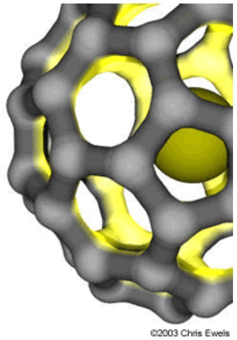


Computational Multiscale Mechanics Laboratory (CMML)

Nanoscale

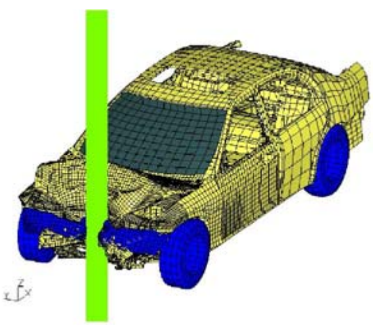
Shaoping Xiao, Assistant Professor

Mesoscale

Microscale

Department of Mechanical and Industrial Engineering
Center for Computer-Aided Design
The University of Iowa
TEL: 319-335-6009 FAX: 319-335-5669
Email: shaoping-xiao@uiowa.edu
Website: www.engineering.uiowa.edu/~sxiao

Macroscale



Research assistants:

Weixuan Yang, PhD student
Maciej Rysz, Undergraduate student

Former student:

Wenyi Hou (PhD, Caterpillar)

Meshfree particle methods (Macro-scale ~1m)

- Treatment of large deformations and fractures
- Stability Analysis
- A coupling method of meshfree particle method with finite element method

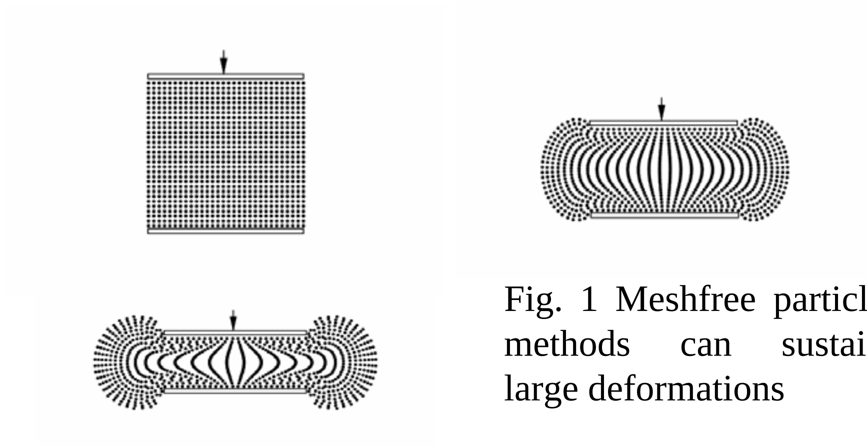


Fig. 1 Meshfree particle methods can sustain large deformations

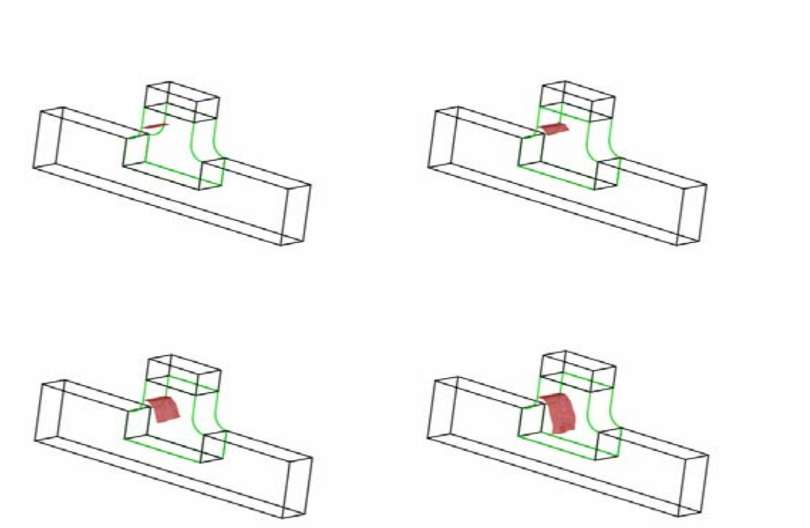
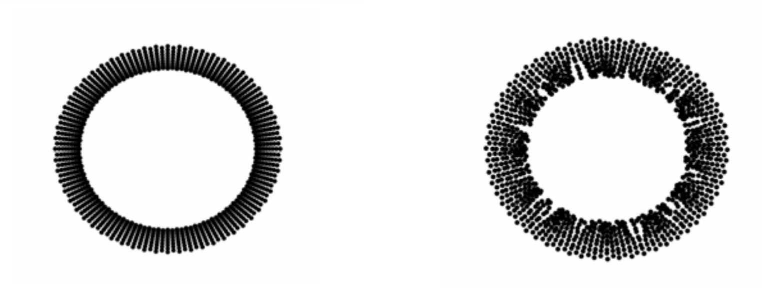


Fig. 2 Meshfree particle method coupled with FEM for 3D crack propagation



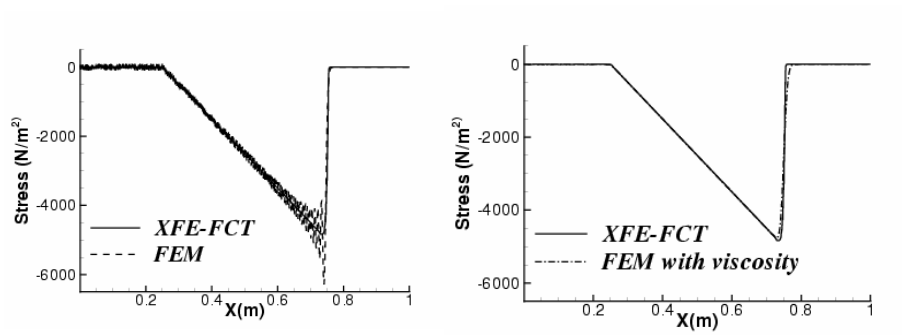
(a) Lagrangian kernel (b) Eulerian kernel

Fig. 3 Rubber ring extension shows that meshfree particle method with Lagrangian kernel (a) is more stable than with Eulerian kernel (b)

- Rabczuk, *et. al.*, *Communications for Numerical Methods in Engineering*, Vol 22(10), 2006, pp 1031-1065
- Xiao and Belytschko, *Advances in Mathematical computation*, Vol 23, 2005, pp 171-190
- Rabczuk, *et. al.*, *Computer Methods in Applied Mechanics and Engineering*, Vol. 193, 2004, pp. 1035-1063
- Belytschko and Xiao, *Computers and Mathematics with Applications*, Vol. 43(3-5), 2002, pp.329-350

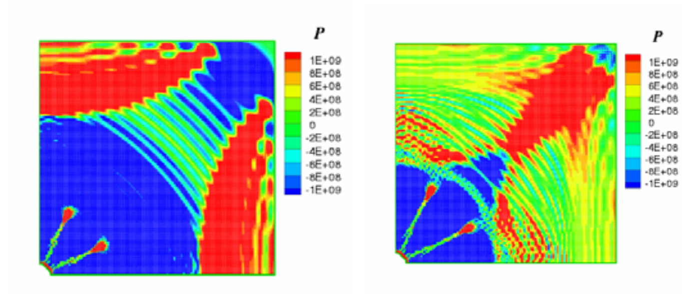
FE-FCT method and dynamic fracture (Macro-scale ~1m)

- Treatment of shock wave propagation and interaction as well as dynamic fracture such as spallation
- A total Lagrangian FE method with structured mesh
- An implicit function is used to describe the arbitrary boundaries
- The flux-corrected transport (FCT) algorithm is used to eliminate the oscillations behind shock wave fronts

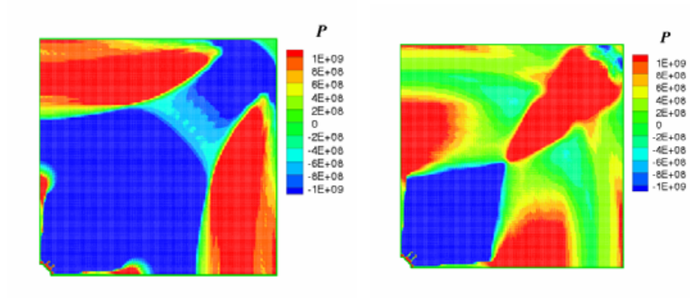


	Theoretical analysis	FE-FCT method	FE with viscosity	FE method
Spall thickness	0.225m	0.226m	0.230m	0.201m

Fig. 4 The FE-FCT method can eliminate the fluctuations as well as keep strong discontinuities. This non-oscillatory method can accurately predict spallation and spall thickness.



(a) FE method



(b) FE-FCT method

Fig. 5 A plate with a central hole with explosion occurring along the circumference of the hole. The fluctuation behind shock wave fronts is observed when performing the conventional FE method. However, the FE-FCT method can eliminate the fluctuation and accurately describe the shock wave propagation and interaction.

- Xiao, *Communications for Numerical Methods in Engineering*, Vol 23, 2007, pp 71-84
- Xiao, *International Journal for Numerical Methods in Engineering*, Vol 66, 2006, pp 364-380
- Xiao, *Wave Motion*, Vol 40, 2004, pp 263-276

Topological optimization (Meso-scale ~1mm):

- Structured extended finite element method
- An implicit function is used to describe the boundary
- The method can describe hole creation and emerging

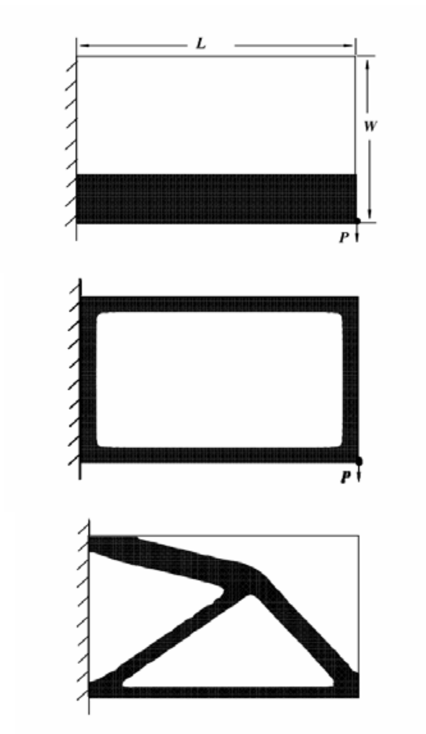


Fig. 6 optimal design can be obtained no matter what initial design is given

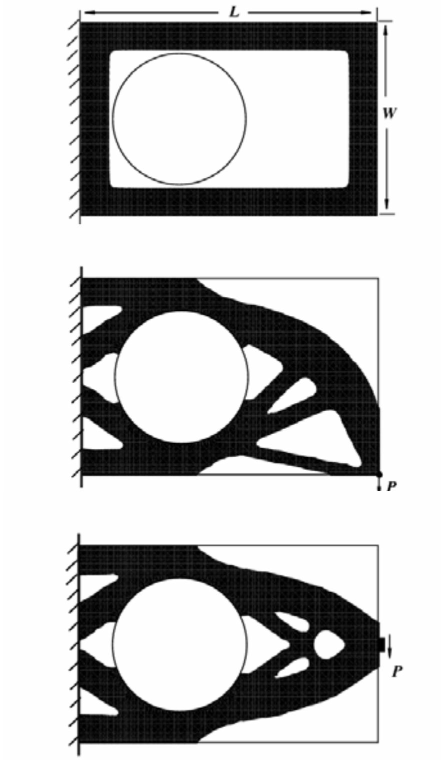


Fig. 7 optimal designs of structures contain a hole with different loads

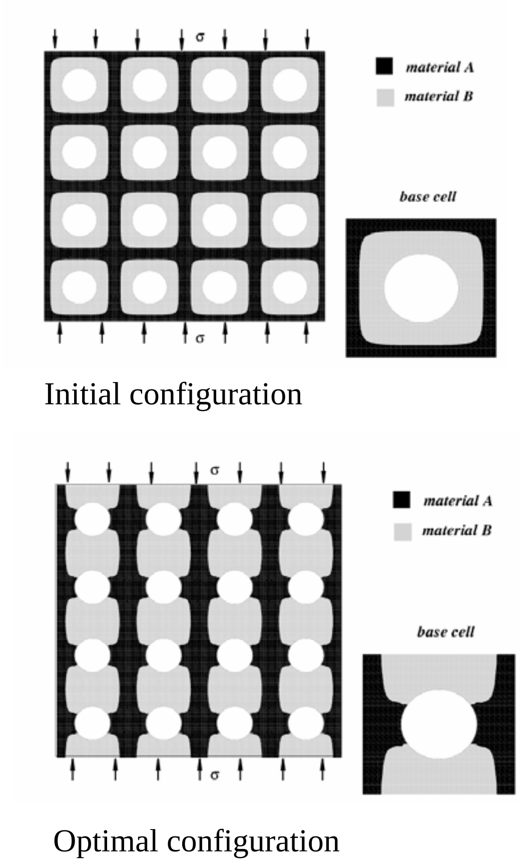


Fig. 8 optimal design of a composite with holes. The simulation is performed on a unit cell

- Belytschko, *et. al.*, *International Journal for Numerical Methods in Engineering*, Vol. 57, 2003, pp.1177-1196

Cell mechanics (Micro-scale ~1μm)

- Understanding mechanics of cultured endothelial cells in response to PKC activation.
- The tensegrity model ignores the contributions of the cell shell, the cytoplasm and the nucleus .
- A structural model of the filamentous cytoskeleton that integrates and considers additional elements, such as the cell shell, the cytoplasm and the nucleus, is proposed.

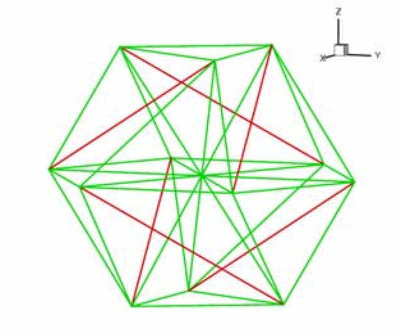


Fig. 9 Tensegrity model of a single cell

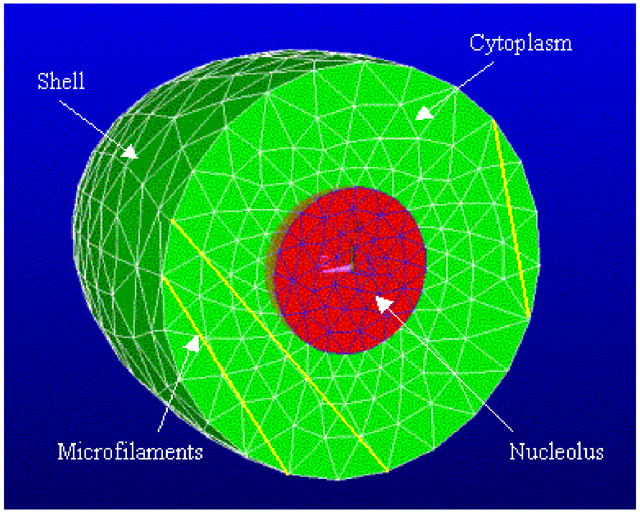


Fig. 10 A finite element model of living cells

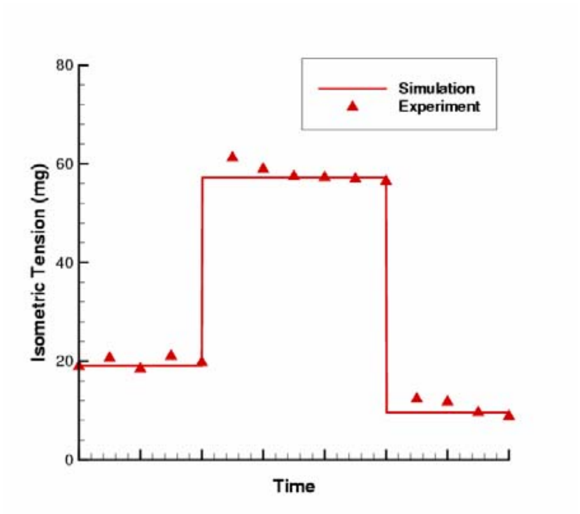


Fig. 11 evolution of isometric tension of a cell sheet in response to thrombin and cytochalasin activation

Temperature-related homogenization (Micro-scale ~1μm)

- Temperature-related Cauchy-Born (TCB) rule considering the free energy instead of the potential
- Assumptions: 1) atoms have locally homogeneous deformation; 2) atoms have the same local vibration modes; 3) the vibration of an atom is harmonic; and 4) coupled vibration of different atoms is negligible
- Verifications and material stability analysis

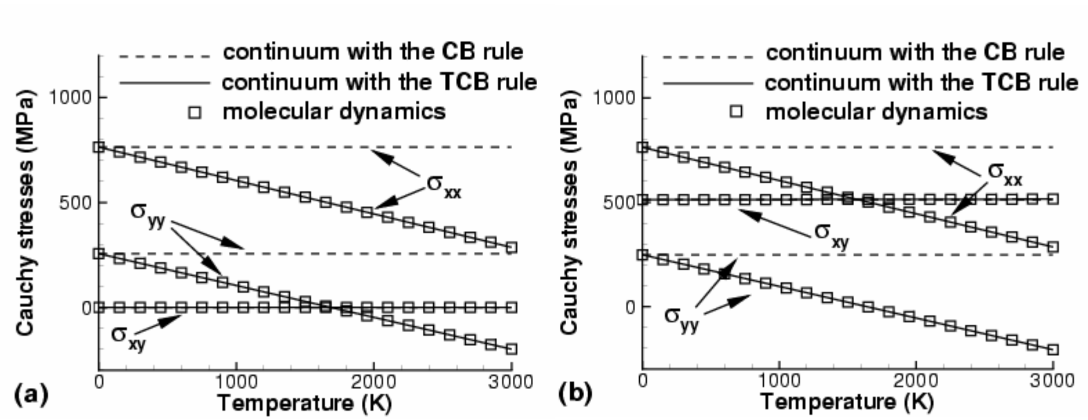


Fig. 12 Comparison of Cauchy stress components at various temperatures in a two-dimensional Lennard-Jones crystal subjected to the following deformation gradients: (a) F11 = 1.001, F12=F21 = 0.0, F22 =1.0; and (b) F11=1.001, F12 = 0.002, F21=0.0, F22=1.0

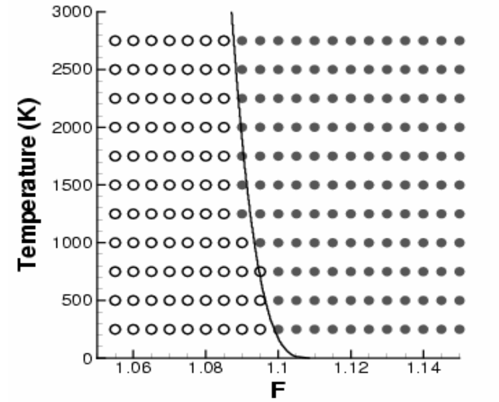


Fig. 13 Stable domain of 1-D molecular chain

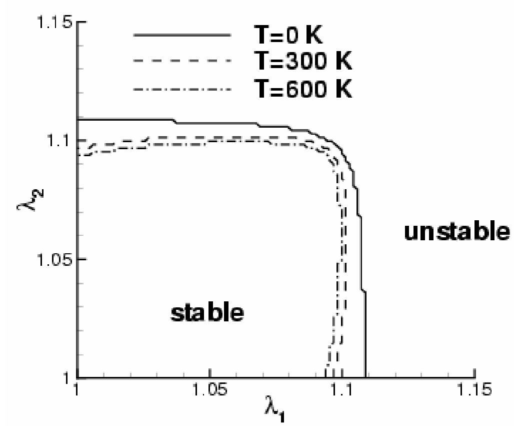
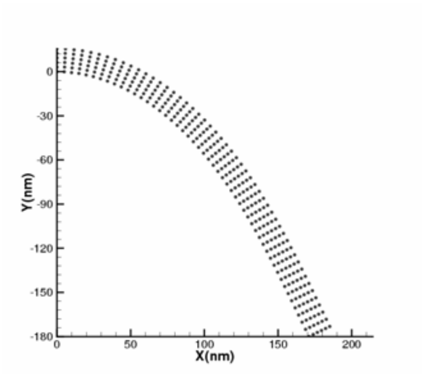


Fig. 14 Stable domain of 2D LJ crystal

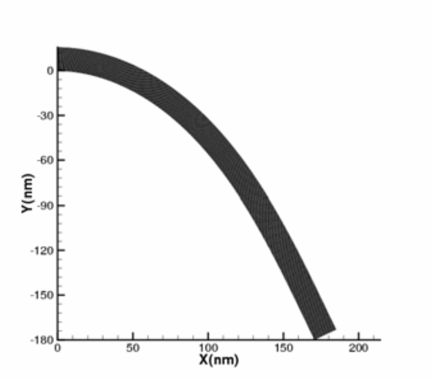
- Xiao and Yang, *International Journal for Numerical Methods in Engineering*, Vol 69, 2007, 2099-2125
- Xiao and Yang, *Computational Materials Science*, Vol 37, 2006, pp 374-379

A hierarchical multiscale method (Micro/Nano-scales ~1μm-1nm)

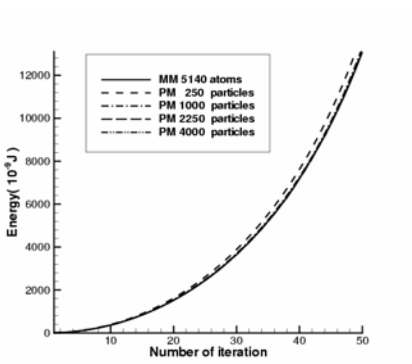
- The meshfree particle methods with the implementation of a homogenization technique
- A temperature-related Cauchy-Born rule



(a)



(b)



(c)

Fig. 15 Bending of a nanobeam. The meshfree particle method result (a) compares well with the molecular mechanics result (b). The comparison of the potential evolution (c) supports the above conclusion

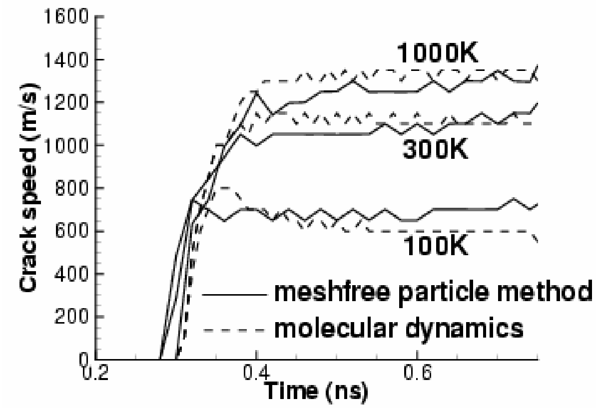


Fig. 16 The calculated temperature-dependent crack speeds are compared well with the results of MD simulations.

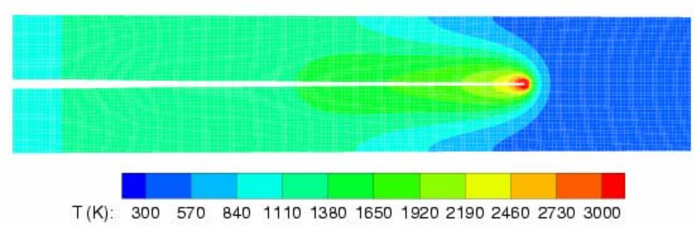


Fig. 17 temperature profile when the crack propagating

- Xiao and Yang, *International Journal for Numerical Methods in Engineering*, Vol 69, 2007, 2099-2125
- Xiao and Yang, *The International Journal of Computational Science and Engineering*, Vol 2(3-4), 2006, 213-220
- Xiao and Yang, *International Journal of Computational Methods*, Vol. 2(3), 2005, pp. 293-313

A concurrent multiscale method (Micro/Nano-scales ~1μm-1nm)

- A bridging domain coupling method
- Molecular domains and continuum domains are overlapped via bridging domains
- An explicit algorithm is developed so that the nonphysical spurious reflection phenomena can be avoided.

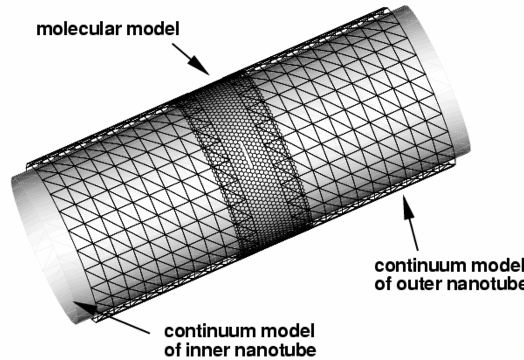


Fig. 19 Bridging domain multiscale modeling for multi-walled carbon nanotube fracture

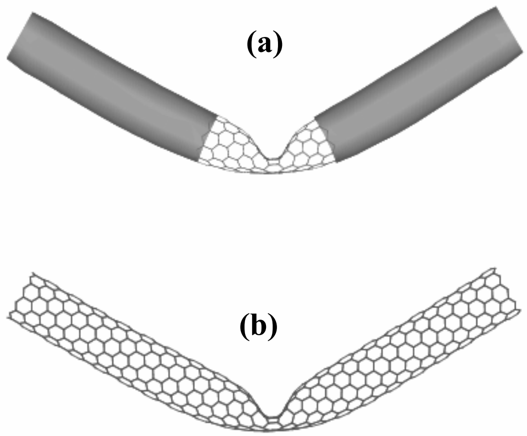
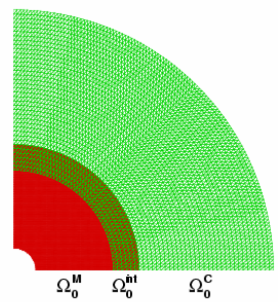
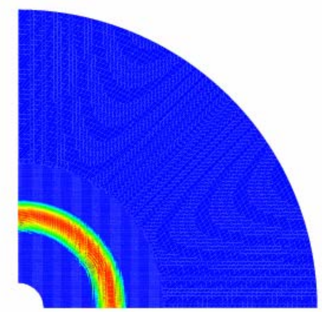


Fig. 18 Bending of a single-walled carbon nanotube: (a) Bridging domain coupling method simulation; (b) molecular mechanics calculation





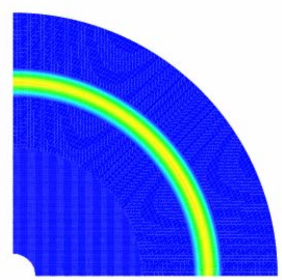


Fig. 20 A circular plate with a central hole with a pulse loaded along the hole. No spurious wave reflection is observed when waves propagate from molecular domain (red) to continuum domain (green)

- Xiao and Belytschko, *Computer Methods in Applied Mechanics and Engineering*, Vol. 193, 2004, pp. 1645-1669
- Belytschko and Xiao, *Journal of Multiscale Computational Engineering*, Vol. 1(1), 2003, pp.115-126

Mechanics of nanotubes (Nano-scale ~1nm)

- Size effects on carbon nanotubes' mechanical properties
- Mechanics of Defect-free and defective carbon nanotubes (CNTs)
- Vacancy defects can dramatically reduce nanotube strength

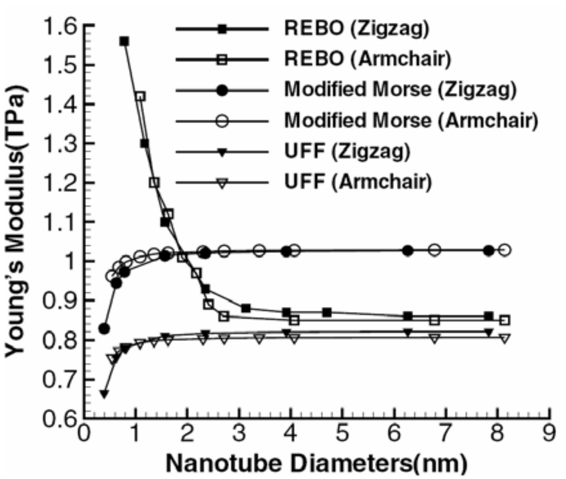


Fig. 21 Studies of size effects on the Young's modulus of a single-walled carbon nanotube. Three potential functions are used in atomistic simulations. The trend confliction is observed for different potential functions.

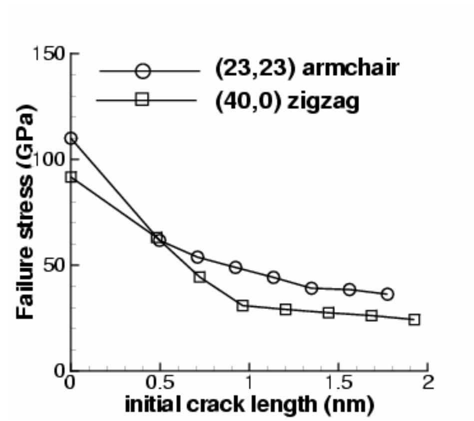
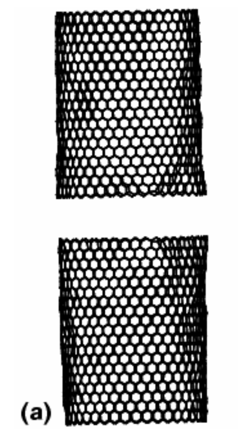


Fig. 22 Failure stresses of defected nanotubes at 300K



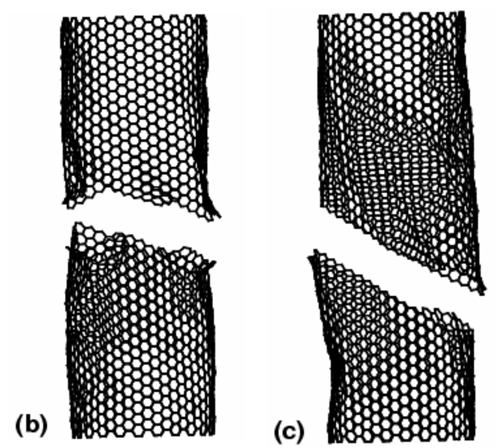


Fig. 23 Fracture modes of (a) a (40,0) zigzag nanotube with an initial crack of length 0.48 nm (Mode I fracture); (b) a (23,23) armchair nanotube with an initial crack of length 0.48nm (Mode I fracture); (c) a (23,23) armchair nanotube with an initial crack of length 0.92nm (Mixed Mode I/II fracture).

- Xiao and Hou, *Physical Review B*, Vol 73, 2006, 115406
- Xiao and Hou, *Fullerenes, Nanotubes, and Carbon Nanostructures* , Vol 14, 2006, pp 9-16
- Mielke *et. al.*, *Chemical Physics Letters*, Vol 390, 2004, pp 413-420
- Belytschko et. al., *Physical Review B*, Vol 65, 2002, 235430

Mechanics of defected nanotubes (Nano-scale ~1nm)

- Vacancy defects are randomly located on nanotubes
- Reliability analysis of nanotubes is conducted
- Bending and torsion of nanotubes are also studied

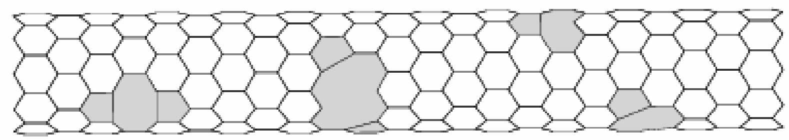


Fig. 24 Configuration of a (10,0) nanotube containing randomly located vacancy defects

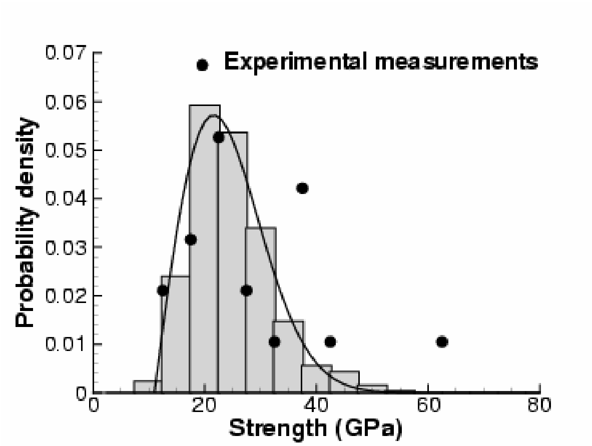


Fig. 25 Probability distribution of nanotube strength at the room temperature of 300K

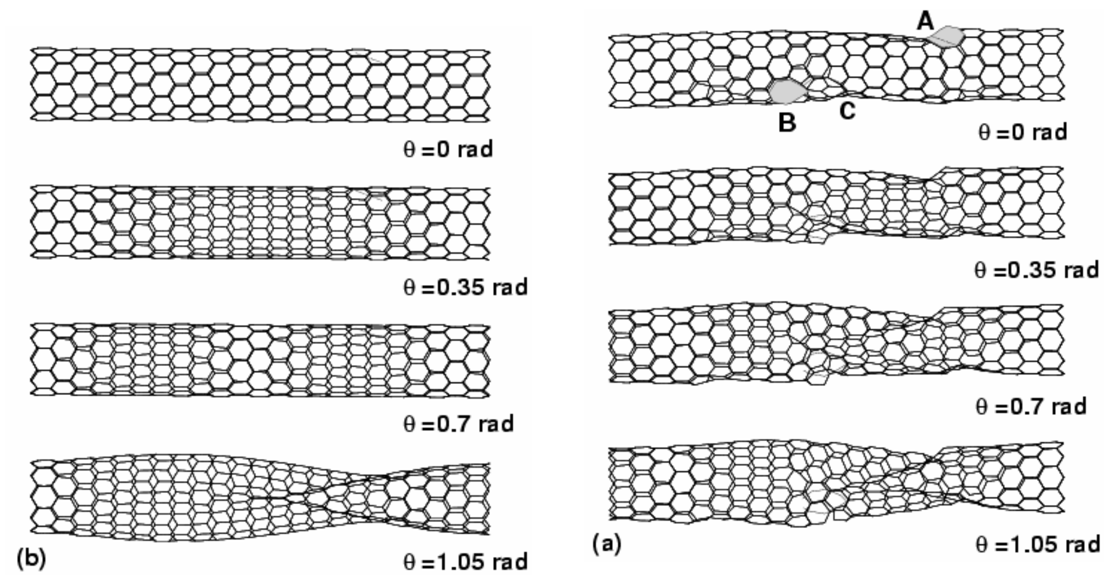


Fig. 26 The evolutions of the configuration of (a) a vacancy-defected (10,0) nanotube and (b) a pristine (10,0) nanotube

- Xiao and Hou, submitted to *Journal of Nanoscience and Nanotechnology, 2007*

Mechanics of nanotube reinforced composites (Nano-scale ~1nm)

- Embedded nanotubes are supposed to reinforce strength of composites
- Effects of the volume fraction of embedded nanotubes are significant
- Occurrence of defects weaken instead of reinforce nanocomposites

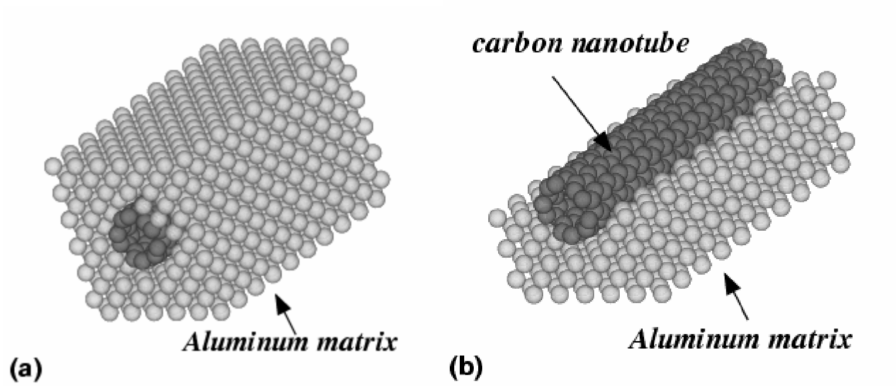


Fig. 27 Computational model of carbon nanotube/aluminum composites

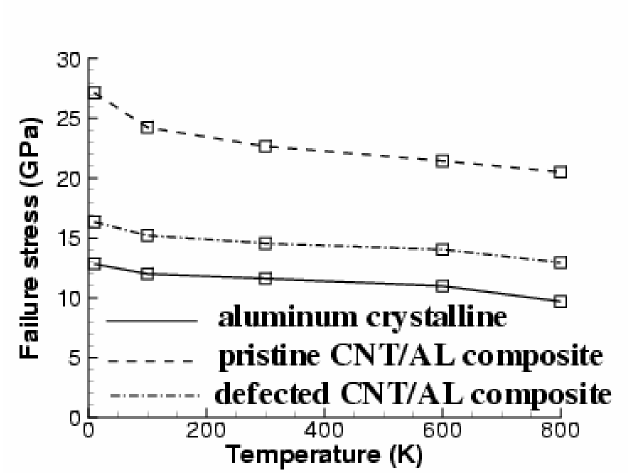


Fig. 28 Failure stresses of nanocomposites compared with those of aluminum crystalline

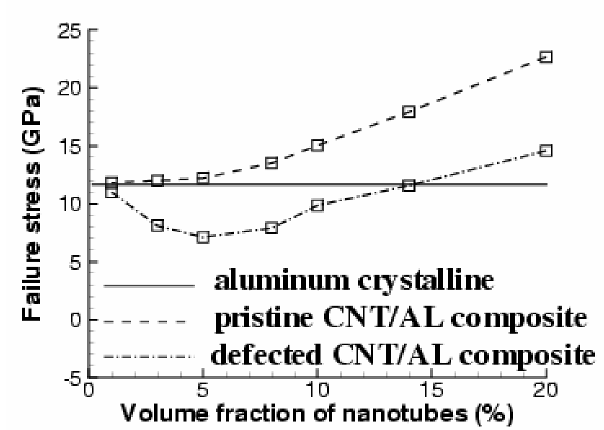


Fig. 29 Effects of volume fraction of embedded nanotubes on strength of CNT/Al composites

- Xiao and Hou, *Physical Review B*, Vol 73, 2006, 115406

Mechanics of nanotube reinforced composites (Nano-scale ~1nm)

- Multiscale modeling and simulation
- SWNT, MWNT, and SWNT bundles are considered

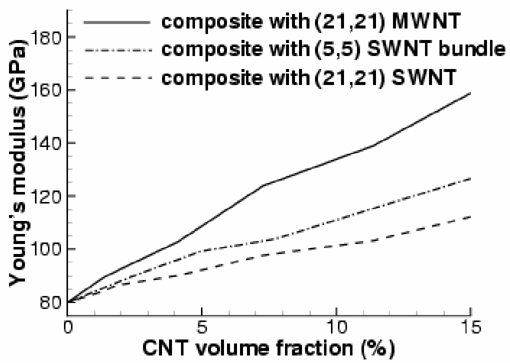


Fig. 31 Young's moduli of composites

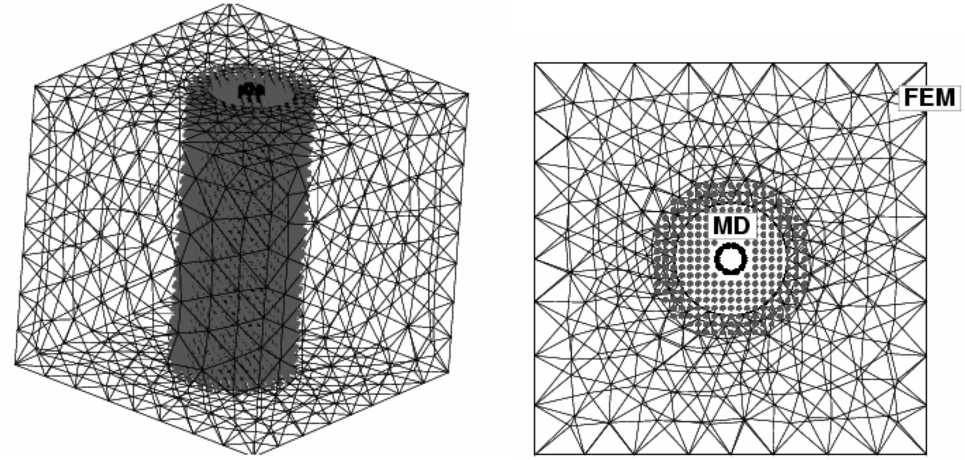


Fig. 30 multiscale model of CNT/Al composites

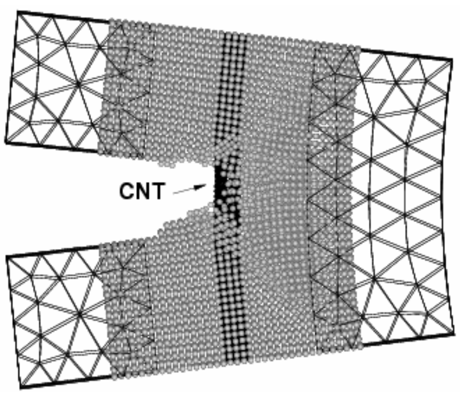


Fig. 32 CNT can resist crack propagation in composites

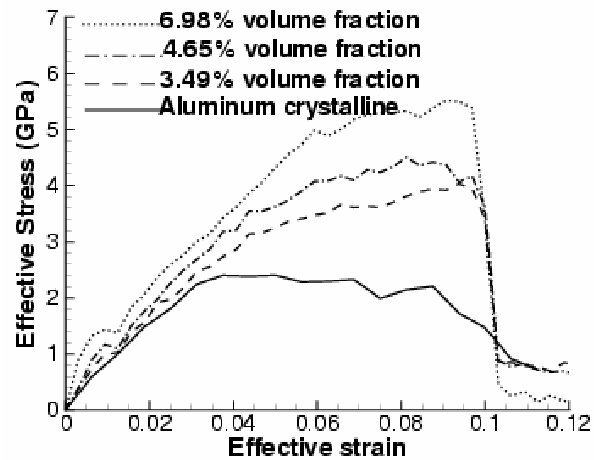
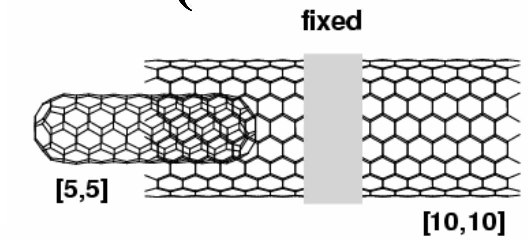


Fig. 33 stress-strain relations when materials subject to mode I fracture

- Xiao and Hou, *International Journal for Multiscale Computational Engineering,* submitted, 2007

Nanoelectromechanical systems (Nano-scale ~1nm)

- Nanotube-based oscillators can have high frequency
- They may stop at finite temperatures
- A NEMS design as memory cells is proposed



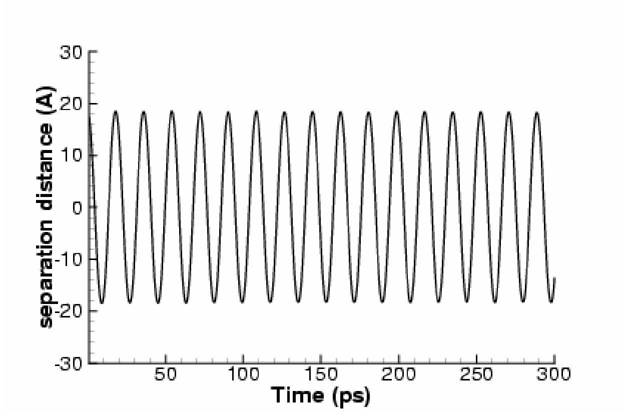


Fig. 34 A [5,5]/[10,10] nanotube-based oscillator can have a frequency of 55 GHz when it is isolated with a zero initial temperature

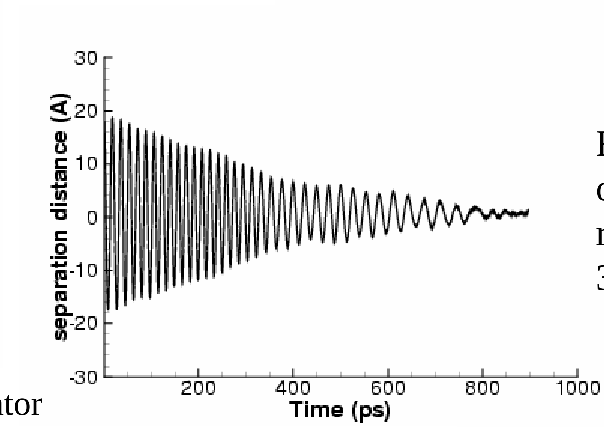


Fig. 35 The nano-oscillator stops at the room temperature of 300K

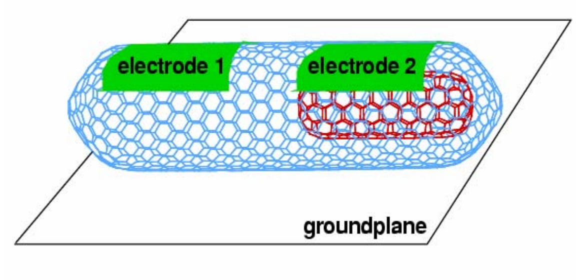
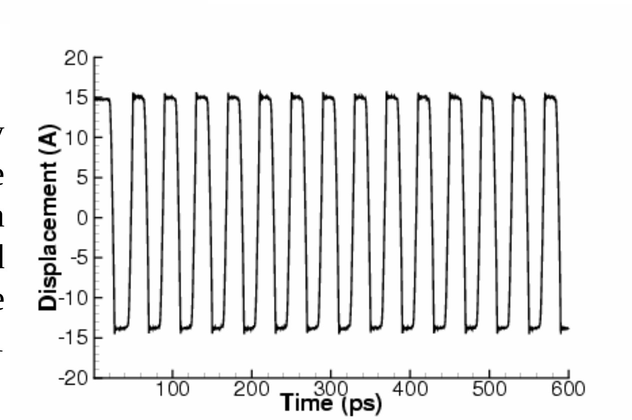


Fig. 36 A NEMS for memory cells (above). When a voltage pulse applied on electrodes, a stable oscillation can be observed (right). Such mechanism can be read as switchable logic 0/1 signals.



- Xiao *et. al.*, *International Journal of Computational and Theoretical Nanoscience, Vol. 3, 2006, pp 142-147*
- Xiao *et. al.*, *International Journal of Nanoscience*, Vol 5(1), 2006, pp 47-55

Nanotube-based resonant oscillator (Nano-scale ~1nm)

- Multiscale modeling and simulation of nanotube-based resonant oscillator
- Comparing well with experimental results
- Energy dissipation depending on the resonance frequency

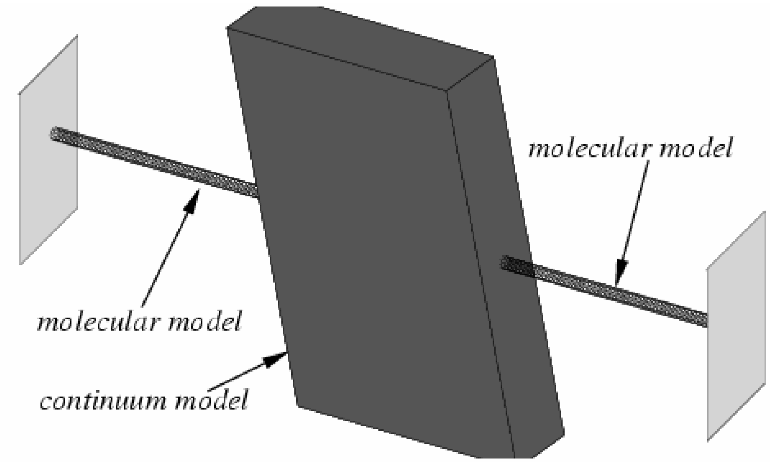


Fig. 37 Multiscale modeling of resonant oscillators

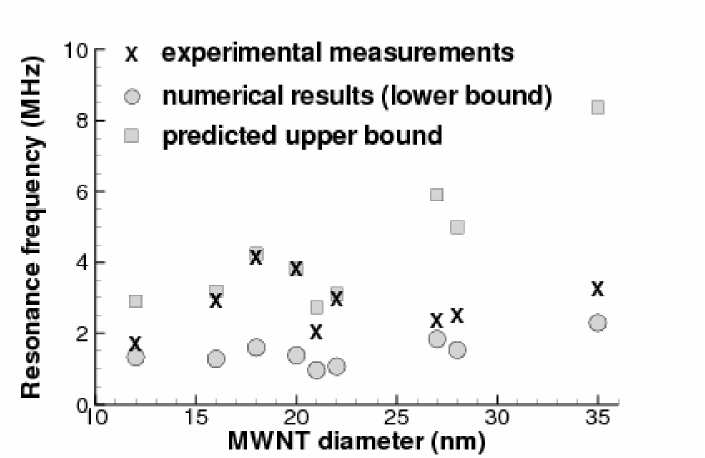
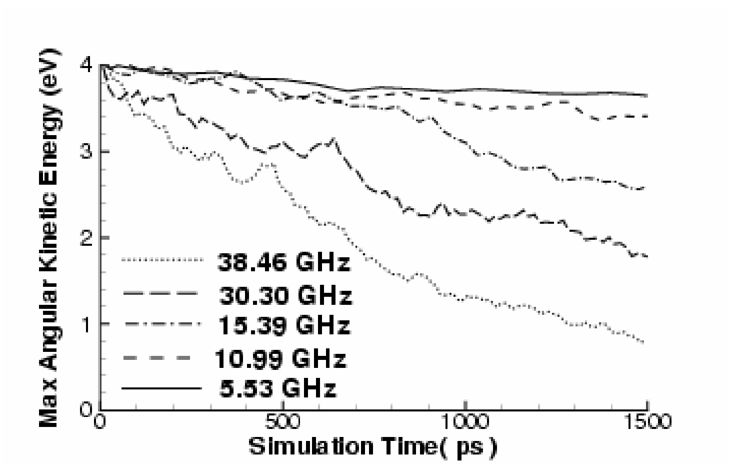


Fig. 38 Comparison with experiments (Papadakis et. al. 2004)

Fig. 39 Effects of resonance frequencies on energy dissipation (right)



- Xiao and Hou, *Nanoscale research letters, Vol 2(1)*, 2007, 54-59
- Xiao and Hou, *Physical Review B, Vol 75*, 2007, 125414