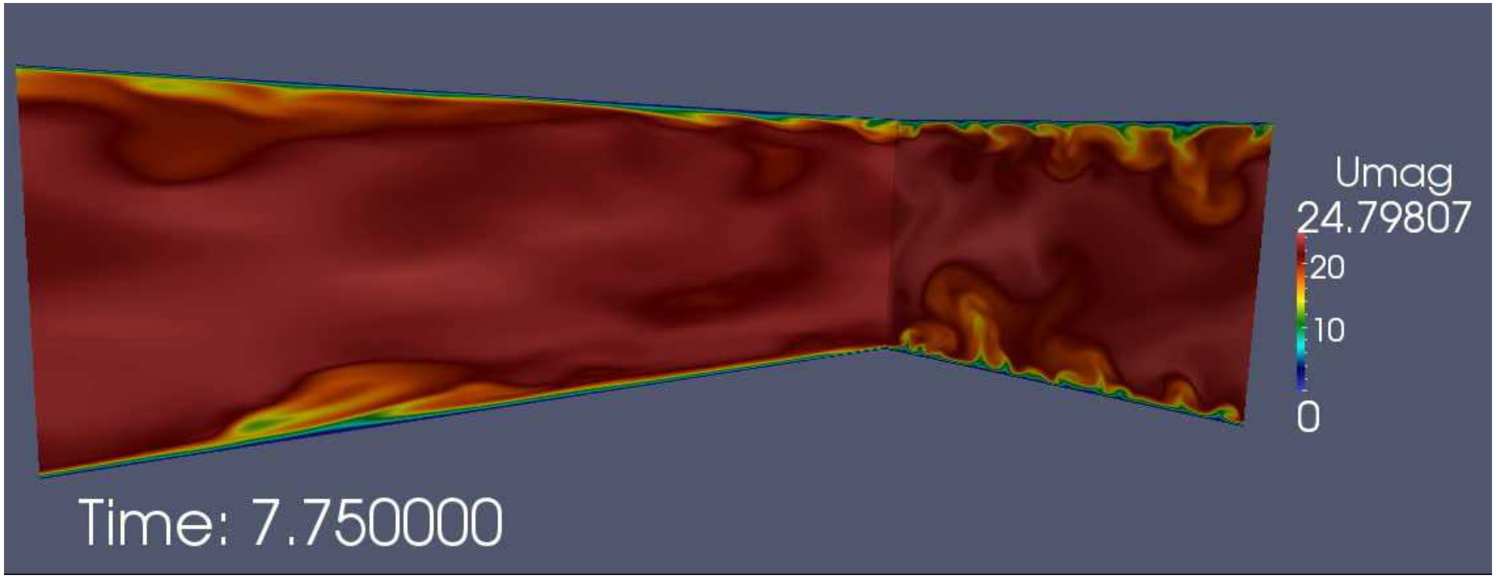
# Projects at Sandia, Livermore

- Started Dec. 2012 in the Thermal/Fluid Sciences & Engineering Dept. (Computer modeling and analysis)
- Several projects using Sandia's in-house CFD codes
  - Uncertainty Quantification of Engineering Level Large Eddy Simulations (LES)
  - Safety, Codes, and Standards
    - Hydrogen Fuel Cell Vehicles
    - Natural Gas Vehicles
    - Using CFD to look at leaks and explosions
  - Underexpanded Jet Simulations
  - Wind turbine modeling for the National Rotor Testbed

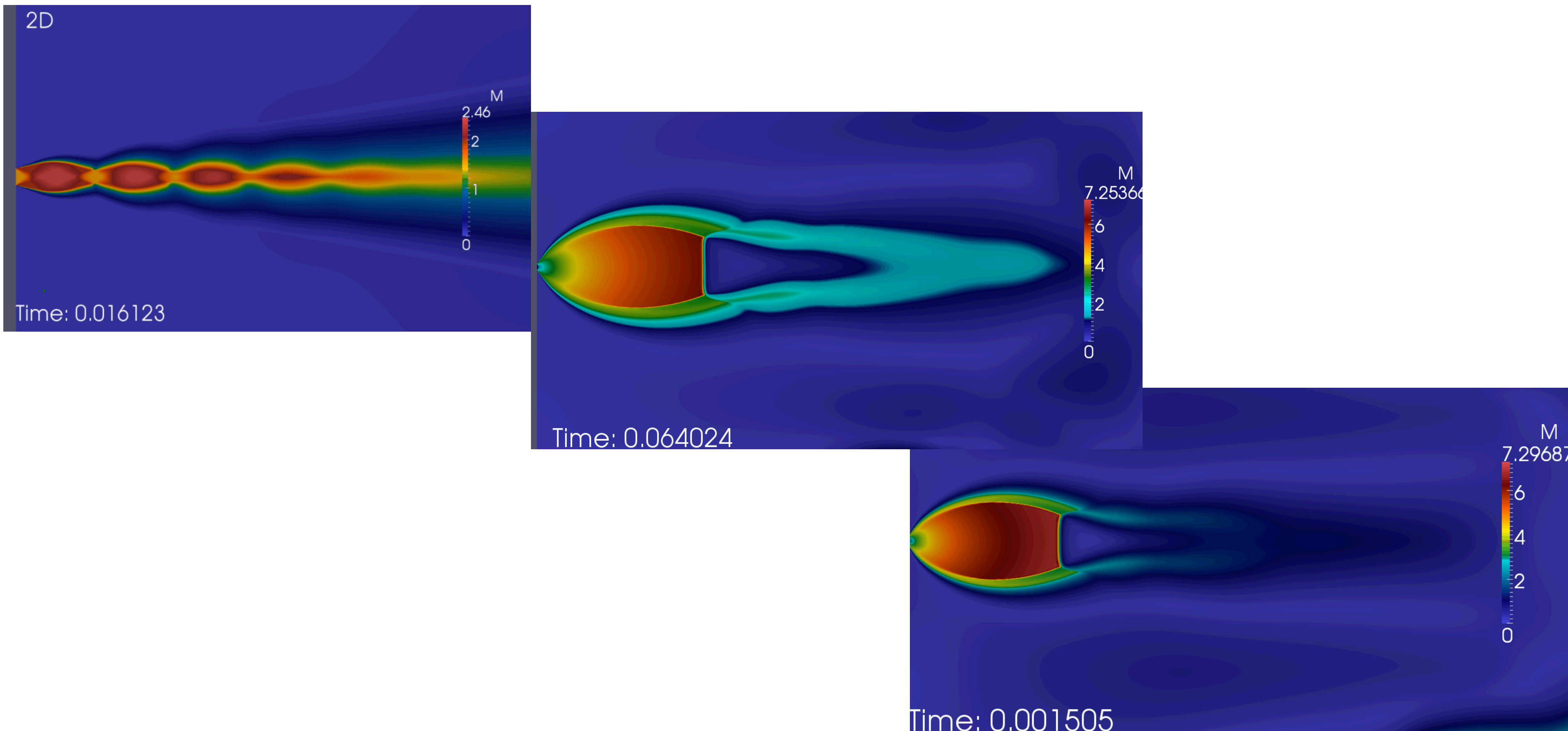
# Large Eddy Simulations (LES)

- Comparing high fidelity LES with "engineering level" LES that can be done more quickly for industry turn-around deadlines
- Starting with simple flows: Channel flow, backward facing step, jet in cross-flow



# Underexpanded Jet

- Supersonic jet shock down to sub-sonic (Mach Number is shown)
- Starting with 2D case, will work up to 3D
- Pressure Ratios of 2, 50 and 100 between outflow and ambient



# Joe Cordaro, Ph.D.

- BA Chemistry
  - University of San Diego (1999)
- PhD Chemistry
  - University of California, Berkeley (2004)
- Post-Doc
  - ETH Zurich
  - University of California, Santa Barbara
- Joined Sandia in 2007
  - Materials Chemistry Dept.
- Research Interests:
  - Polymers and materials for diverse applications
    - Membranes
    - Printed electronics
    - Photovoltaic devices
    - Flexible coatings

# Optoelectronic Devices Based on Semi-Conducting, Flexible Polymers

**Step 1**, excitation on D:

$$D + A \longrightarrow {}^{1,3}D^{*} + A$$

**Step 2**, excitation delocalized on the D-A complex:

$$^{1,3}D^{*} + A \longrightarrow {}^{1,3}(D\text{-}A)^{*}$$

**Step 3**, Charge transfer Initiated:

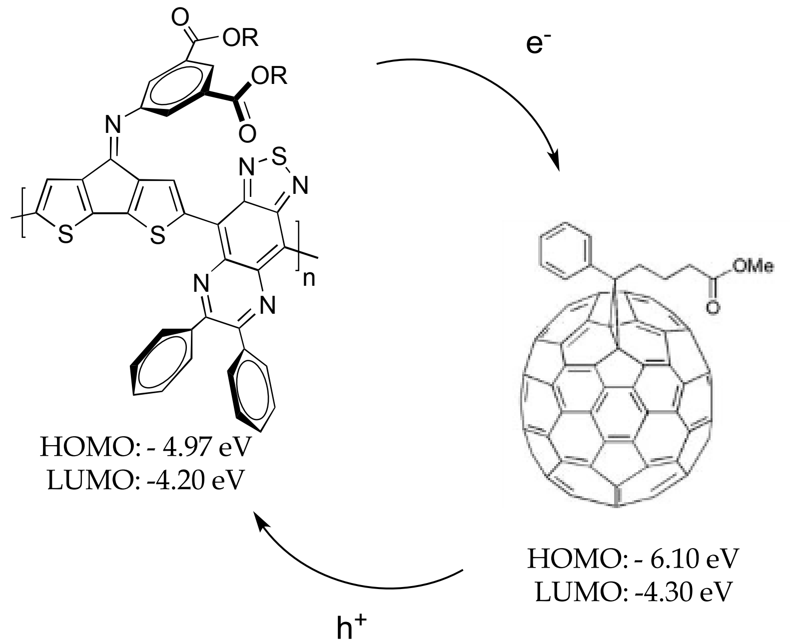
$$^{1,3}(D\text{-}A)^{*} \longrightarrow {}^{1,3}(D^{\delta+}\text{-}A^{\delta-})^{*}$$

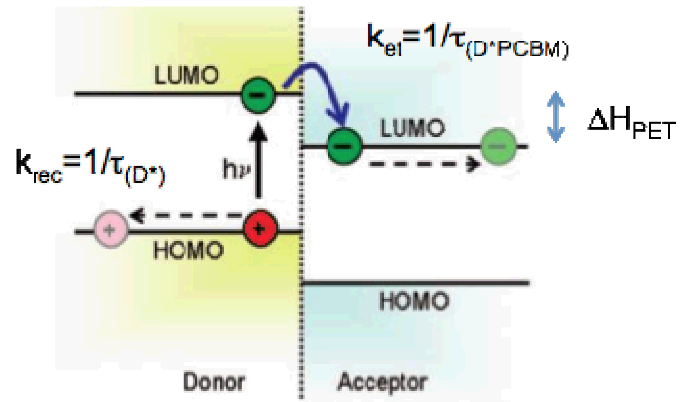
**Step 4**, Ion radical pair formed:

$$^{1,3}(D^{\delta+}\text{-}A^{\delta-})^{*} \longrightarrow {}^{1,3}(D^{+\cdot}\text{-}A^{-\cdot})$$

**Step 5**, Charge separation:

$$^{1,3}(D^{+\cdot}\text{-}A^{-\cdot}) \longrightarrow D^{+\cdot} \quad A^{-\cdot}$$



# New Materials Made at Sandia

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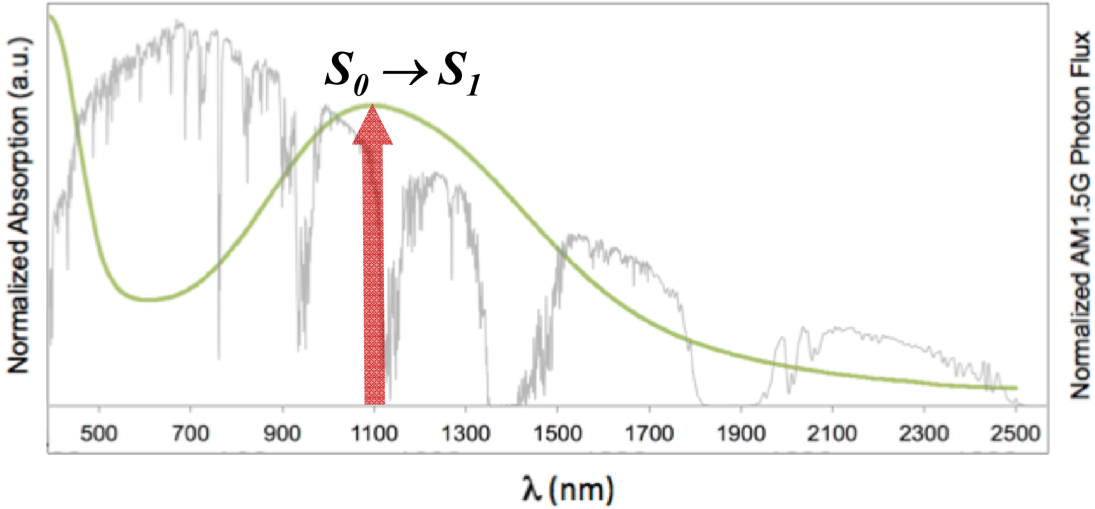
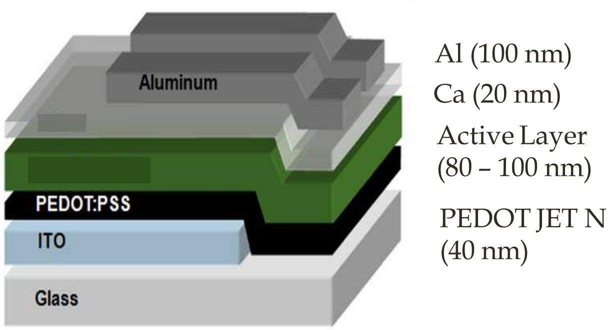
R = $C_{12}H_{25}$
$E_g^{DFT}$: 0.55 eV
$E_g^{opt}$: 0.55 eV




Preliminary calculations indicate that accurate band gaps can be obtained with nonlocal hybrid functionals (i.e. B3LYP), TD-DFT accurately predicts primary photoexciation ($S_0 \rightarrow S_1$).

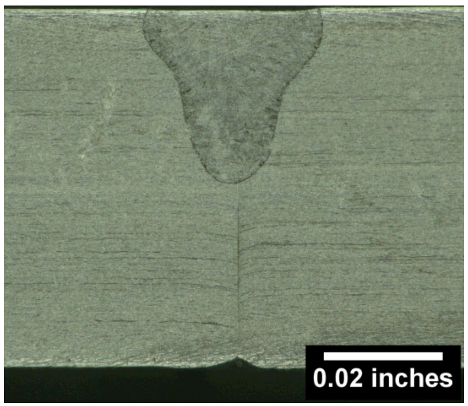
# Sharlotte Kramer, Ph.D.

- BS Aerospace Engineering
  - University of Virginia (2004)
- MS Aeronautics
  - California Institute of Technology (2005)
- PhD Aeronautics
  - California Institute of Technology (2009)
- Joined Sandia in 2011
  - Structural Mechanics Lab
- Research Interests:
  - Experimental structural mechanics

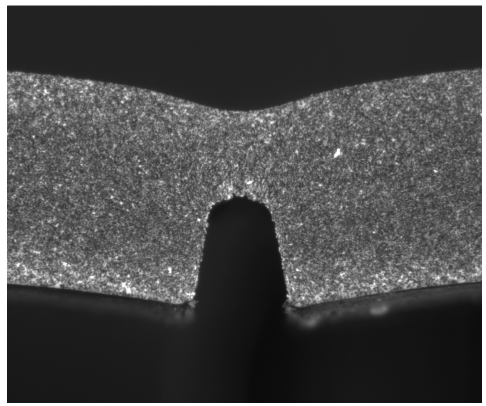
# Laser Weld Characterization: Motivation

Sandia National Laboratories

**Laser Weld:**
Metallic joint formed by fusing of two metal surfaces using a high-power laser without any additional material, i.e. the weld is directly formed using the native material of the two surfaces (often the weld does not penetrate the entire thickness of the surfaces)

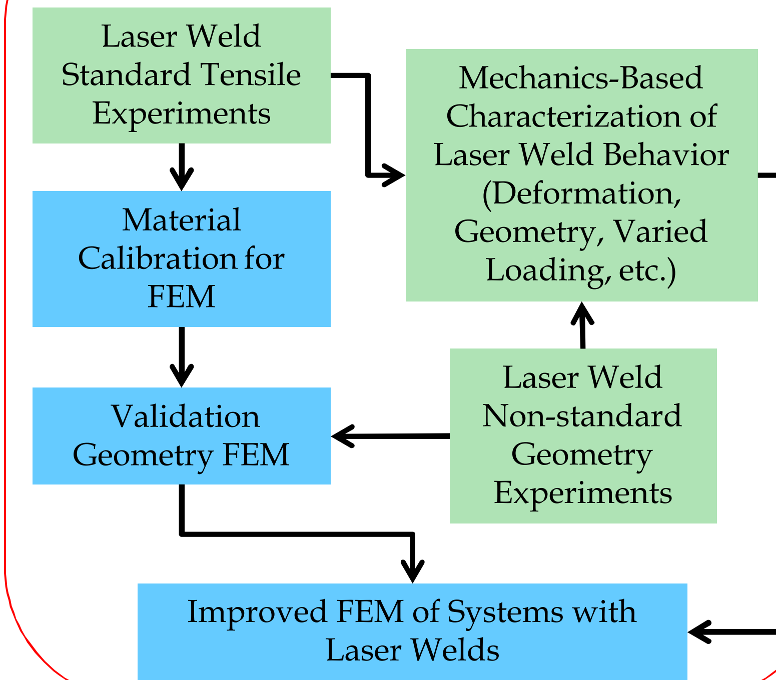



*Side Profile of a 304L SS to 304L SS Partial Penetration Laser Weld*



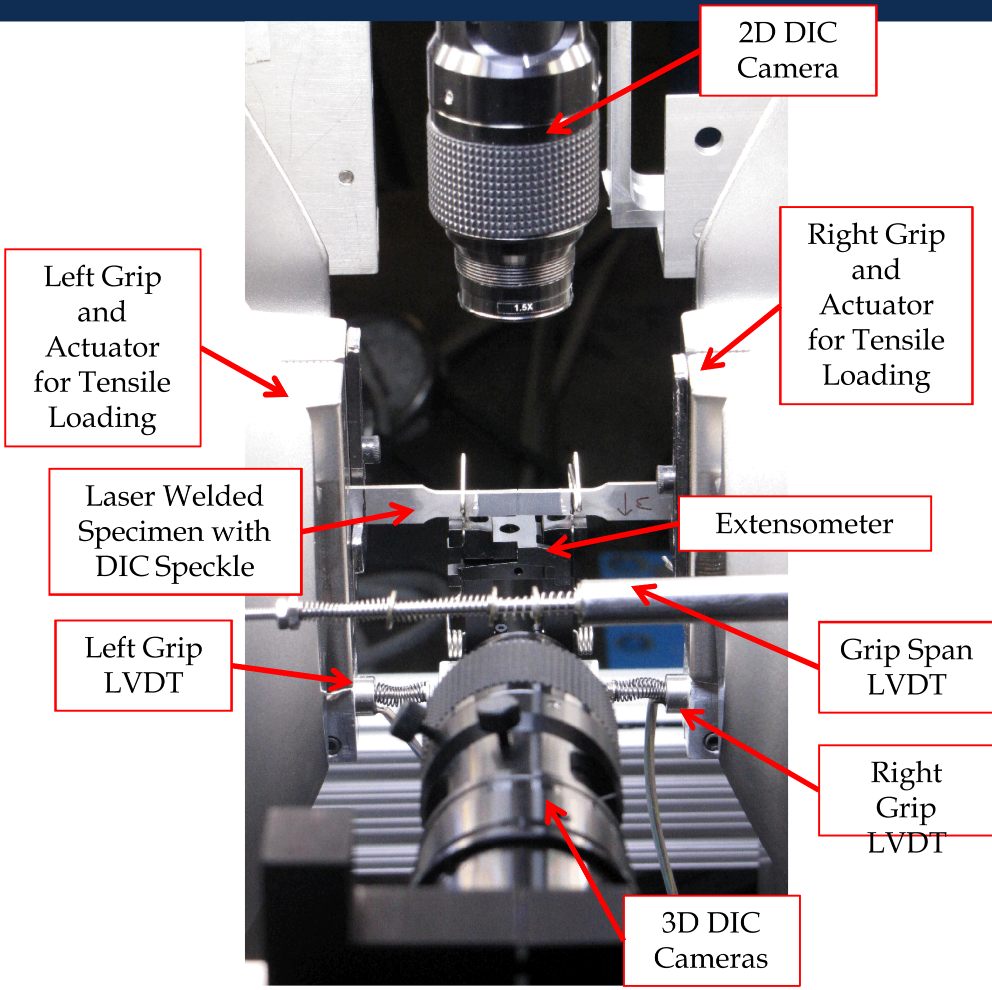
*Laser Welded Specimen with Significant Bending Before Failure Under Tensile Load*

**Research Approach (Collaboration with Modelers in Blue):**




**Issue:**
**Thousand of feet of 304L stainless steel laser welds in critical systems are not well characterized experimentally and computationally, but we must make critical decisions and evaluations of our systems.**
**We need fundamental and practical understanding of how laser welds deform and fail to improve how we model these critical systems.**

# Laser Weld Characterization: Experiments




*Experimental setup for dual-actuator loading of dog-bone shaped tensile specimen with laser weld with 2D DIC (Upper) and 3D DIC (lower) cameras and global extensometer and LVDT measurements*

**Digital image Correlation (DIC): Full-field optical method to measure surface displacements and strains**

- Random speckle patterns on a surface are imaged during the experiment
- Correlation algorithms measure the *displacements* of the speckles with *resolution on the order of 0.01 pixels of the CCD camera*

**"Standard" Tensile Experiments: Material Properties**

- Base material dog-bones
- Base material dog-bones with a cut notch to characterize raw material with a geometry similar to a partial penetration laser weld
- Dog-bones with a central straight laser weld

**"Non-Standard" Geometry Experiments**

- Plate with a straight laser weld
- Plate with a circular weld in the center
- Plate with a central hole (no laser weld)

# Laser Weld Characterization: Observations

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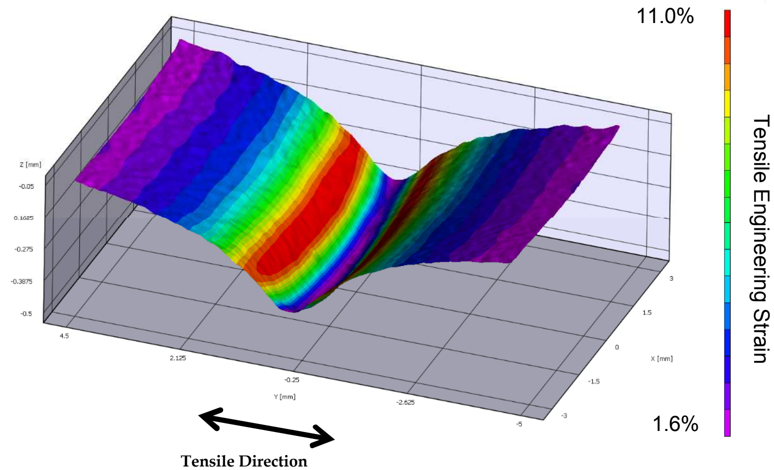
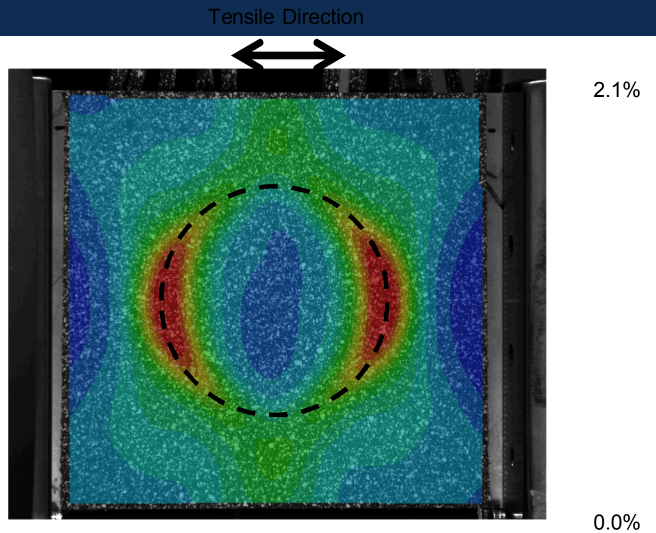



*Highly Non-Uniform 3D Deformation Measurements on Surface of Dog-Bone Shaped Laser Welded Specimen*




*In Situ Image of a Deforming Plate with a Central Circular Laser Weld (Outlined with Dashed Line) With Overlaid Color-map of the Full-Field DIC Tensile Strain Data*

## Observations:

- Dog-bone specimens with laser weld behave similarly to dog-bone specimens with a notch instead of a laser weld.
- Circular welds in a plate behave similarly to the straight welds in a plate until the weld starts to fail (large strain regions in right full-field map). Then, the weld "unzips" half way around circle. After the weld crack stops propagating, specimens behave similarly to plates with circular holes.
- **Both experiment types demonstrate that 304L SS laser weld material is similar to the base material and that large non-uniform deformations are mostly due to geometry.**
- **We need to improved computational techniques to manage the effects of geometry for better predictive models of large systems.**

# Francois Leonard, Ph.D.

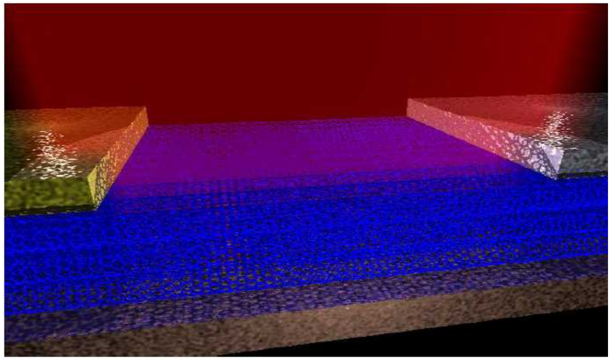
- BS Physics
  - McGill University (1994)
- MS Physics
  - University of Toronto (1995)
- PhD Physics
  - University of Toronto (1998)
- Joined Sandia in 2000
  - Material Physics
- Research Interests:
  - Nanoelectronics
  - Nanophotonics

# Broadband Carbon Nanotube Photodetectors with Intrinsic Polarimetry

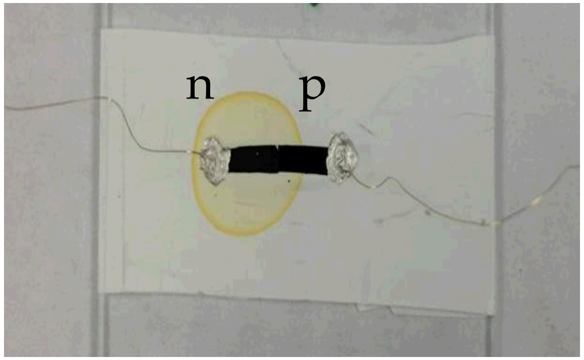
*Xiaowei He, Sébastien Nanot, Xuan Wang, Kankan Cong, Qijia Jiang, Robert H. Hauge, Junichiro Kono*
*Rice University*

*Akira Ikeuchi, Takafumi Akiho, Kazuhisa Sueoka*
*Hokkaido University*

*Aron Cummings, Alexander Kane, John Goldsmith, François Léonard*
*Sandia National Laboratories*

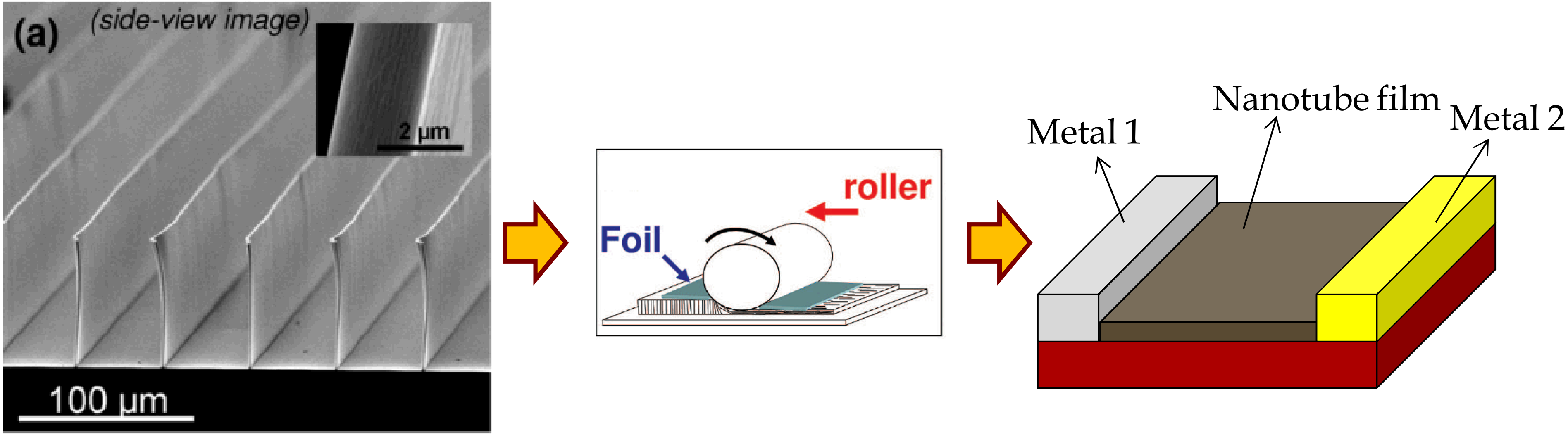


*Scientific Reports* **3**, 1335 (2013).

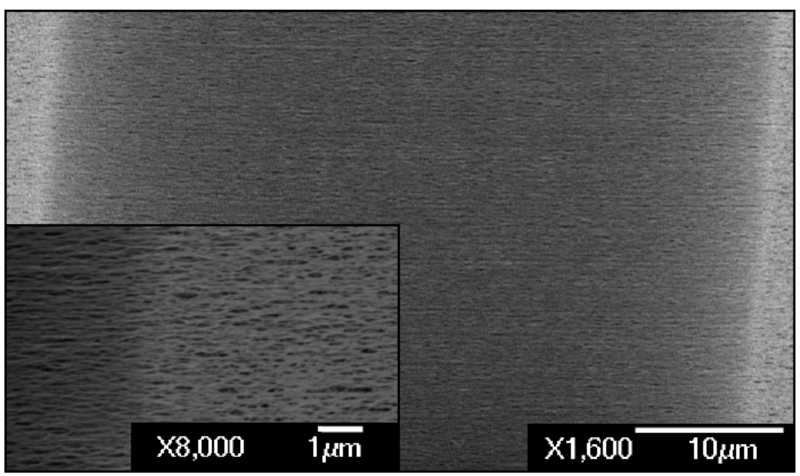



*ACS Nano* **7**, 7271 (2013).

# Device Assembly

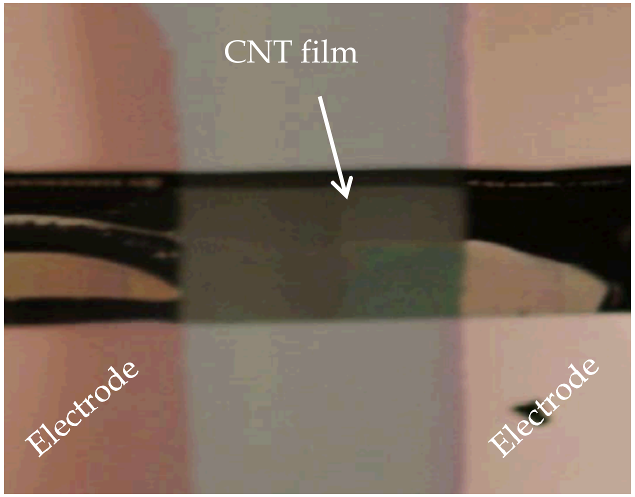



C. Pint *et al*., *ACS Nano*. **2(9)**, 1871 (2008)



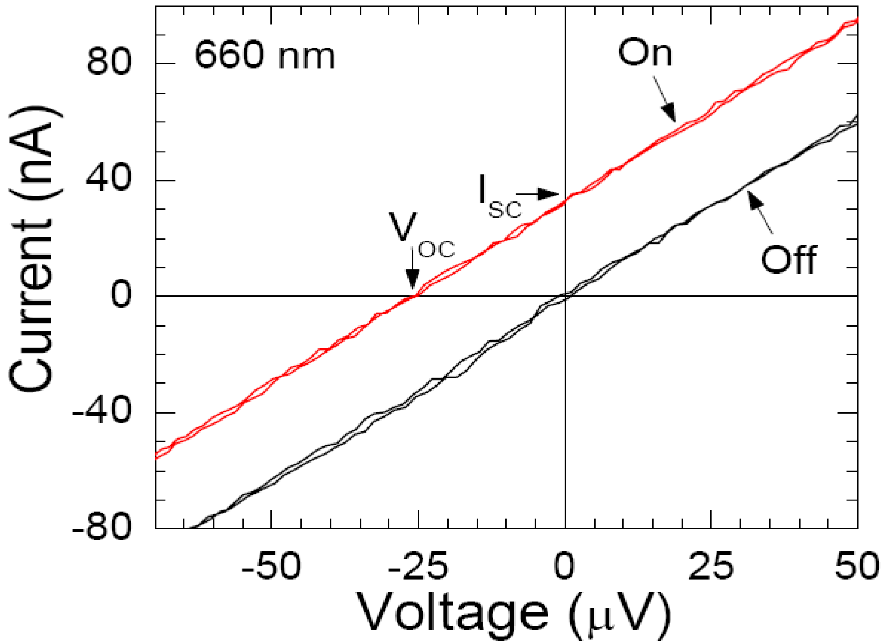

- Optically-thick film (1 micron)
- Aligned CNTs
- Long channel (several hundred microns realized)
- Dense CNTs (average spacing 10 nm)

# Macroscopically aligned CNT thin film devices generate photocurrent under global illumination




0.5 mm

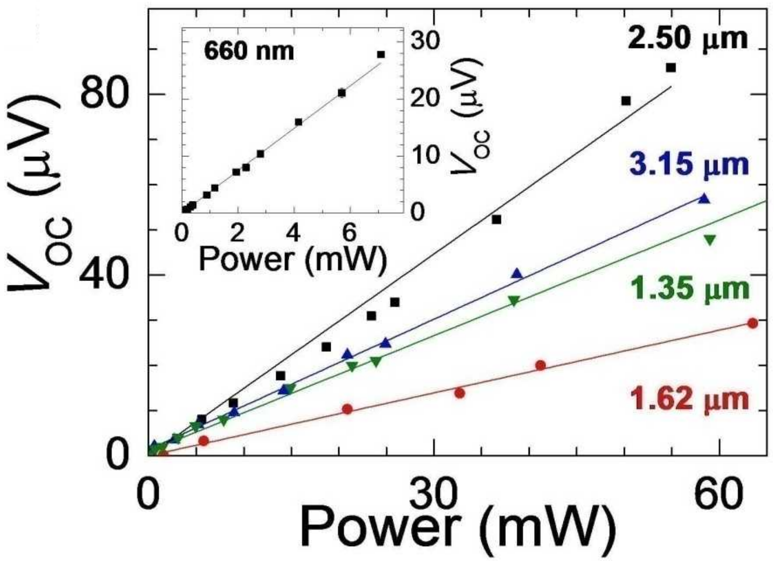
Global illumination

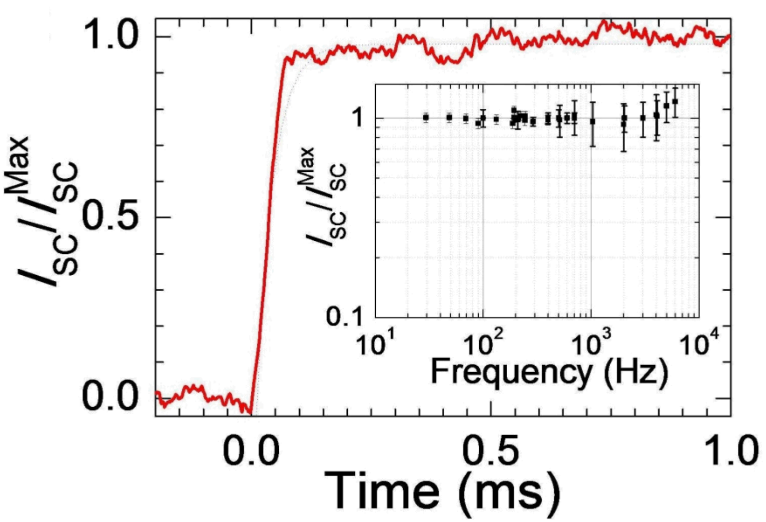



S. Nanot *et al.*, *Scientific Reports* **3**, *1335 (2013).*

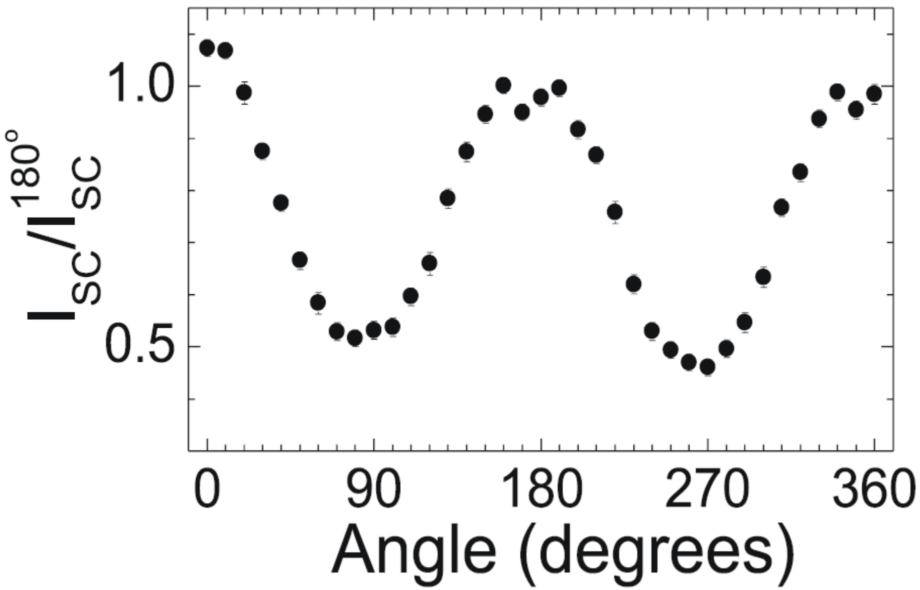
# Device Performance

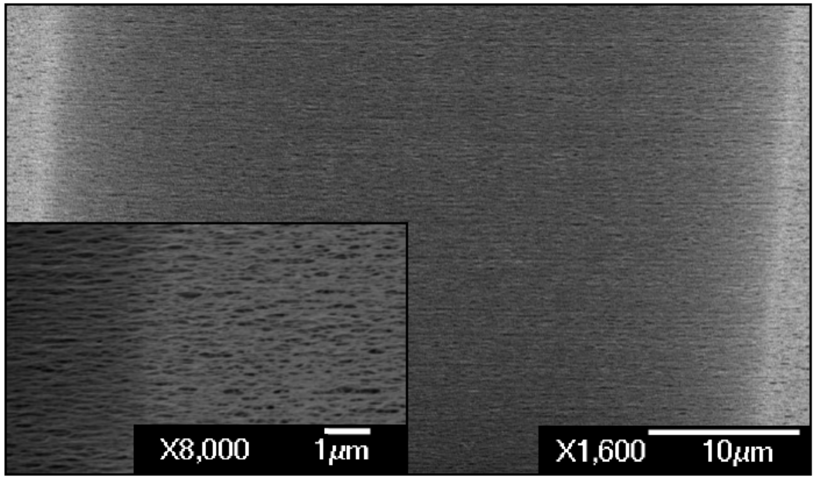
**The detector is broadband...** **...and is fast:**



# Polarimetry




The unique aligned-nanotube material allows polarimetry directly integrated in the detector.


S. Nanot *et al.*, *Scientific Reports* **3**, *1335 (2013).*

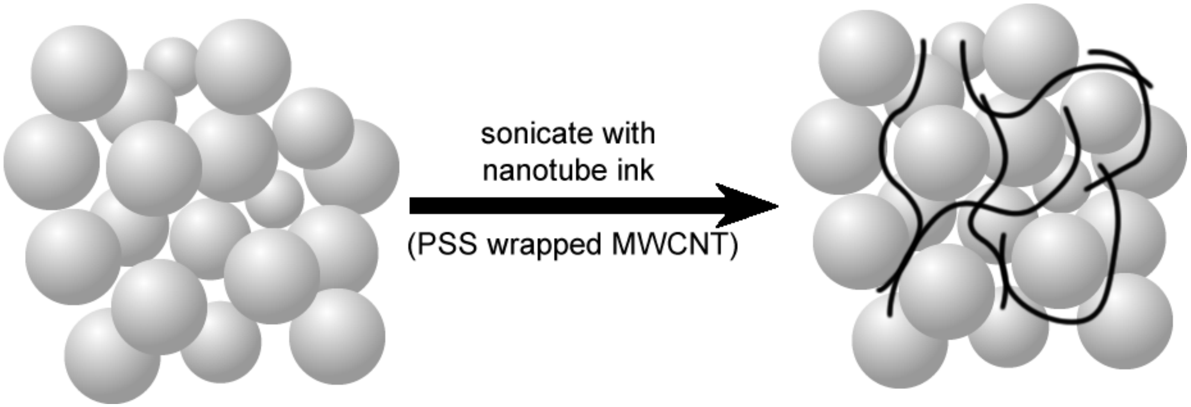
X. He *et al.*, *ACS Nano* **7**, 7271 (2013).

# Bryan Loyola, Ph.D.

- BS Physics
  - University of California, Davis (2005)
- MS Mechanical and Aeronautical Engineering
  - University of California, Davis (2010)
- PhD Mechanical and Aeronautical Engineering
  - University of California, Davis (2012)
- Joined Sandia in 2012
  - Center for Critical Application Sensing
- Research Interests:
  - Characterization of CNT-based sensors
  - Sensor development
  - Structural health monitoring
  - Electrical impedance tomography

# Sprayable MWNT-Latex Thin Film

- Rapid large-scale deposition
  - Required for mass deployment of methodology
- MWNT-PSS/Latex paint formulation
  - Collaborated to improve initial Sandia formulation
  - Sub-micron PVDF creates mold for MWNT organization
  - Off-the-shelf deposition method




Kynar Aquatec™ latex solution (avg. particle size 150nm)

Forms segregated MWCNT network

# MWNT-Latex Morphology

- Creation of MWNT networks:
  - Electrical percolation above 1 wt% MWNTs
- Fiber-reinforced polymer deployment:
  - Surface applied to post-cured composites
  - Applied to fiber weaves for embedded sensing

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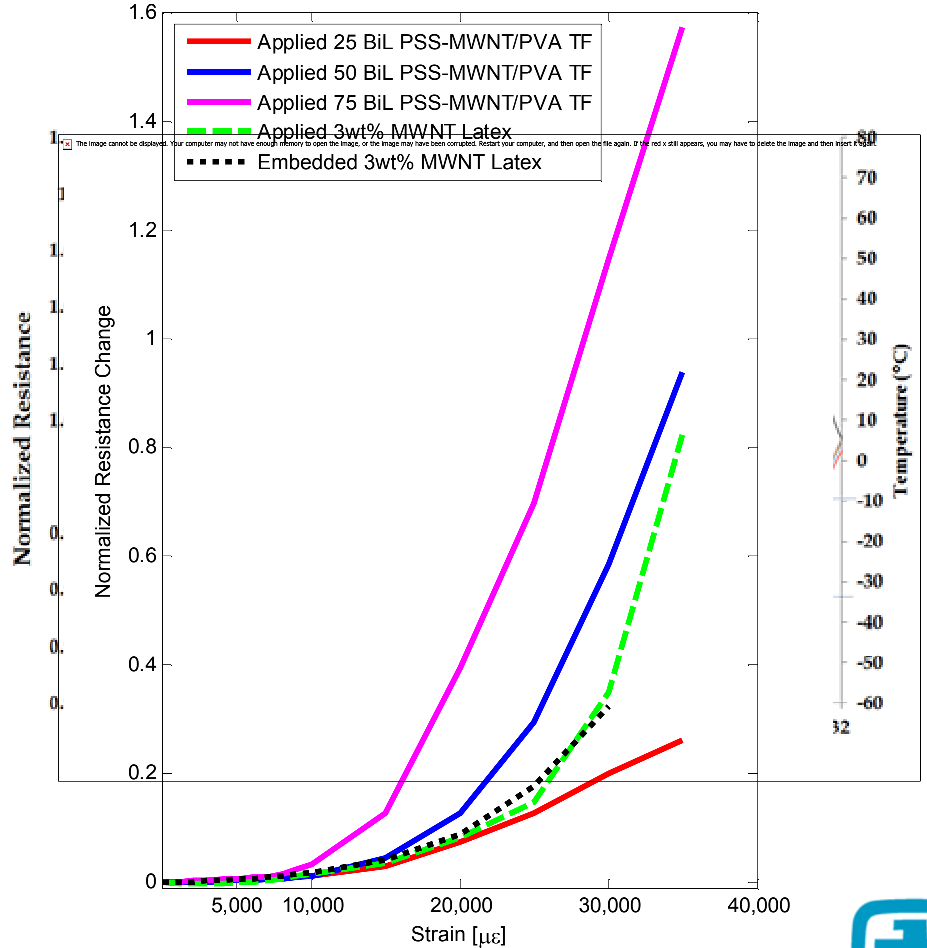
Cross-section and MWNT network SEM images of 3wt% MWNT-Latex film

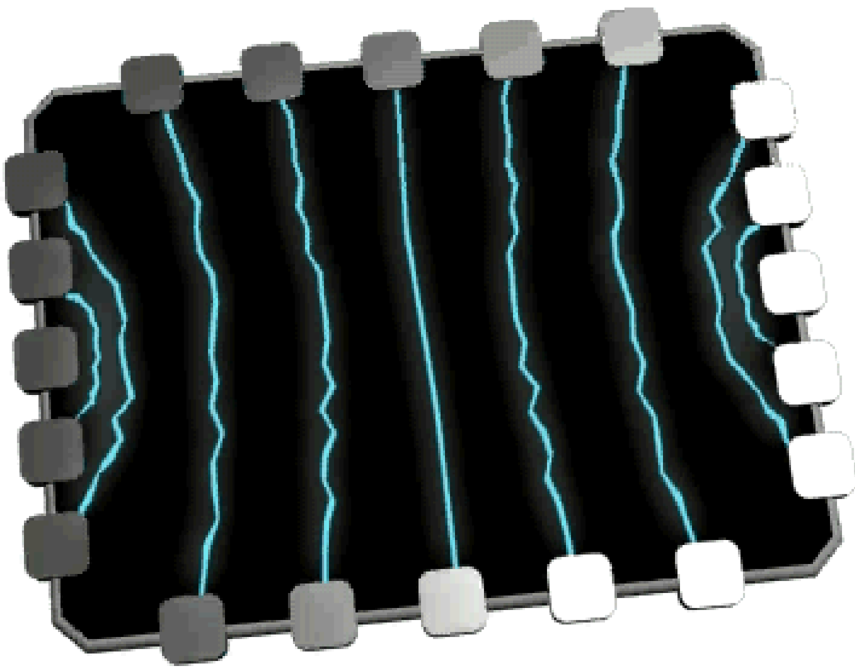
# MWNT-Latex Characterization

- Electromechanical characteristics:
  - Quasi-static testing
    - Nearly same sensitivity as LbL
  - Bi-functional strain response
    - Linear
    - Quadratic
      - Cracking of film
- Thermo-resistance coupling:
  - -50°C to 80°C over 2 hours
  - 2 hour holds
  - Inversely linear relationship
  - Non-linear response @ -30°C
    - ~ $T_g$ of PVDF
    - Restructuring of MWNTs



# Electrical Impedance Tomography

- Overview of spatial conductivity mapping
  - Since film impedance calibrated to strain, conductivity maps can correspond to 2-D strain distribution maps



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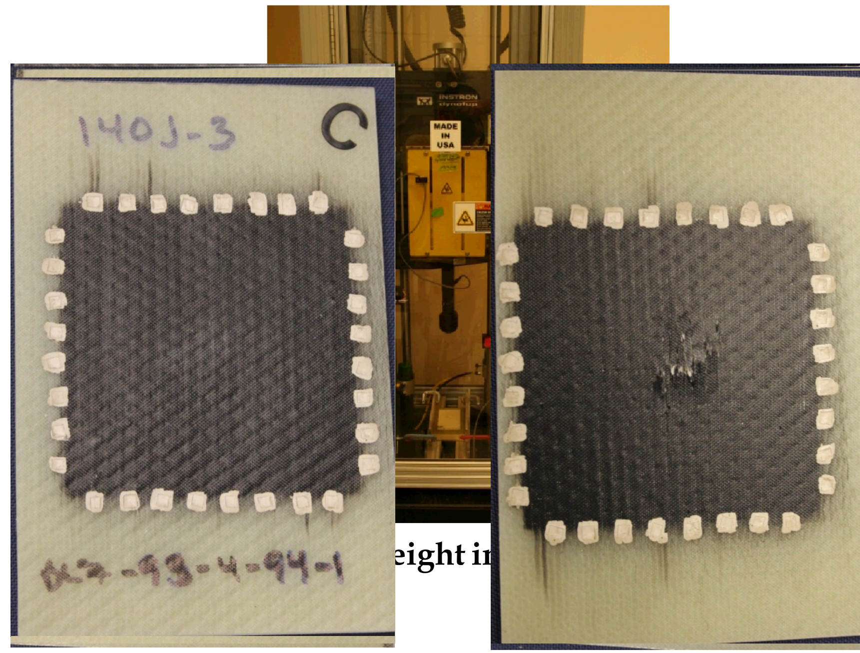
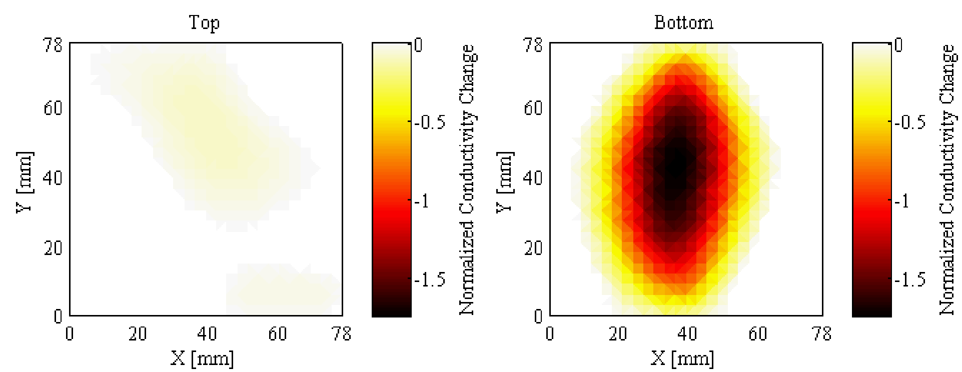
# Impact Damage Detection

- Drop-weight impact tests
  - **ASTM D7146**
  - 78 mm by 78 mm sensing region
  - MWNT-latex on glass fiber weave
  - Impact energy: 20, 60, 100, 140 J
  - Before/after EIT measurements
- Verification:
  - Thermography
    - Matrix Cracking
    - Delamination
  - Photographic Imaging
    - Surface damage





# My Time at Sandia

- Joined on July 16, 2012
- Three projects
  - Characterization of carbon-nanotube thin film
  - Development of sprayable-ceramic-free piezoelectric sensor
  - Subject matter expert (SME)
    - Non-destructive testing and structural health monitoring
      - Acoustic methods
        - Ultrasonics
        - Ultrasonic resonance
        - Acoustic emission
      - Fiber-optics
        - Fiber bragg gratings
          - Densely instrumented strain measurements
          - Embedded strain measurements in composites
      - Electrical impedance tomography
        - Impact damage detection

# My Time at Sandia

- Funding
  - Mostly internal
    - LDRD/RTBF
    - Programmatic
  - External (except NSF)
- Mobility
  - Free to decide the direction of my career, considering funding.
  - Could really change positions and focuses every ~5 years
- Work-Life balance
  - 9/80 schedules
  - Can take off time for personal/family appts in the middle of the day
- Experience
  - Work closely with a group of dedicated individuals
  - Numerous experts in a wide range of fields allows for quick progression of technologies

# Thank You!

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*Exceptional service in the national interest*

## Questions?

## Acknowledgements:

Sandia National Laboratories