HPC Innovation for Nanotechnology

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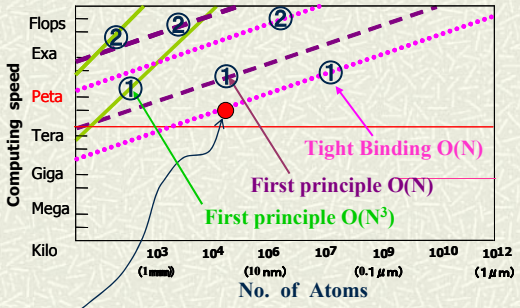
Nanotechnology: Complex System

- **Nanotechnology**: Manipulating atoms and molecules, and creating noble materials and devices
  - >> Synthesizing: Nanotubes, fullerenes--- strategic materials.
  - >> Self-Assembling : Emerging Engineering-Process
- **Multi-Scale, -Disciplinary** : Nano → Our real scale
- **Complex** combination of classical physics and quantum mechanics.
- At each stage in hierarchy, new laws and concepts are needed.

Nature is not a simple extrapolation from the properties of a few atoms or molecules !

- **Fast, Large–scale simulation is indispensable for multi-scale and disciplinary, complex-system.**

Large-Scale Simulation in Nanotechnology: Fast computing is required for Quantum MD Simulation.



Iterative steps : 10^6 (①) , 10^{12} (②)
>> Cal. volume

CPU time : One month

CPUtime=Cal. Volume /Computer speed

As a actual example, thermal conductivity simulation is plotted …

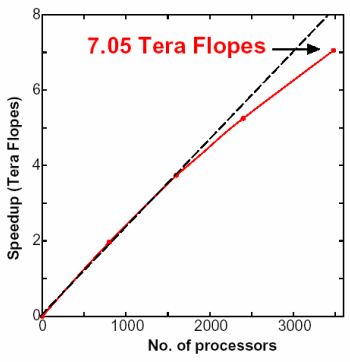
CNT Len.(nm)	Atoms	Requirement Resource	Days
140	48,000	128nodes × 12h × 69	35

Earth Simulator

10^6 iterations

Speed: A Big Tool for LS Simulation !

Example: Thermal Conductivity of CNT



Optimization up to 3480 processors
Vector ratio : 97.7%
Parallel ratio : 99.99%
Total Performance : 7.05TeraFlops

PC: 3 years → ES: 2 hours

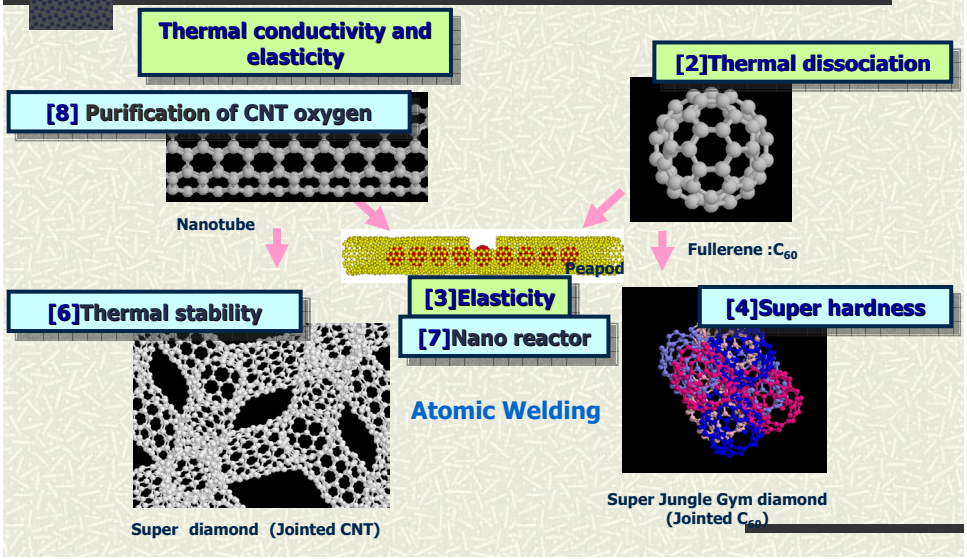
18,000 times faster

Surprise !

Speed of Earth Simulator

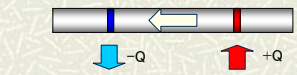
→ A Big Tool for Nanotechnology !

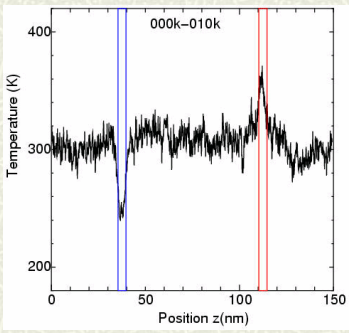
Simulations of Nanocarbons on Earth Simulator



Thermal Conductivity on CNT

Ballistic conductance



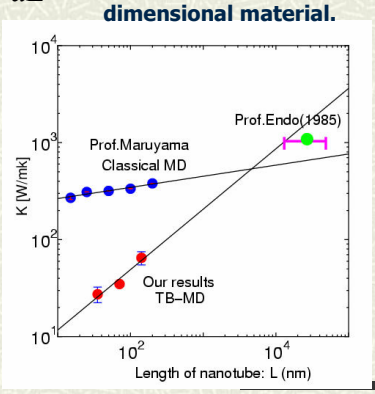


Power-low Dependence:

$$\kappa_L = aL^{\alpha}$$

(1) The thermal conductivity increases as dose the length.

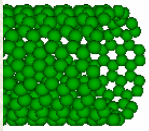
(2) Power low dependency shows the character of the one dimensional material.



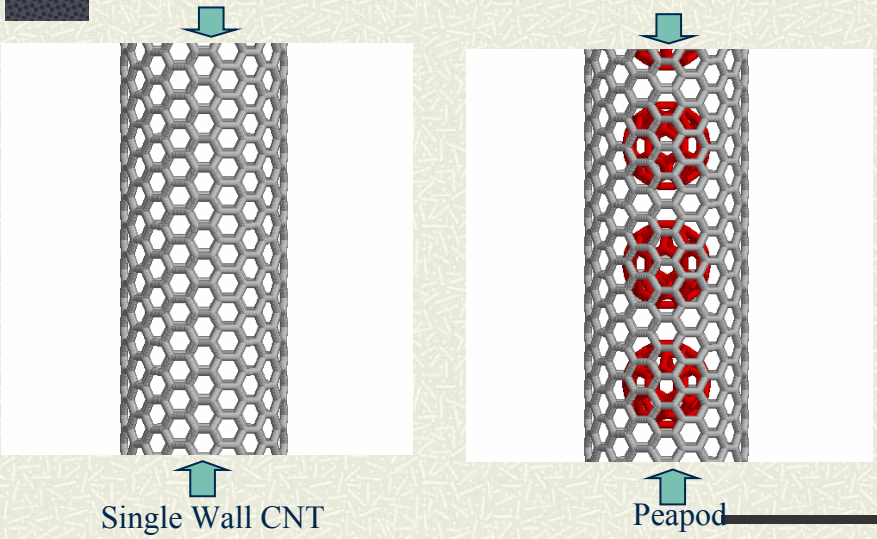
Elasticity on CNTs

Axial Compression of CNT and Peapod

- Computational procedure
  - ① Stretch CNT and fix it's length.
  - ② Relax atoms with given length until $\vec{F} \fallingdotseq \vec{0}$.
  - Reiterate the procedure ① and ②. Potential energy goes down due to change structure



Axial Compression of CNT and Peapod



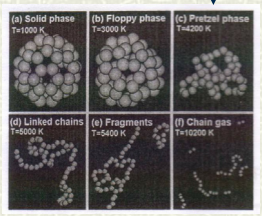
Thermal Dissociation of Fullerene

(1) Simulation was carried out until 150ps each temperature.
(16 Nodes × 12h × 10 samples)

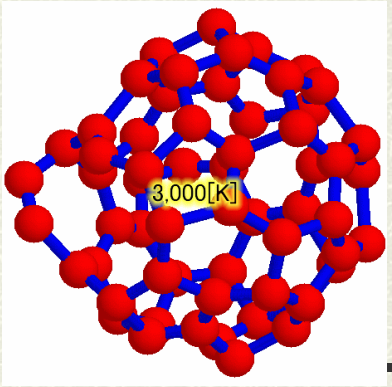
(2) Our results agree with that of experiment, 3550k.

(3) Enough simulation time is needed for the reliable estimation on thermal stability

4200K



PRL1994、S.G.Kim and D. Tomanek

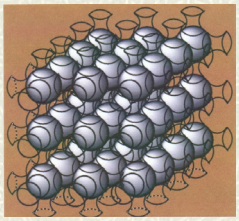


Application:
Electronic devices

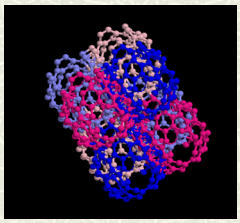
Super Diamond with Jungle Gym Structure

Negative Gaussian Curvature of the surface !

First-Principles Method（DFT-PW、RIST）



(1) Bulk Elastic modulus
(25 % of natural diamond)
(2) Mass density
(20 % of natural diamond)
(3) Band Gap
(0.5eV)



Light and hard 3-d semi-conductor!

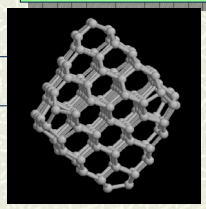
ES:80PEs × 40h

Application:
・lubricant / bearing surface / hard coating /corrosion protection

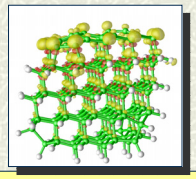
Nanodiamond Processing

How to promote the diamond growth to the micron scale from nanodiamonds ?

Diamond Structure



Diamond structure is stabilized by electron charging

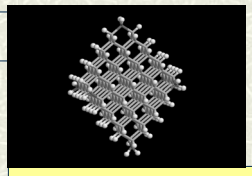


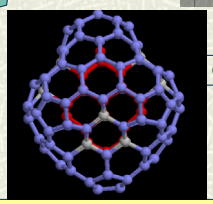
Continuous growth of diamond

ES:10nodes×40h

By hydrogen

Hydrogen covered





Onion structure

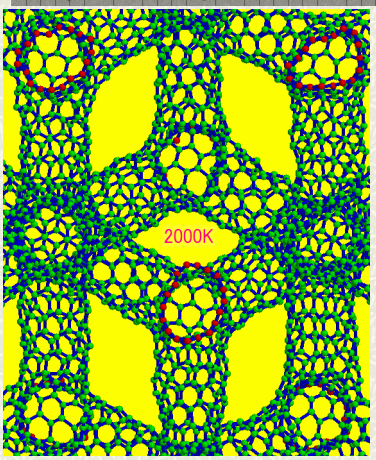
Diamond surfaces reconstruct into fullerene-like sp^2 surface

ES:10nodes×40h

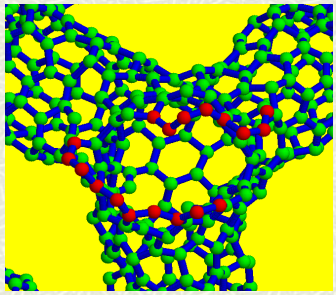
Growth Stop!

Thermal Stability on Joints of Super-diamond Structure

Are joints of Super-diamond stable at high temperatures ?



No. of atoms :3372



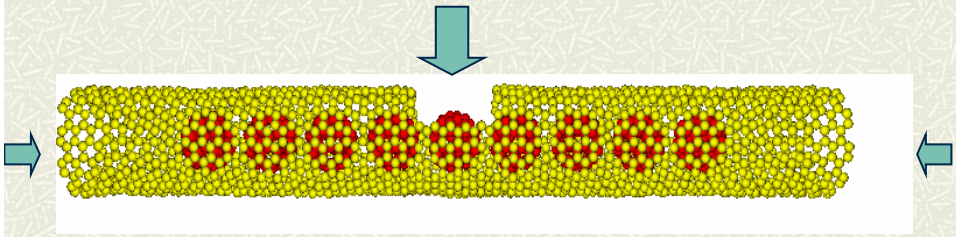
3, 500K

Super-diamond is stable up to 3500k.

Application:
・Nano Reactor

Mechanical Stability of Peapod

Is CNT useful as nano scale reactor ?



⇒The encapsulation of fullerenes are stable even if the wall and cap has defect and opening.

Ignite HPC Innovation

For solving complex & large scale problems and unseen models of noble phenomena in nano science & technology,

- Need new HPC machines,
  - With sufficient speed & memory and flexible architecture.
- Igniting new HPC machines, step by step,
  - Through contemporary and emerging **nanotechnology**
- ***A new machine Makes next new machines !!***

Nanotechnology: It may be Our Ground !

- HPC boosts Nanotechnology
  - with Fast & Large-Scale Simulations.
- Nanotechnology improves HPC Innovation
  - Through powerful & new horizontal nano-electronic devices…
- Collaborations are indispensable
  - Between HPC folks and Nanotechnologists,
  - Internationally

Proposals for *Bridging Communities*

- Nanotechnology as world-class challenge problems:
- Next BOF meeting: SC2004 Pittsburgh,
- Need to exchange recent progresses between HPC and Nanotechnologist
- Through computational nanotechnology,
- For bridging communities.
- *If possible, International Conference on Computational Nanotechnology*