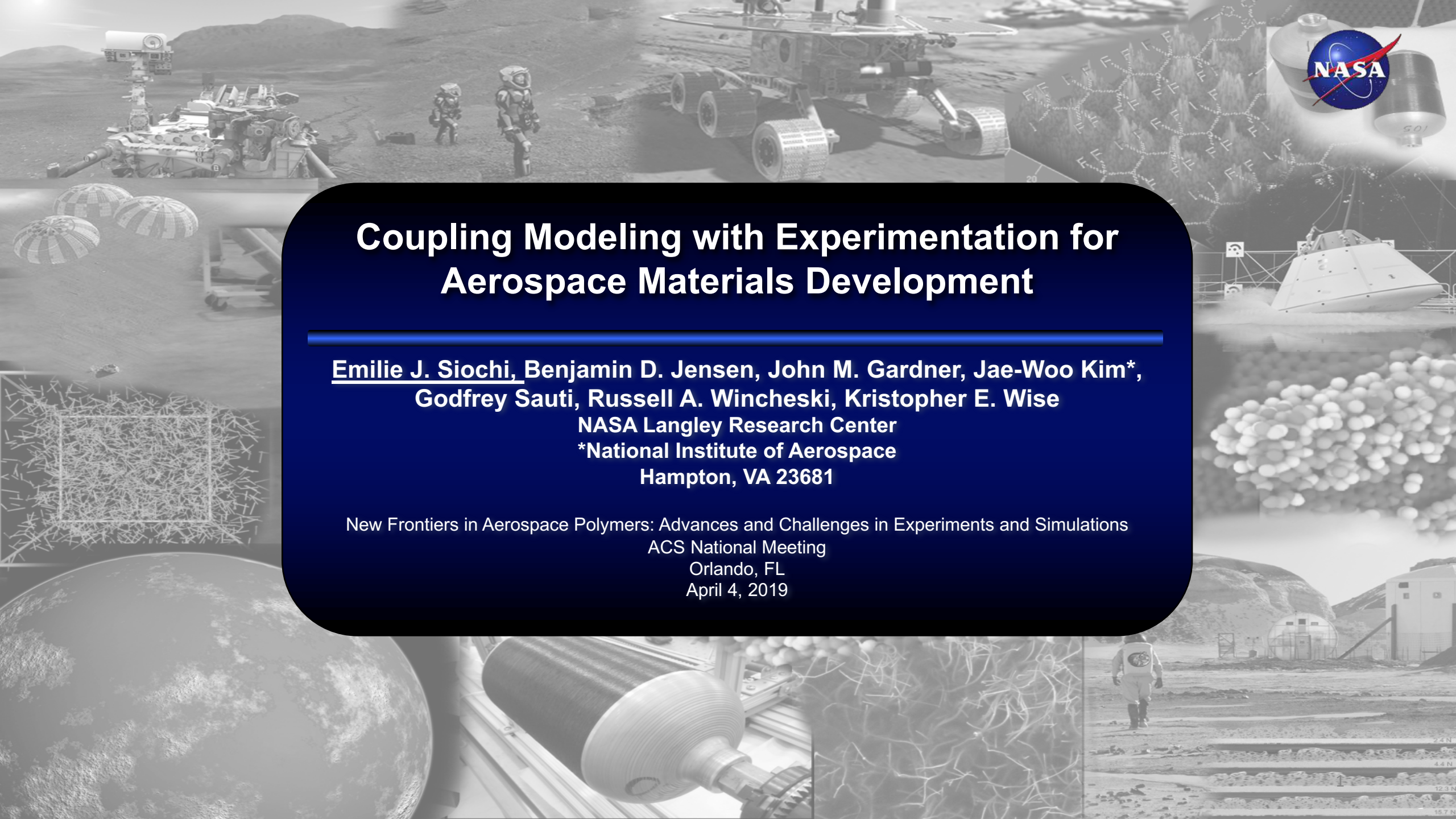




Coupling Modeling with Experimentation for Aerospace Materials Development

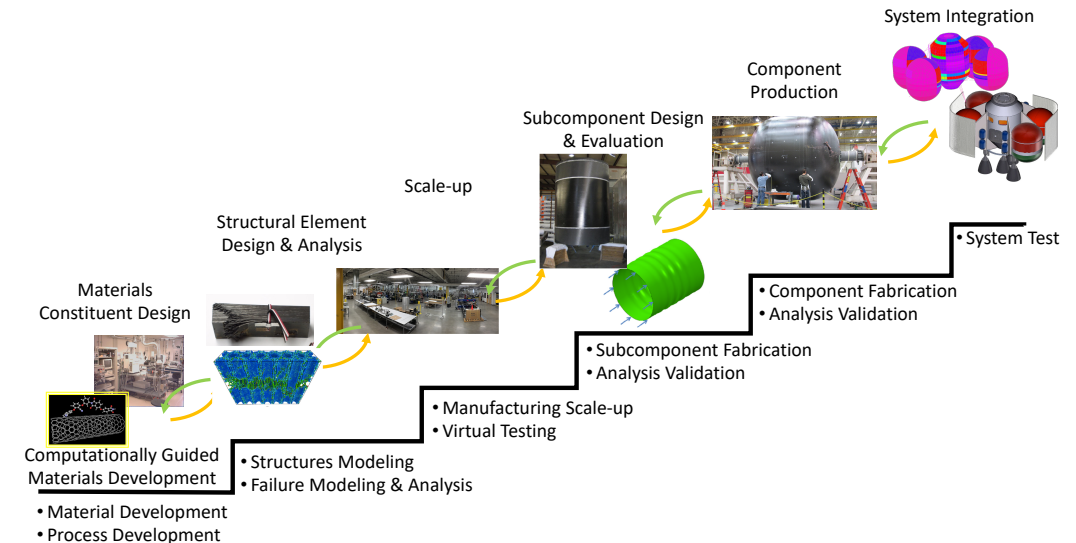
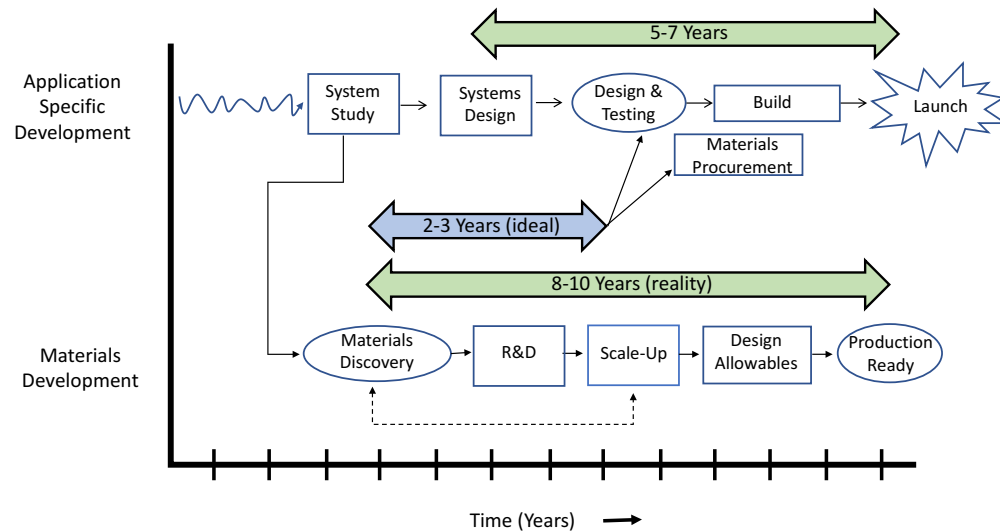
Emilie J. Siochi, Benjamin D. Jensen, John M. Gardner, Jae-Woo Kim*,
Godfrey Sauti, Russell A. Wincheski, Kristopher E. Wise
NASA Langley Research Center
*National Institute of Aerospace
Hampton, VA 23681

New Frontiers in Aerospace Polymers: Advances and Challenges in Experiments and Simulations
ACS National Meeting
Orlando, FL
April 4, 2019

The Problem



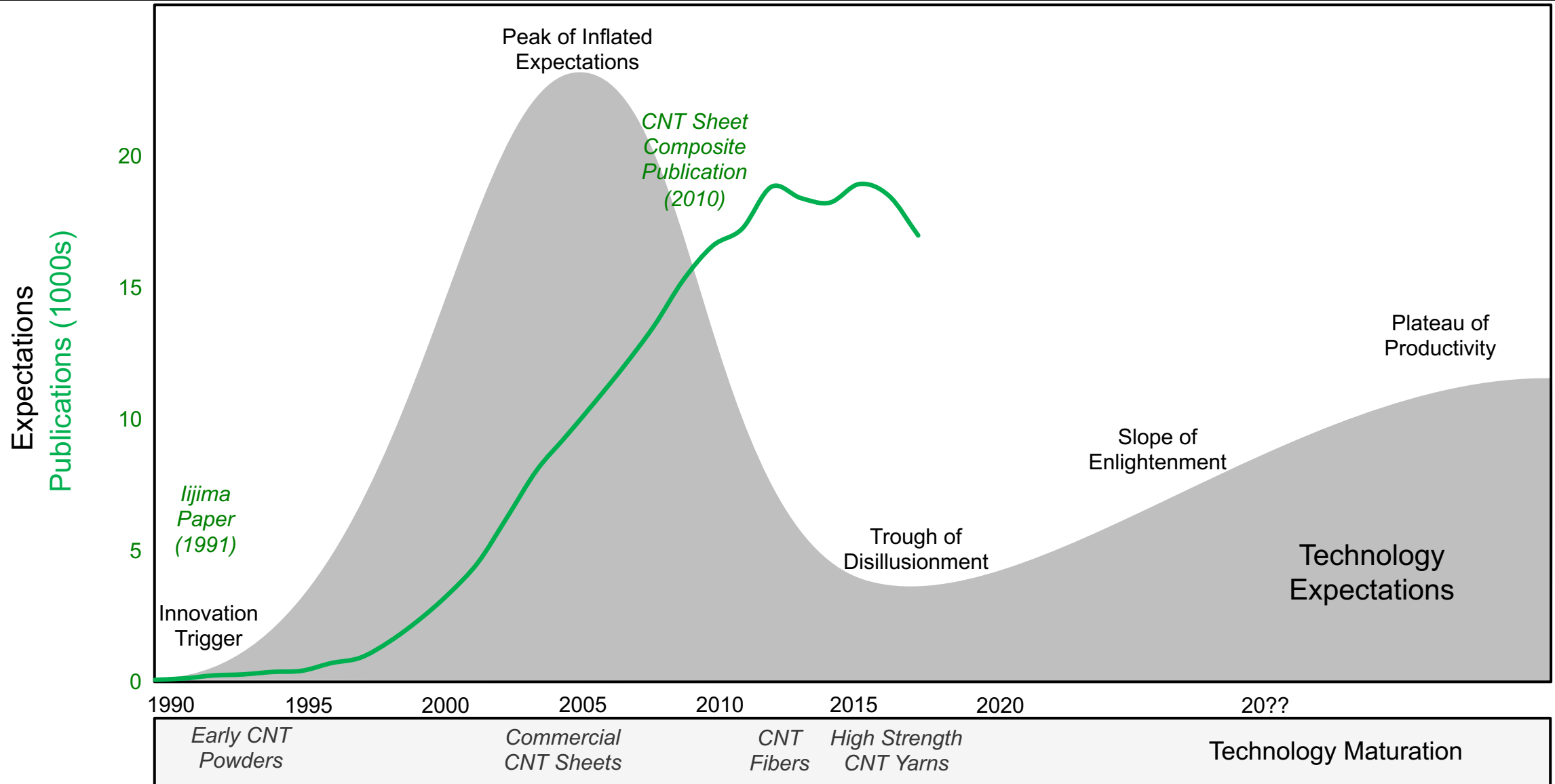
Typical Approach



Modified From: Gerould Young, "The Challenge of New Materials in the Aerospace Industry," Presentation at Georgia Tech, May 15, 2013

- Typical materials development tends to take decades.
 - Conventional approach is not guided by application pull early in the development.
 - Materials maturation elements such as research and development, scale-up and designing for application occur serially, and largely by trial and error.
- In order to accelerate materials development:
 - Recognize that the aerospace materials ecosystem has to be engaged early.
 - Leverage resources to develop technologies with broad impact.
 - Computationally guided materials maturation to address relevant materials issues tied to application requirements.
 - Focus efforts targeted to solving manufacturing and design issues to accelerate technology maturation and insertion.

Carbon Nanotube (CNT) Gartner Hype Cycle



Challenges/Barriers to Coupling Modeling with Experimentation

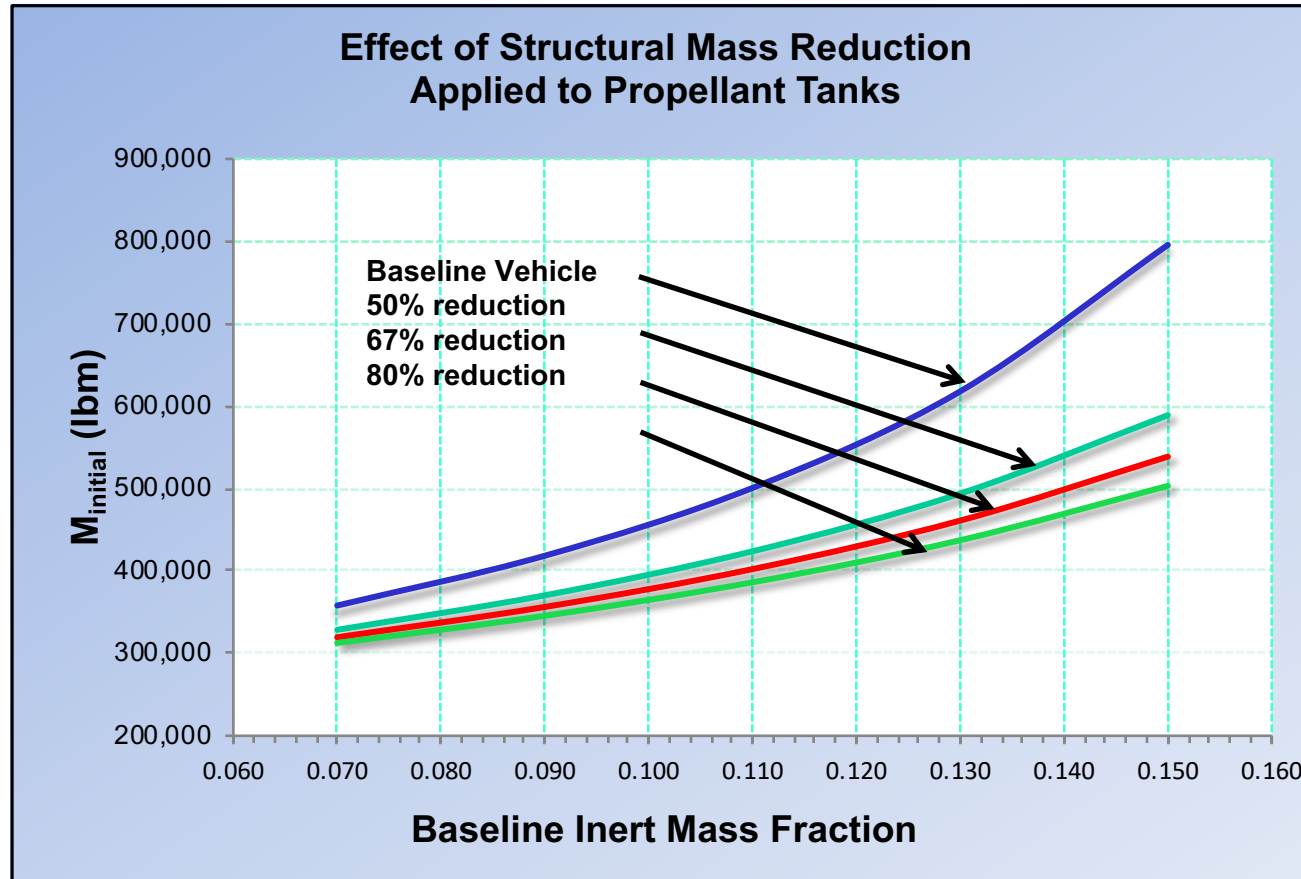


- **Modeling – presumes understanding of the physics.**
 - Takes a long time to lay foundations.
 - Inclined towards modeling of simpler model systems.
 - Verification/validation requires experimental capabilities that are not always available at the scale being modeled.
 - Macroscale properties require multiscale modeling.
- **Multiscale requires collaboration among many scientists towards common technical objective.**
- **Experimentalists rely on experience-based trial and error.**
- **Considering complexity of experiments, and how long it takes to develop models, judicious decisions about what to model need to be made.**
 - Requires clear definition of questions that need to be addressed.

Examples of Computationally Guided Materials Development

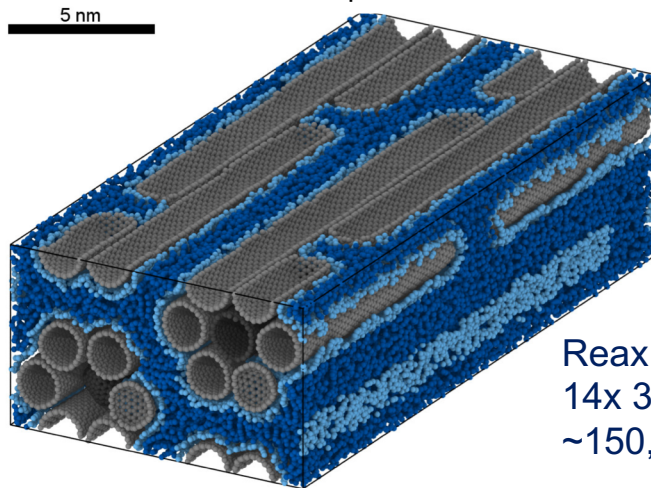
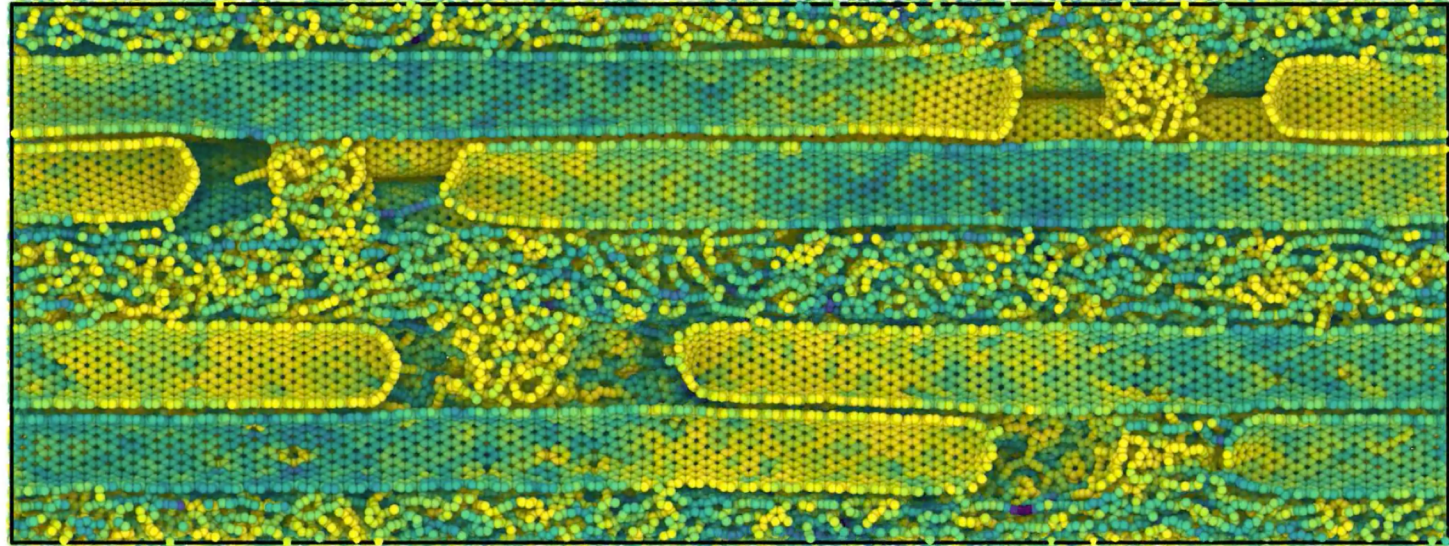
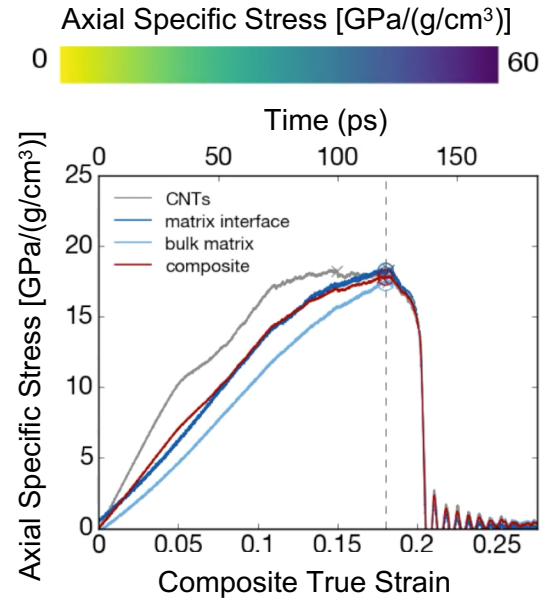


- **Carbon Nanotube Composite Development**
- **Carbon Nanotube Manufacturing**
- **3D Printing**

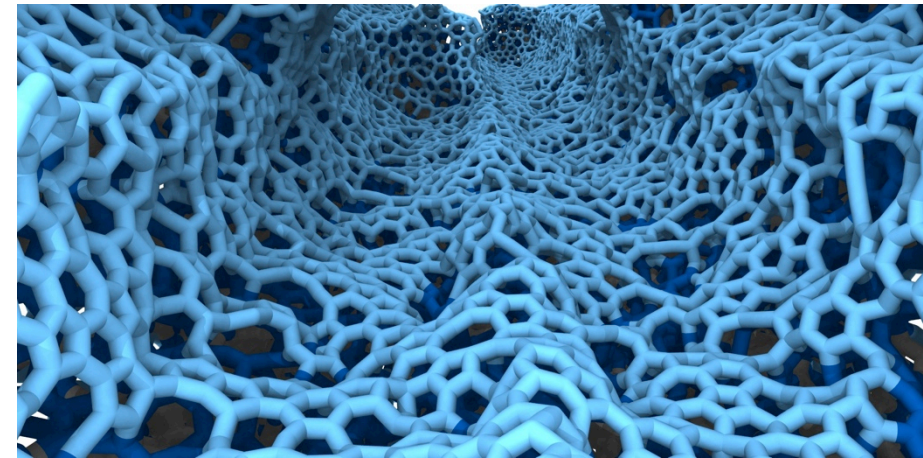


- A 2-3x improvement in specific mechanical properties will permit substantial mass reduction in structural and non-structural components.
- Mass savings are potentially large enough to change design concepts.

Molecular Simulation of Carbon Nanotube Composites



ReaxFF
14x 3.2 nm diameter CNTs
~150,000 atoms

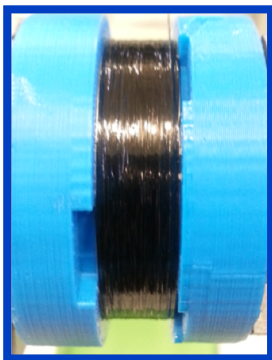


CNT/matrix interface structure

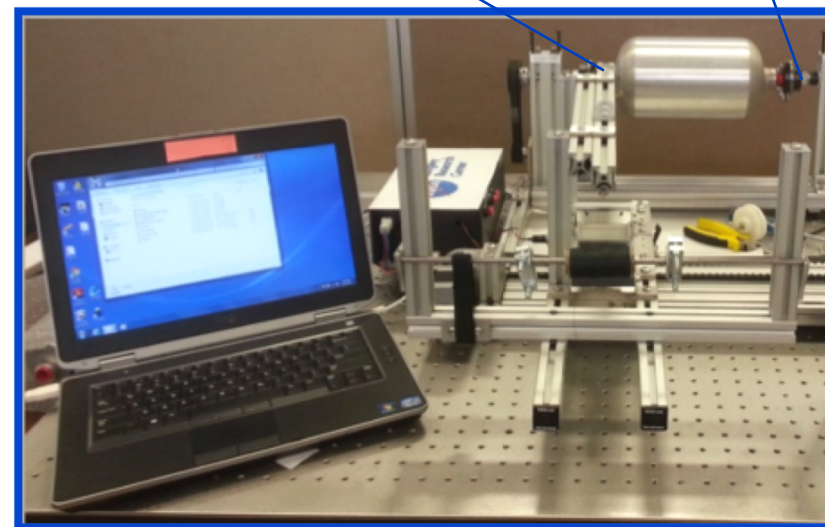
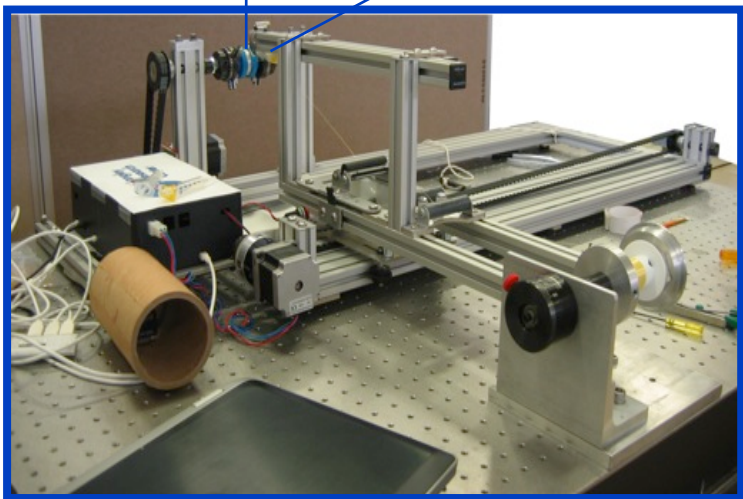
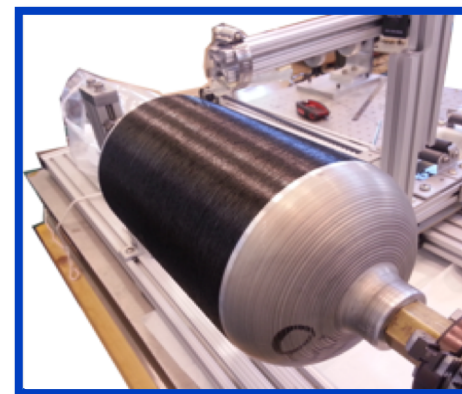
Rapid Prototyping of CNT Composite Fabrication

Tabletop Filament Winder for Rapid Prototyping of Composite Processing

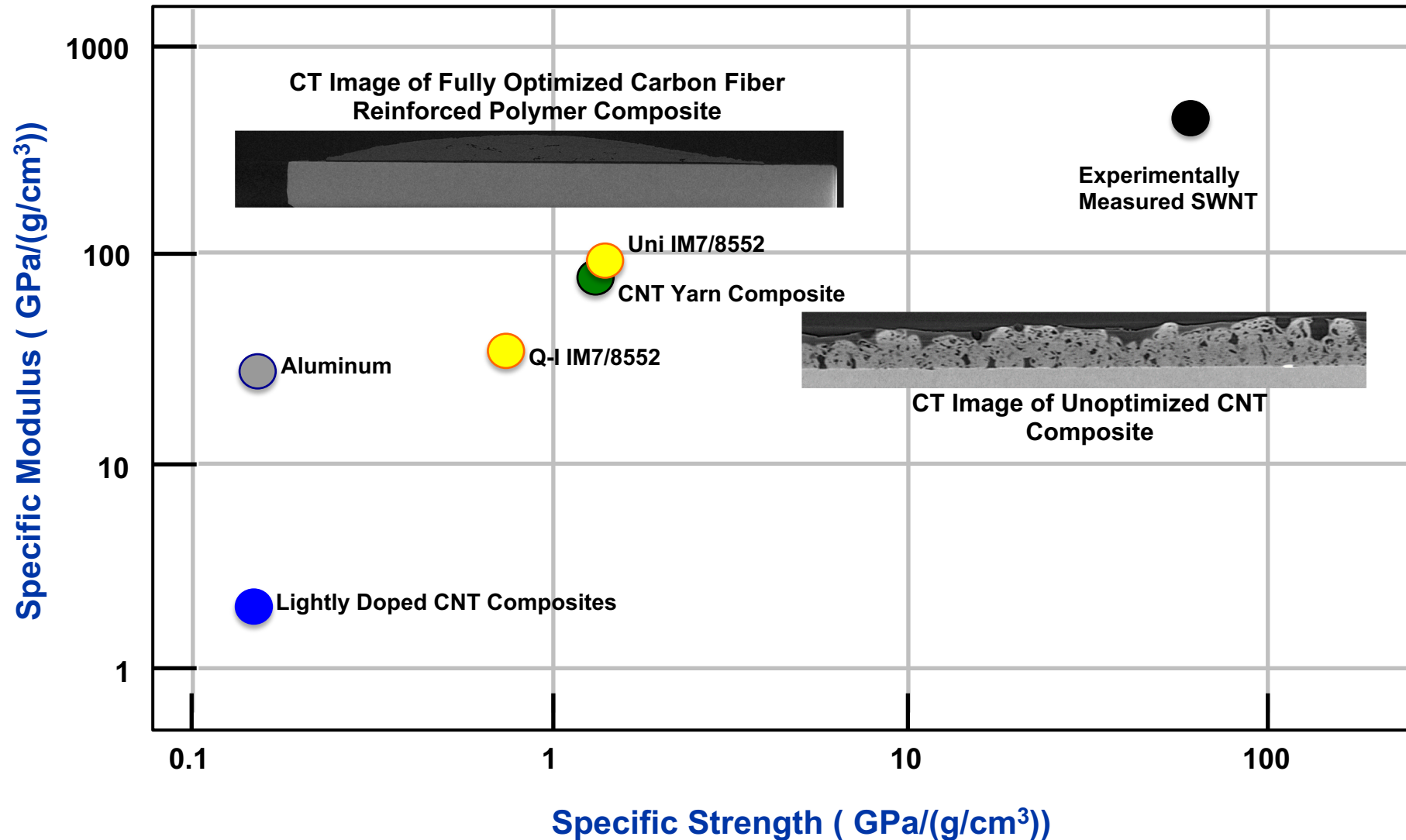
Aluminum Ring



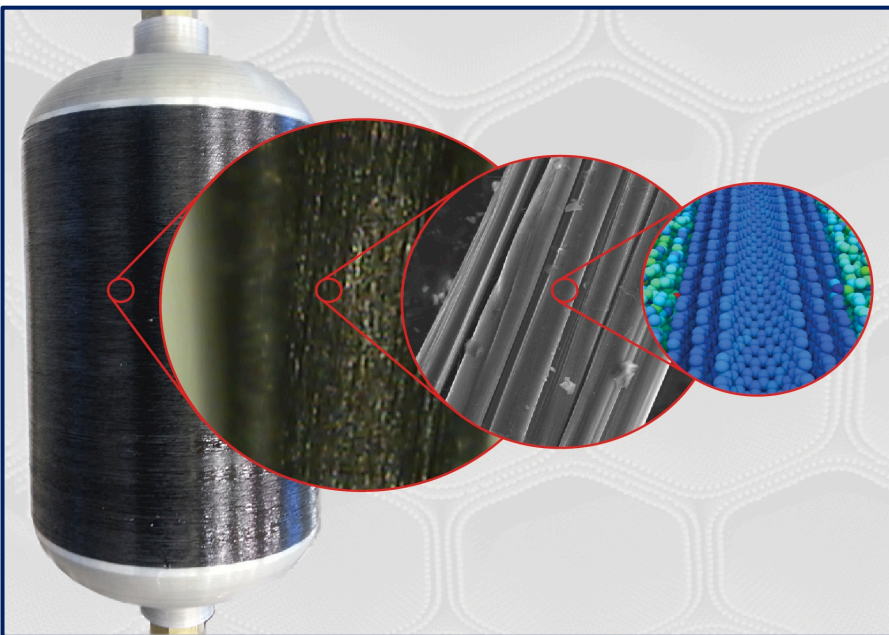
CNT Composite Overwrapped Pressure Vessel



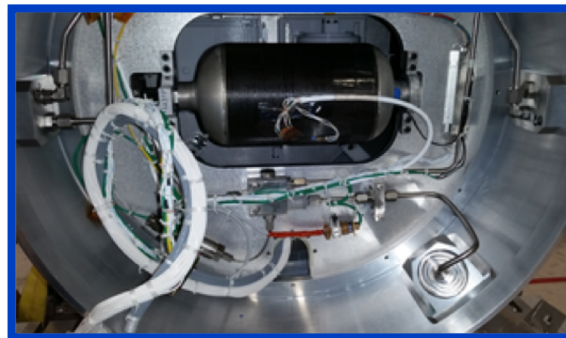
Structural CNT State of the Art



Computationally Guided Use Driven Materials Research



October 2013 – September 2015



October 2016



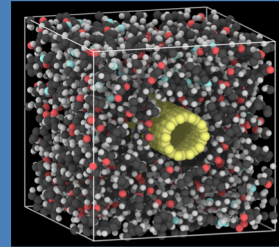
May 2017

Technical Advisory Board (TAB)

Simulation & Design Team (SDT)

Team lead: Greg Odegard

- Force field development
- Atomistic/molecular modeling
- Meso-scale modeling
- Continuum modeling



Testing
feedback &
model
validation

Material
structure

Optimized
material
design

Synthesis
feedback

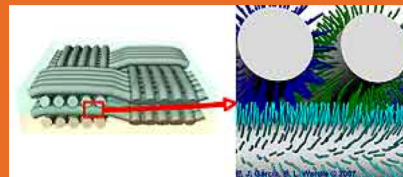
Validation

Characterization

Material Synthesis Team (MST)

Team lead: John Hart

- Small-scale material prototyping
- Material screening



Manufacture
feedback

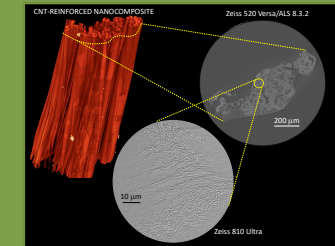
Material
prototypes

Leadership Team

Testing & Characterization Team (TCT)

Team lead: Mike Czabaj

- Materials characterization
- Thermo/electro/mechanical properties



Prototypes

Structure data

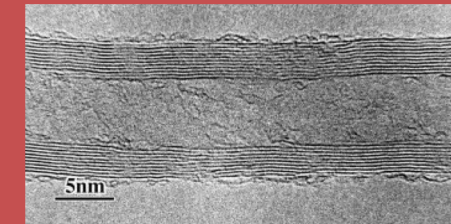
Quality
feedback

Test
panels

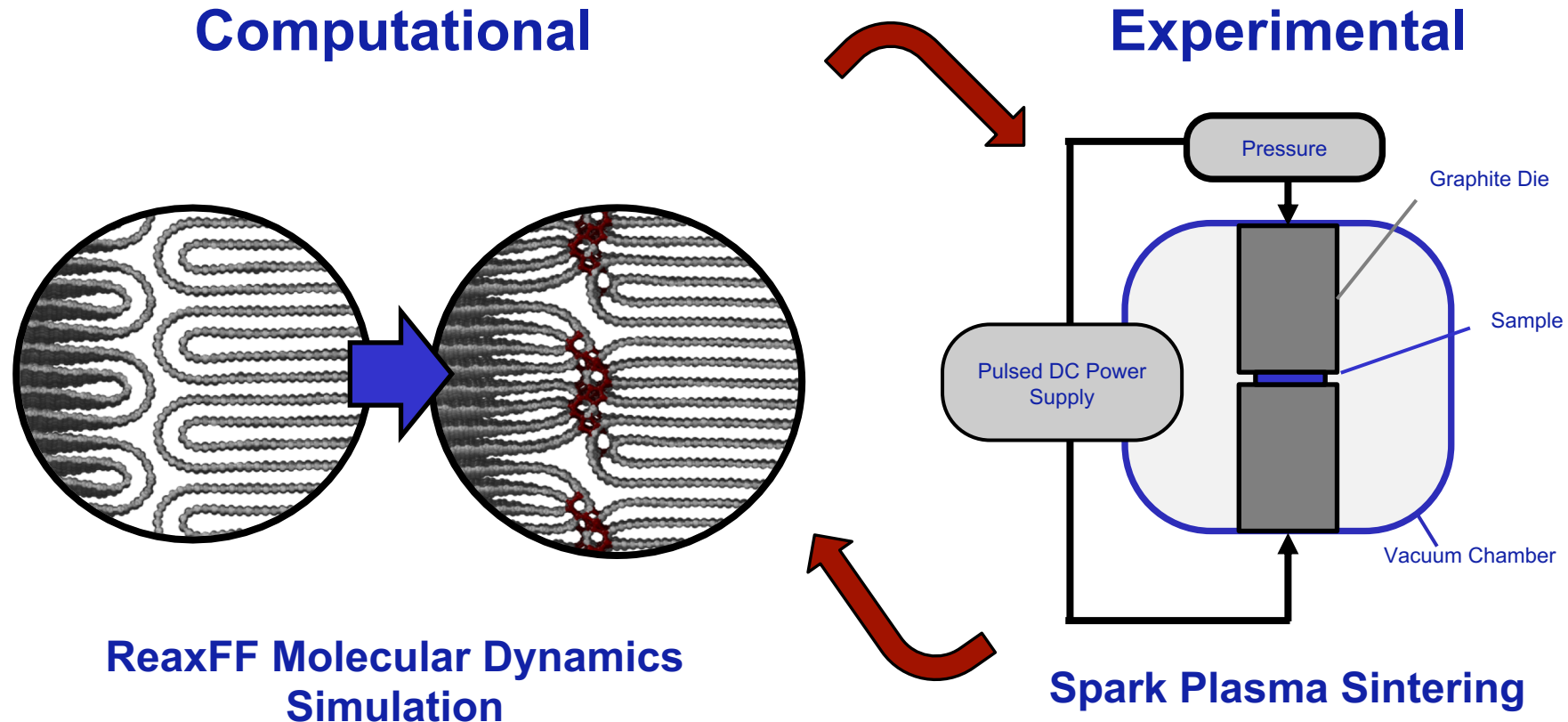
Material Manufacturing Team (MMT)

Team lead: Richard Liang

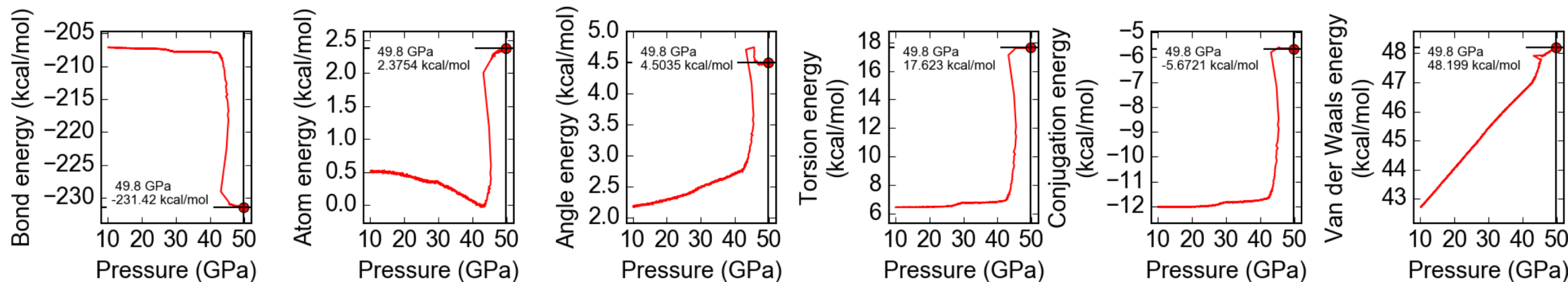
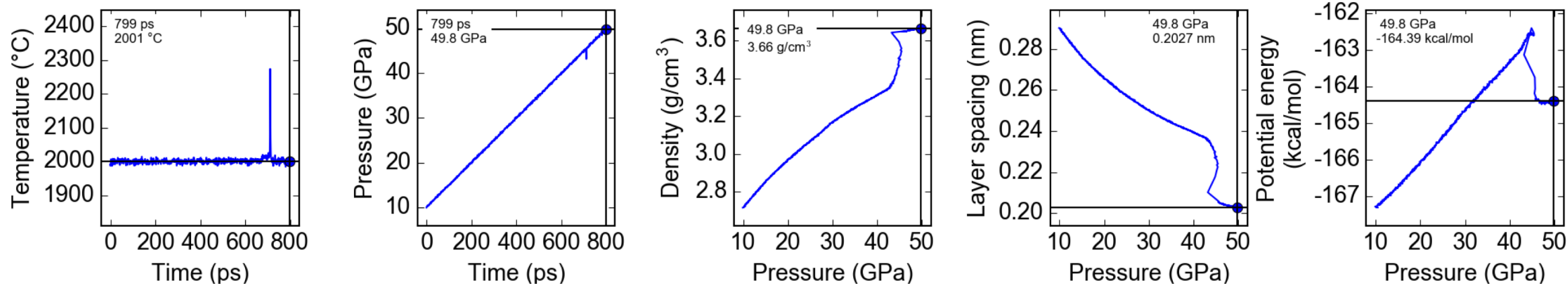
- Manufacturing scale-up
- Materials characterization



High Strength CNT Structures via Covalent Bonds



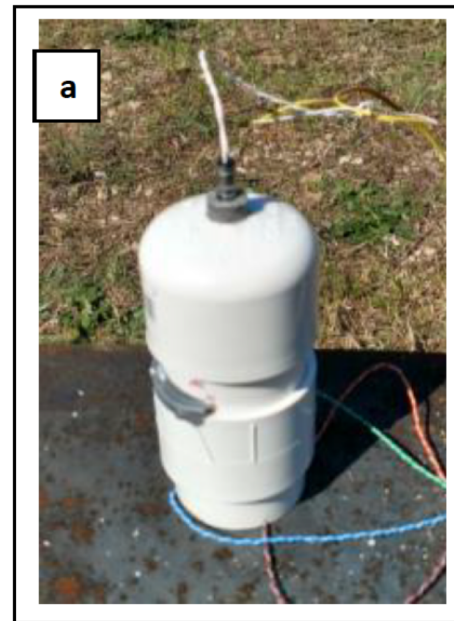
Representative Simulation



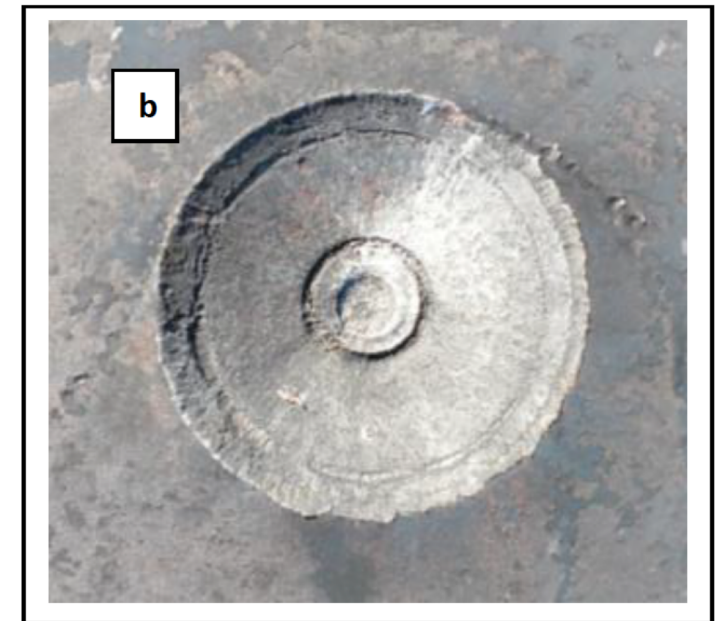
High Strain Testing



Coin cells with CNT in
4" Tall Test Cylinders

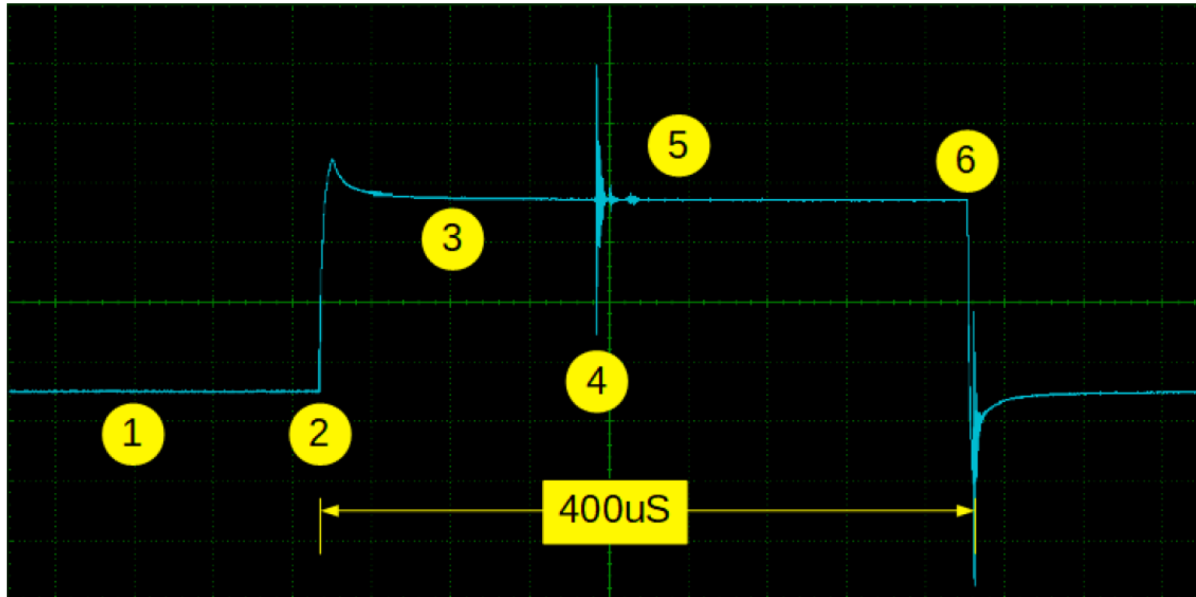


Explosive Charge
Assembly

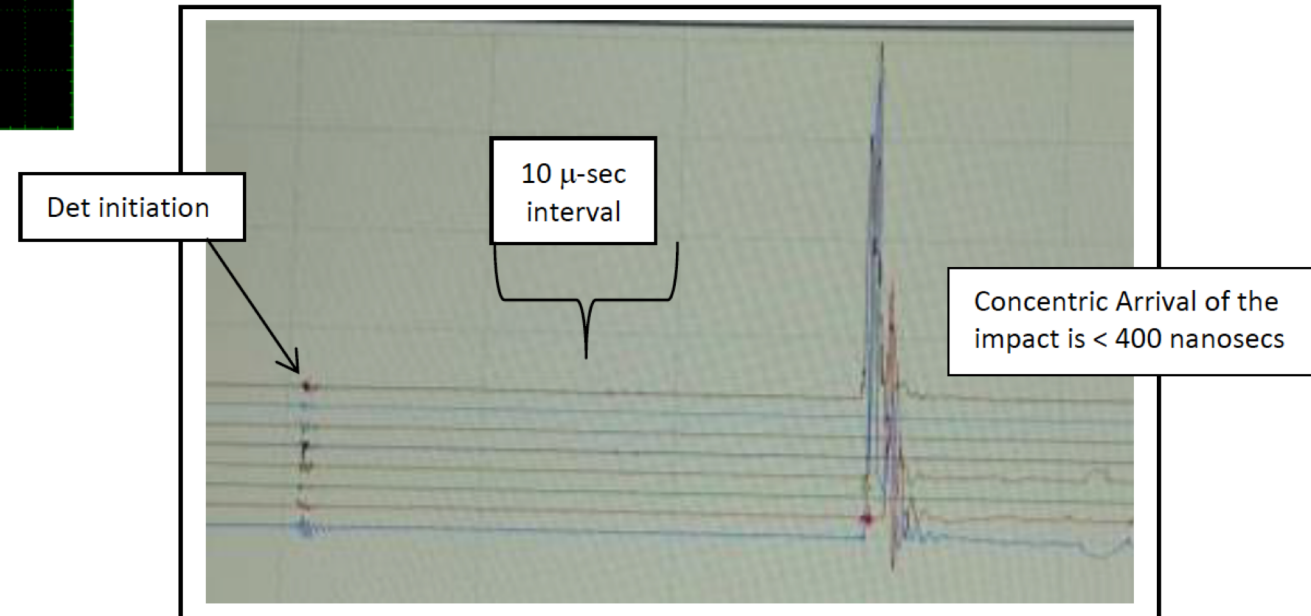


Coin Cell Embedded in
Steel Plate

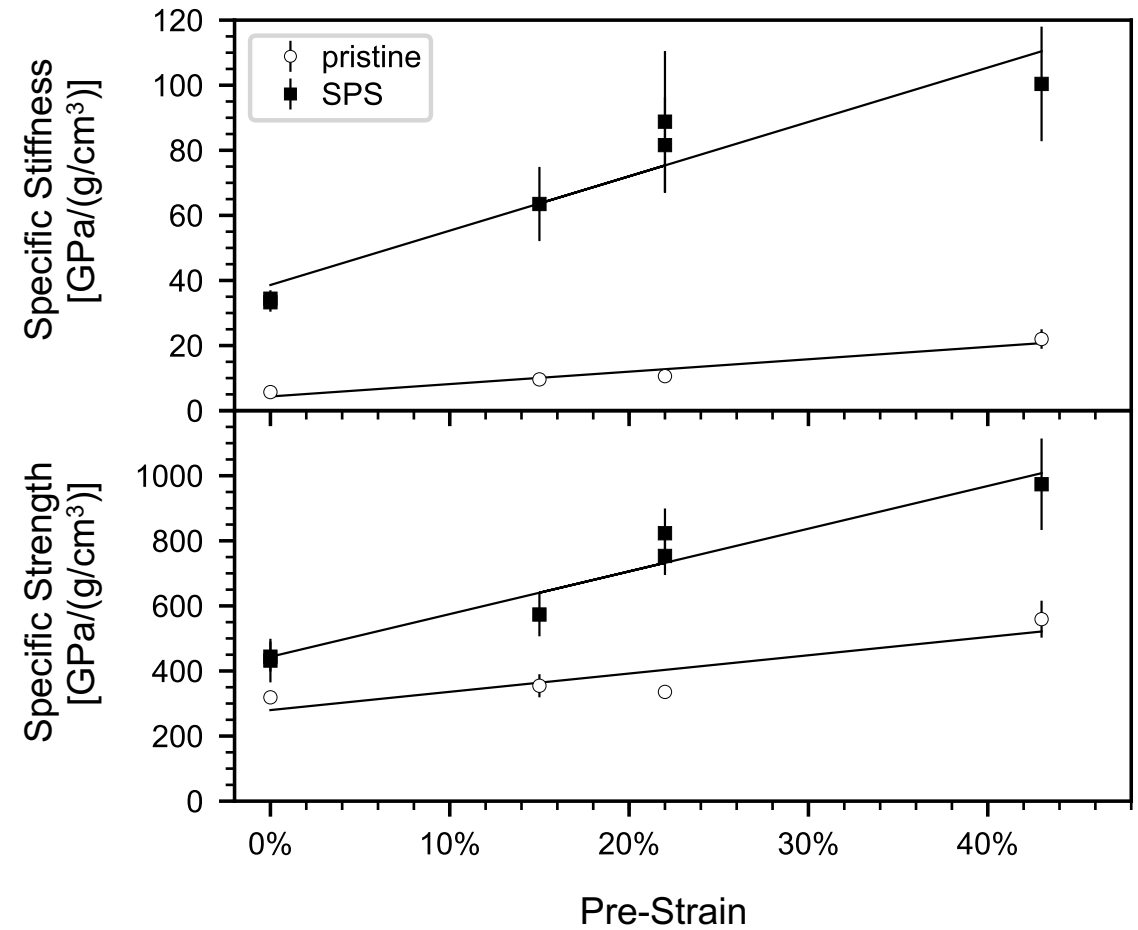
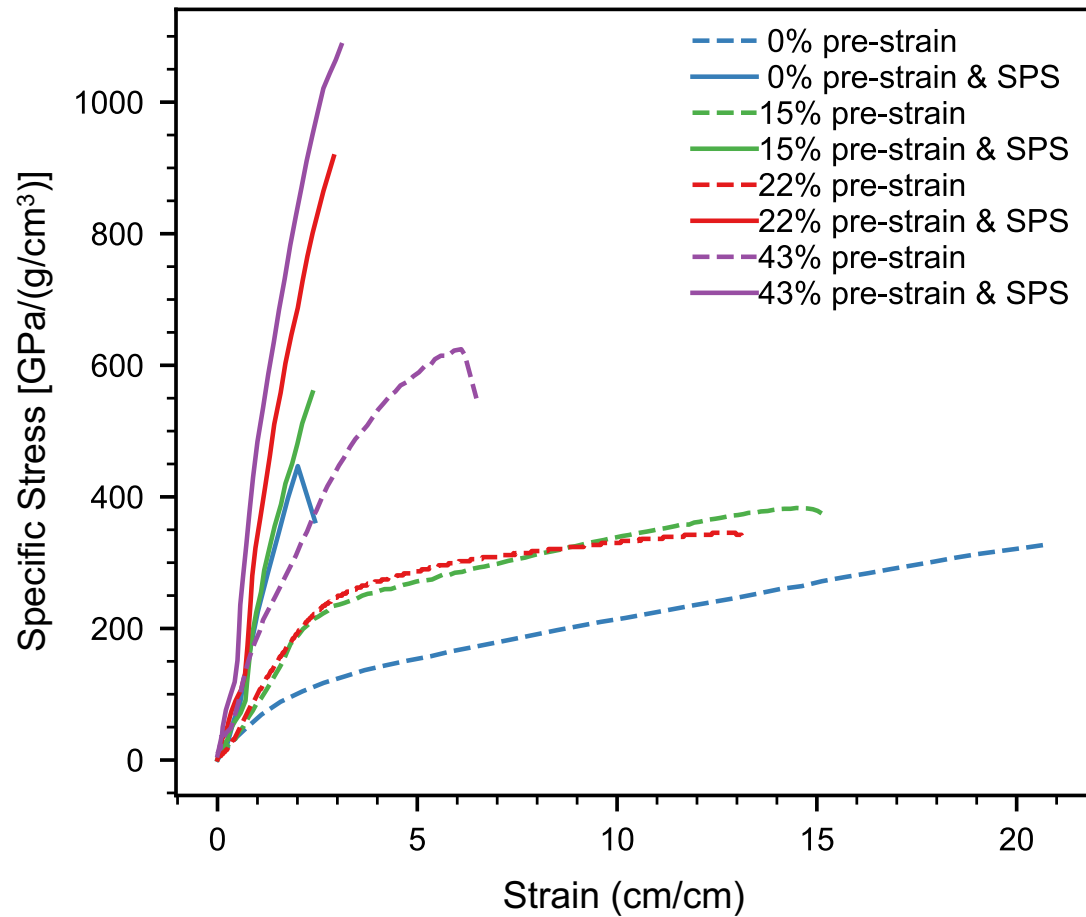
Timing Check Signal Trace



Data Acquisition for High Strain Testing



Mechanical Response of Processed CNT Sheets



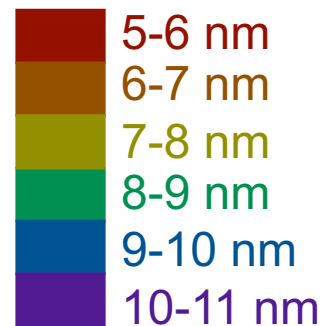
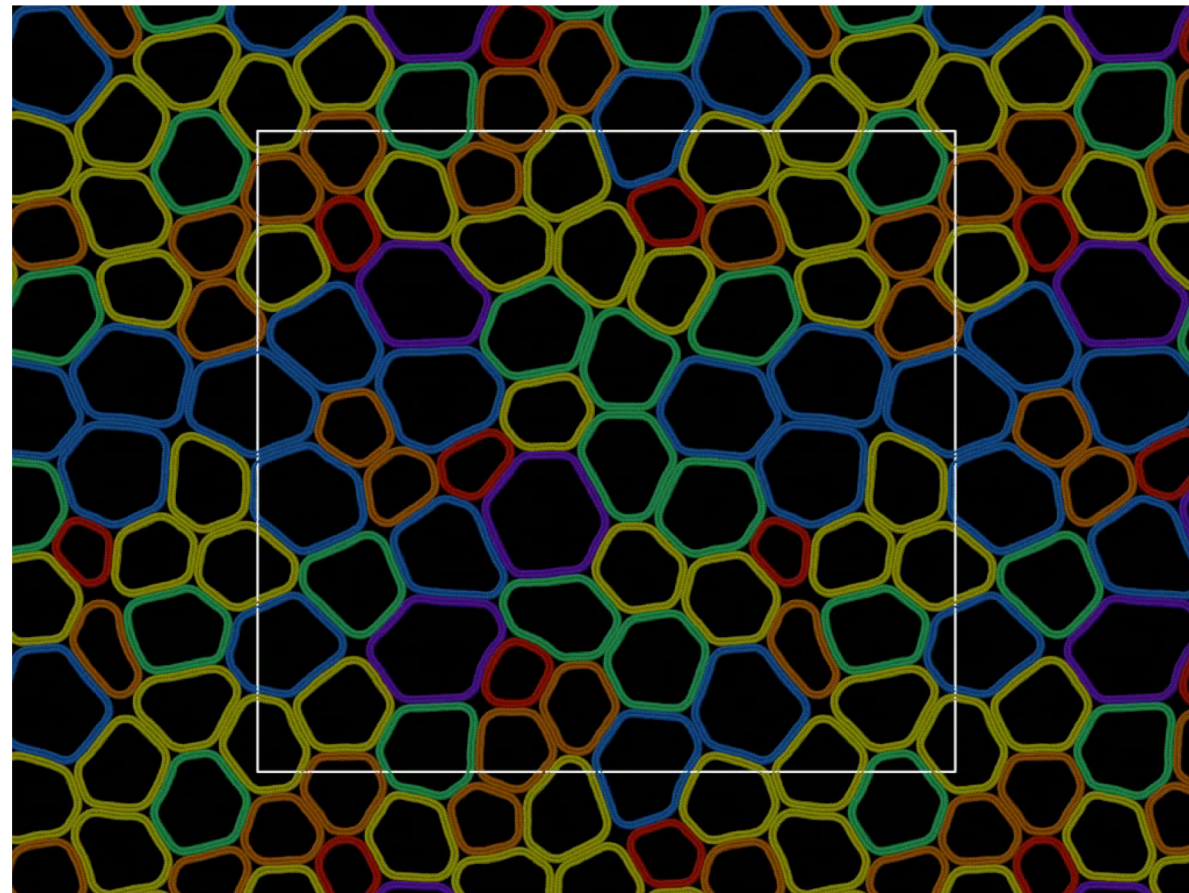
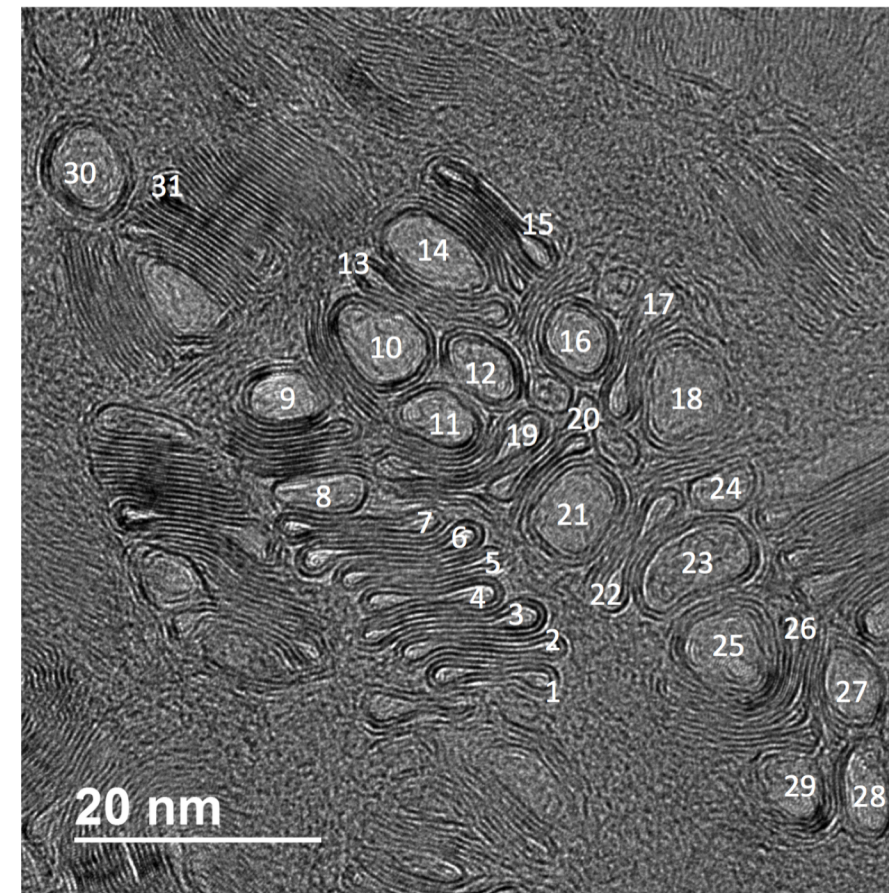
Examples of Computationally Guided Materials Development



- Carbon Nanotube Composite Development
- **Carbon Nanotube Manufacturing**
- 3D Printing

Molecular Dynamics Simulations of CNTs

Modeling the flattening process for much larger systems with experimental diameter distribution

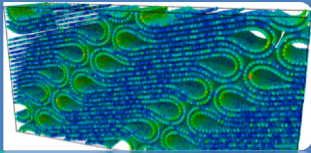


Examples of Computationally Guided Materials Development

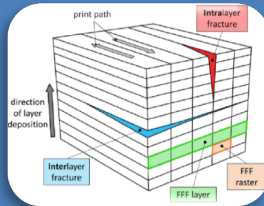


- Carbon Nanotube Composite Development
- Carbon Nanotube Manufacturing
- **3D Printing**

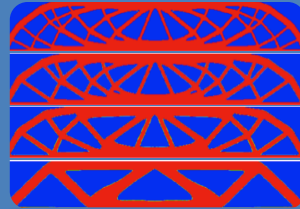
3D Printing for Aerospace Applications



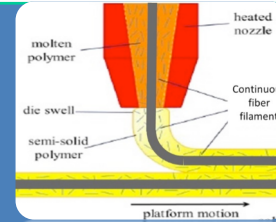
Atomistic Modeling



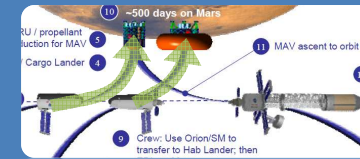
Mechanics of Materials Modeling



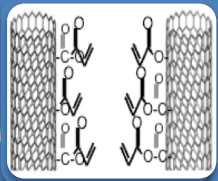
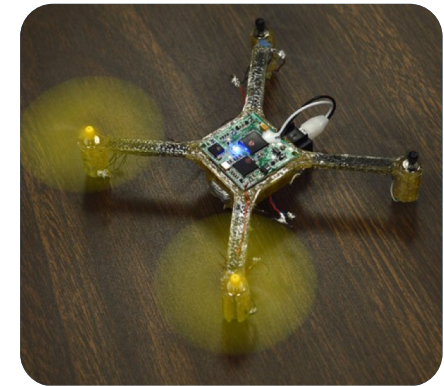
Topological Optimization



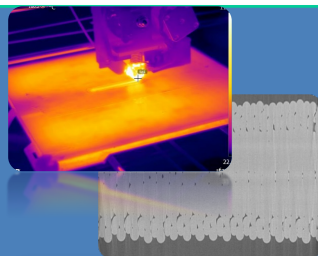
Process Modeling



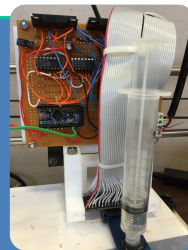
Systems Analysis



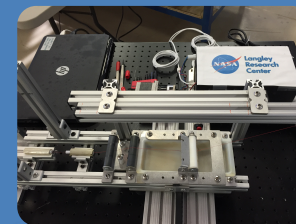
Chemistry



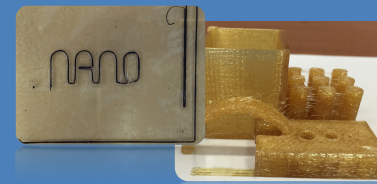
Materials Characterization



Sensor Fab and Characterization

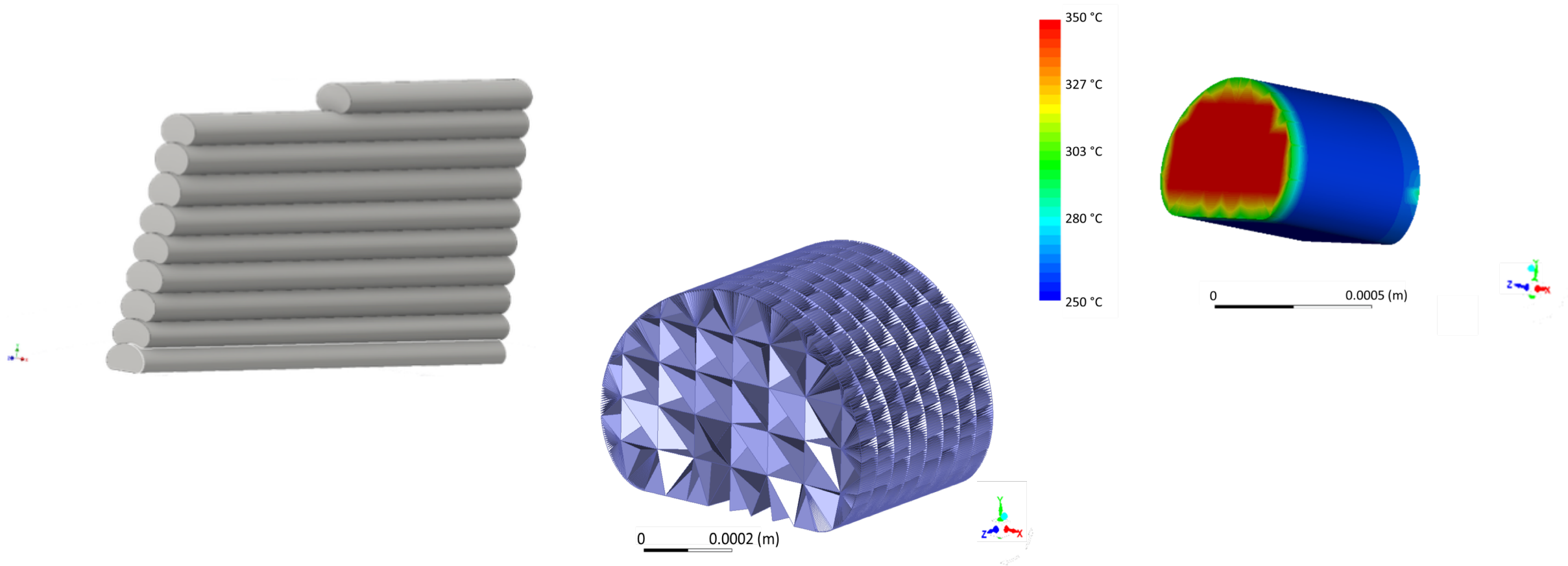


Composite Processing



3d Printing

Process Modeling of 3D Printing Process



Machine Learning Steps

Error Identification & Classification

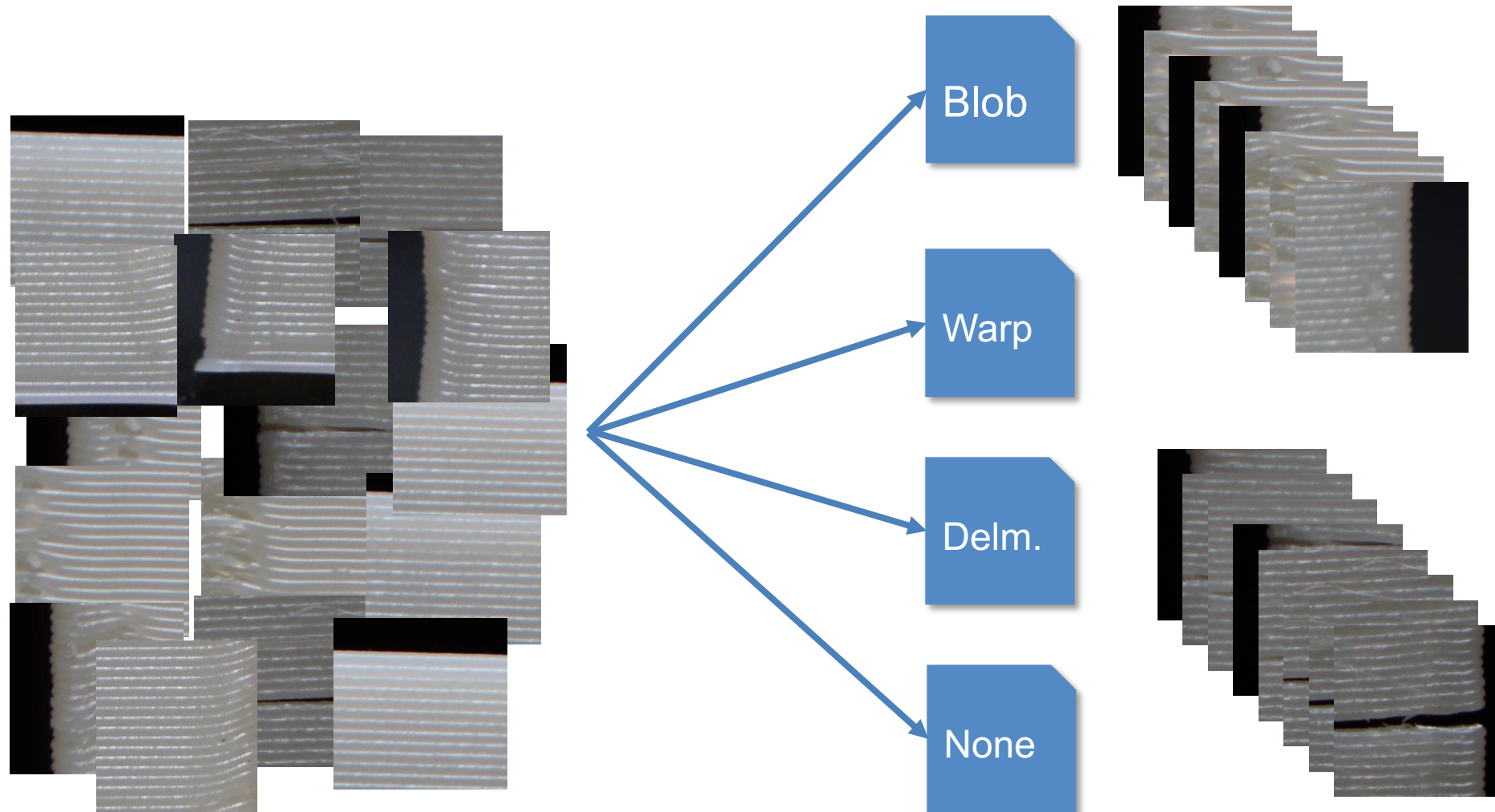


Error Prediction
(Parameter Selection)

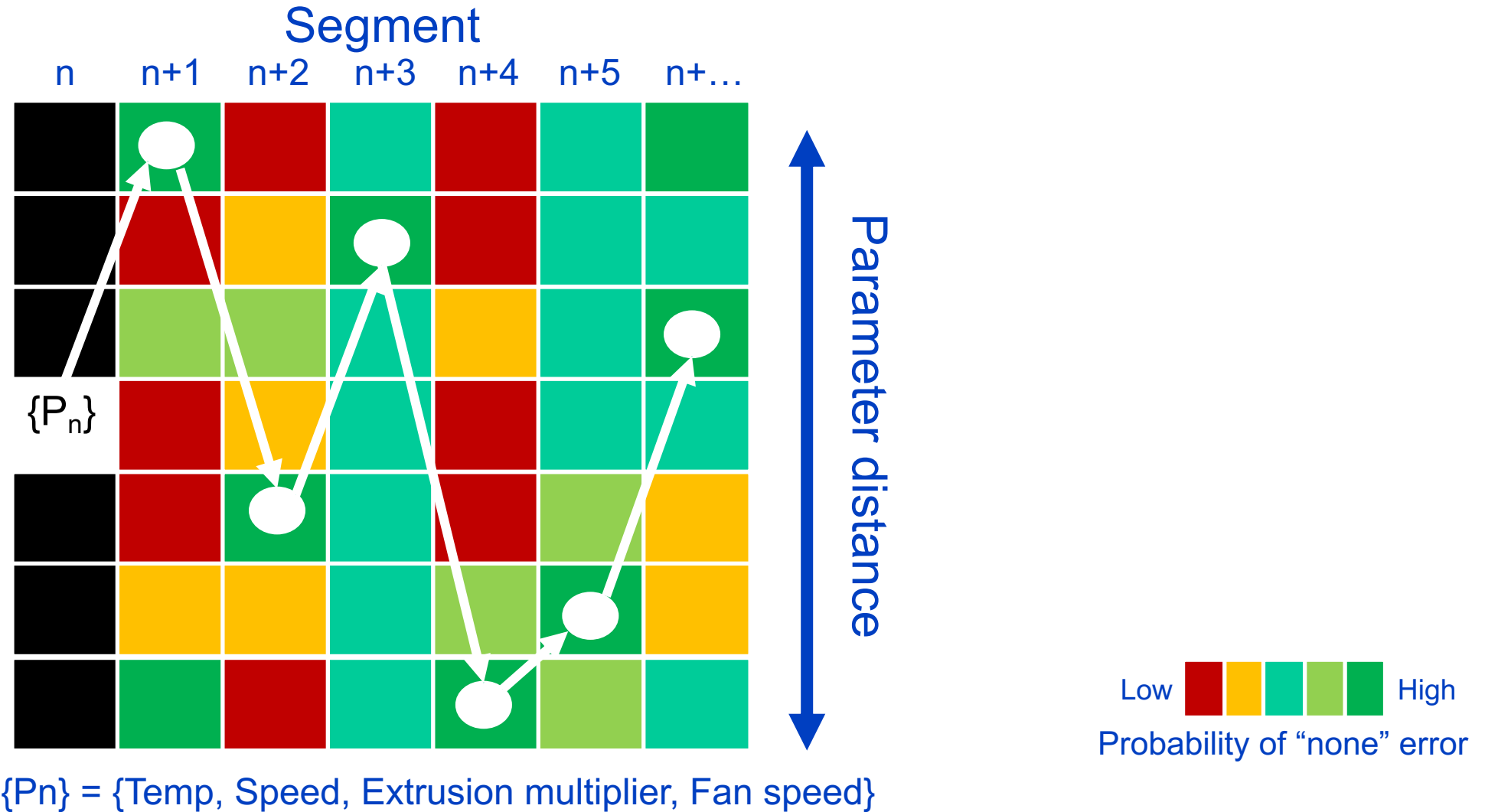


Parameter Smoothing

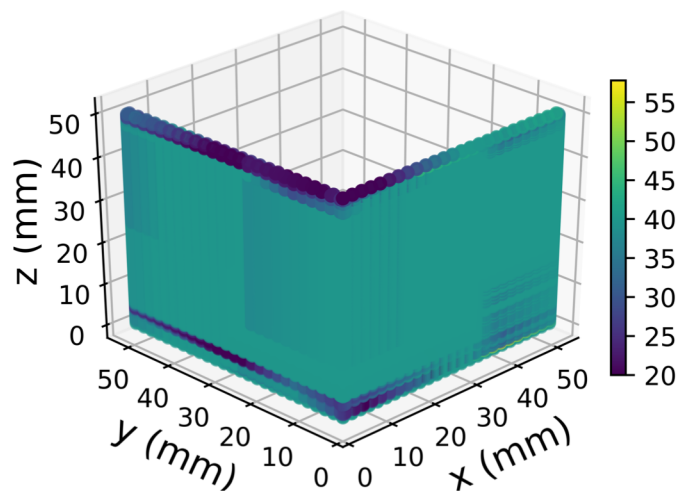
Sorting by Error Types



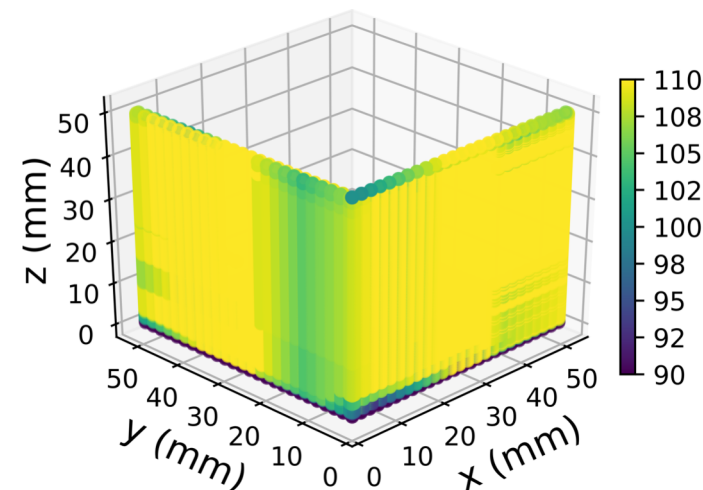
The “Best” Parameter Picks



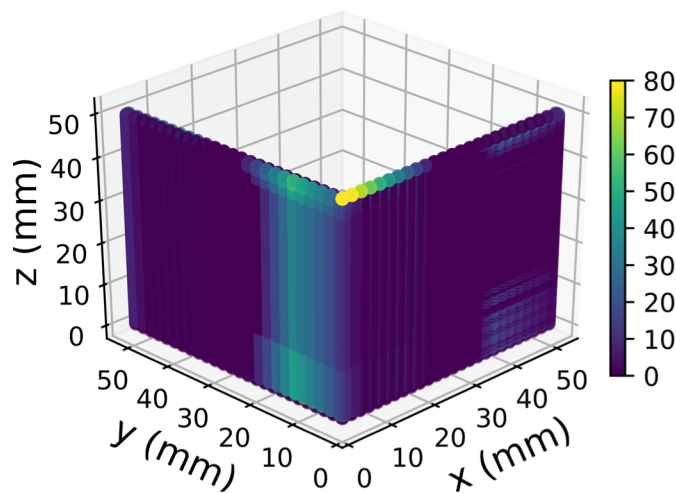
Optimizing for Best Quality



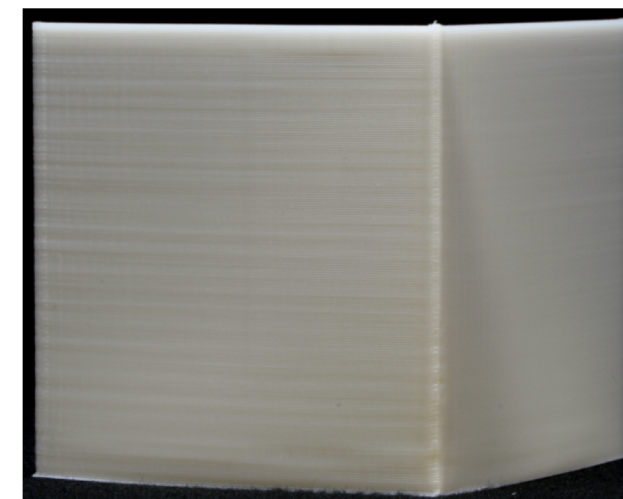
Print speed



Extrusion multiplier



Fan speed



- **Systems analysis can provide concrete goals for fundamental research.**
- **Iterative coupling of modeling with experimentation can advance both modeling tools and experimental approaches to accelerate materials development.**
- **Rapid prototyping is an effective tool for exposing necessary areas of research to advance emerging materials towards insertion in applications.**
- **Use inspired materials development requires engagement of the materials ecosystem to guide research paths for fastest payoff.**



EXPLORESPACE TECH

TECHNOLOGY DRIVES EXPLORATION

Thank You