

## ABSTRACT OR SUPPORTING INFORMATION

**Presentation/Publication Information:**

A contributed talk to be given by Deepak Srivastava of the Computational Nanotechnology task at the American Physical Society March 99 meeting in Atlanta, GA (March 22-26, 1999).

A copy of the presentation is attached.

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**Abstract:**

Nanomechanics of single-wall C, BN and BC<sub>3</sub> and B doped C nanotubes under axial compression and tension are investigated through a generalized tight-binding molecular dynamics (GTBMD) and *ab-initio* electronic structure methods. The dynamic strength of BN, BC<sub>3</sub> and B doped C nanotubes for small axial strain are comparable to each other. The main difference is in the critical strain at which structural collapse occurs. For example, even a shallow doping with B lowers the value of critical strain for C nanotubes. The critical strain for BN nanotube is found to be more than that for the similar C nanotube. Once the structural collapse starts to occur we find that carbon nanotubes irreversibly go into plastic deformation regime via the formation of tetrahedral (four-fold coordinated) bonds at the location of sharp pinches or kinks. This finding is considerably different from the classical MD simulation results known so far. The energetics and electronic densities of states of the collapsed structures, investigated with *ab-initio* methods, will also be discussed.





### Plasticity of Carbon and CxByNz Nanotubes: via a Quantum Molecular Dynamics Method

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#### Motivation:

- Carbon and other nanotubes could be useful as:
  - reinforcing phase in novel composite materials
  - nanomechanical and nanoelectromechanical system components.

#### Status:

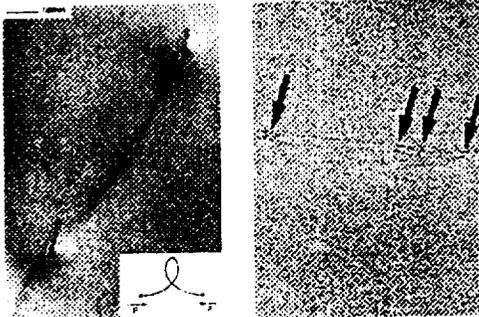
- Nanomechanics of Nanotubes:
  - Youngs modulus ~ 1 - 5 TPa range (expt, theory)
  - Yacobsen et. al. Phys. Rev. Lett. (1996) - Shell model and classical MD simulation description of nanomechanics.
- Route to Plasticity and Fracture of Axially Stressed Nanotubes
  - linear response followed by non-linear response
  - kinks, pinches and morphological buckled configurations but the tube remains completely elastic
  - route to plasticity is via Stone-Wales bond rotation (5,7 pair) defect formation.

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#### Status:

- Experiment : Buckling and Collapse of Embedded Carbon Nanotubes  
O. Lourie et. al. Phys. Rev. Lett. Vol. 81, 1638 (1998).



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

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### Compression of Nanotubes with a Quantum Molecular Dynamics Method

#### Methodology:

$$U = U_{el} + U_{rep} + U_0$$

$$U_{el} = \text{Sum [one electron energies]}$$

$$U_{rep} = \text{Sum [repulsive pair potential]}_{\text{occupied}}$$

- Non-orthogonal atomic basis GTBMD method

$$\text{Secular Eq. } \det( h_{ij} - E s_{ij} ) = 0$$

The forces on atomic coordinates are given by

$$F_x = - dU/dx$$

Molecular Dynamics : system is dynamically evolved at each time step

Previous Parametrization : Silicon and carbon  
M. Menon and K. R. Subbaswamy, Phys. Rev. B (1993-94)

Extended to heteroatomic systems including: Si, C, B, N

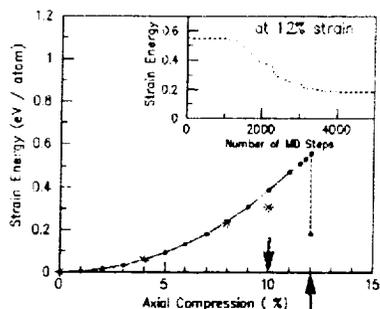
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### Compression of Carbon Nanotubes I



- Energetics of collapse-plasticity of (8,0) CNT at 12% compression strain.



Quantum GTBMD Method  
classical atomistic (with Tersoff-Brenner potential)

- Linear response regime ( $Y = 1.3 \text{ TPa}$ ) followed by pinching/buckling (classical MD) or collapse/plasticity (quantum MD).

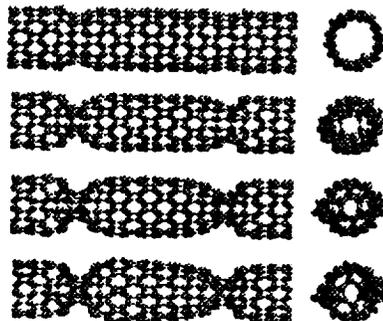
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### Compression of Carbon Nanotubes II



- Spontaneous collapse-plasticity of (8,0) CNT through graphite ( $sp^2$ ) to diamond like ( $sp^3$ ) type transition.



(a) side view

(b) top view

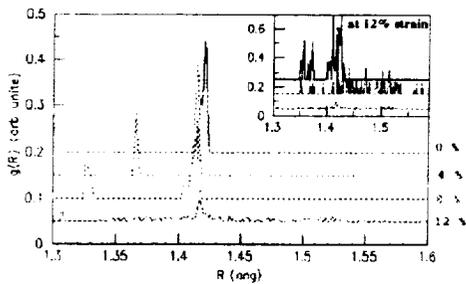
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### Compression of Carbon Nanotubes III



- Radial Distribution Function Analysis



at 12% strain



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### Compression of Carbon Nanotubes IV



- DFT-LDA analysis of (8,0) CNT collapse

#### Simulation Parameters

- 64 C atoms in Supercell:  $13 \times 13 \times L_z$  [ $\text{\AA}$ ]
- $L_z = 6.1 - 8.7 \text{ \AA}$
- K-points, two special points
- $E_{\text{cut}} = 40 \text{ Ry}$
- Plane Waves up to 36 GPa basis functions
- Up to 370 Mbytes CPU on T90 @ SDSC

#### Simulation Results

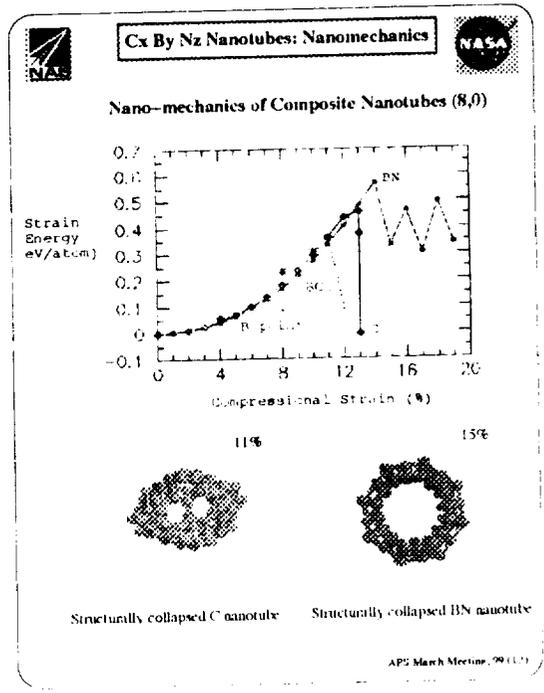
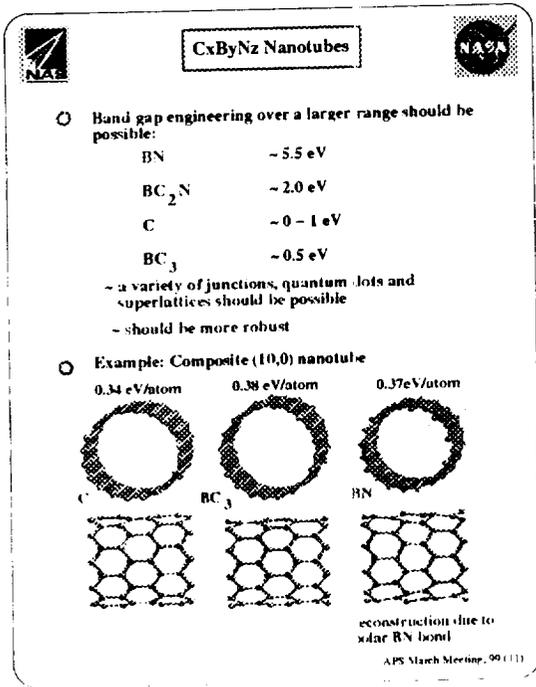
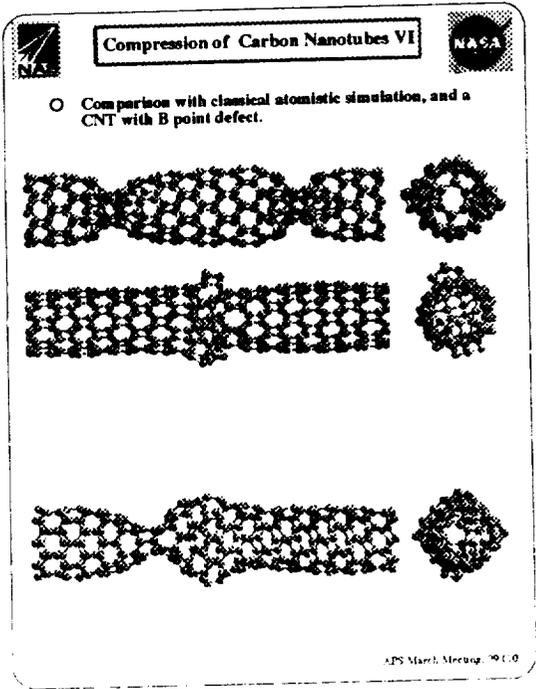
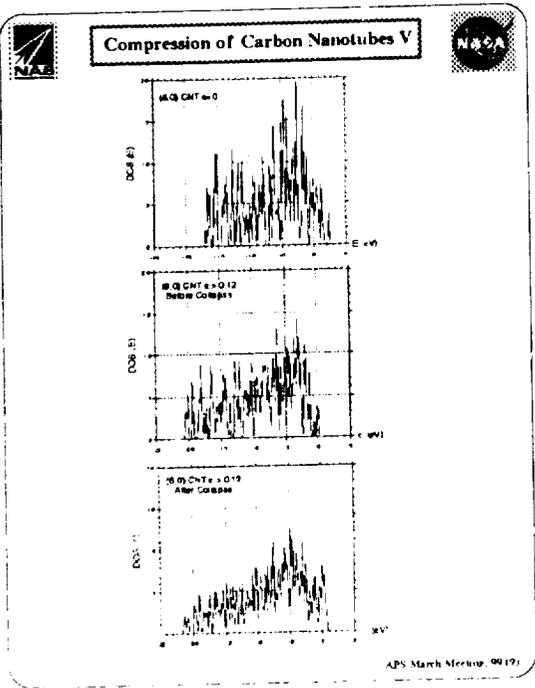
- Energy per C atom:

$$\epsilon = 0, \quad E(\text{C atom}) = -154.72 \text{ eV}$$

$$\epsilon > 0.12, \quad \begin{array}{l} \text{Before Collapse} \\ E(\text{C atom}) = -153.81 \text{ eV} \\ \text{After Collapse} \\ E(\text{C atom}) = -153.76 \text{ eV} \end{array}$$

- $K = 80.80 \text{ eV}$  in  $E(\text{C atom}) = K\epsilon^2/2$
- Equivalent Young's modulus:  $Y = 1.3 \text{ TPa}$
- Energy increase of collapsed section: 3.0 eV
- Strain energy decrease:  $58.2 (2n-1)/n$  [eV], where  $n$  is the number of center CNT units

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**Comments:**

o **Compression of 'thin' Carbon nanotubes:**

- a novel route to plasticity of carbon nanotubes via collapse of nanotube is observed which is in agreement with recent experimental findings.
- the plasticity occurs via graphitic (sp<sup>2</sup>) to diamond like (sp<sup>3</sup>) transition at the location of the collapse.
- this limits the elastic behavior of compressed nanotubes to within 12% strain (120 GPa critical stress) before the tube collapses plastically.
- these results have implications in engineering of nanotube based composite materials as well as nano-electromechanical systems.

o **Compression of heterotomic nanotubes:**

- B point defect tends to localize the position of the collapse at the position of the defect.
- equivalent BN nanotube has similar strength and higher elastic limit than carbon nanotubes.

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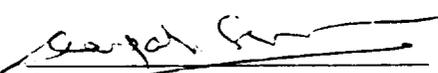
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Deepak Srivastava

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**Nanomechanics of Carbon and CxByNz Nanotubes: via a Quantum Molecular Dynamics Method**

Title

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Author(s)

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