Computational Nanotechnology of Materials, Electronics and Machines: Carbon Nanotubes

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NASA Mission Needs

• Onboard computing systems for future autonomous intelligent vehicles
  - powerful
  - compact
  - low power consumption
  - radiation hard
• High performance computing (Tera- and Peta-rops)
  - processing satellite data
  - integral space vehicle engineering
  - climate modeling
• Smart, compact sensors
• Light weight devices
• Advanced instrumentation for space astronomy

http://www.ipf.nasa.gov/index.html

Research Focus

• Large Scale Classical Molecular Dynamics on a Shared Memory Architecture Machine
  - Parallel implementation on a shared memory Origin2000 machine
  - Srivastava and Barnard — IEEE SuperComputing '97

• Quantum Molecular Dynamics Methodology
  - Tight-binding molecular dynamics in a non-orthogonal atomic basis (GTBMD) method.
  - Previous Parametrization: Silicon and carbon
  - Extended to heteratomic systems including: C, B, N
    M. Menon and D. Srivastava

Techniques

http://www.nasa.gov/search.jsp?R=20010108004 2019-07-16T14:17:16+00:00Z
Technique Development Focus I

Large Scale Classical Molecular Dynamics on a Shared Memory Architecture Machine

- Brenner's reactive many-body potential for hydrocarbons
- Long Range (6-12) Van der Walls interactions
- Parallel implementation on a shared memory Origin 2000 machine
  - Cell method
  - Spatial Decomposition for neighborlist
  - Lexical Decomposition for Force Calculations
    - better load balancer

![Graph](image)


Technique Development Focus II

Quantum Molecular Dynamics Methodology:

\[ U = U_{el} + U_{rep} + U_{b} \]

- \( U_{el} \) = Sum of one electron energies
- \( U_{rep} \) = Sum of repulsive pair potential

- Non-orthogonal atomic basis
- GTBMD method

Secular Eq.: \( \det [ [h_{ij} - E] ] = 0 \)

The forces on an atomic coordinates are given by

\[ F = -dU/dx \]

Molecular Dynamics: system is dynamically evolved at each time step

Previous Parametrization: Silicon and carbon


Extends to heteratomic systems including: Si, C, B, N, and H

Research Focus I

Nanotube - Nanomechanics/materislis

- Nanotubes are extremely strong highly elastic nanofibers
  - high value of Young modulus:
    - steel - 0.2 TPa
    - swol - 1.2 TPa

- Dynamic response of nanotubes to ballistic deformation:
  - axial compression, bending and torsion
  - comparison between SWNT and MWNT behavior

![Graph](image)

- redistribution of strain, and side ways buckling


![Graph](image)

**FIG. 1.** MD-simulated nanotube of length \( L = 6 \) nm, diameter \( d = 1 \) nm, and armchair helicity (7,7) under axial compression. The strain energy plot displays four singularities
Under Compressional strain two modes are observed:

- (a) - long multi-wall nanotubes behave as elastic rods that buckle, bend and loop
- (b) - thin walled nanotubes locally collapse or fracture rather than buckle

**Spontaneous collapse-plasticity of (8,0) CNT through graphitic (sp2) to diamond like (sp3) type transition.**

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(a) side view  (b) top view
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**Energetics of collapse-plasticity of (8,0) CNT at 12% compression strain.**

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Quantum GTPSMD Method
classical atomistic with Trueloff-Brenner potential
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**Comparison with classical atomistic simulation, and a CNT with B point defect.**

- With a single B point defect
- Symmetric pinching deformation (elastic) with Brenner potential
Band gap engineering over a larger range should be possible:
- BN: 5.5 eV
- BC$_2$N: 2.0 eV
- C: 0.1 eV
- BC$_3$N: 0.5 eV

A variety of junctions, quantum dots and superlattices should be possible
- should be more robust

Example: Composite (10,0) nanotube

Young's modulus and plasticity of a compressed BN nanotube.

$Y_{(BN)} = 1.2 \text{ TPa}$ - BN is 92% as strong as CNT
$Y_{(C)} = 1.3 \text{ TPa}$

BN nanotube plastically collapses at even higher strain than C nanotube.
BN Nanotubes - Nanomechanics

- BN nanotubes reinforce composites with anisotropic plasticity

Nanostructured Skin Effect I

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Carbon-based Electronics

- Molecular wires
- Topological defect mediated hetero-junctions - switching tunneling devices
- C nanotubes doped with B and N
- BN nanotubes (insulator - 5eV gap) heterojunctions superlattices
- Combination of the above two - to tailor the probable device characteristics
- Interconnects - Carbon/metal junctions

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Carbon Nanotube Electronics Band Structure (basics)

- Hexagonal Lattice of a Graphene Sheet - (2 unit cell)
- First Brillouin zone for an armchair tube
- Chiral vector \( ch = n a + m b \)

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2-point Nanotube Heterojunctions
Molecular Electronic Switches

Chico et al. Phys. Rev. Lett. 96
Lambert et al. Chem. Phys. Lett. 96
M. Meenon and D. Srivastava, J. Mat. Res., 96

We studied the effect of capping the tubes and relaxing the junctions with a quantum GTPMD method.

Research Focus III
BxCyNz Composite Nanotubes and Junctions
- Band gap engineering over a larger range should be possible:
  - BN: -5.5 eV
  - BC$_2$N: -2.0 eV
  - C: -0.1 eV
  - BC$_3$: -0.5 eV
- A variety of junctions, quantum dots and superlattices should be possible
- Should be more robust

Example: Composite (10,0) nanotube
0.34 eV/atom
0.28 eV/atom
0.37 eV/atom

reconstruction due to polar BN bond
**Composite Nanotubes and Junctions**

- B doping of Carbon Nanotubes
  - Random
  - Island (BC3)
  - Superlattice (BC3)
  - 0.000
  - 0.013
  - 0.016 eV/atom

  Phase separation of doped and undoped regions is thermodynamically stable?

- BN/C Junctions

  Interface Energy = 2*BN/C - BN - C
  Interface Energy = 0.33 eV/CB bond
  Stable interfaces should be possible!


**Nano-Mechano-Electronics**

- Mechanical deformations alter the Electronic Characteristics of Nanotubes

  Nano-mechano-electronics effects are "strongly" dependent on tube chiralities?


**Functionalization of Nanotubes**

- Predictions of enhanced chemical reactivity in regions of local conformational strains: Kinky Chemistry

  Kink on a bent tube

  Ridge on a twisted tube

  Binding Energy
  Cohesive Energy
  Electronic Energy

**Nano-Mechano-chemistry**

- Torsionally twisted SWNT equilibrated in an H bath

2000 - D Srivastava
SEM images of MWNTs dispersed on a V-ridge substrate
(a) Before Reaction
(b) Same sample after exposure to nitric acid vapor at room temperature


Comments:
Nanotechnology Materials and Applications.
- compressed C nanotubes in composites
- Nanostructured skin effect
- Functionality of a smart material
- Nano Electronomechanical Sensors (NEMS)
- Components of Molecular Electronices
- mechanical kink catalyzed chemistry
- kinky chemistry

Mechanical
Chemical
Electronic