Multiscale Modeling for Characterization of Damage Resilient Nanocomposites

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Presentation outline

1. Company overview
2. Damage resilient nanocomposites
3. Multiscale modeling
4. Problem objective
5. Conclusions and future work

NextGen Aeronautics facilities

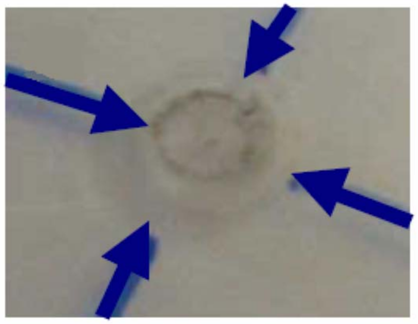
Torrance, California 4th floor offices

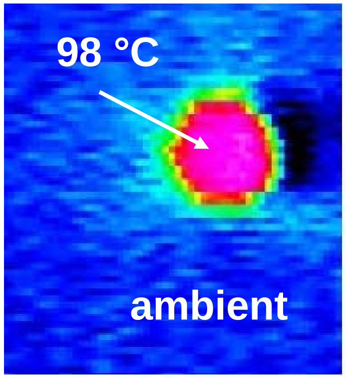
Torrance, California Fabrication Facility

Danville, Virginia Facility, IALR Main Building

NextGen R&D focus areas

Smart materials & adaptive structures





Morphing / multifunctional UAVs

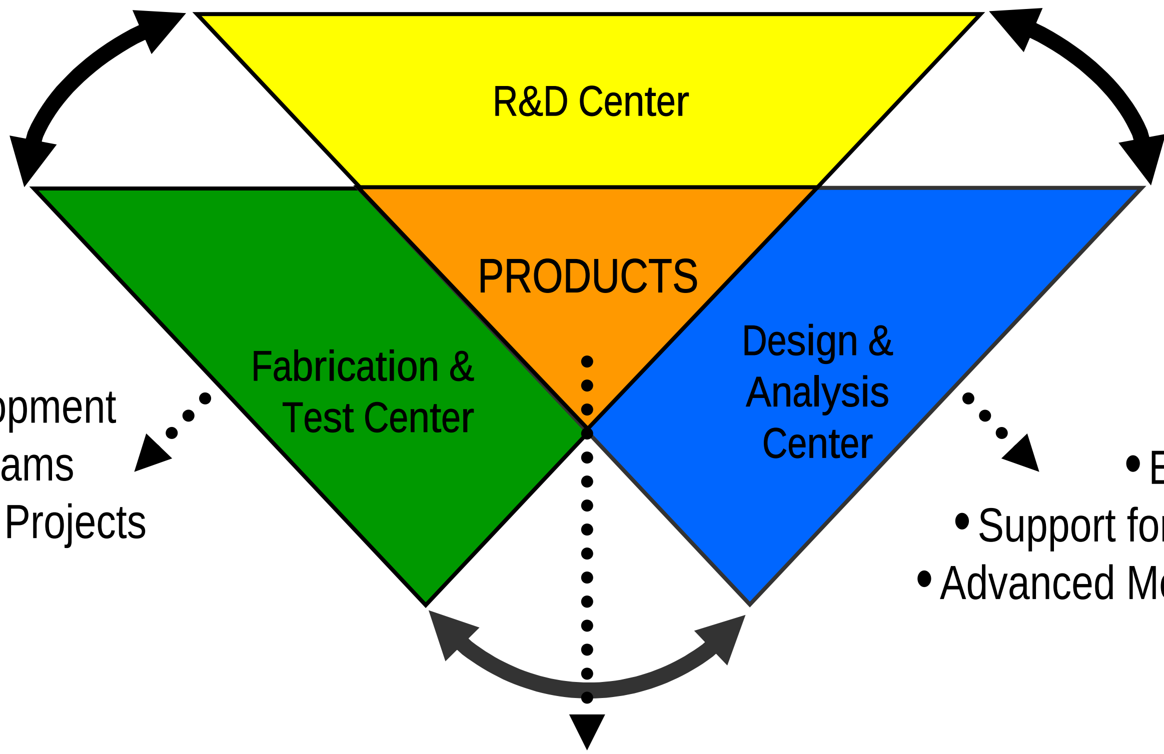
Integrated antennas

Health and structural state monitoring

Rapid design / analysis

Our approach is multi-disciplinary and interative

NextGen strategy



- Prototype Development
- Production Programs
- Support for R&D Projects

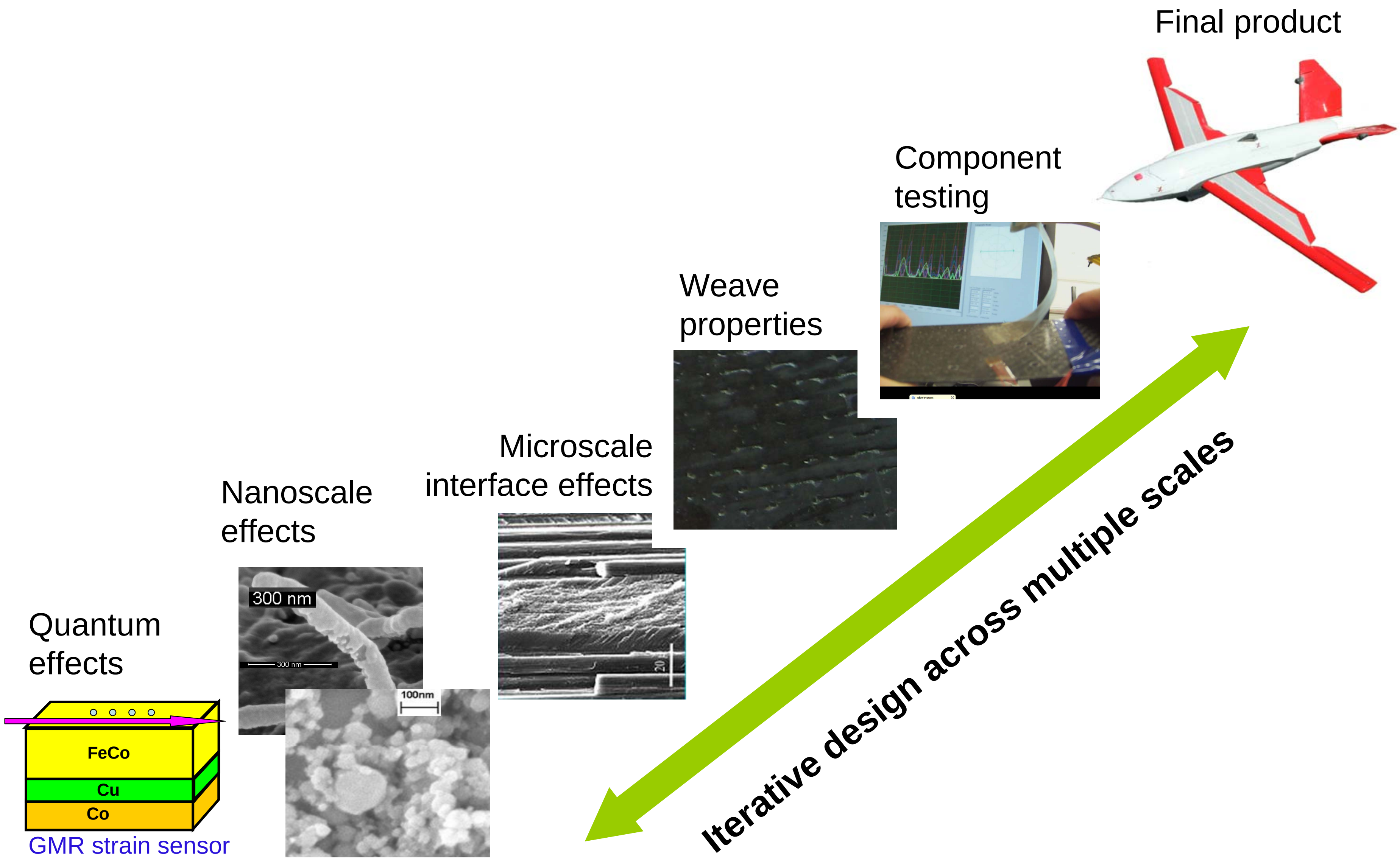
- Engineering Services
- Support for NextGen Programs
- Advanced Methods Development

- Multifunctional UAVs
- Morphing Structures
- Smart Materials

- Actuators/Sensors
- Integrated Antennas
- Rapid Design/Analysis Tools

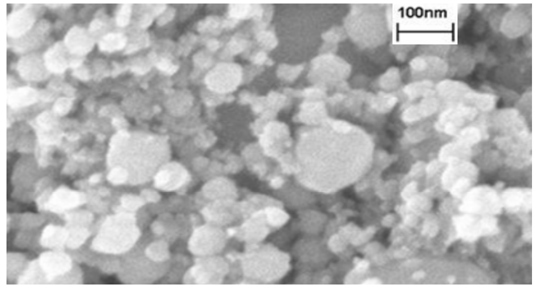
Using an integrated approach how do we develop damage resilient nanocomposite technology?

NextGen multifunctional composite design



Inspired by Prof. Jacob's Fish Lecture at WCCM 2007

Damage resilient composites



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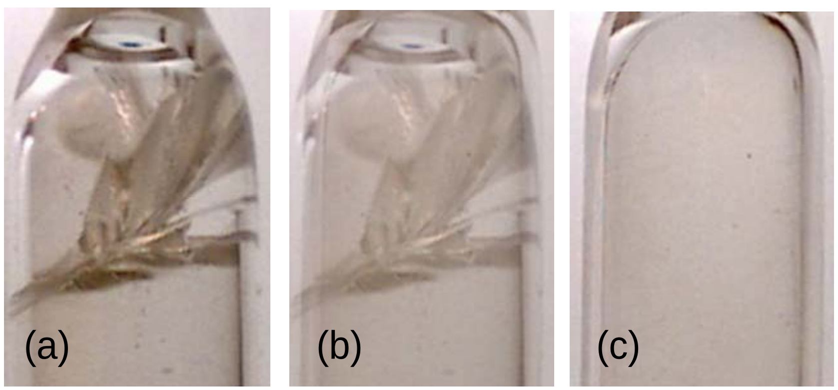
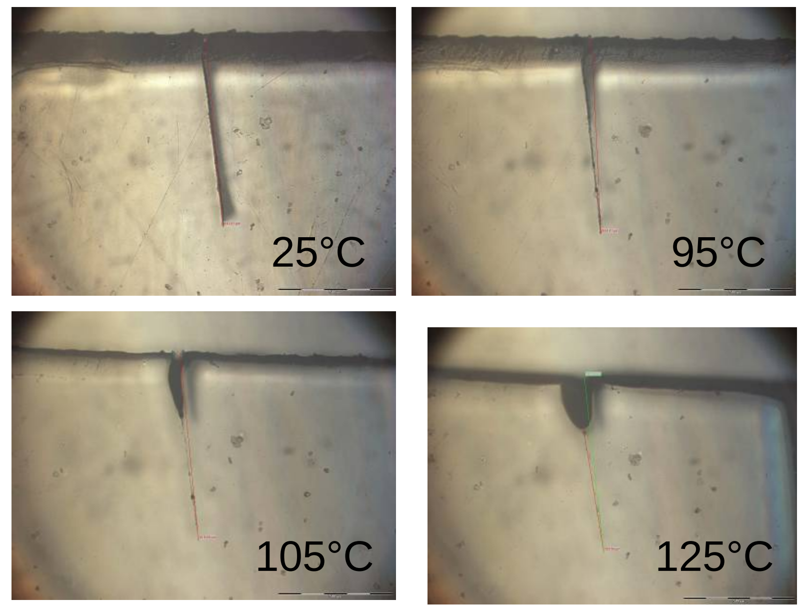


Structural Mendomer (2 GPa)

or

Initial cut width = 10 microns

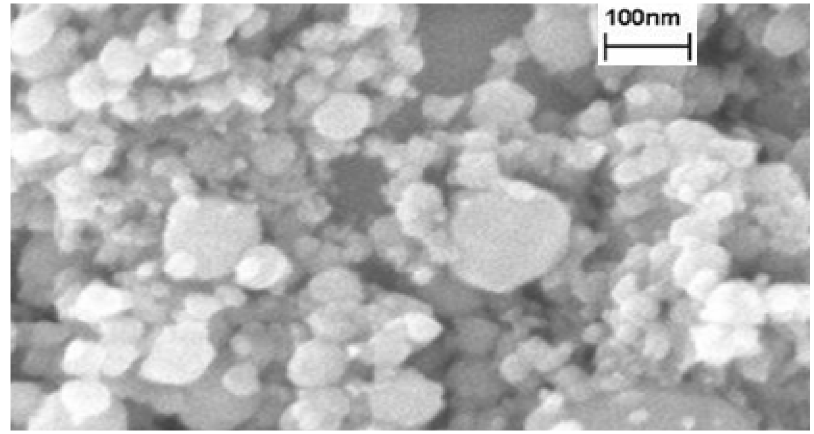


Compliant ionomer (200 MPa)

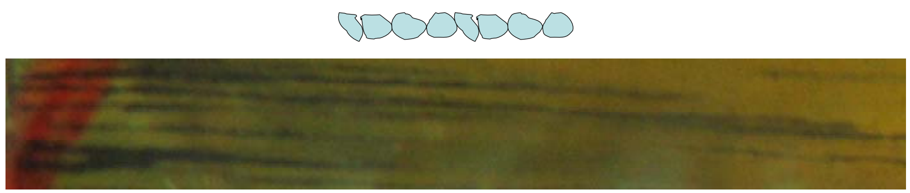
= Damage resilient composite (self-healing)

Damage resilient nanocomposites

Nanoparticle sample is brittle (iron oxide)



Coarse and nano polydisperse with “tuned” ferromagnetic temperature is currently best option (ferrite)



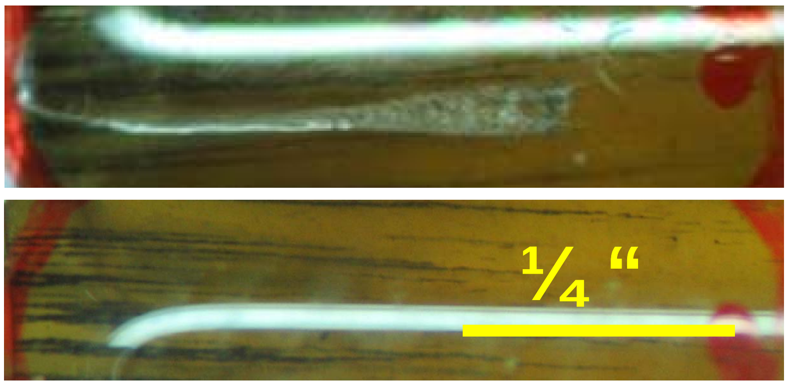
Ordered structures can focus healing

- Also are being developed for active self-healing
- Other than magnetic particles, we’re also using CNTs and carbon fibers for resistive heating

Nanocomposites results

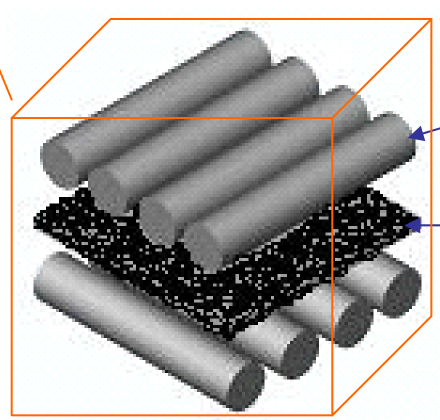
Matrix cracks and delaminations can be healed in-situ

Nanofibers improve average critical strain energy release rate



360 micron x 5000 micron crack

healed crack



nanofibers

carbon fiber

Results for 2 different Mendomer samples

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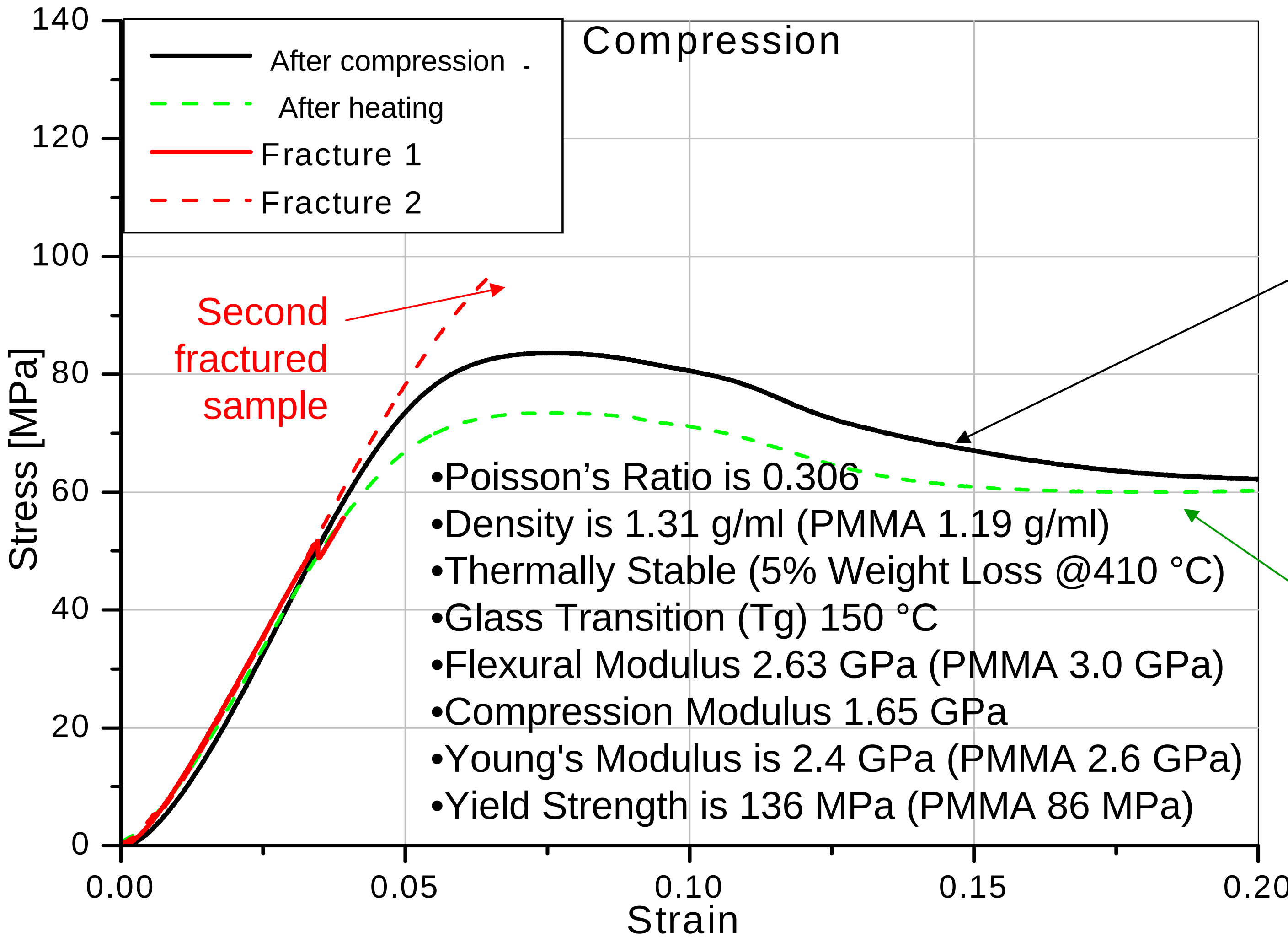


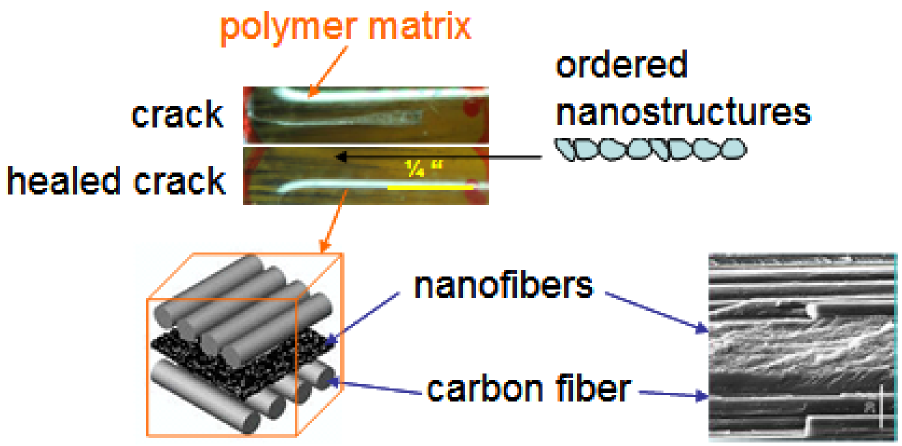
After Compression

After Heating

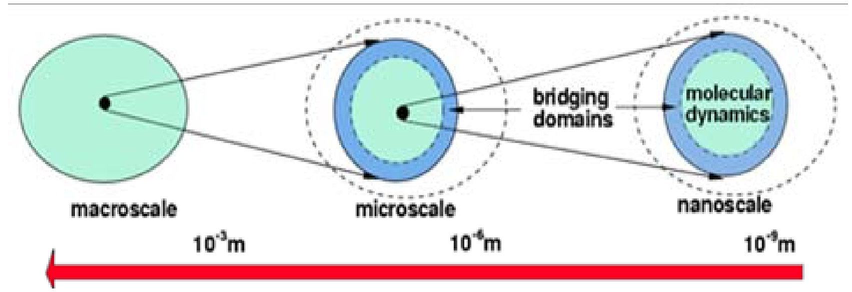
The Mendomer can be healed back to its initial compressive modulus after both fracture and yielding.

Duenas, T. et al. "Multifunctional Self-healing Morphing Composites", Proceedings for the 25th Army Science Conference, Orlando, Florida November 27-30, 2006

Ultimate problem objective



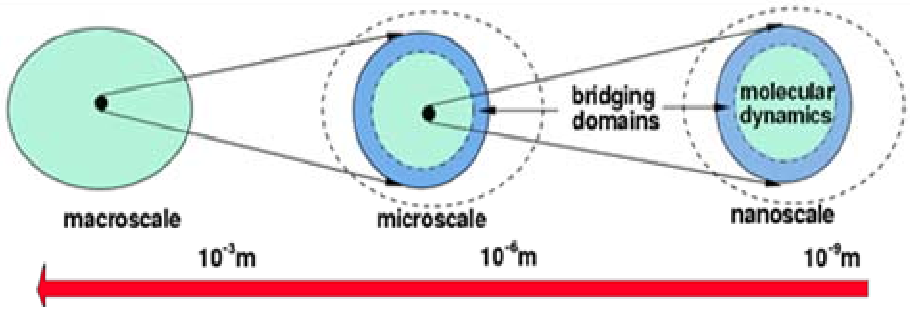
Damage resilient nanocomposites



Multiscale modeling

Modeling and experimentation converge to govern characterization of coupons

Multiscale modeling



1. **A molecular dynamics or quantum mechanical simulation of a real-life structure is not feasible because of the extremely small length and time scales.** For example, a cubic volume of 10^{-3} μm^3 contains billions of atoms, and a typical time-step in MD simulations is about a femtosecond ($\sim 10^{-15}$ s).

2. **Such simulation would lead to extremely vast amount of information, which is not needed in majority of cases.**

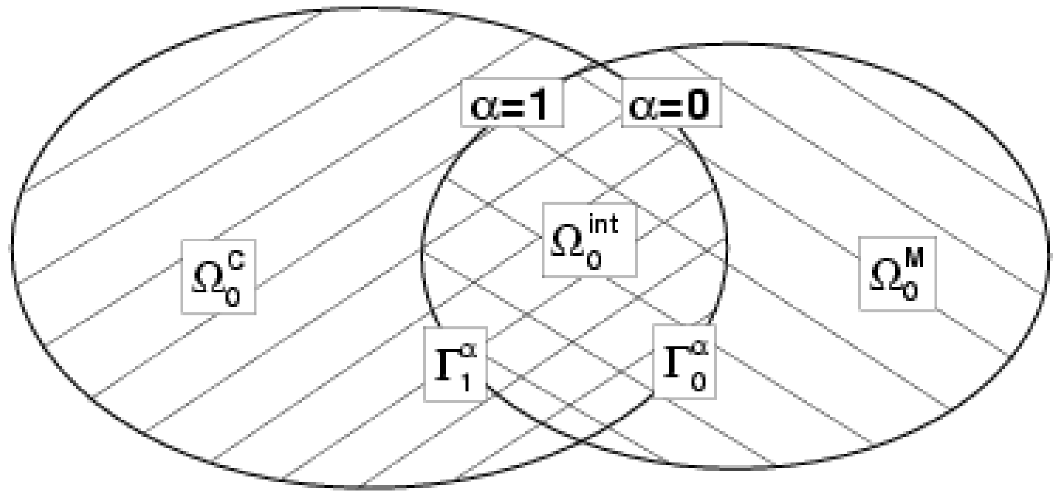
3. **A multiscale method tries to keep a balance between computation expense and accuracy of simulation by using appropriate physics at different scales.**

Bridging Domain Multiscale Method

The total Hamiltonian of the system can be expressed as

$$H = \int_{\Omega^C} \alpha(\mathbf{X})\left(K^C + U^C\right) d\Omega^C + \sum_I \left(1-\alpha(\mathbf{X}_I)\right)\left(K_I^M + U_I^M\right) + \sum_{I\in\Omega^{\mathrm{int}}} \lambda(\mathbf{X}_I)\left(\mathbf{u}^C(\mathbf{X}_I,t) - \mathbf{u}_I^M(t)\right)$$

$$\alpha = \begin{cases} 1 & in \quad \Omega_0^C - \Omega_0^{int} \\ [0,1] & in \quad \Omega_0^{int} \\ 0 & in \quad \Omega_0^M - \Omega_0^{int} \end{cases}$$



The discrete equations can be obtained based on classical Hamiltonian mechanics as:

$$\overline{M}_I \ddot{\mathbf{u}}_I^C = \mathbf{f}_I^{extC} - \mathbf{f}_I^{intC} - \mathbf{f}_I^{LC} \qquad in \quad \Omega^C,$$

$$\overline{m}_I \ddot{u}_I^M = \mathbf{f}_I^{extM} - \mathbf{f}_I^{intM} - \mathbf{f}_I^{LM} \qquad in \quad \Omega^M$$

Bridging Domain Multiscale Method

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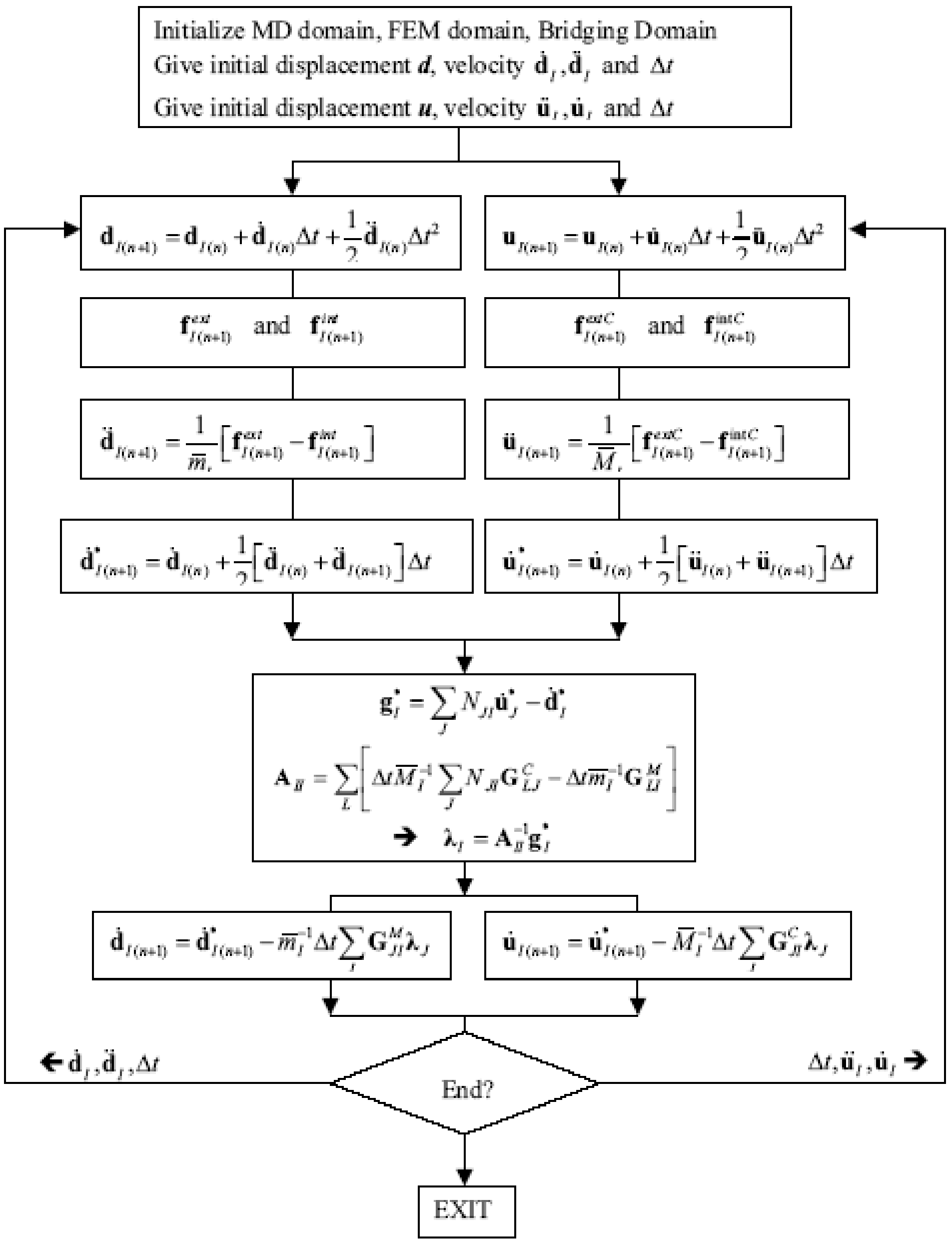


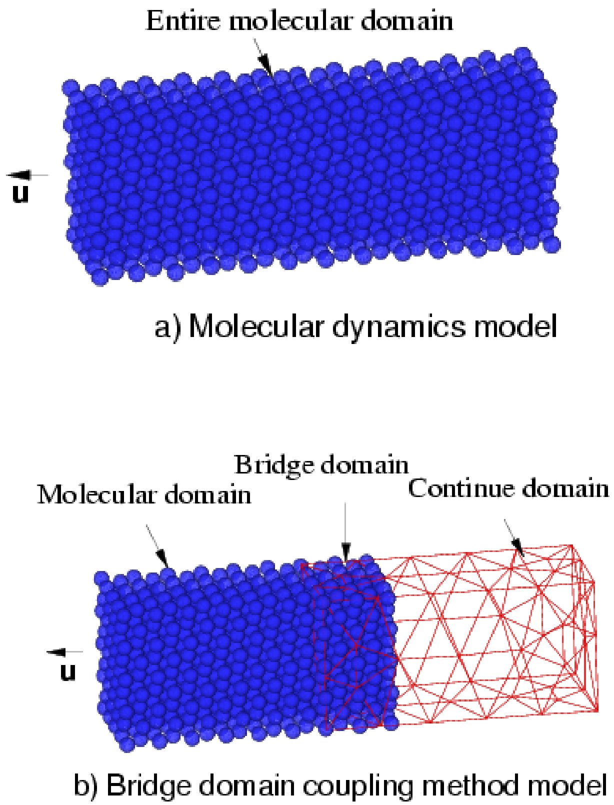
1. The trial velocities are obtained independently in the continuum and molecular domains without the consideration of constraints.

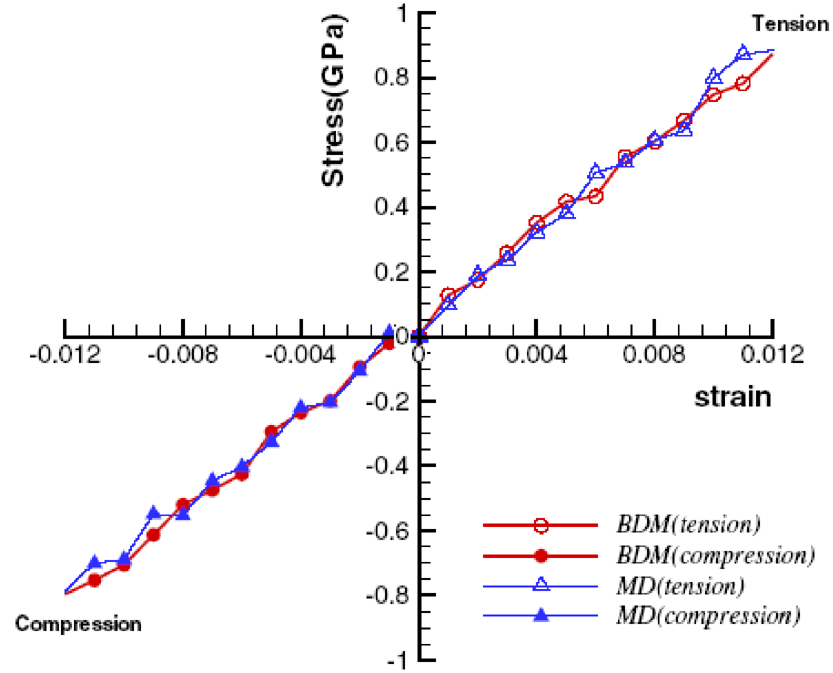
2. Constraints are applied to calculate the Lagrange multipliers.

3. The constraint forces are then used to correct the nodal/atom velocities in the bridging domain.

4. The method is then iterated.

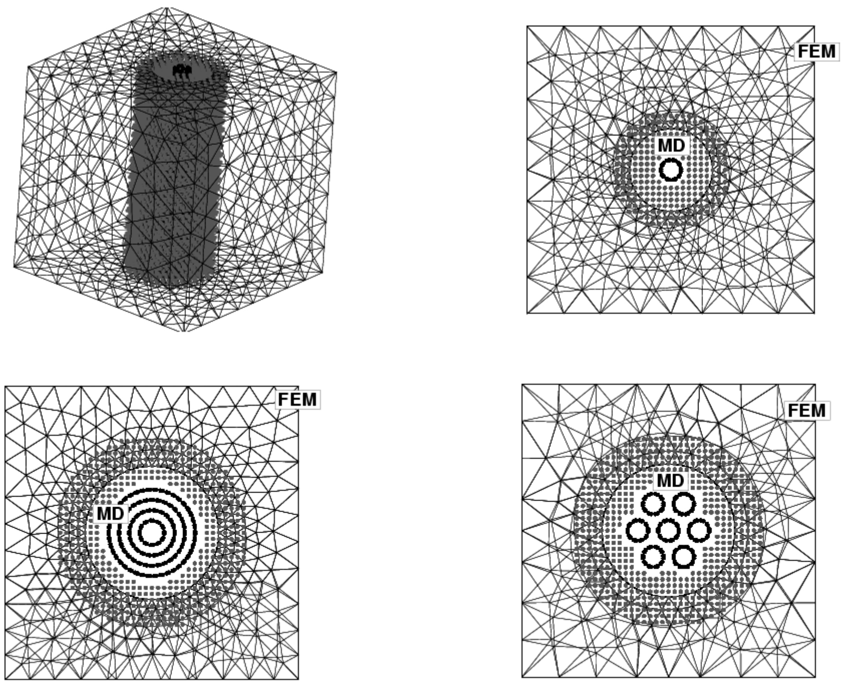
3-D Verification

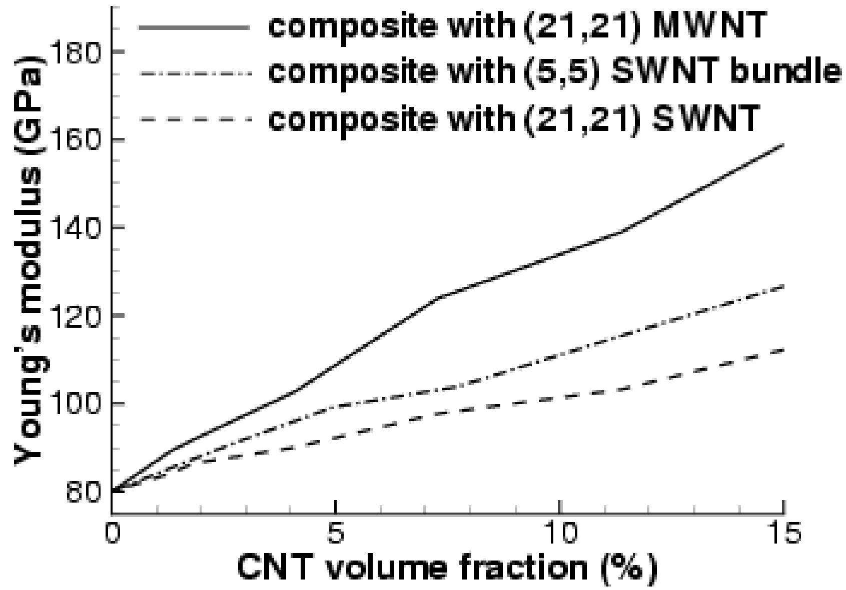




Comparison of stress-strain behavior as predicted from a molecular dynamics simulation and bridging domain multiscale method.

Elastic Moduli of CNT/AL Composites



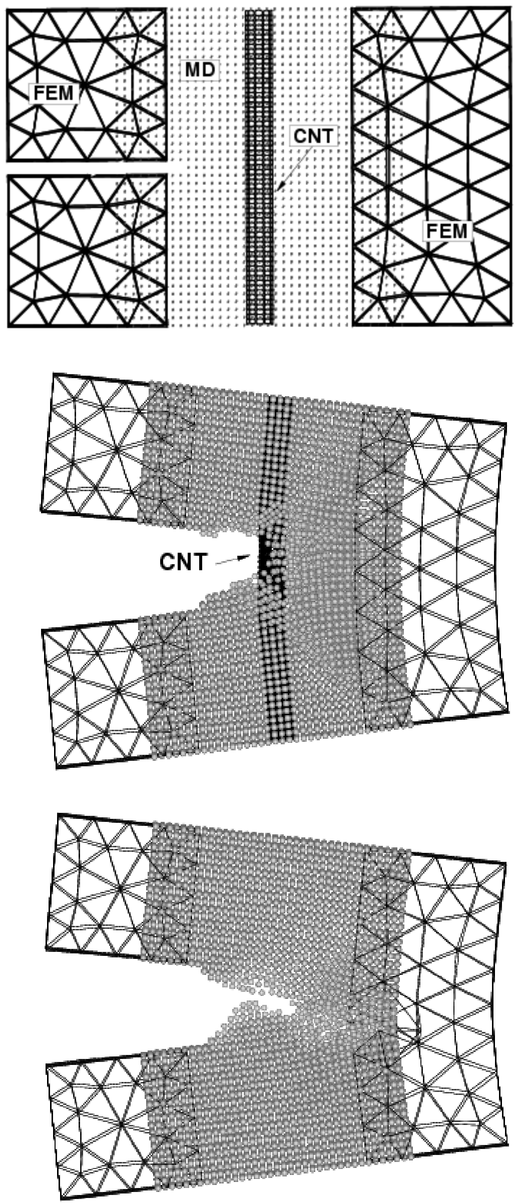


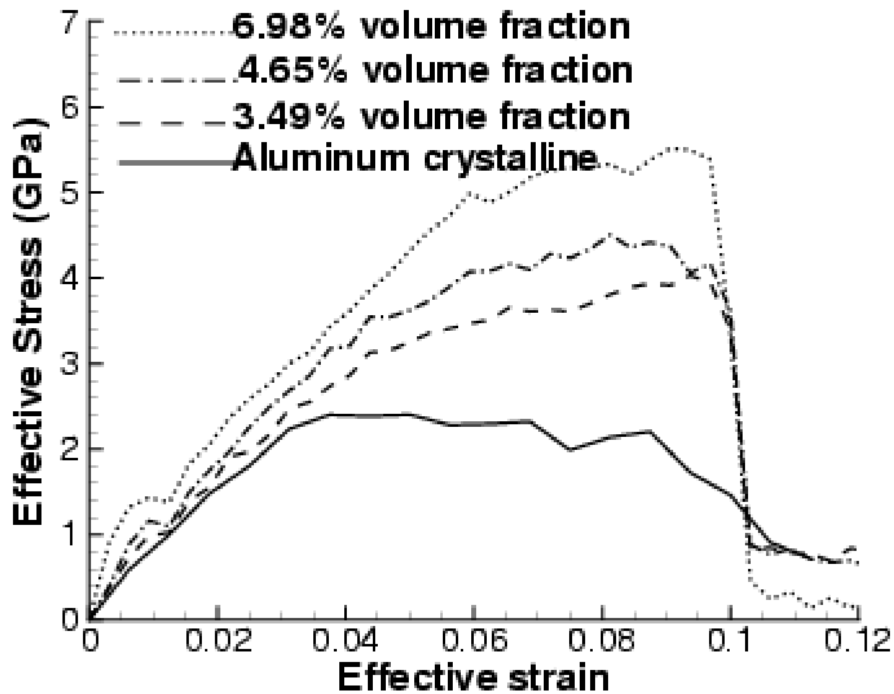
1. Modified Morse potential function to describe interatomic interaction between bonded carbon atoms in SWNT.

2. Lennard-Jones potential as follows is used to describe nonbonded interaction between the embedded carbon nanotube and the aluminum matrix.

3. The tube is considered to be long and the periodic boundary condition is employed. The prescribed displacement is applied on both the nanotube and the Al matrix.

Fracture of CNT/AL Composites





1. The initial edge crack is modeled in the molecular domain.

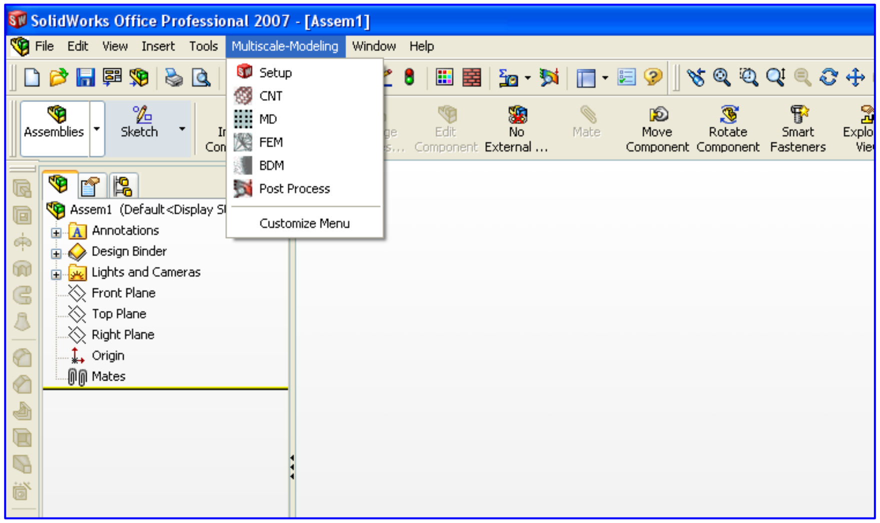
2. While Al crystalline exhibits ductile material characteristics, the nanocomposite shows brittle characteristics.

3. The tube is considered to be long and the periodic boundary condition is employed. The prescribed displacement is applied on both the nanotube and the Al matrix.

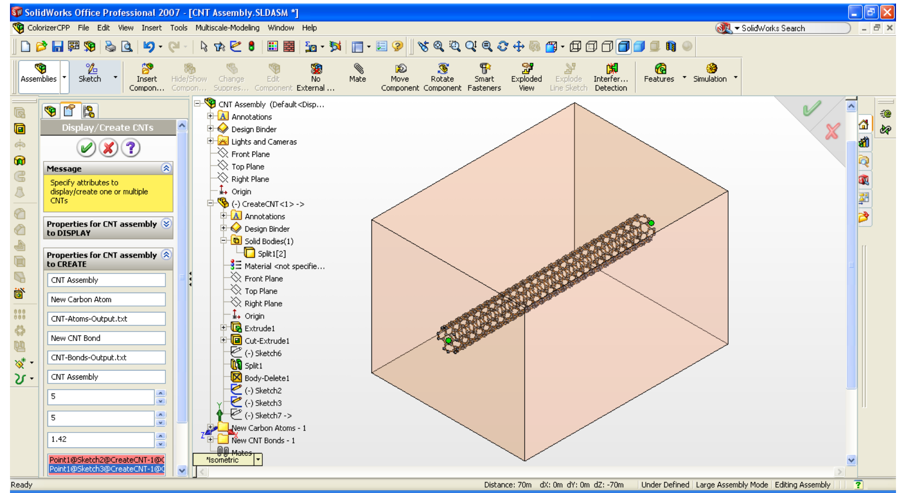
Summary of available software tools

Software Name	Purpose	Organization	Multiscale	Multiphysics	User Interface	Success
TINKER	MD simulation		No	No	Poor	Limited
GAMESS	Ab initio quantum chemistry package		No	No	Some	Limited
NEMO 3-D	Quantum dot simulation	Jet Propulsion Lab	No	No	Poor	None
OCTA	Multiscale model of material		Yes (under dev)	Yes (under dev)	Average	Limited
Insight II	MD for drugs	Accelrys	No	No	Average	Good
Junius Tech	Fullerenes, CNTs, quantum dots	Junius Tech Inc	No	No	Unknown	Limited
nanoXplorer	Molecular devices	nanoTITAN	No	No	Average	Limited
Nanosteller	Nanocatalysts	Nanosteller, Inc.	No	No	Unknown	Limited
HyperChem	MD targeted for chemical analysis	Hypercube, Inc.	No	No	Good	Very good
CoventoWare	MEMS design and analysis	Coventor, Inc.	No	Yes	Good	Very good
ANSYS	FEA and MEMS	ANSYS, Inc.	No	Yes	Very good	Excellent

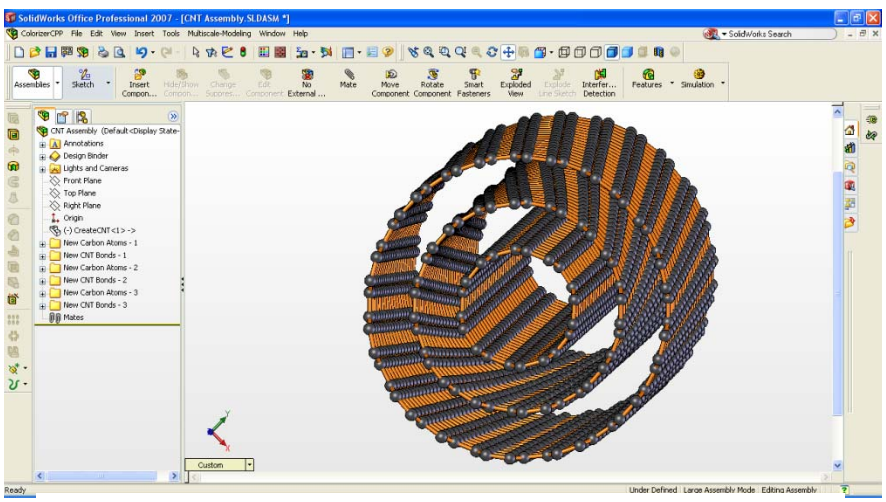
SolidWorks-Based Preprocessor



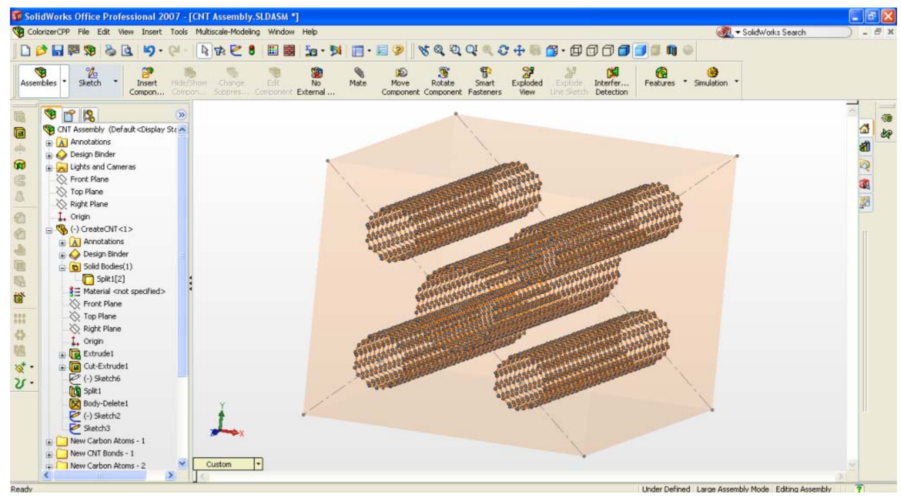
SolidWorks-based multiscale menu.



A single nanotube in a matrix.

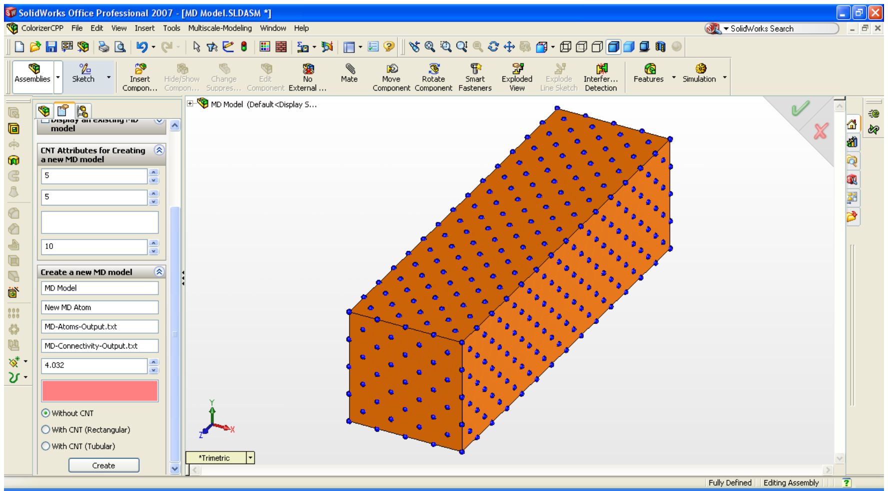


Creating a multi-walled nanotube.

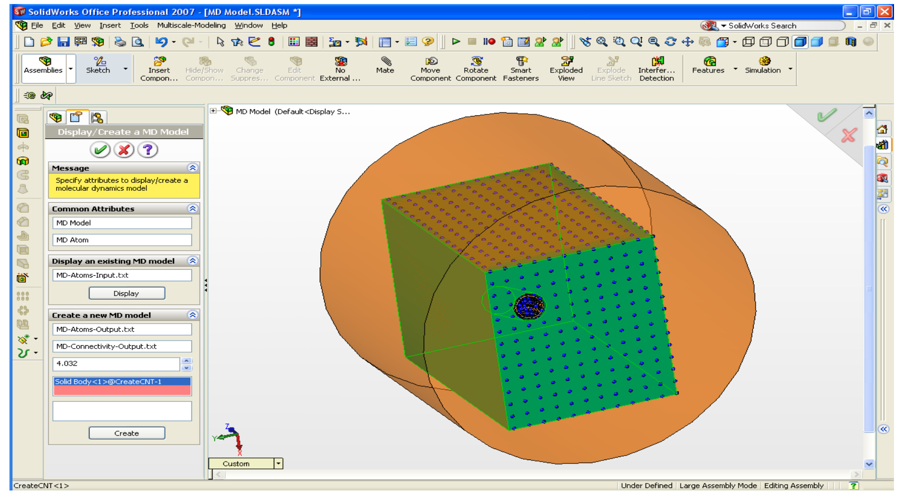


Creating a bundled nanotube in a matrix.

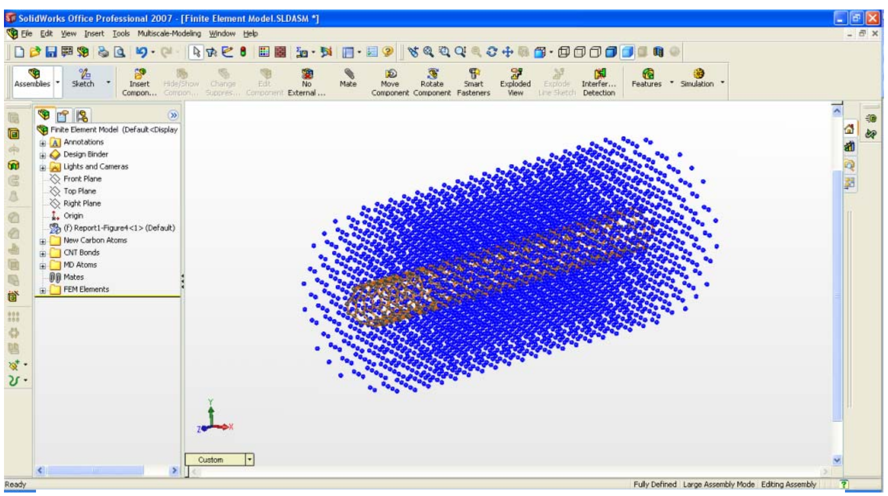
Molecular Dynamics Model



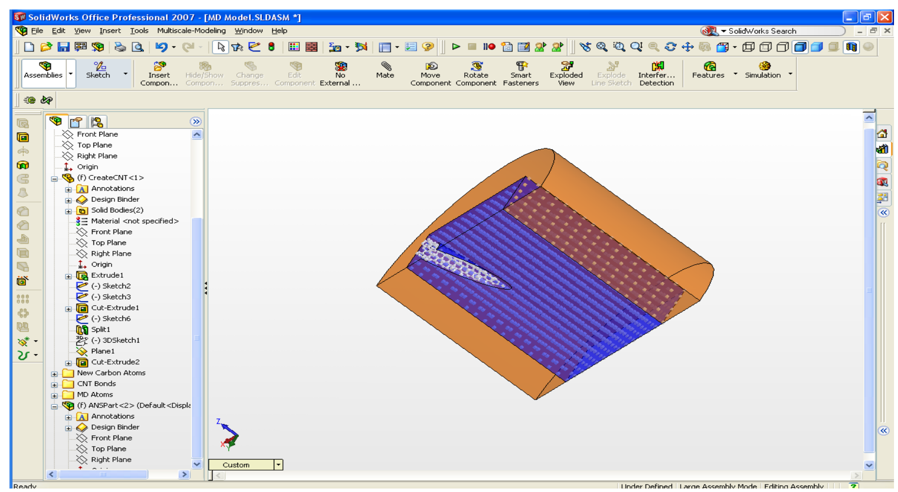
MD Model for a rectangular solid.



MD model when a CNT is present.



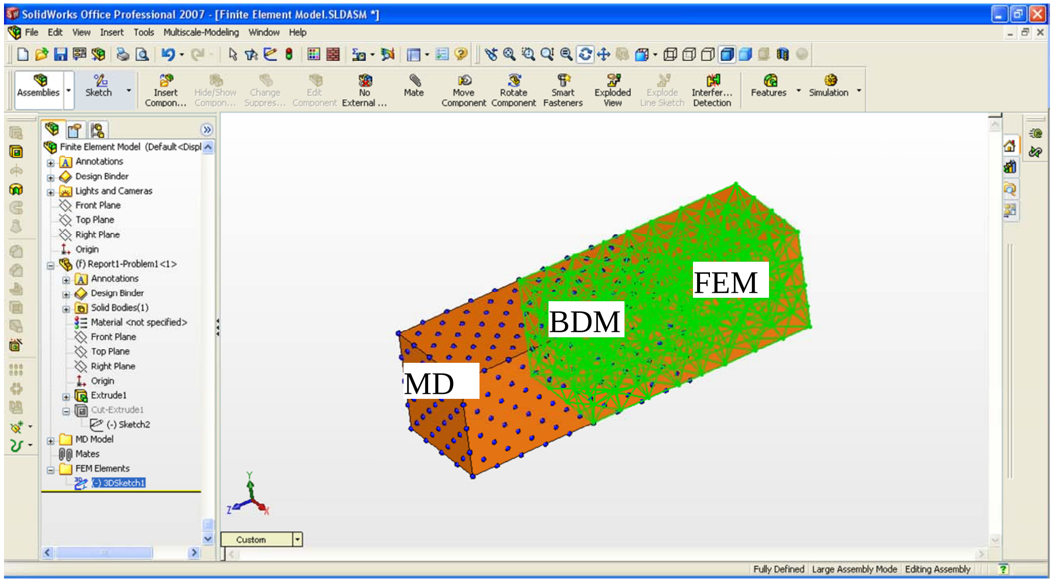
Tubular MD model.

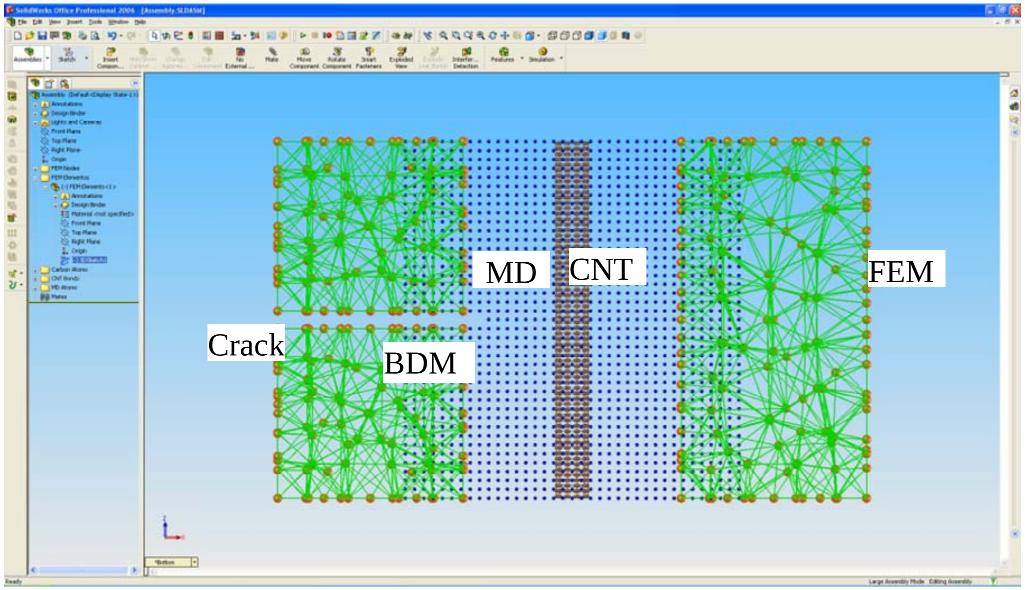


Demonstrating SolidWorks-based menus.

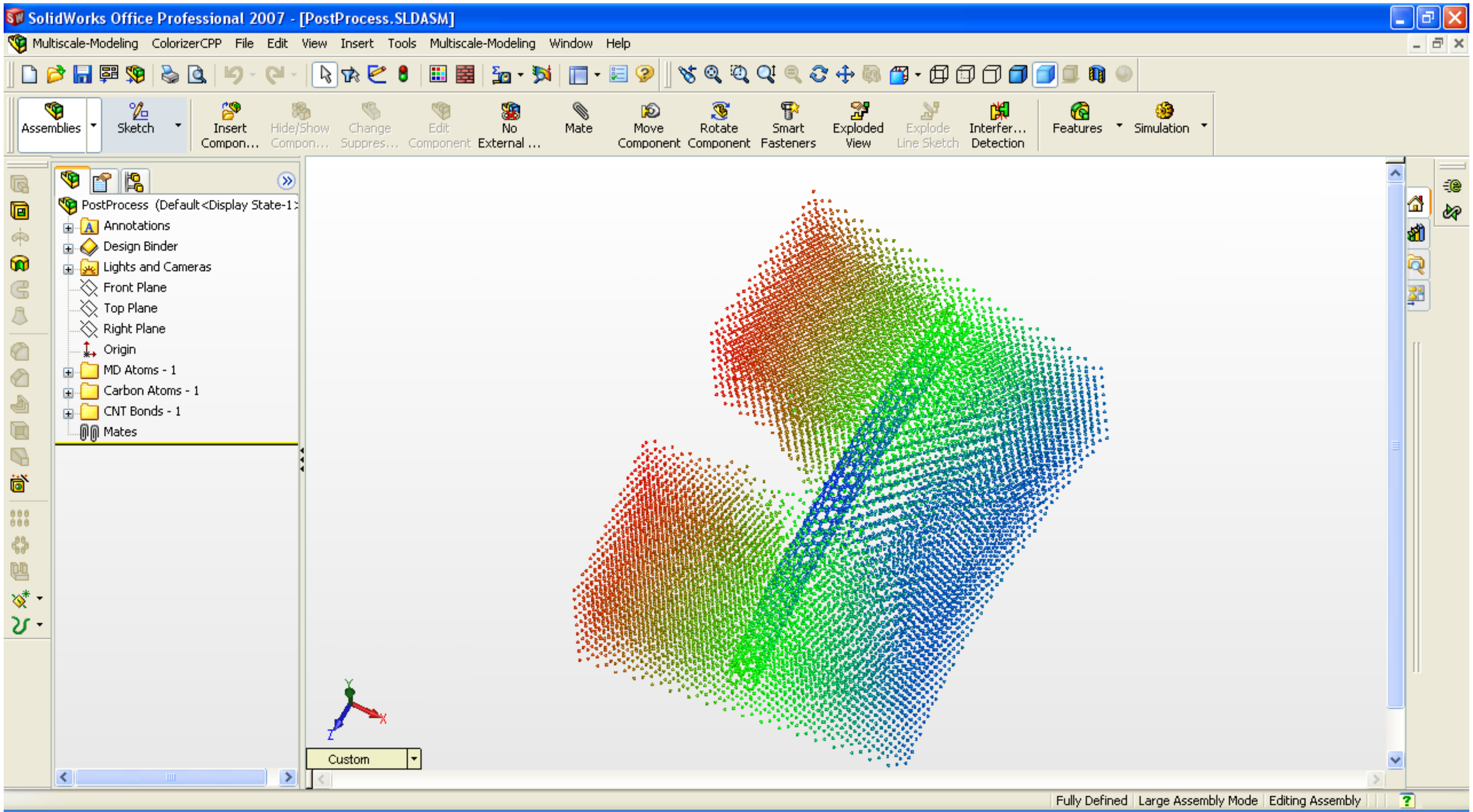
Bridging Domain Model

- Divide a Solid in Two Parts or, Create Two Solids for MD and FEM
- Define End Points in Solid for MD and Chirality to Create Nanotubes
- Choose a Solid for MD Model and Define Atomic Dist to Create MD Model
- Choose another Solid to FEM and Define Element Density to Create FEM
- Define Bridging Domain and Export the Entire Model Data
- Submit the Model Data Files to Solution Engine Developed at UI
- Read the Output File and Display the Result.





Post Processor



Conclusions and future work

Proof of concept was demonstrated to show that a small volume-fraction of magnetic particles is sufficient for self-healing of a crack in a Mendomer.

A feasibility study was performed for interlaminar fracture toughness improvements in nanomodified carbon-epoxy composites for missile systems.

Literature survey in the area of multiscale modeling software tools showed that there is almost no commercially available tool in this area.

Multiscale modeling indicates that Al/CNT composites are more brittle when compared with crystal Al.

A CAD-centric approach to developing pre- and post- processor for multiscale modeling was demonstrated.

Use multiscale approach to predict modulus for nanoscale monodisperse particles versus coarse polydisperse particles for low-volume (<10%) fraction in a polymer matrix.

Use multiscale modeling to self-healing properties of Mendomer magnetic particle composite.

Develop analytical models that describe and predict the energy dissipation potential at matrix nanoscale interfaces such as the potential energy of absorption and surface energy of nanofibers. Using a multiscale approach, use this to predict critical strain energy release rate.

Acknowledgements

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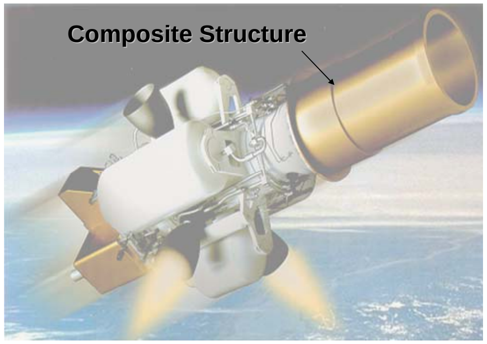
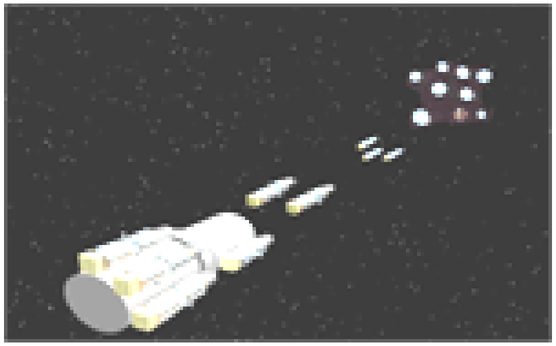


Exo-atmospheric Kill Vehicle (EKV)
Structure is made of composite materials
Source: Raytheon



Missile Defense Agency MKV
Source: Raytheon

Interceptor and launcher parts of the KEI
Source: Raytheon

Questions

NextGen Aeronautics
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