National Aeronautics and
Space Administration

Space Technology Research Institutes 2016

Computationally Accelerated Materials Development for Ultra High Strength Lightweight Structures

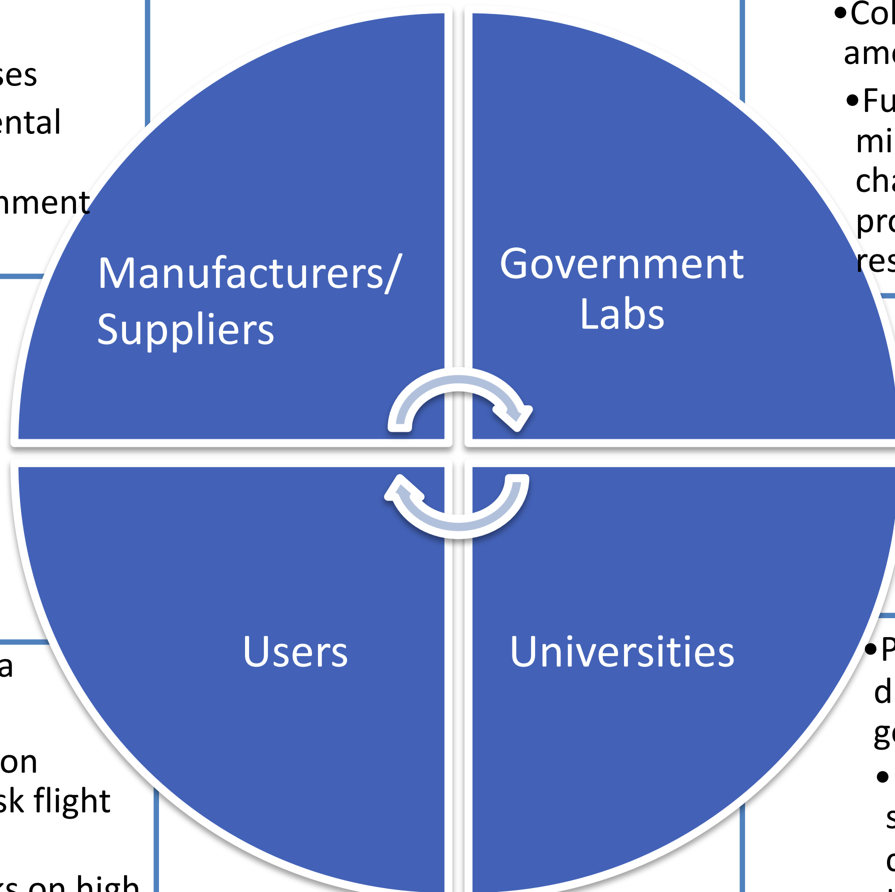
Mia Siochi

NASA Advisory Committee Meeting
December 7, 2018

Collaborative Partnerships in Materials Ecosystem

- Scale up of materials
- Optimization of manufacturing processes
- Capitalize on fundamental science provided by universities and government research labs

- Technical leadership
- Collaborative partnerships among government labs
- Fund focused efforts on mission relevant challenging technical problems – use-inspired research



- Early engagement via advisory role
- Provide demonstration opportunities, low risk flight opportunities
- Provide reality checks on high payoff applications

- Professors working across disciplines toward common goals
- Provide fundamental science understanding for challenging technical issues toward technology adoption

Accelerated technology adoption through engagement of key players to enable a sustainable advanced aerospace materials ecosystem

Challenge

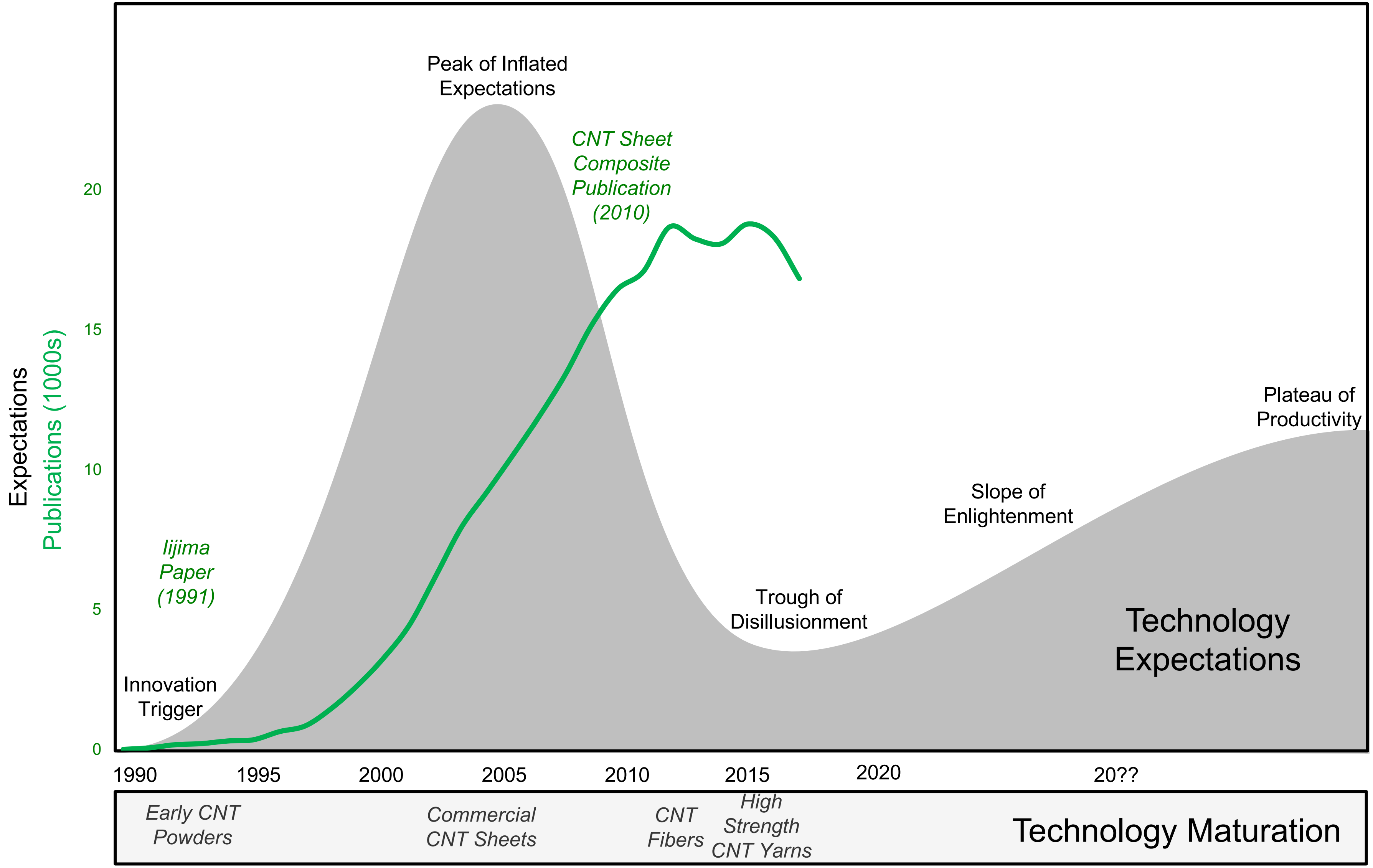
- Cost increases in proportion to the mass ratio
- Mass ratio increases linearly with the dry mass and exponentially with Δv
- Reducing structural mass reduces mission cost at constant payload or increases mission capability at constant cost

	Mass Ratio*	Cost per pound*
Low Earth Orbit	20	$4,000
Earth to Moon	200	$40,000
To Moon, Return to Earth	500	$100,000
Earth to Mars	500	$100,000
To Mars, Return to Earth	5000	$1,000,000

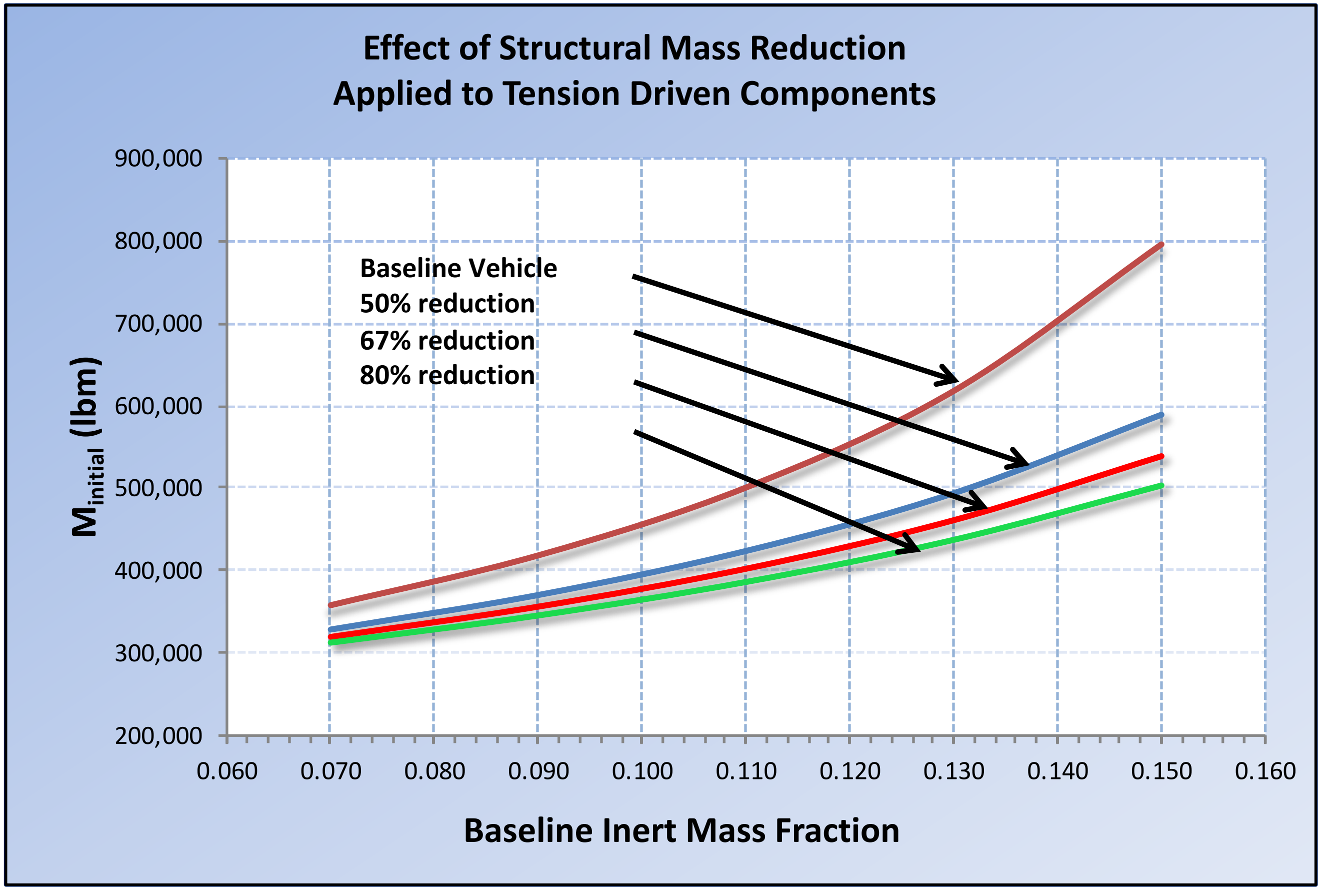
* Order of magnitude estimates for mass ratios and costs.

G. Gordon, AIAA SPACE 2007, paper 6278.

Carbon Nanotube (CNT) Gartner Hype Cycle



Setting Goals using Systems Analysis



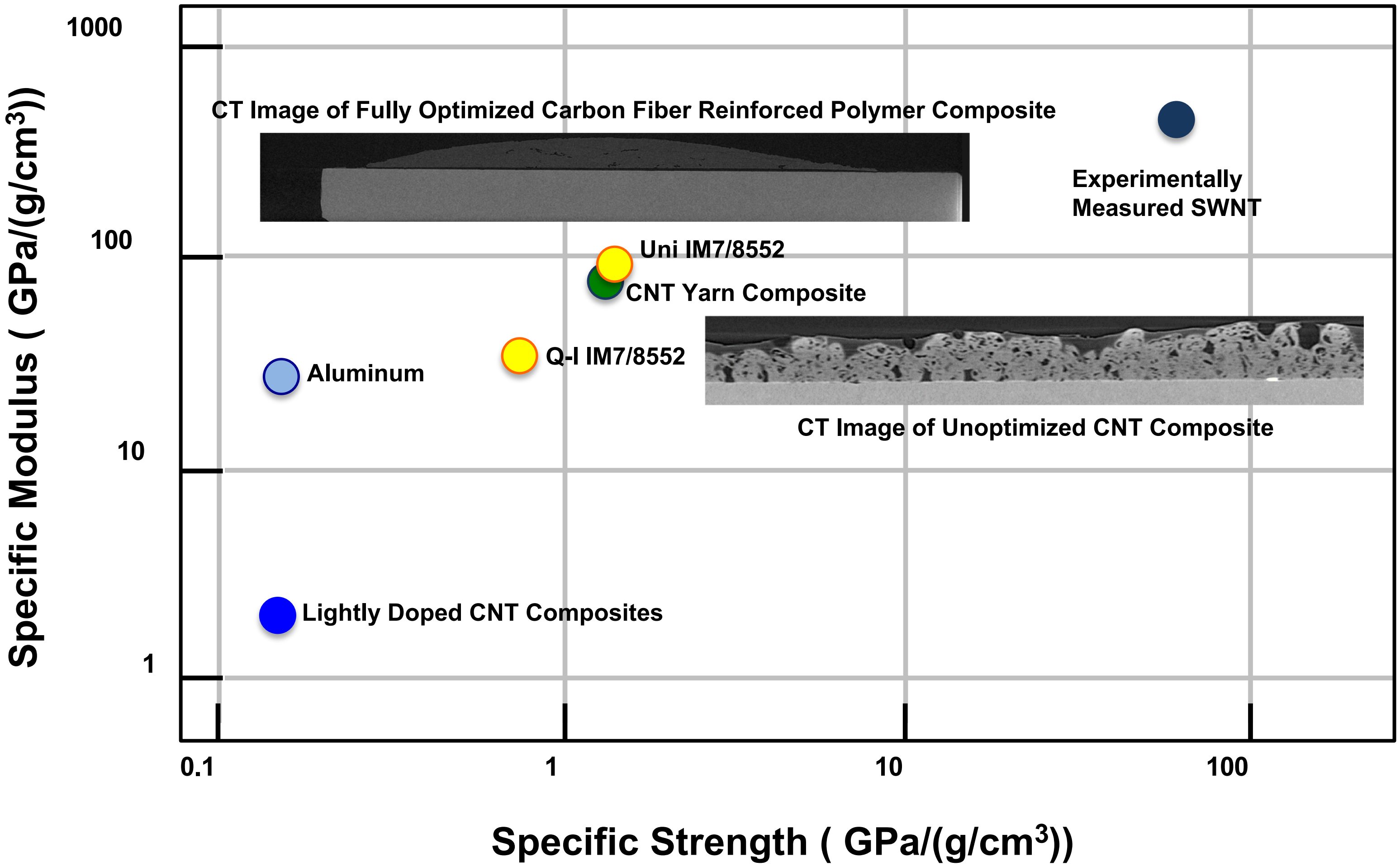
- A 2-3x improvement in specific mechanical properties will permit substantial mass reduction in structural and non-structural components
- Mass savings are potentially large enough to change design concepts

McMillan, M., System Level Impact of High Strength Carbon Nanotube Materials Applied to Launch Vehicle Concepts, White Paper, March, 2013.

State of the Art Lightweight Structural Material

Image Credit: NASA

Structural CNT Potential



Computationally Accelerated Materials Development for Ultra High Strength Lightweight Structures

Topic Focus

Ultra high strength lightweight structural material enabled by Materials Genome Initiative (MGI) inspired computational guidance

Distinctive Features of Topic

- MGI approach that spans entire materials development cycle
- Requires demonstration article with challenging property targets at the end of performance period
- Panel properties specified are at least double that of state of the art carbon fiber composite properties
- Properties defined with systems guidance on overall payoff in mass reduction for aerospace systems

Computational Guidance Spans Materials Development Cycle

- Application-guided structural materials design – predictive modeling of material properties including load transfer mechanisms that will influence material and structure design
- Computationally guided design, synthesis, and processing to enable macroscale fabrication of ultra high strength composite
- Accelerated testing and evaluation of material properties to inform iterative advancement of materials design, synthesis, and processing

University of Utah

Michigan Tech University

Florida State University

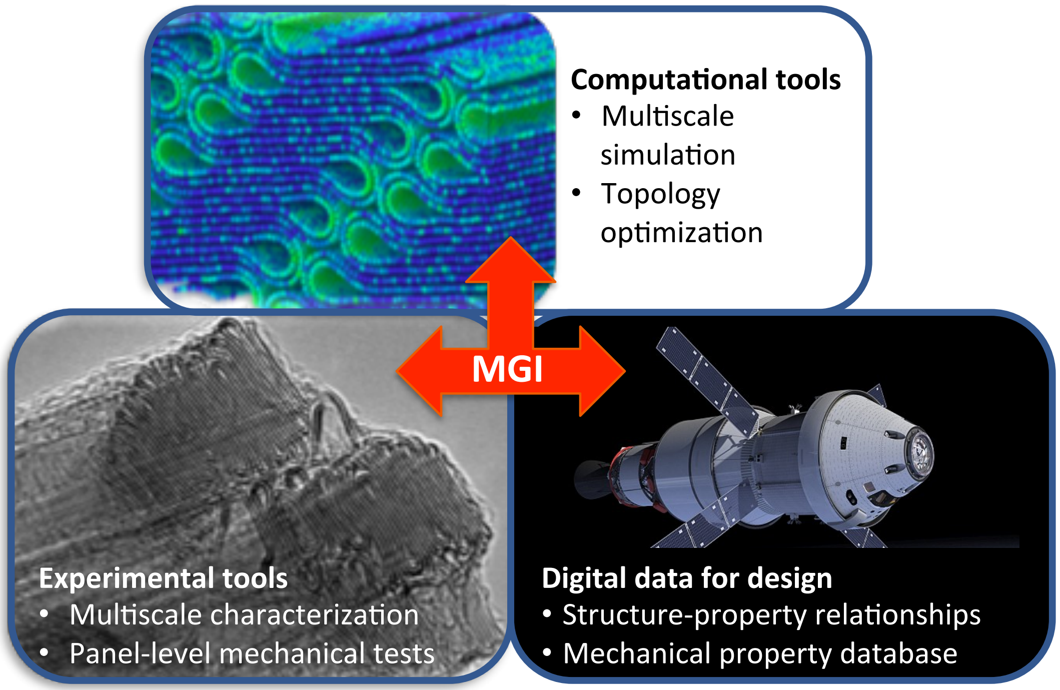
Massachusetts Institute of Technology

Pennsylvania State University

Virginia Commonwealth University

University of Minnesota

Georgia Tech



University of Colorado

Florida A&M University

TECHNOLOGIES, INC.

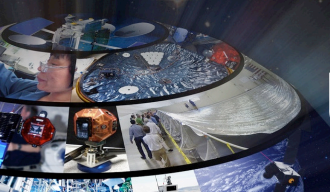
SOLVAY

Johns Hopkins University

https://www.nasa.gov/press-release/nasa-selects-proposals-for-first-ever-space-technology-research-institutes

Research Objectives

- Develop novel Ultra-high strength lightweight (UHSL) structural material per NASA requirements
- Establish new computationally-driven material design paradigm for rapid material development
- Develop modeling, processing and testing tools and methods for CNT assemblage-based UHSL materials
- Train a pool of highly skilled scientists and engineers to contribute to the materials development workforce



US-COMP Organizational Structure

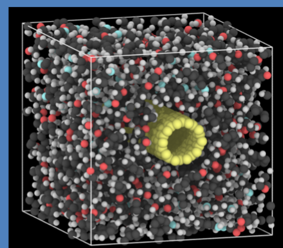
Technical Advisory Board (TAB)

Leadership Team

Simulation & Design Team (SDT)

Team lead: Greg Odegard

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



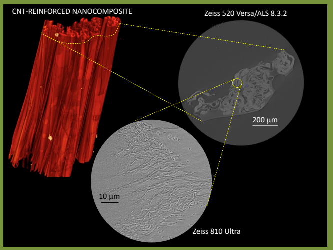
Testing feedback & model validation

Material structure

Testing & Characterization Team (TCT)

Team lead: Mike Czabaj

- Materials characterization
- Thermo/electro/ mechanical properties



Optimized material design

Synthesis feedback

Validation

Characterization

Prototypes

Structure data

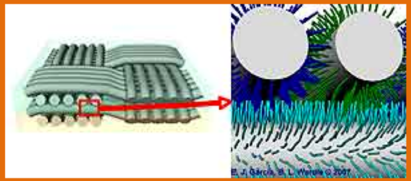
Quality feedback

Test panels

Material Synthesis Team (MST)

Team lead: John Hart

- Small-scale material prototyping
- Material screening



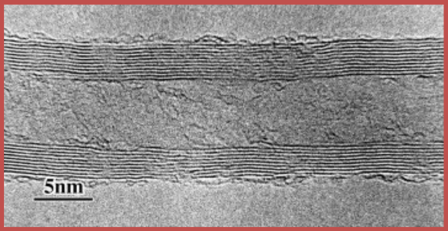
Manufacture feedback

Material prototypes

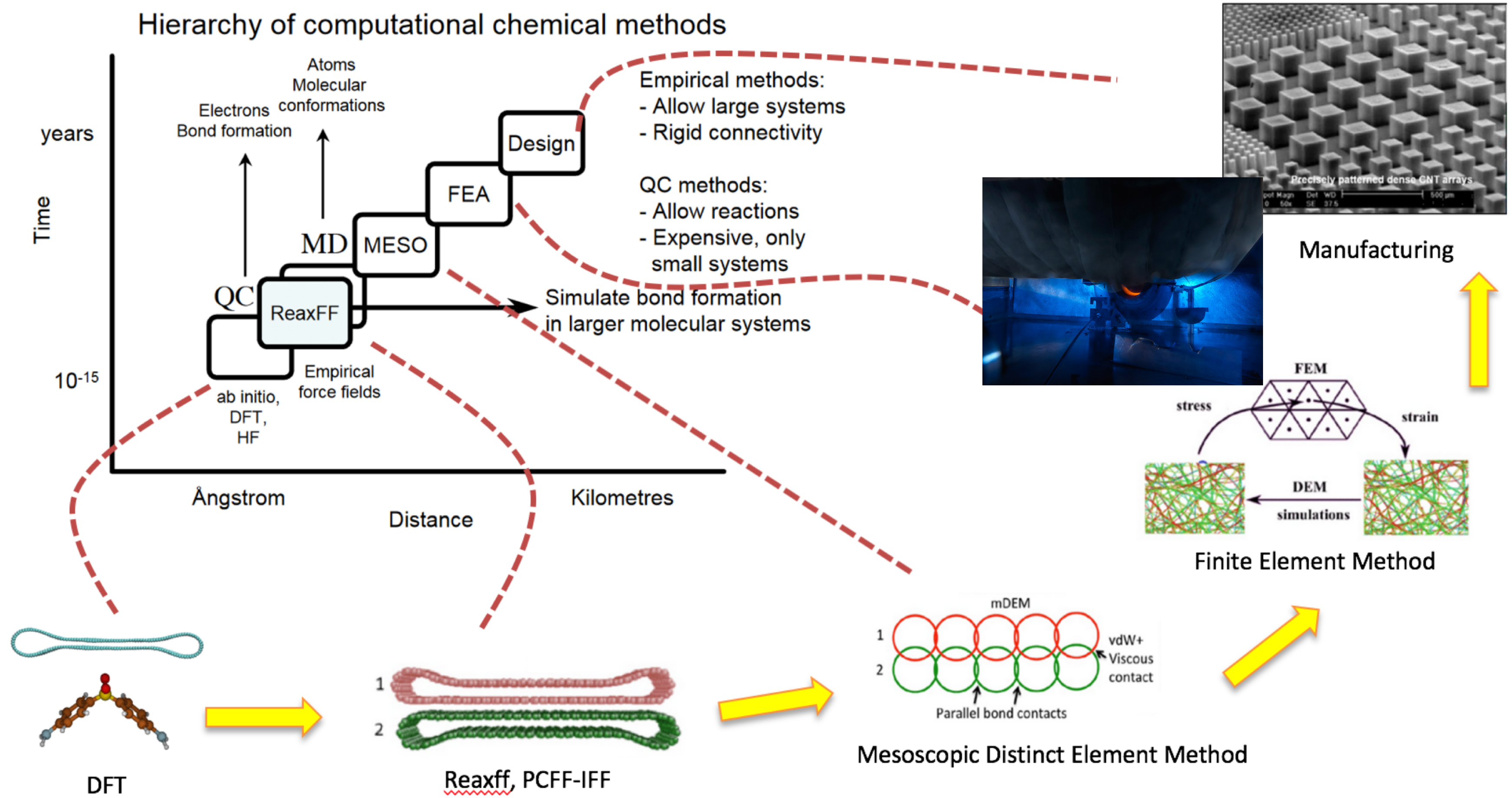
Material Manufacturing Team (MMT)

Team lead: Richard Liang

- Manufacturing scale-up
- Materials characterization



Multiscale CNT Composite Modeling



Simulation & Design Team (SDT)

Team lead: Greg Odegard

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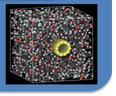
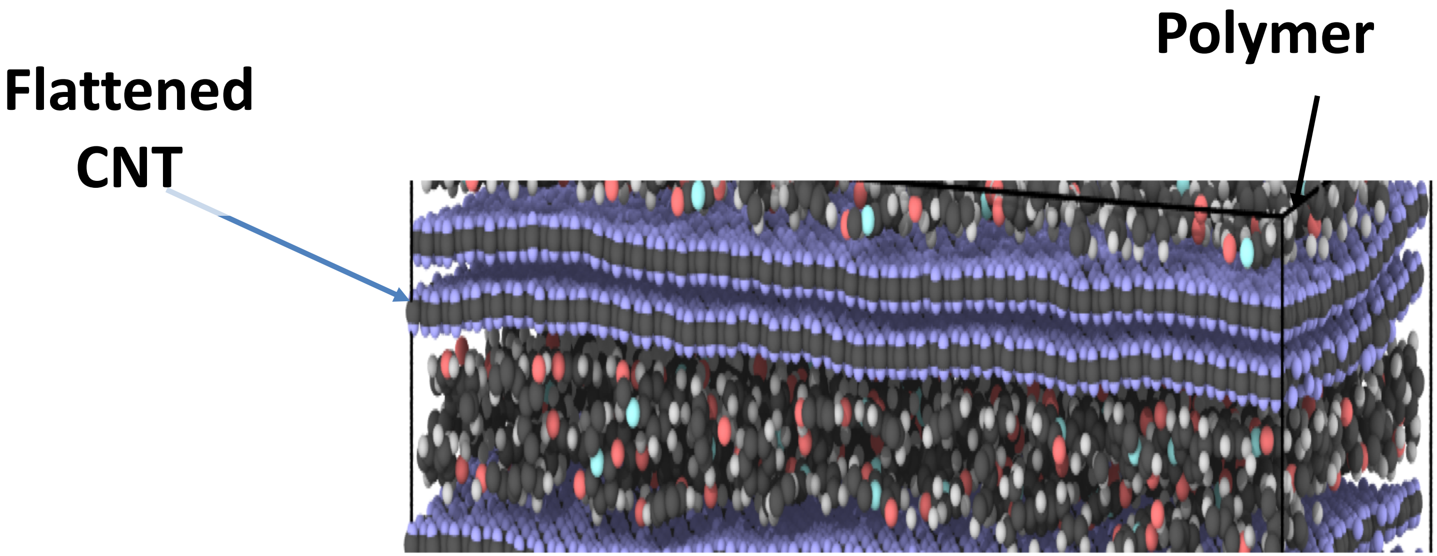


Molecular Modeling

- **Understanding the interaction characteristics between CNTs and polymers (for optimal load transfer)**
  - **Most compatible CNT/polymer combinations**
  - **Influence of polymer crosslinking/polymerization**
  - **Optimal levels of polymer content**



Molecular dynamics model

Simulation & Design Team (SDT)

Team lead: Greg Odegard

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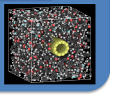
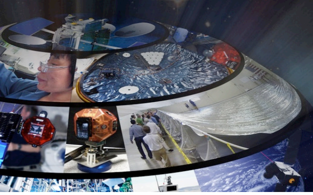
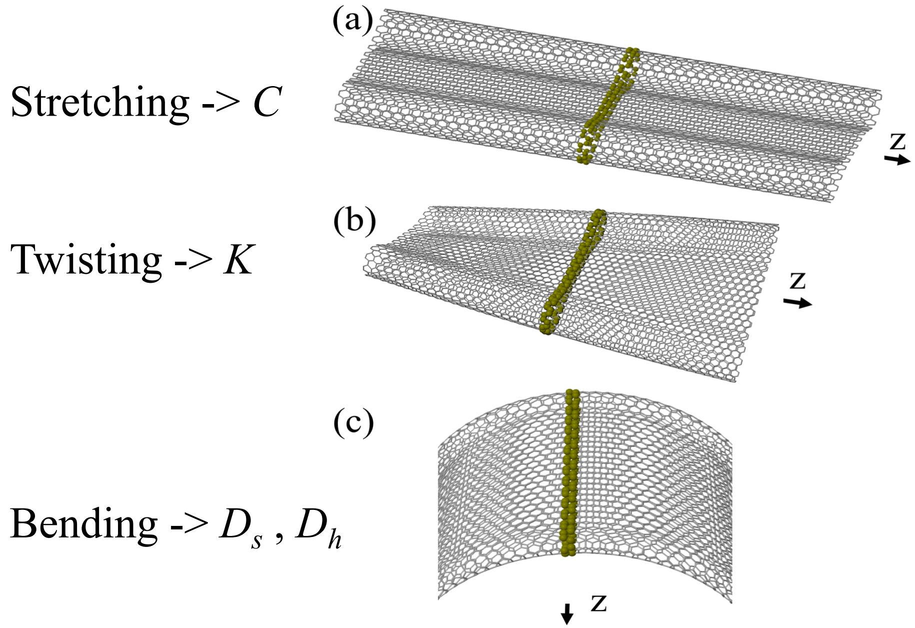
- Continuum modeling

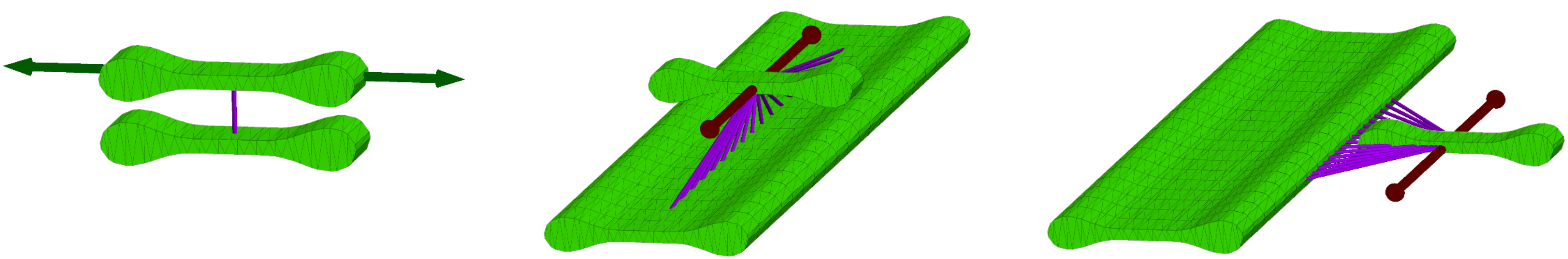




Meso-Scale Modeling

- **Meso-scale (atomistically informed) models can now predict the CNT-CNT interaction at larger length scales**
- **The failure behavior of CNT bundles can be predicted**





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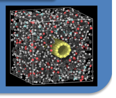
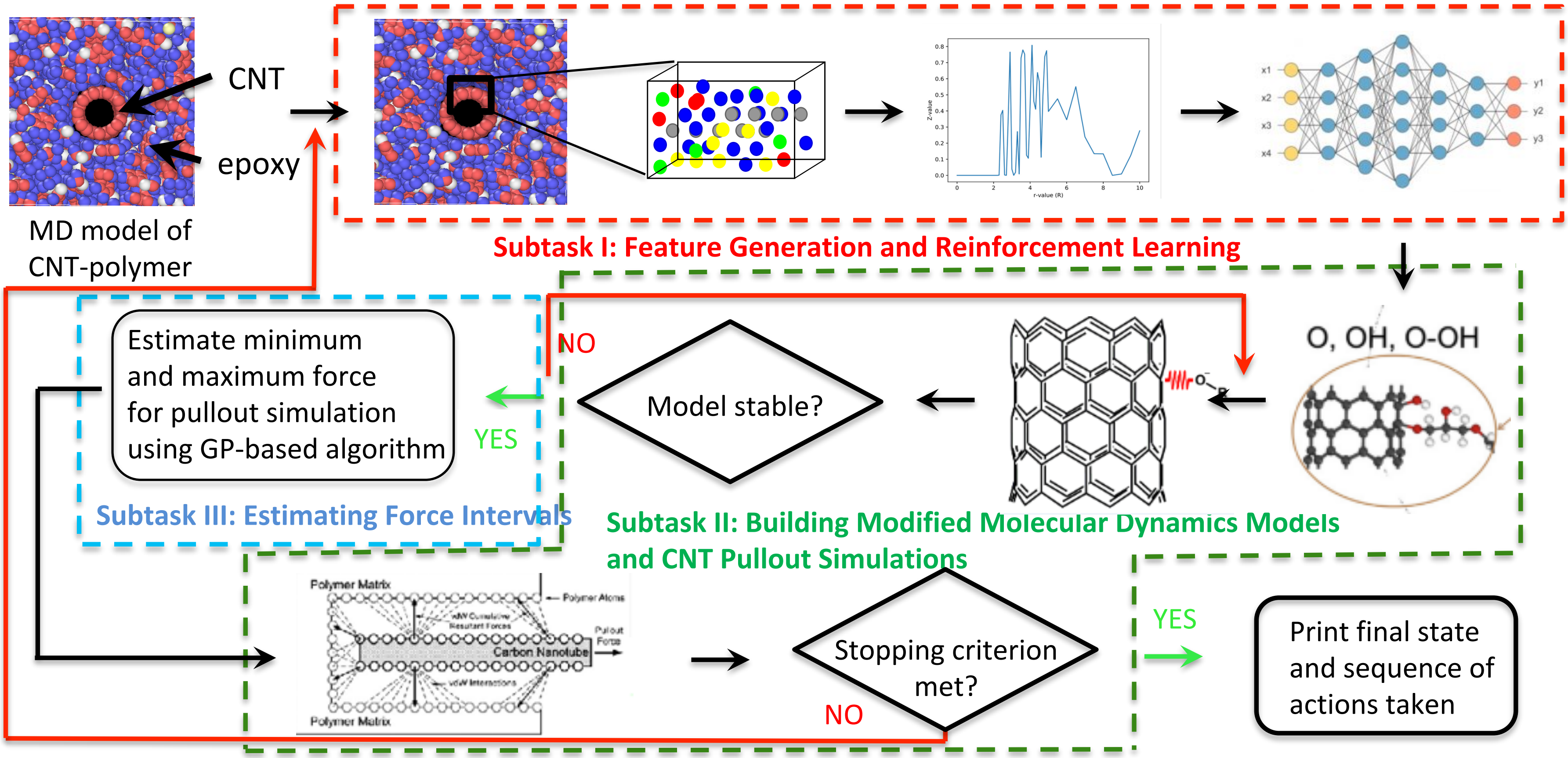
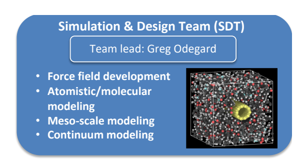
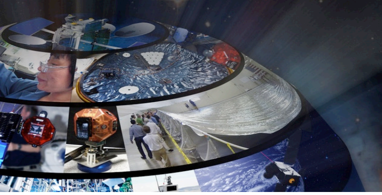


Machine Learning for Materials Design

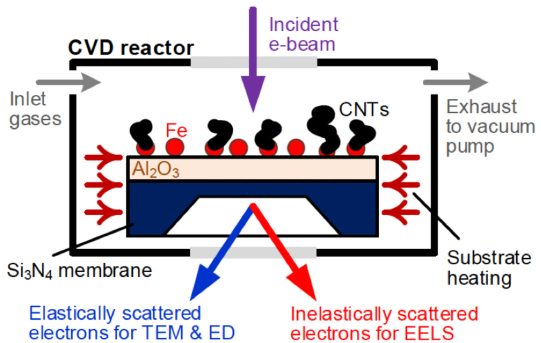


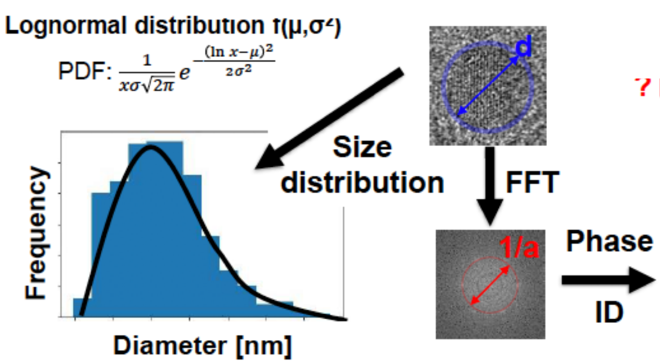
Proof-of-concept ML algorithm for designing simple CNT/polymer composites with optimal interfaces

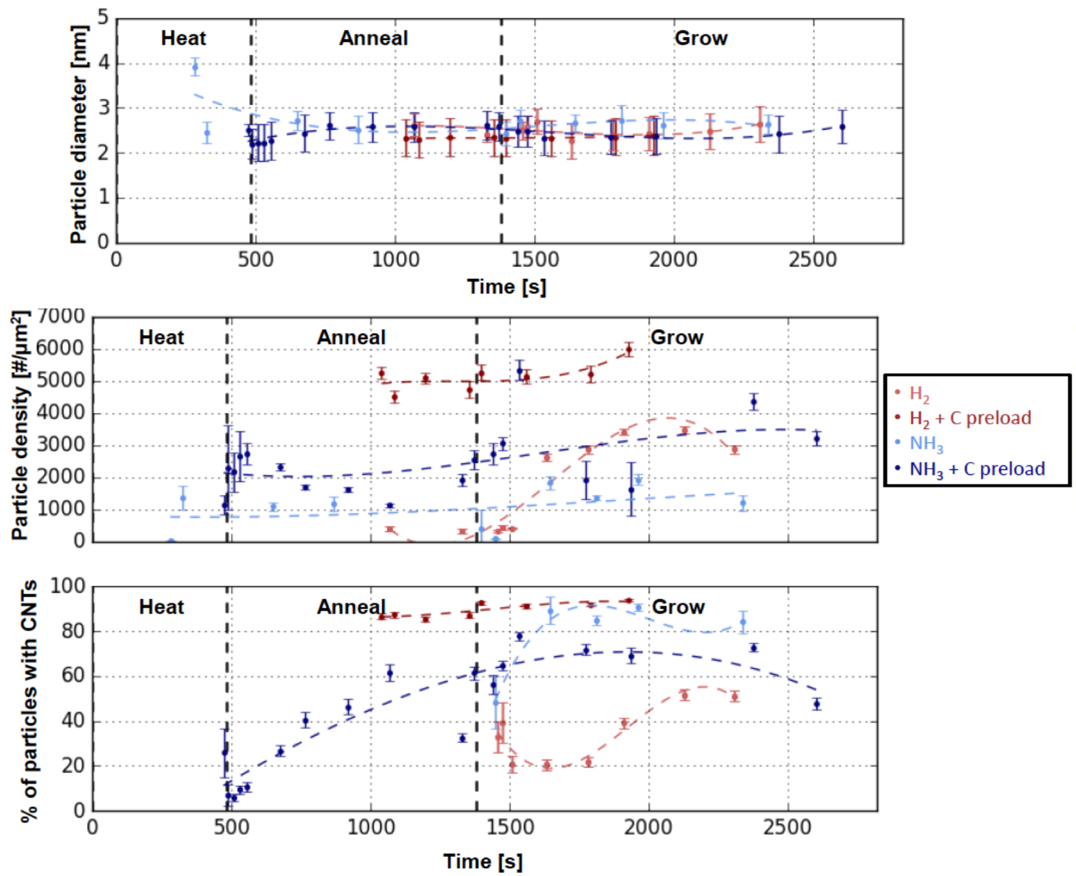




Identification of High-Yield CNT Growth Conditions



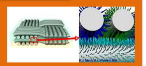




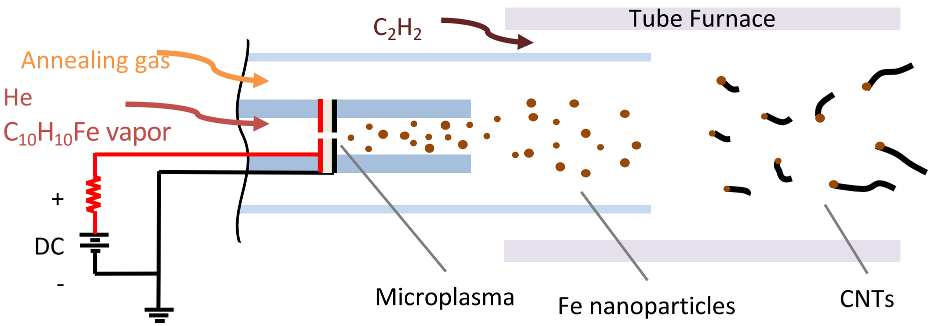
Material Synthesis Team (MST)

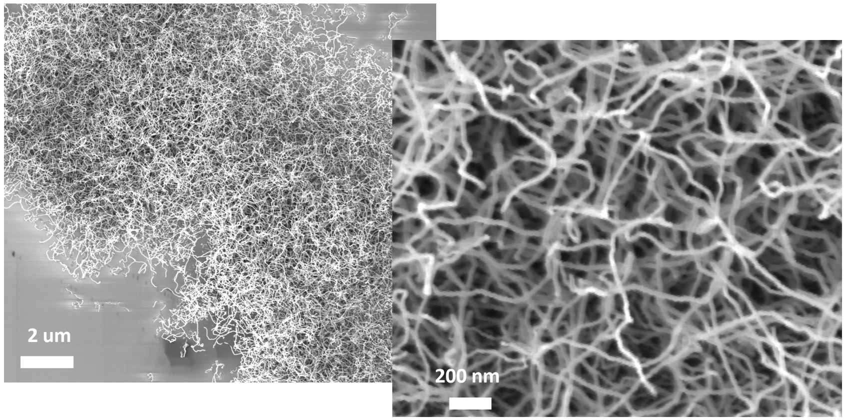
Team lead: John Hart

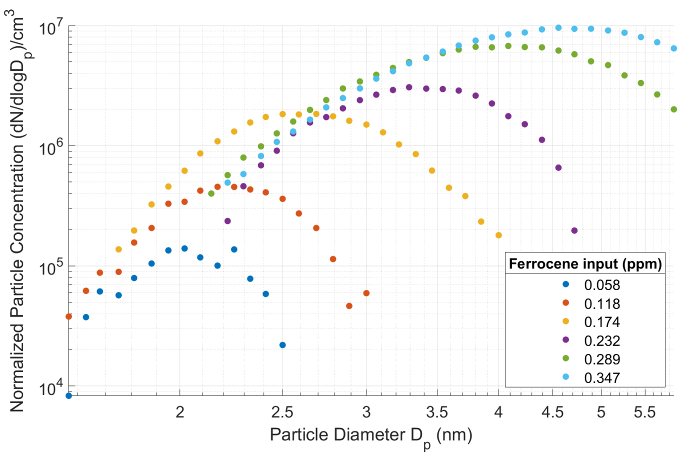
- Small-scale material prototyping
- Material screening

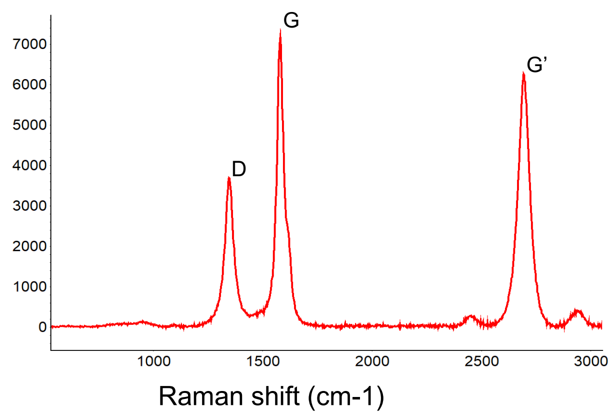


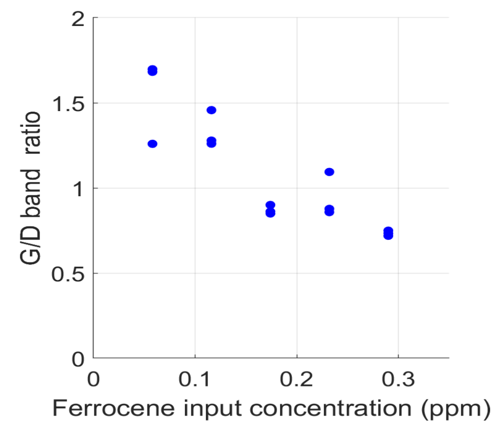
Efficient Gas-Phase Production of High-Quality CNTs

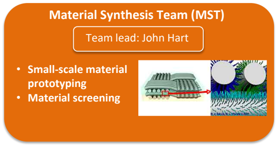








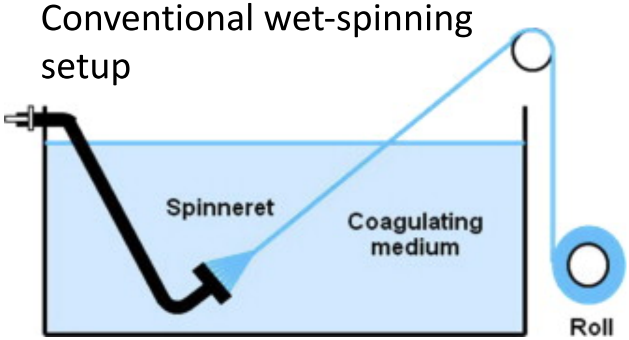




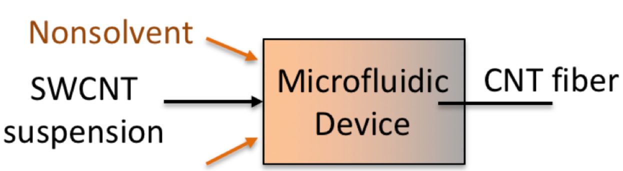
Microfluidic Spinning of CNT Fibers for Composites

- Using microfluidics, we spin continuous CNT fibers with controlled density
- Fiber properties are currently limited by CNT length (aspect ratio) and alignment

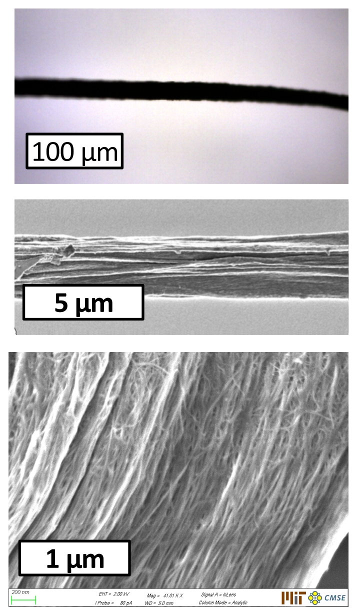
Conventional wet-spinning setup



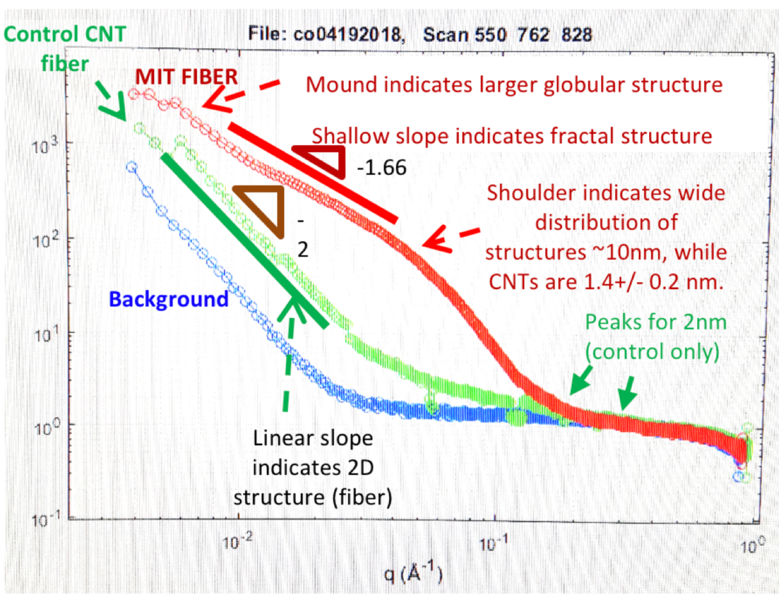
Microfluidic spinning (MIT)

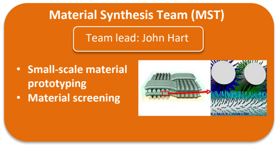


CNT fibers spun at MIT



Small-Angle X-Ray scattering

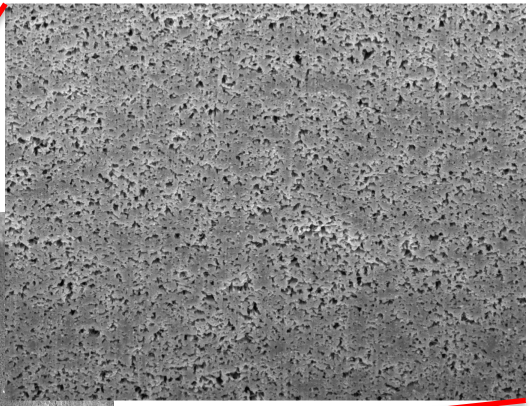


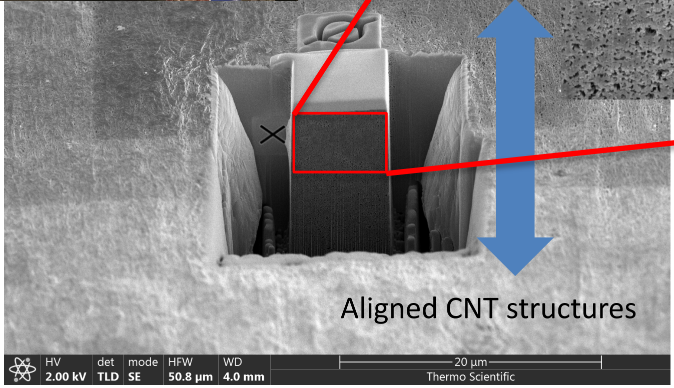


Fundamental Understanding of Material Characteristics

FIB for Multiscale 3D Tomography Analysis

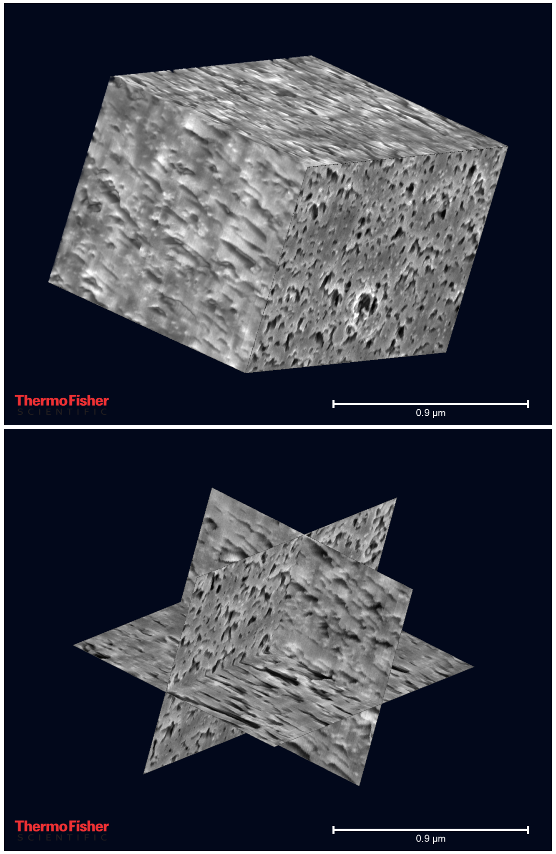
Cross-section of Aligned CNT Networks





W=6.5 µm

Stretching-induced alignment in CNT tape



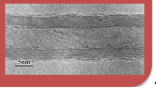
Pixel resolution
3.14 nm X 3.14 nm X 5 nm

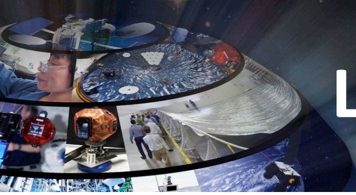
Fundamental understanding of structures within CNT materials provides guidance for synthesis and manufacturing

Material Manufacturing Team (MMT)

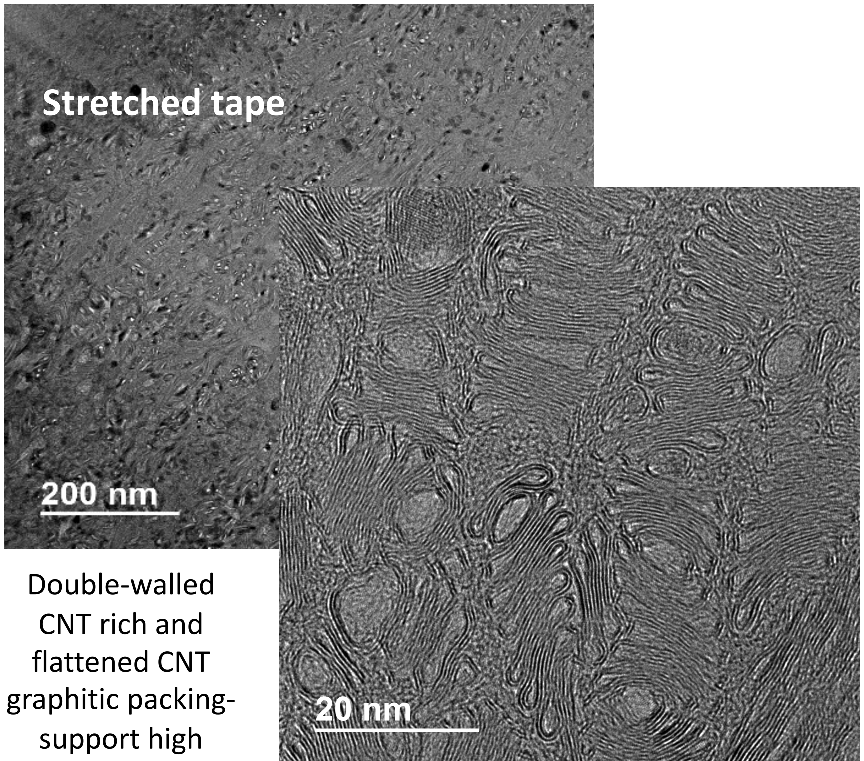
Team lead: Richard Liang

- Manufacturing scale-up
- Materials characterization

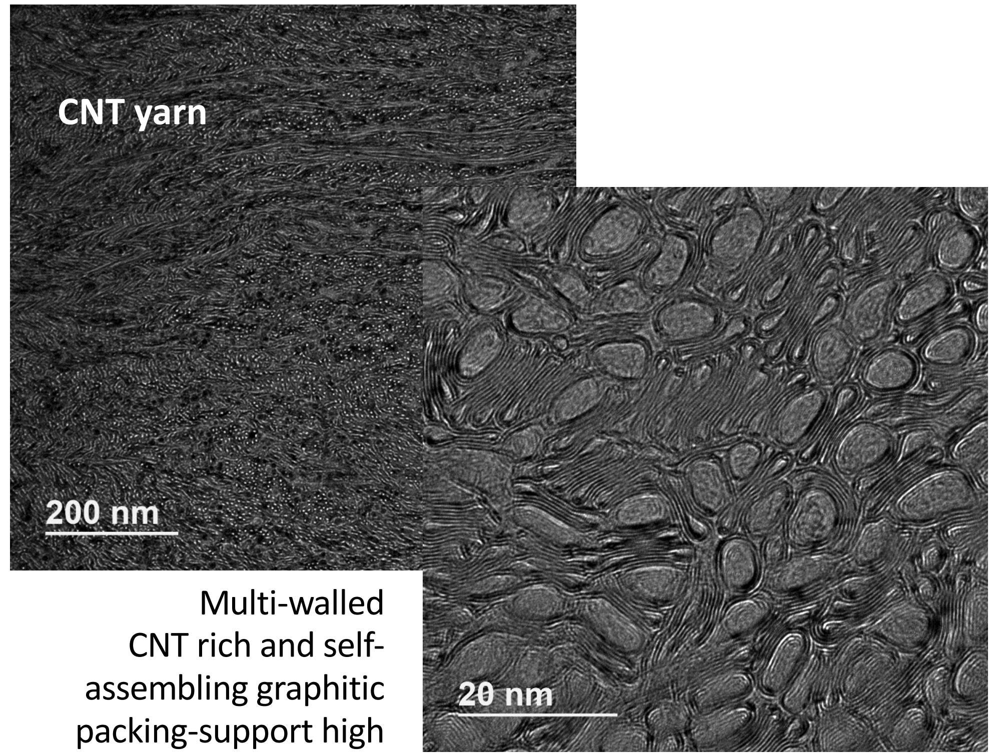




Load Transfer by CNT Reinforcement



Double-walled CNT rich and flattened CNT graphitic packing-support high modulus



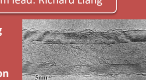
Multi-walled CNT rich and self-assembling graphitic packing-support high strength

Microstructures provide insight on load transfer mechanism for high strength CNT composites

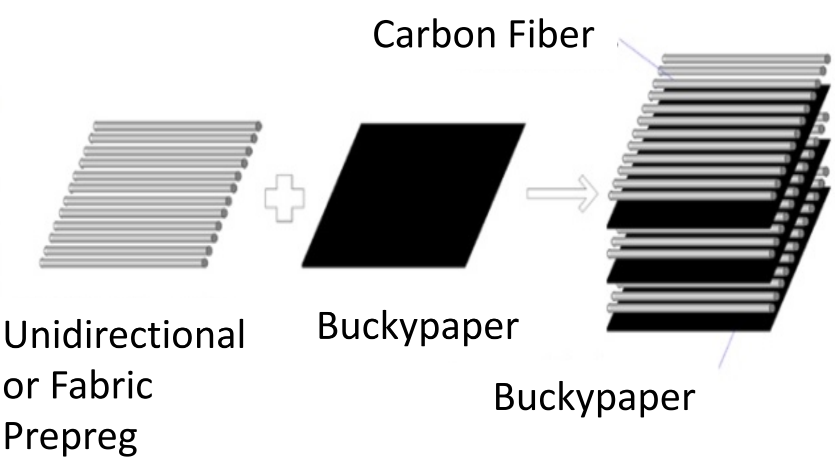
Material Manufacturing Team (MMT)

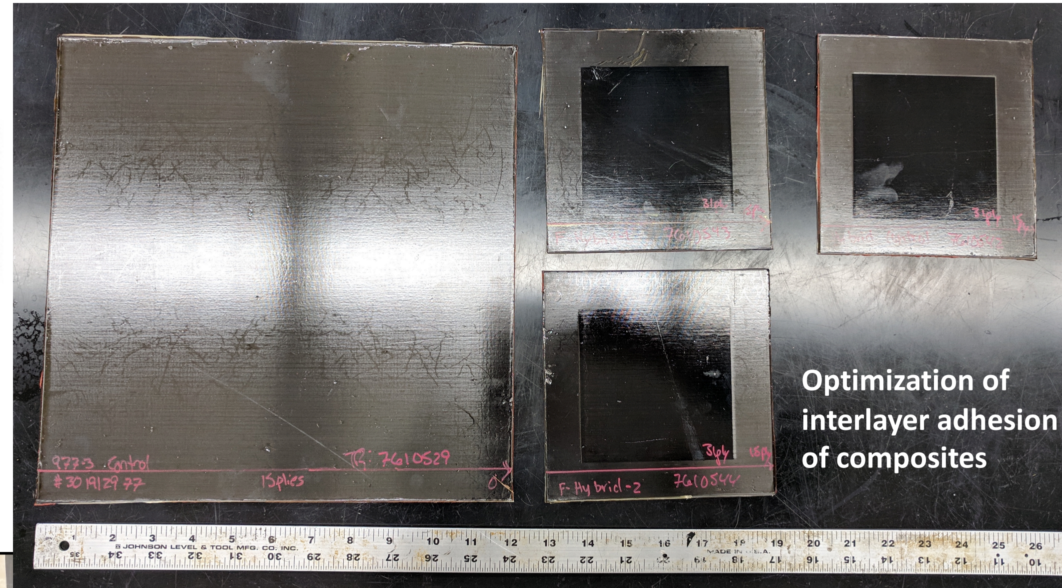
Team lead: Richard Liang

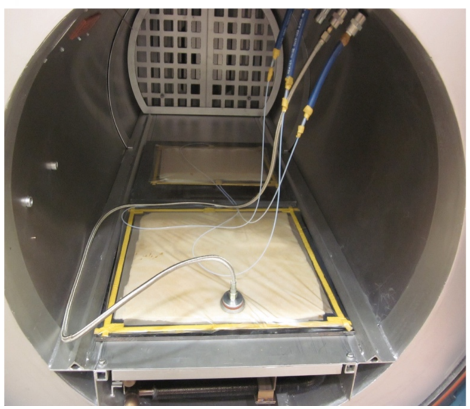
- Manufacturing scale-up
- Materials characterization

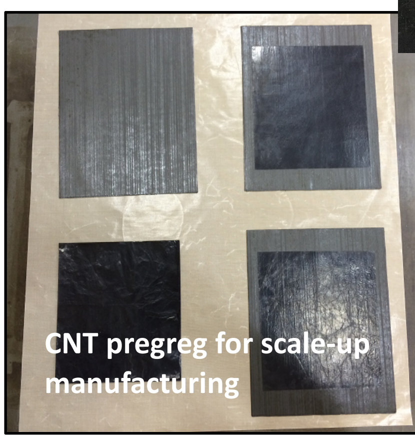


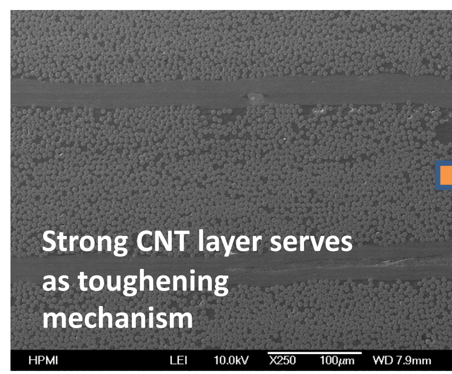
Fabrication of Aerospace Quality Hybrid Composites

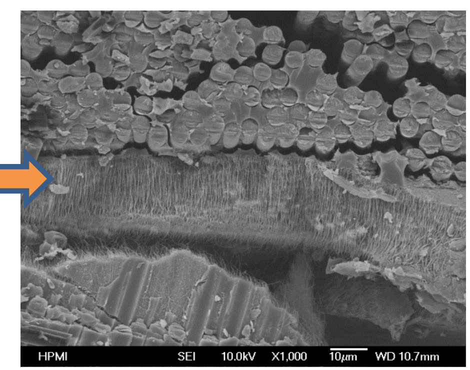


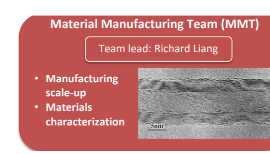








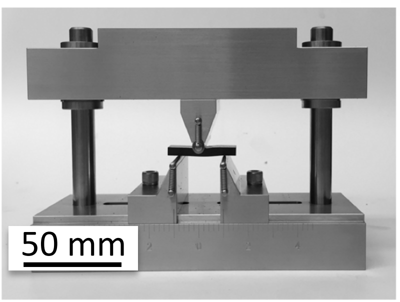




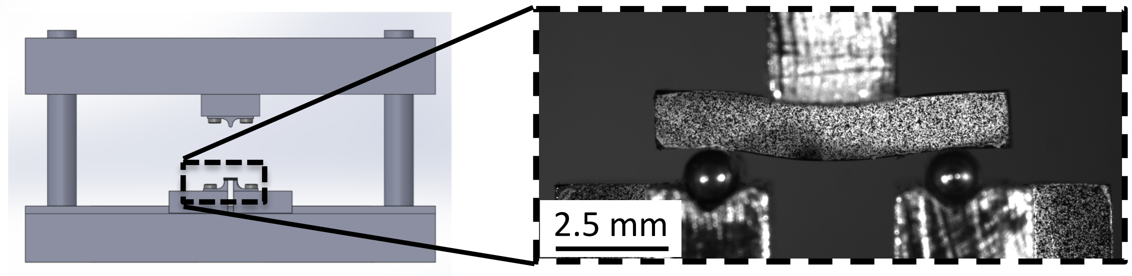
Experimental Characterization

Short Beam Shear Tests for Laminates with Thickness ~1 mm

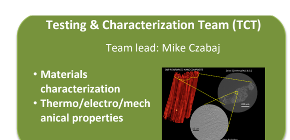
ASTM D2344



Miniature D2344

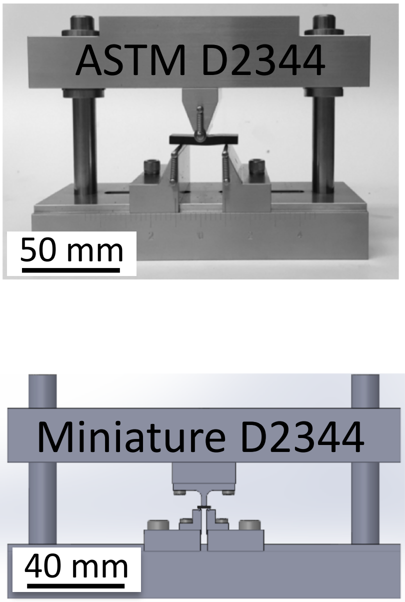


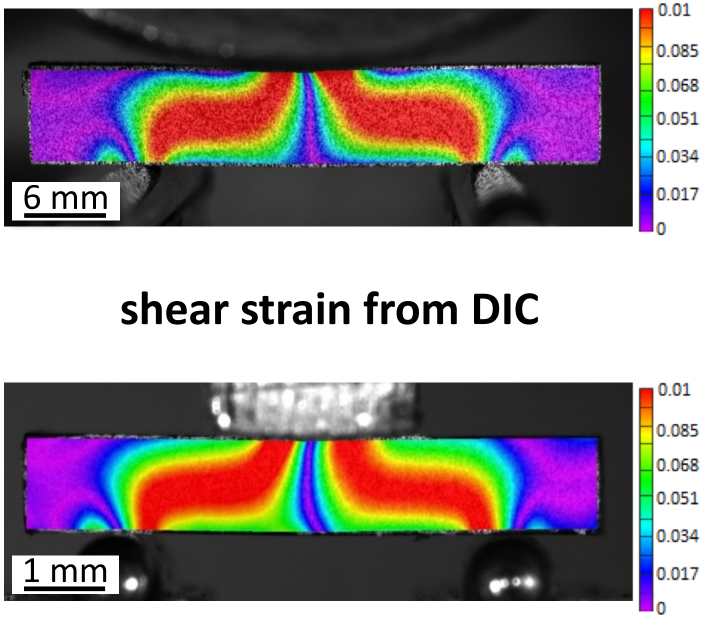
Development of new composite systems can be accelerated by using scaled-down structural characterization tests



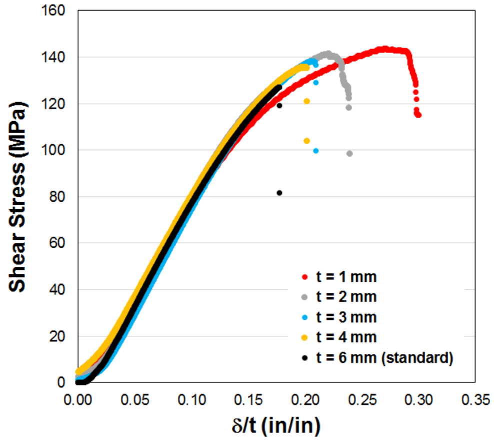
Experimental Characterization

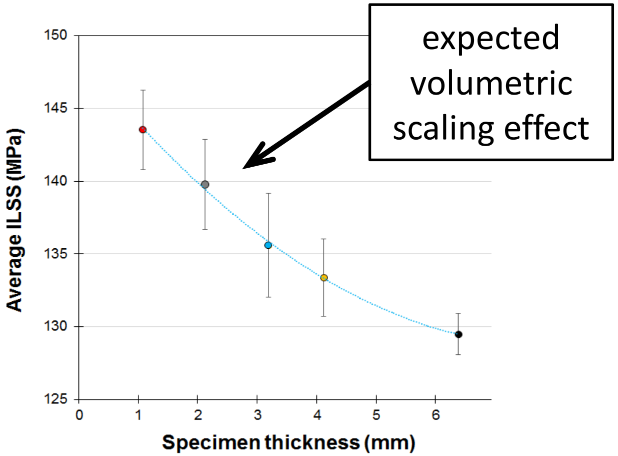
Validation of Miniaturized Mechanical Test

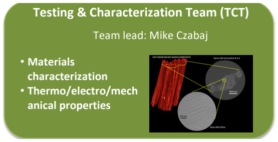




shear strain from DIC







MGI efforts – Modeling & Characterization

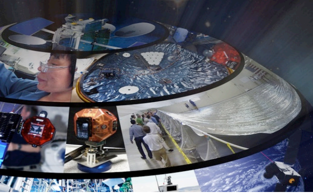
- US-COMP registered at repositories
  - CDMHub
  - NanoHub
- Data sharing and IFF website update in progress
  - Integration in CHARMM-GUI (with Adri van Duin, Wonpil Im)
  - New automatic conversion utilities for using IFF with NAMD and GROMACS released
- Received Special Creativity Award in NSF-MGI initiative (DMREF)
- Sharing and remote/real-time viewing of tomographic image data (Czabaj)
  - Initiated a new collaboration with the University of Utah ***Scientific Computing and Imaging*** (SCI) Institute to enable remote and real-time access to large quantities of image data collected during in situ experiments
- Sharing of image processing and SAXS analysis codes (Hart)
- Opportunity for HPC ETEM video analysis (Hart)

Publications

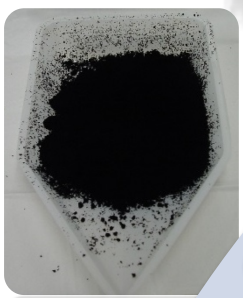
Special Issue

Carbon Nanotube Composites for Structural Applications, Odegard, G., Liang, Z. and Wise, K. E. (eds.), Composites Sci. and Technol., **166**, 1-182, September, 2018.

- Radue, M. S., Odegard, G. J., “Multiscale Modeling of Carbon Fiber/Carbon Nanotube/Epoxy Hybrid Composites: Comparison of Epoxy Matrices,” *Composites Sci. and Technol.*, **166**, 20-26, 2018.
- Nakarmi, S., Unnikrishnan, V. U., Varshney, V., Roy, A. K, “Computer-Aided Design of Three Terminan (3T) Zia-Zag SWCNT Junctions and Nanotube Architectures,” *Composites Sci. and Technol.*, **166**, 36-45, 2018.
- Pramanik, C., Nepal, D., Nathanson, M., Gissinger, J. C., Heinz, H., “Molecular Engineering of Interphases in Polymer/Carbon Nanotube Composites to Reach the Limits of Mechanical Performance,” *Composites Sci. and Technol.,* **166**, 86-94, 2018.
- Gair, J. L., Lambeth, R. H., Cole, D. P., Wardle, B. L., “Strong Process-Structure Interaction in Stoveable Poly(Urethane-Urea) Aligned Carbon Nanotube Nanocomposites,” *Composites Sci. and Technol.,* **166**, 115-124, 2018.
- Jolowsky, C., Sweat, R., Park, J. G., Hao, A., Liang, R., “Microstructure Evolution and Self-Assembling of CNT Networks During Mechanical Stretching and Mechanical Properties of Highly Aligned CNT Composites,” *Composites Sci. and Technol.,* **166**, 125-130, 2018.
- Kalfon-Cohen, E., Kopp, R., Furtado, C., Ni, X., Wardle, B. L., “Synergetic Effects of Thin Plies and Aligned Carbon Nanotube Interlaminar Reinforcement in Composite Laminates,” *Composites Sci. and Technol.,* **166**, 160-168, 2018.

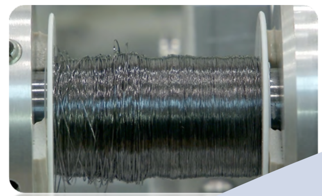


Computationally Accelerated Materials Development for Ultra High Strength Lightweight Structures

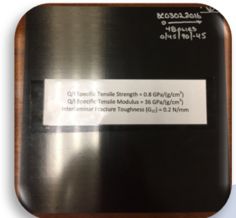


CNT Powder

CNT Sheets



High Strength CNT Yarn



Ultra High Strength Composite Panel

1991-Early 2000s

- Early national investments in CNT research
- NASA interest in structural properties
- Powder form CNT unable to enhance mechanical properties to compete with state of the art structural materials

2004

- CNT sheets first became available
- Manufacturing maturation heavily supported by DoD, including Title III funding
- Property enhancements were focused on electrical properties
- CNT sheets for electrostatic charge dissipation were used on Juno which launched in 2011

2015

- NASA Game Changing Development Program supported efforts in structural CNT resulted in mechanical property improvements to commercially available CNT yarn for composite application
- NASA's internal efforts supported 500% increase in specific strength and 1600% increase in specific modulus of CNT composites over 3 years despite non-optimal CNT composites
- CNT composites at tipping point, needing better understanding of mechanisms for load transfer to continue improvements in mechanical properties

2022

- 5-year Space Technology Research Institute (STRI) funding expected to yield fundamental understanding of CNT composite mechanical properties to reach panel level properties that will enable systems level mass reduction
- Materials Genome Initiative accelerated panel properties development required by STRI will yield both models to enhance understanding of CNT composites and continued maturation of CNT materials manufacturing
- Vision for STRI includes complementary internal NASA efforts to assure timely integration of this technology in systems architecture concepts

Collaborative Partnerships for Advancement of Structural CNT

NASA Centers
LaRC
MSFC

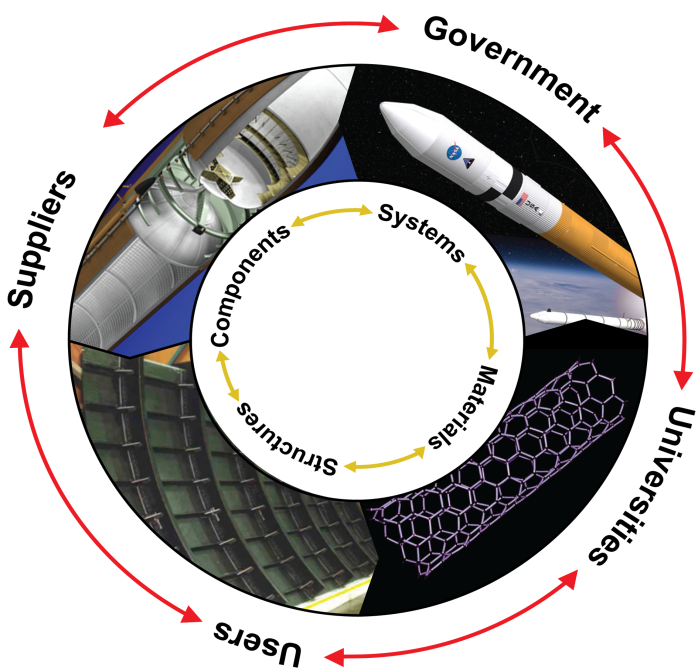
ESI
U of Minnesota
U of Virginia

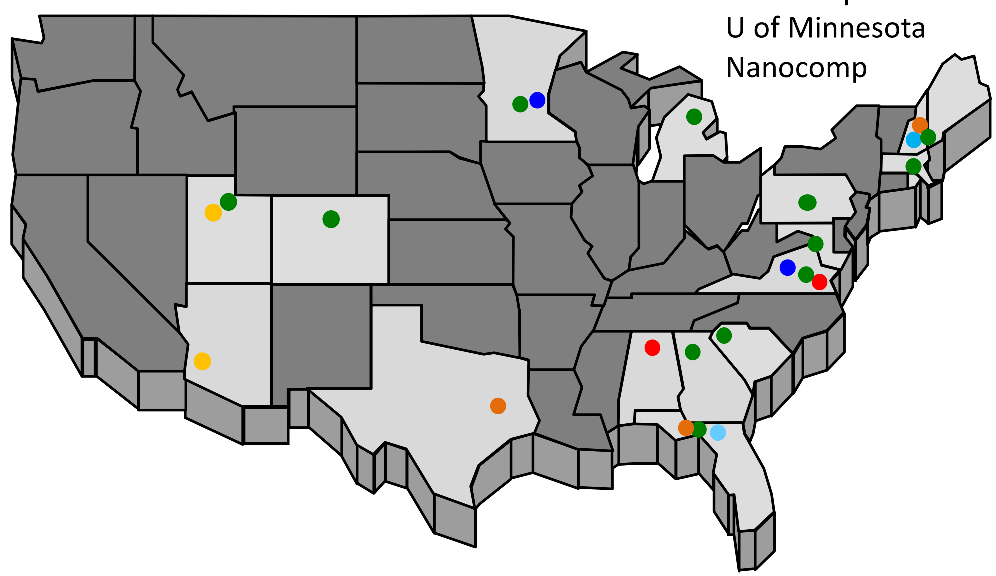
Public/Private Partnerships
Northrup Grumman/Orbital ATK

OGA Partnerships
AFOSR
AFRL – STTR,
ManTech

SBIR/STTR
Florida State U
Dexmat, Inc.
Nanocomp Technologies, Inc.

NSTRI
Florida State U
MIT
VCU
Ga Tech
Penn State U
FL A&M U
Solvay
Michigan Tech
U of Utah
U of Colorado
Johns Hopkins
U of Minnesota
Nanocomp





Collaborative multidisciplinary partnerships to leverage fiscal resources, ideas, knowledge & expertise

Complementary Manufacturing Development of High Strength CNT

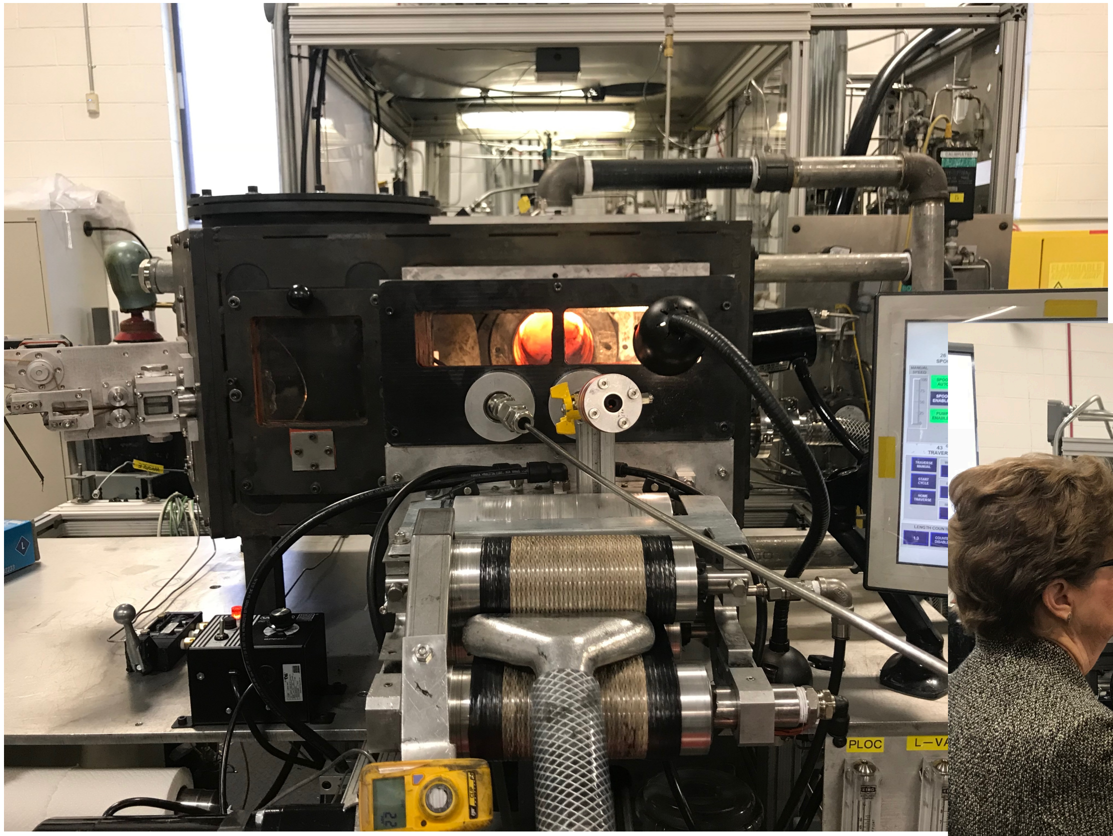


Image Credits: NASA

NASA awarded Phase III SBIR for scale-up of high strength CNT as part of Game Changing Program to develop superlightweight aerospace composites.