Molecular Modeling of Nanocomposites

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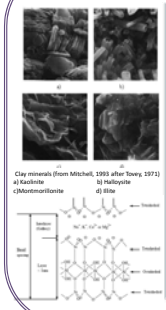
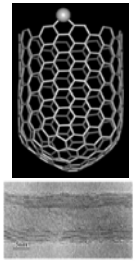
1D- Clay Minerals



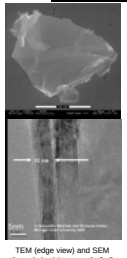
- Clay Minerals are hydrous aluminum phyllosilicates
- Have variable amount of iron magnesium alkali metals and other cations
- Typical MMT have net charges distributed within the octahedral layer or tetrahedral layer
- Bulk Modulus: ~ 20-50 GPa
- Young's Modulus:~ 6.2 GPa

2D-Carbon nanotube



- Singlewalled Carbon Nanotubes & Multiwalled Carbon Nanotubes
- Diameter: ~ 1 *nm*
- Length: ~ 100 *μm*
- Superior Mechanical Properties
  - Elastic Modulus: ~ 1 TPa
  - Density:~ 1/6th of steel
  - Conductive Ability is:~ 100,000 times that of copper
  - Yield Strain:~ More than 4%
  - Buckling Strain: ~ 5% (aspect ratio of 1/6)

2D-Graphite & Graphene

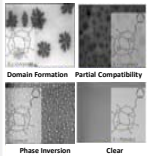


TEM (edge view) and SEM (lateral view) images of xGnP

- Single carbon Layer and multi carbon Layers
- Thickness: ~ 5-10 *nm*
- Length: ~ 0.86-15 *μm*
- Superior Mechanical Properties
  - Elastic Modulus: ~ 1 TPa
  - Intrinsic Strength: ~ 130 GPa

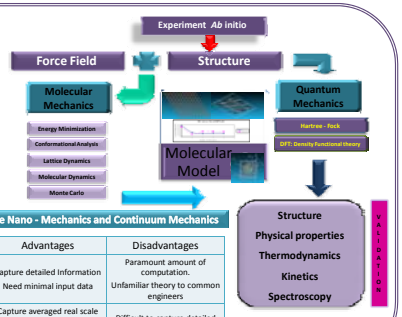
(Experiments conducted for a monolayer graphene by Lee et al. 2008, reported that graphene is strongest material ever measured)

3D-POSS Organic- Inorganic



POSS dissolving in a polymer
http://www.hybridplastics.com/pdf/paper.pdf

- A new class if organic – inorganic nanocomposites containing POSS monomers which have been copolymerized with organic monomers.
- POSS hybrid chemical composition
- POSS molecules span 1~3 *nm* size range.
- Improve impact resistance.
- Reduce friction and improve flow.
- POSS can dissolve in polymers.

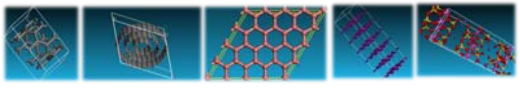


Need to bridge Nano - Mechanics and Continuum Mechanics

Items	Advantages	Disadvantages
Nano-mechanics	Capture detailed Information Need minimal input data	Paramount amount of computation. Unfamiliar theory to common engineers
Conti-nuum mechanics	Capture averaged real scale behavior. Familiar theory	Difficult to capture detailed information

Molecular Dynamic Simulation of Nanocomposites and their Constituents

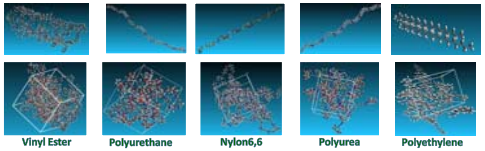
Nano- Reinforcement



Eng. Constants	SWCNT	MWCNT	Graphene	Graphite	MMT
E_{11} (GPa)	878	690	1373	461.4	354
E_{22} (GPa)	23.2	27.5	831	31.7	84.1
v_{12} (GPa)	0.16	0.33	0.30	0.012	0.23
G_{23} (GPa)	7.6	8.6	340.5	216	198.4
K_{23} (GPa)	24.6	57.6	624.1	248.6	267.6

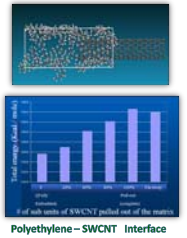
POSS

Nano- Matrix



Eng. Constants	Vinylester	Polyurethane	Nylon6,6	Polyurea	Polyethylene
E_{11} (GPa)	3.7	5.5	3.4	5.5	1.2
v_{12} (GPa)	0.31	0.32	0.37	0.29	.37
G_{23} (GPa)	1.41	2.1	3.6	4.4	.45
K_{23} (GPa)	3.37	3.6	1.6	2.1	1.73

Nano- Composite Interface



Nano- Composites

Eng. Constants	5%	10%	20%
E_{11} (GPa)	5.5	13.6	73.5
E_{22} (GPa)	5	9.6	40.6
v_{12} (GPa)	0.32	0.31	-
G_{23} (GPa)	1.8	6.3	8.6
K_{23} (GPa)	5.3	10.5	18

Eng. Constants	
E_{11} (GPa)	92.18
E_{22} (GPa)	2.31
v_{12} (GPa)	0.33
G_{23} (GPa)	0.97
K_{23} (GPa)	13.55

Eng. Constants	
E_{11} (GPa)	24.62
v_{12} (GPa)	0.36

Eng. Constants	GnP 10%	GnP 20%	xGnP 10%	xGnP 20%
E_{11} (GPa)	11.4	58.3	17.4	13.7
E_{22} (GPa)	81.8	160.7	113.9	140.6
v_{12} (GPa)	-	-	0.05	0.03
G_{23} (GPa)	27.9	56.4	41.8	49.4
K_{23} (GPa)	77	139.7	94.1	124.4

Parametric Evaluation of Multiwalled Carbon Nanotubes (MWCNT) MD

I. Geometrical Parameters

A. Chirality

B. Number of Carbon Nanotube Walls

C. Aspect Ratio

II. Simulation Parameters

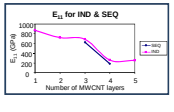
a) Temperature Effect

b) Thermodynamic Ensemble

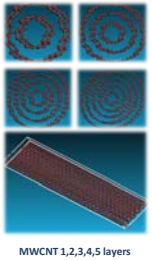
c) Thermostat and Barostat Algorithm

I A . Chirality

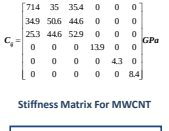
Sequential Individual



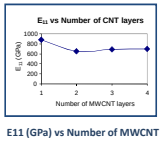
I B . Number of Carbon Nanotube Walls



MWCNT 1,2,3,4,5 layers



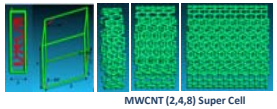
Stiffness Matrix For MWCNT



E11 (GPa) vs Number of MWCNT Layers

Unit cell contains: 3600 atoms
MWCNT: Three layers, Chirality : (5_5, 10_10, 15_15)

I C . Aspect Ratio



MWCNT (2,4,8) Super Cell

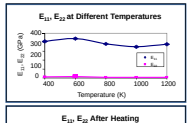
Conditions of The Simulation:
Unit Cell Contains: 120 Atom per Unit Cell
Unit cell size(3D super cell) : 22.5*22.5*73.8A
MWCNT: Three layers, Individual Setup
Chirality : (5_5, 10_10, 15_15)
Dynamic: NPT (Berendsen Thermostat)
Temperature 400K
Elastic Constants: 298K

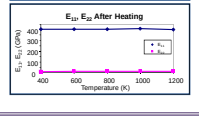
NPT Three Wall	Length A	L/d Ratio Inner tube	L/d Ratio Outer tube	E_{11}	E_{22}	v_{12}	M_{23}	K_{23}
2 Unit	4.92	0.72	0.25	439	36	0.2	11	47.3
4 Unit	9.84	1.5	0.5	493	36	0.26	7.7	47.15
8 Unit	20	3.63	1.2	590	31.1	0.26	9	59.2
20 Unit	49.2	7.3	2.4	687	30	0.26	8.6	57.6
30 Unit	73.8	11	3.6	690	27.5	0.33	7.9	52.6
40 Unit	98.4	14.4	4.8	720	28.6	0.33	8.3	54.9

MWCNT Length Variation

II a) . Temperature Effect

Unit Cell Contains: 2400 Atom
Unit Cell Size(20 super cell): 22.5*22.5*49.2A
MWCNT: Three Layers Individual Setup
Chirality: {(5,5), (10,10), (15,15)}
Dynamic: NPT (Berendsen Thermostat)
Temperature: 400, 600, 800, 1000, 1200K
Elastic Constants: 298K

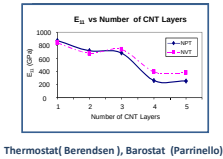




II b) . Thermodynamic Ensemble

a. Isochoric (NVT)
N: Number of Atoms
P: Pressure

b. Isobaric (NPT)
V: Volume
T: Temperature



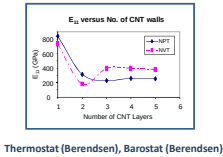
Thermostat(Berendsen), Barostat (Parrinello)

II c) . Thermostat and Barostat Algorithm

a. Berendsen Algorithm

b. Andersen Algorithm

c. Parrinello Algorithm



Thermostat (Berendsen), Barostat (Berendsen)

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