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SAMPE LONG BEACH 2016

Conference: May 23-26, 2016
Exhibition: May 24-25, 2016
Long Beach Convention Center
Long Beach, California

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MICROMECHANICAL STIFFNESS PREDICTIONS AT THE NANO-SCALE: CARBON NANOTUBE REINFORCED COMPOSITES

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Overview

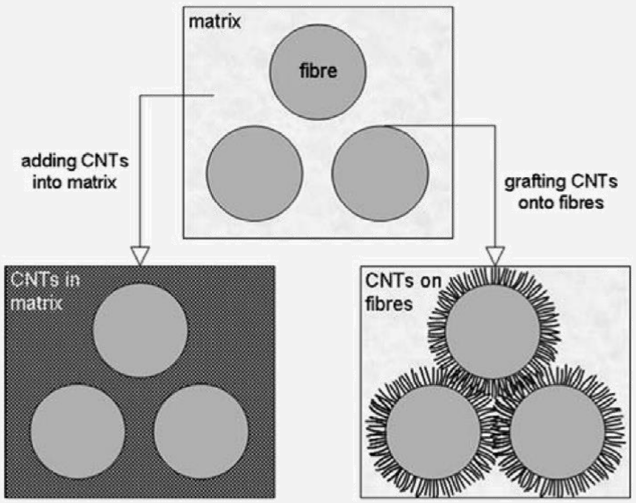
- Overview and focus of this work
- Application of micromechanical models to nanoscale problems
- Modified Anumandla-Gibson model
- Comparison with experimental results
- Issues and future work

Motivation

- Micromechanical models offer simple algebraic relations between composite variables
- Application to CNTs would aid in material decisions (e.g. material trade)
- Bridge to practicality

Nanotube Reinforced Composites

- Two primary types (3-phase)
- Focus on CNTs in matrix
  - Grafting:
    - Not amenable to micromechanic approaches
    - Involves high temperatures (700-1200C)
  - CNTs in matrix:
    - Similar to existing composites (e.g. CSM)
    - Traditional manufacturing methods



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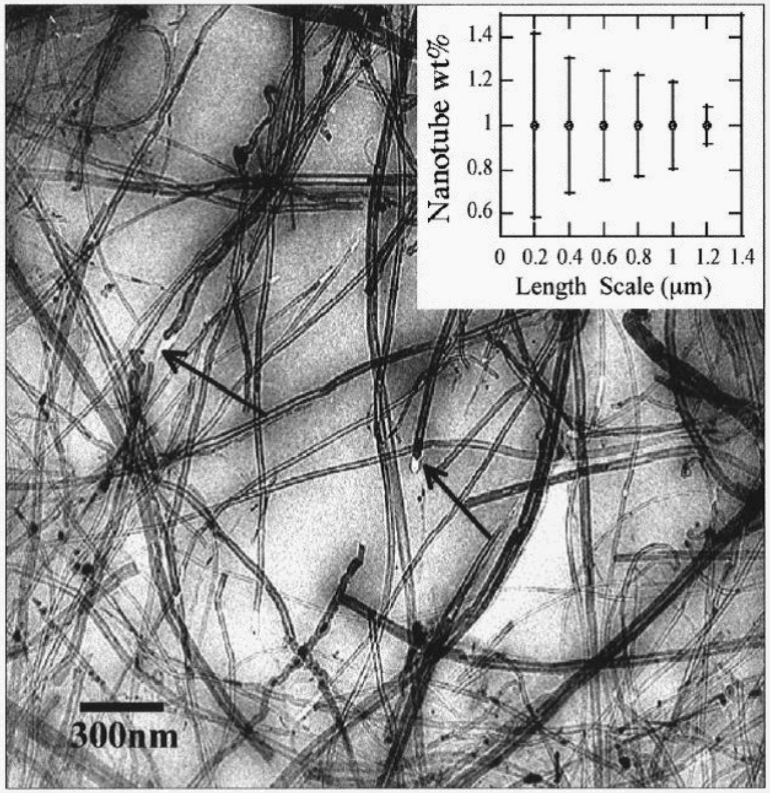
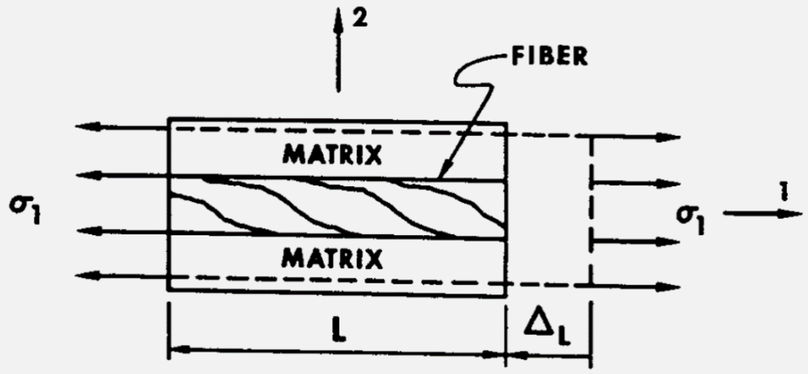
Nanotube Reinforced Composites

- Fundamental issues that must be addressed
  - Waviness
  - Length and aspect ratio
  - Dispersion and agglomeration
  - Orientation



Applying Micromechanics to the Nanoscale

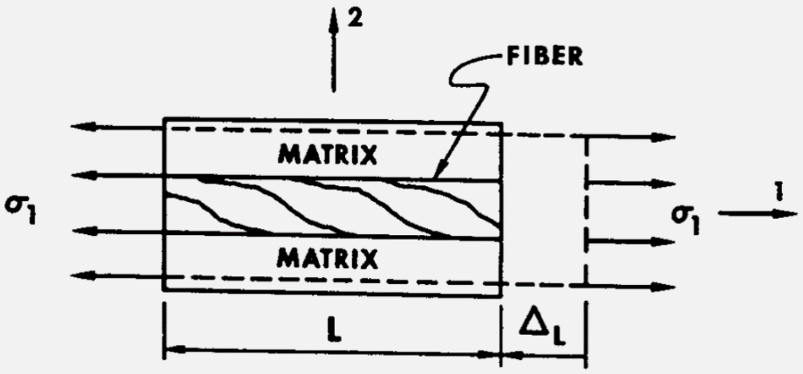
*Micro*mechanics at the *Nano*scale



$$E_{1c} = E_f v_f + E_m(1 - v_f)$$

- Desirable to have simple mathematical relationships
- No assumption is made about type of fiber
  - Can this be applied directly to nanocomposites?

*Micro*mechanics at the *Nano*scale



$$E_{1c} = E_f v_f + E_m(1 - v_f)$$

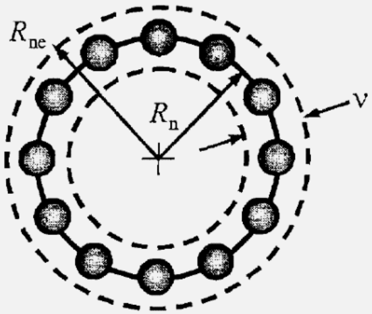
- What is the modulus of the nanotube?
  - Many differing reports from literature
    - Lourie & Wagner: 2.8 – 3.5 TPa
    - Yakobson & Avouris: 1 Tpa
- Why the discrepancy?

*Micro*mechanics at the *Nano*scale

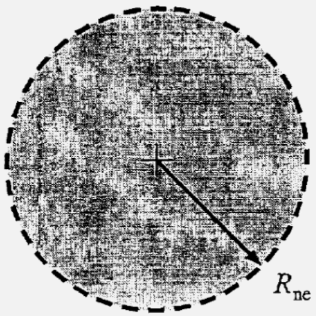
- Discrepancy comes from an assumption in the question
  - Assumes there *is* a nanotube modulus in the traditional sense
- Nanotubes lack a “translational invariance”
  - Characteristic dimensions of tube on same order of carbon atoms
  - More accurate to classify them as structures
    - Geometry dependent properties

Nanotubes as a Structure

- Pipes - Filled Cylinder Equivalency
  - Assign graphite in-plane (1.05 TPa) modulus to open cylinder
  - Scale to cylinder using ratio of areas



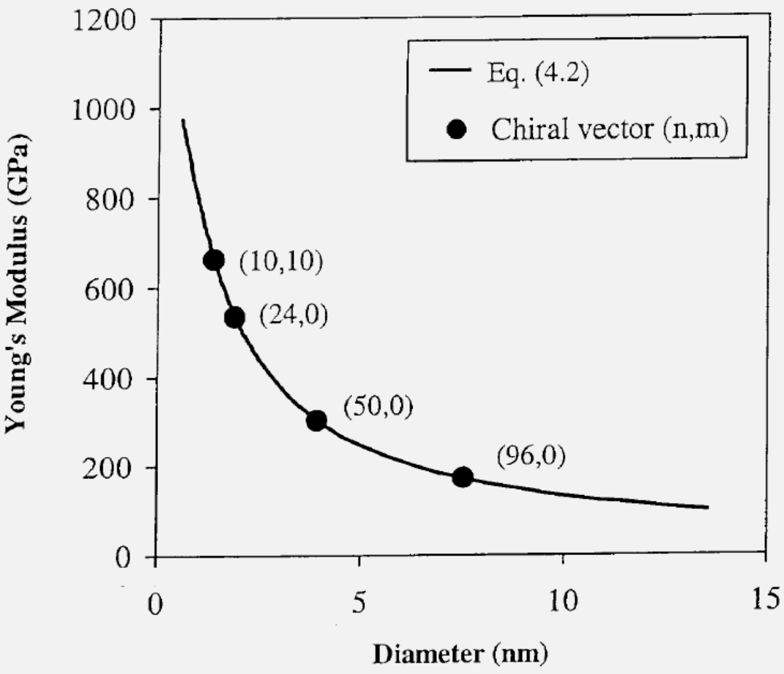
a) Open cylinder model of SWCN



b) Filled cylinder model of SWCN

Nanotubes as a Structure

- Illustrates SWNT "modulus" sensitivity to geometry
  - Concept extends to density as well
- Can select E value given a particular diameter
  - Can we apply micromechanics equations now?



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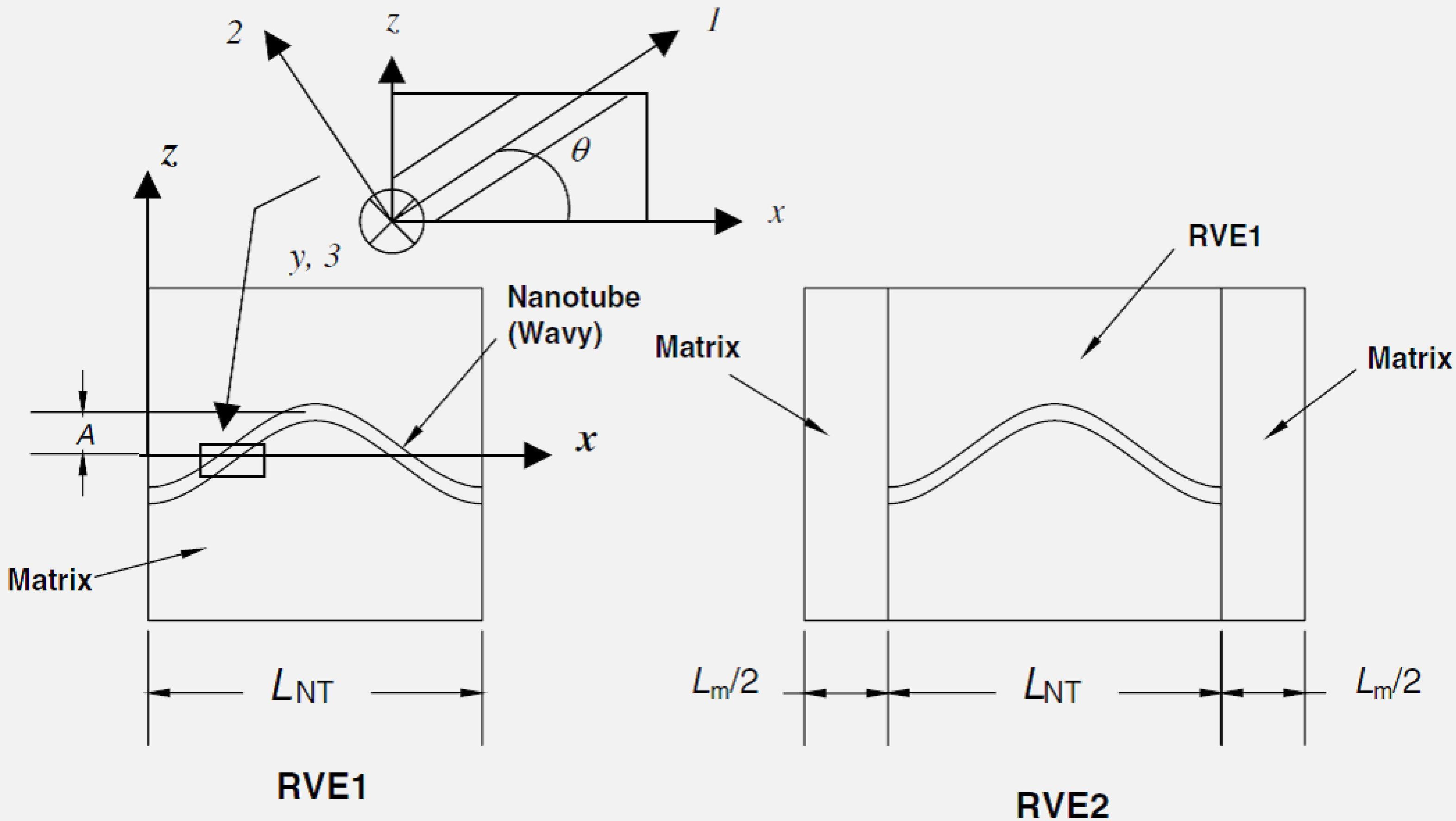
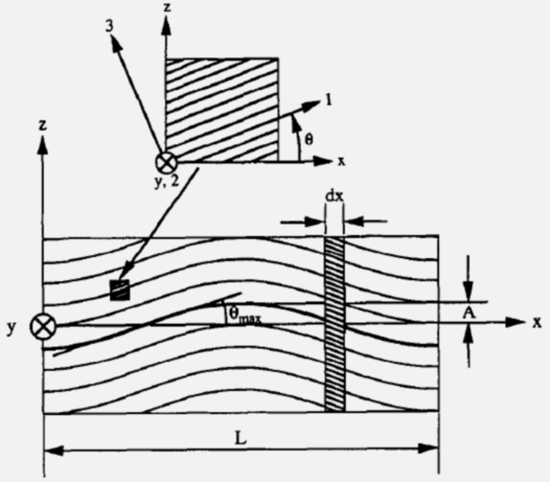
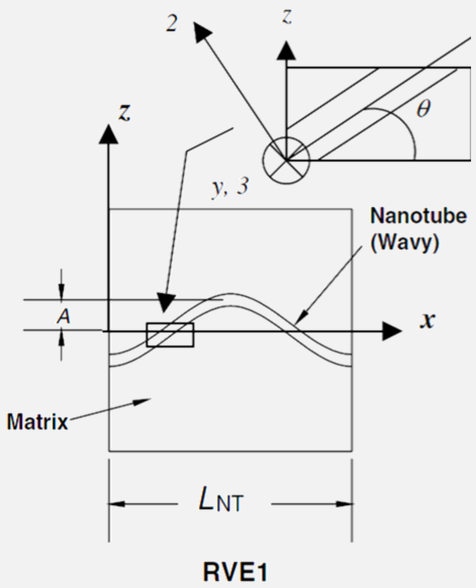
Anumandla-Gibson Model



Waviness

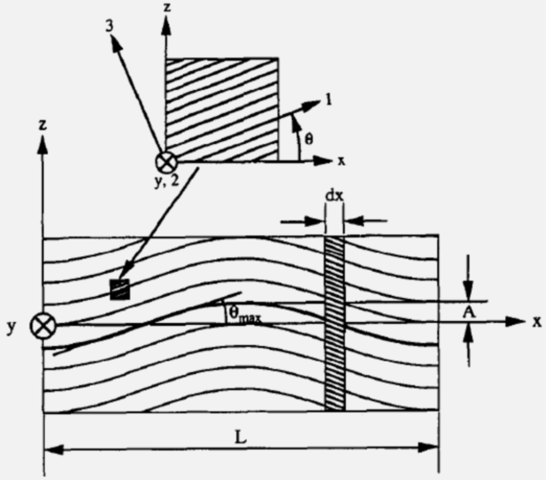
- Borrow micromechanical concepts
- Hsiao & Daniel uniform waviness model
  - Treat each dx slice as off axis lamina
  - Average strains over one wavelength
  - Characterize "waviness" as A/L

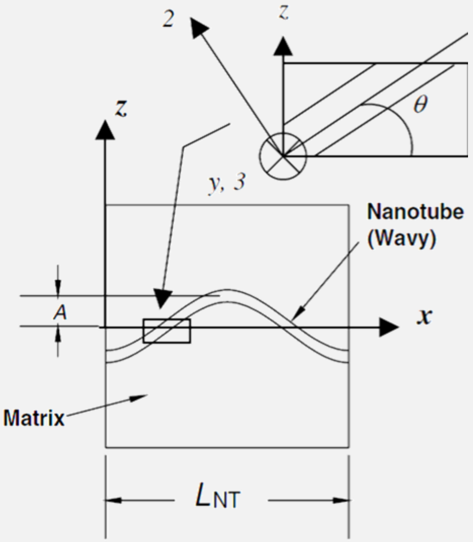




Waviness

- Hsiao & Daniel requires zero-waviness properties
- Use Chamis micromechanical equations inside RVE1
  - Present work modified this to use Halpin-Tsai equations

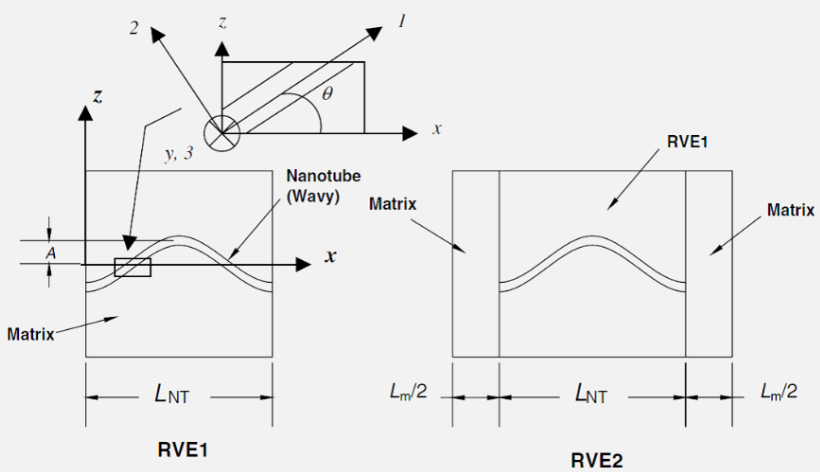




RVE1

Orientation and Length Effects

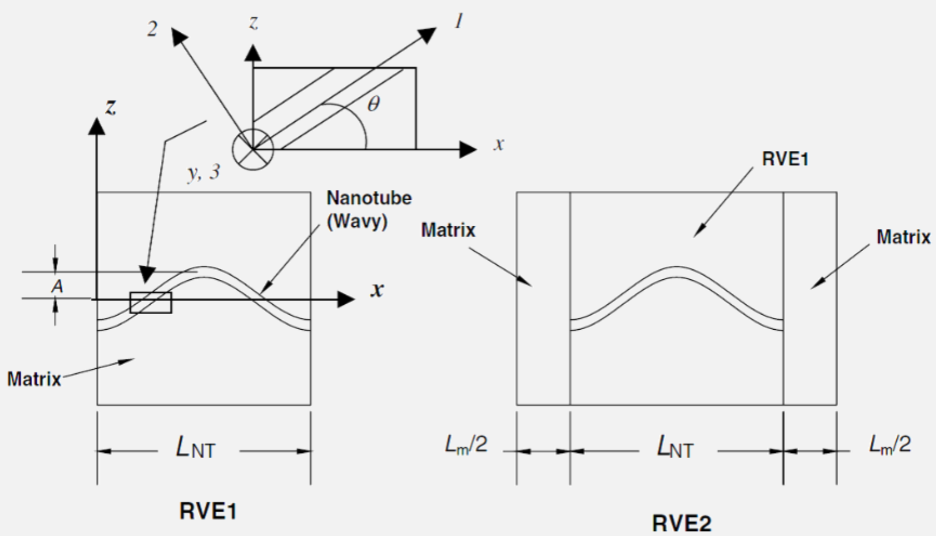
- Christensen & Waals model
  - 3D Randomly aligned reinforcement
  - Yields another effective modulus
- Additional matrix sections added to RVE
  - Makes reinforcement non-continuous



Orientation and Length Effects

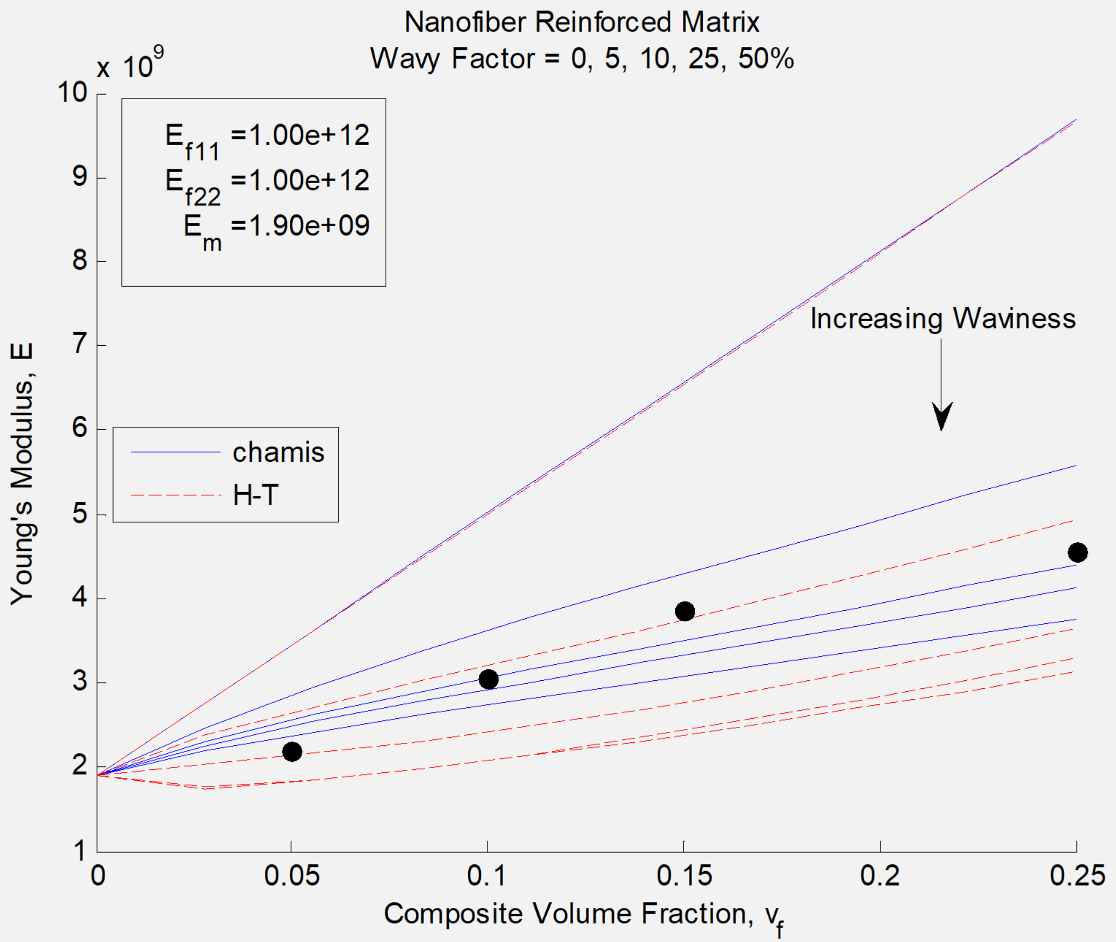
- Must combine all sections to get single RVE2 modulus
  - Inverse rule of mixtures
  - Extension to 3-phase now possible with CLPT

$$\frac{1}{E_{3D-RVE2}} = \frac{1}{E_{3D-RVE1}}\left(\frac{L_{NT}}{L_m + L_{NT}}\right) + \frac{1}{E_m}\left(\frac{L_m}{L_m + L_{NT}}\right)$$

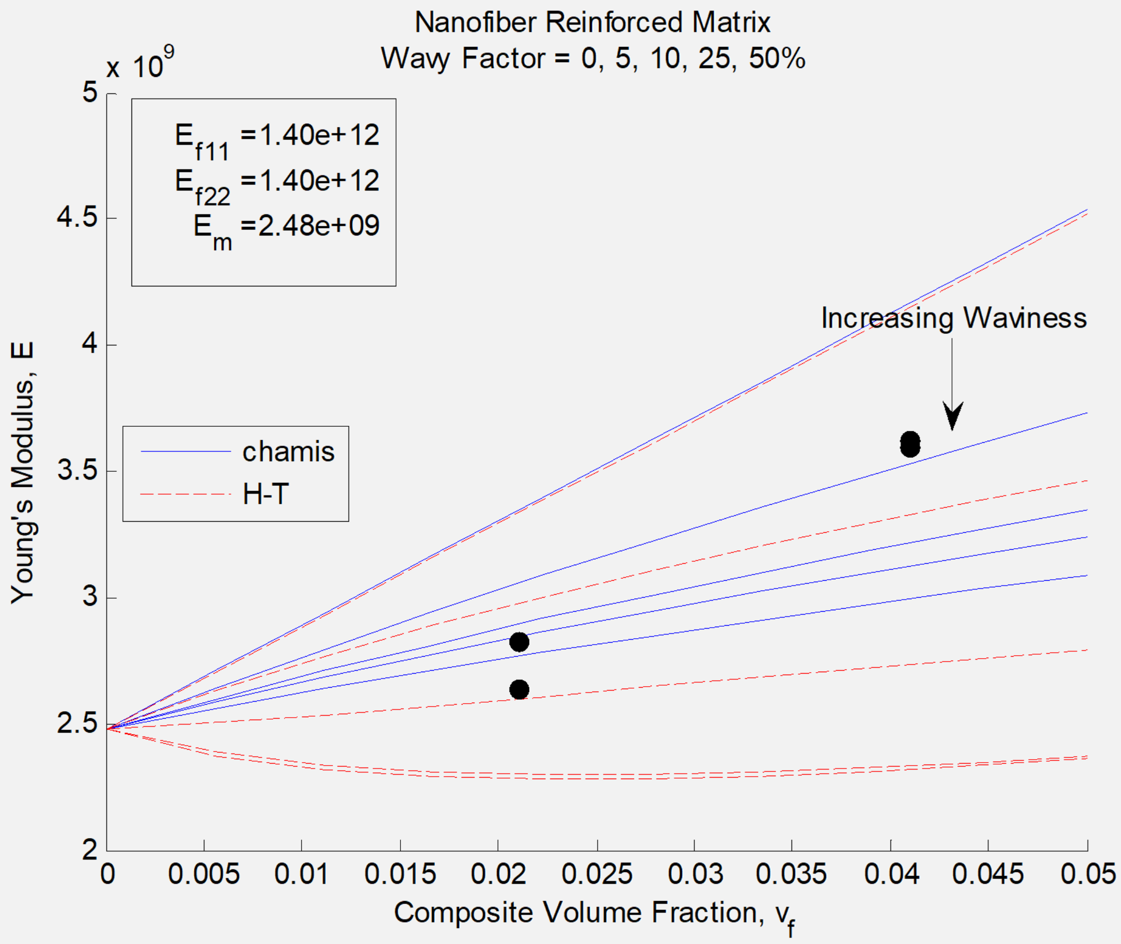


Comparison with Experimental Results

Experimental Comparison



Experimental Comparison



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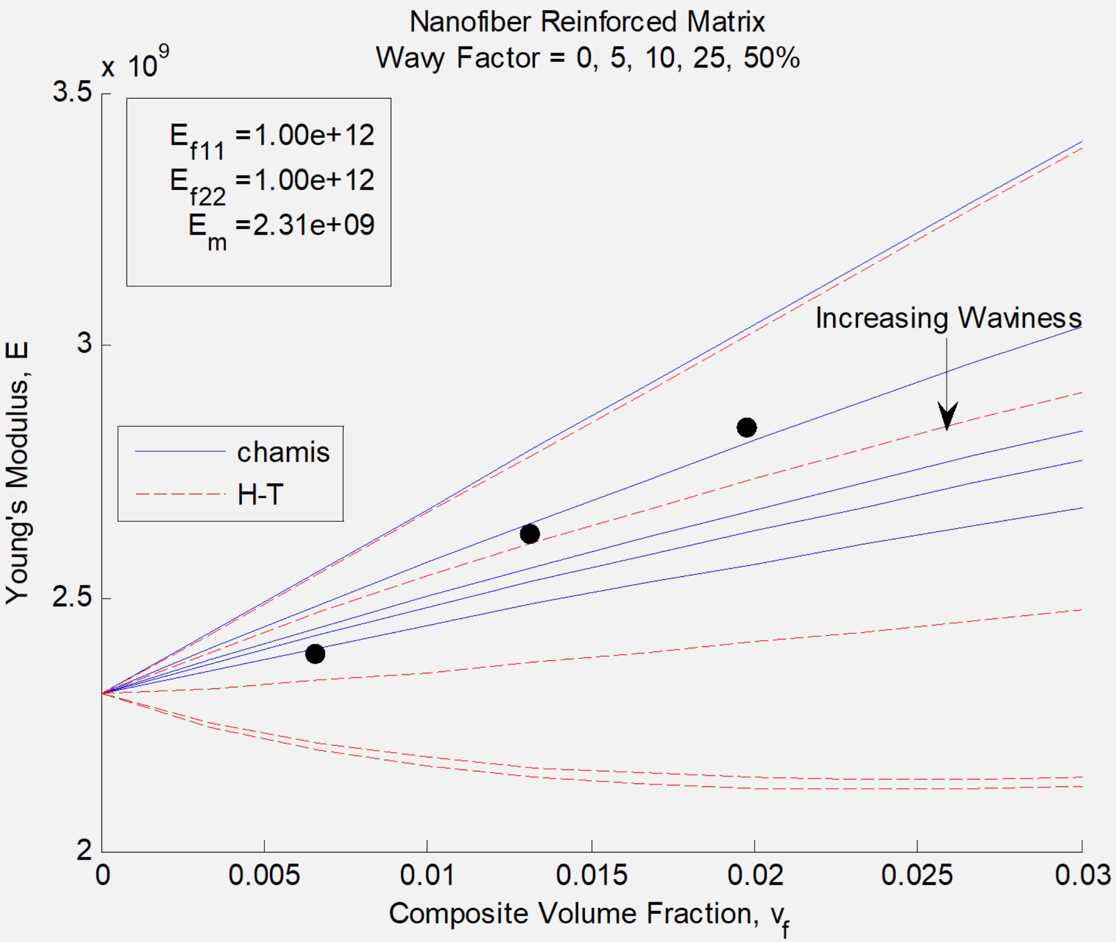

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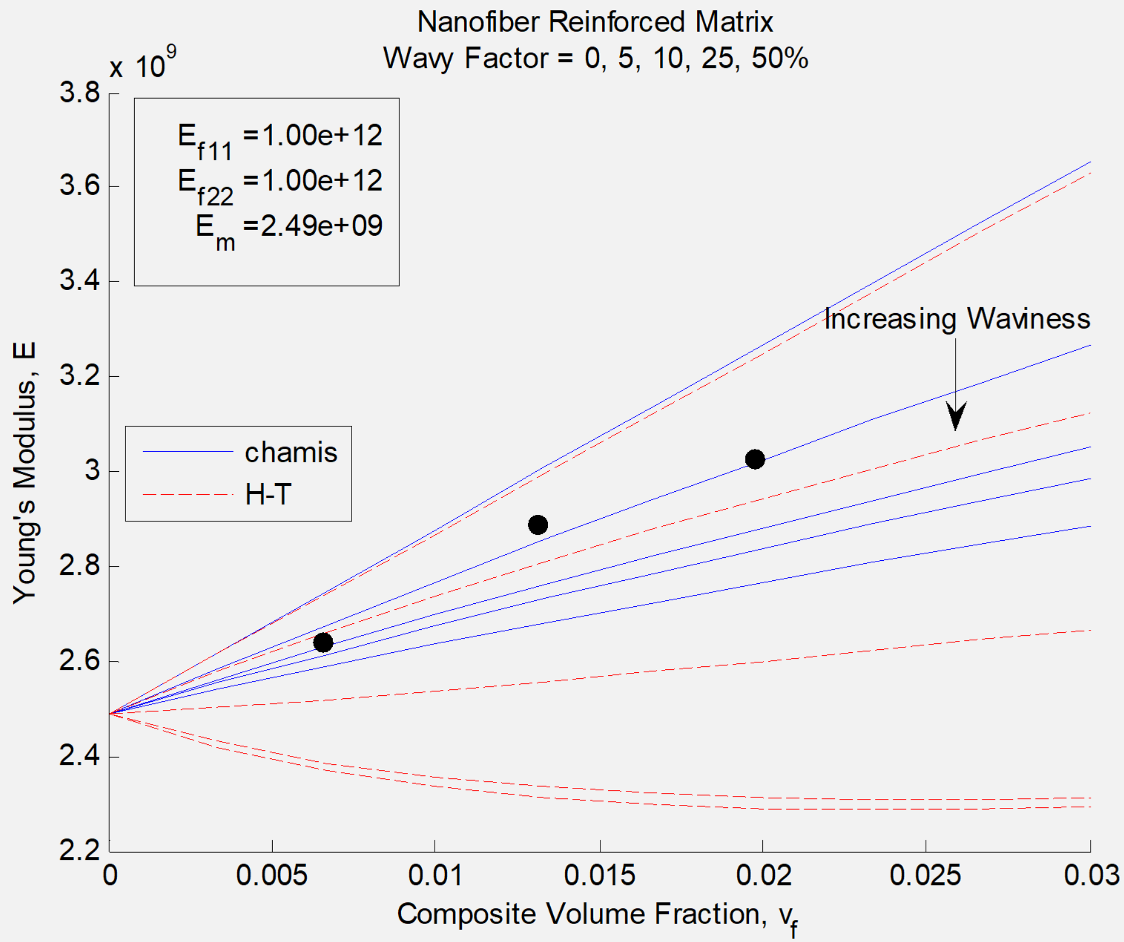

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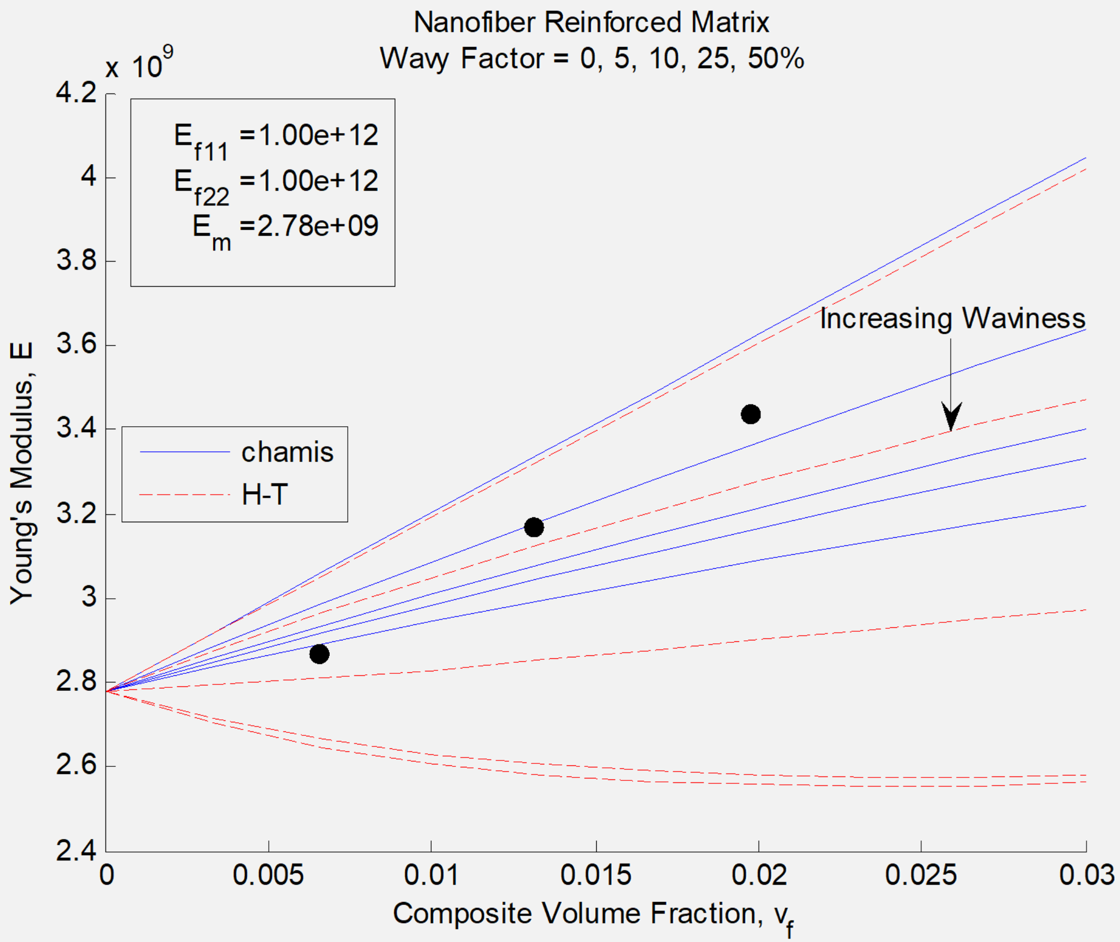

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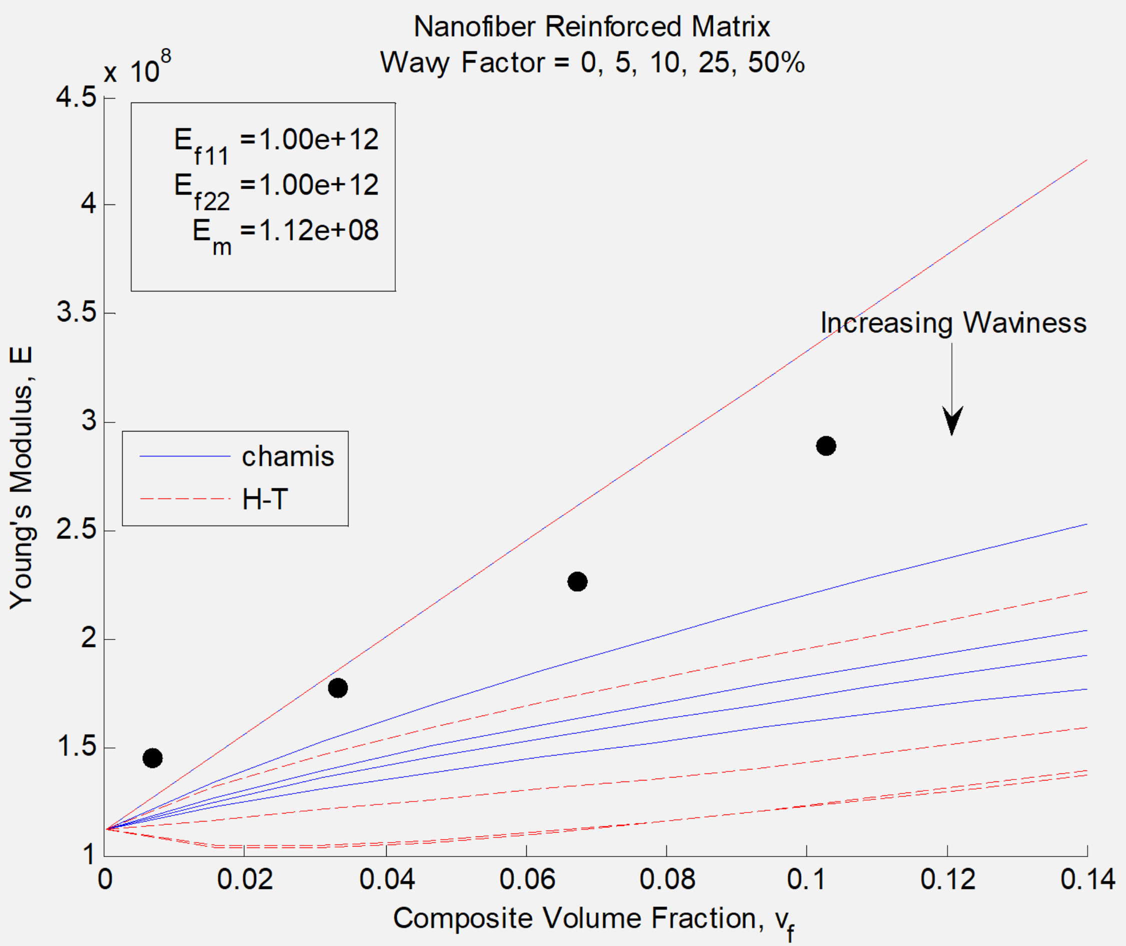

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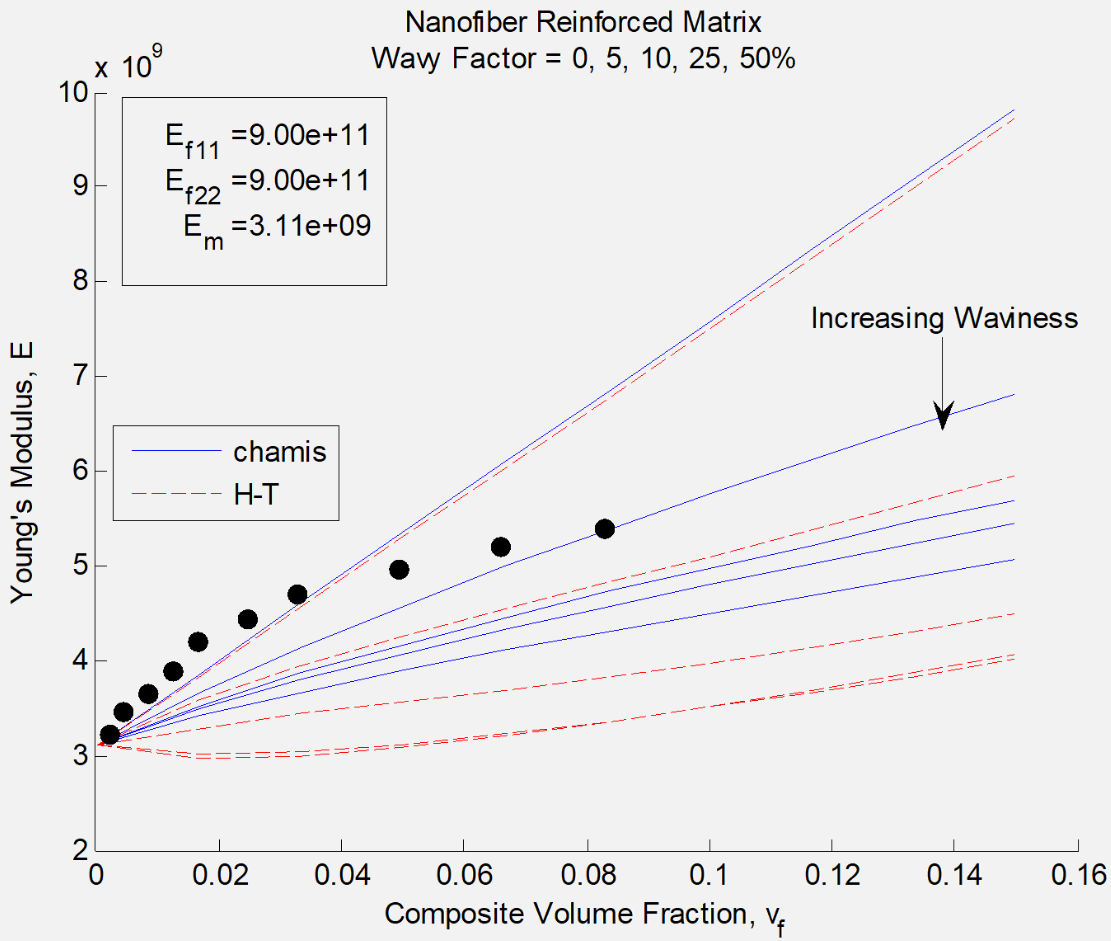

Shortcomings of Data

- Of the 7 data sets presented:
  - 2 reported CNT modulus values
  - 5 reported weight fractions (not volume)
  - 1 reported CNT density
- To Improve:
  - CNT geometry must be reported
    - Parameters are not single valued
  - Attention must be paid to dispersion
  - Better definition of “waviness”

Takeaways

- Micromechanical models are viable for nanoscale problems
- Nanotube geometry is important

THANK YOU