Large Scale Simulations for Carbon Nanotubes

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Carbon nanotubes (CNTs) and fullerenes have a lot of potential applications in nanotechnology. In the stream of efforts to exploit these nanoscale materials, the computational simulations have turned out to be powerful and efficient tools. Especially, as the recent trend in technology made it possible to manipulate a further miniaturized structures, required simulations for emerging material become lager and lager. Aiming at realistic simulations for nanomaterials, we have developed a large-scale computation technique utilizing tight-binding molecular dynamic method, *ab initio* density functional theory (DFT), and time-dependent DFT method.

We have studied various physical properties of nano-carbon material e.g., Mechanical properties of CNT, transformation of structure of fullerens inside CNT and carrier Lifetime in CNT.

During these works, we have realized that the Earth Simulator is very powerful tool for large-scale material simulations.

Keywords: Large scale simulation, TB theory, *ab initio* theory, DFT, Carbon Nanotube, Nano Diamond, Mechanical Properties

1. INTRODUCTION

Carbon materials have been expected to make a breakthrough in material science and nanotechnology. A lot of potential applications of nanotubes and fullerenes e.g., electronic field emitter and electronic devices have attracted scientific community. In the investigation and utilizing their material properties, numerical simulation using supercomputer has turned out to be a very efficient tool. A recent development in nanotechnology has required more efficient supercomputing capable of a large-scale simulation of up to 10^4 atoms.

Aiming at large-scale simulations utilizing Earth Simulator, we have developed computational software package based on *ab initio* DFT theory and parameterized tight-binding (TB) method. The TB code we have developed is shown to be suitable for the very large systems despite of the lack of symmetrical arrangement. We have carried out three subjects in this work, which are described in the next section. Our purpose is to give the clear explanation of properties and phenomena of nano-scale events and deduce guiding principle to design new materials from nano-structures using super-computers.

2. PHYSICAL STUDIES ON NANOMATERIALS

2.1. Mechanical Properties of CNT

It has been suggested that the tensile strength of carbon nanotubes might exceed that of other known fibers because of the inherent strength of the carbon-carbon bond. So nanotubes have beneficial consequences for their application in composite bulk materials and as individual elements of nanometer-scale devices and chip of sensors.

The mechanical properties of nanotubes are predicted to be sensitive to details of their structure and to the presence of defects, which means that understanding on individual nanotubes are essential to examine these properties.

A lot of simulations on compression and stretch of isolat-

ed nanotubes have been carried out. As peculiar phenomena, Young's modulus, bending, collapse, twisting and buckling are investigated on. Almost all the simulations adopt the Young's modulus based on the first principle calculation with a small number of atoms in unit cell, or deformations like an undulation based on the tight binding method under external filed for a short length nanotube. But for an undulation process of nanotube, one can speculate easily that it depends on a length of nanotube.

We investigated the undulation process of long nanotubes under axial pressures by help of a large scale tight binding simulation. For example, the number of atoms for the (10,10) nanotube is 2200. This size is ten times as large as conventional calculations. Undulation structure obtained from our simulations are very different from the previous one [1].

Our first principle calculations of the elastic properties of nanotubes also confirm that they are extremely rigid in the axial direction. The Young's modulus of (10,10) nanotube is equal to 1.06 Tera Pa. We will continue simulations on elastic properties for a variety of materials as double wall nanotube and peapod with different chiral vectors.

2.2. Structure of fullerenes inside CNT

Carbon fullerenes, such as C60, are molecules with a large range of interesting properties. Our previous simulations on thermal stability in carbon materials indicate that C60 melts at about 3500 k, while some nanotubes are still stable at the temperature. Our question raised here is about "peapod", which has a structure of one-dimensional array of C60 inside a nanotube. How fullerenes of "peapod" are changed here to a new phase? Experimental observations tell us that at high temperature fullerenes inside a nanotube connect each other forming an inner nanotube. Thus peapod turns out to be double-wall nanotube. The result indicates a potential of creating new materials by packing more complicated carbon materials, yet, the detailed mechanisms on the phenomenon is not clarified yet. This phenomenon will be deeply affected by the condition of the system temperature and pressures of inter-fullerenes. The structure simulation of fullerenes inside a nanotube is performed up to 4ps with 80,000 time steps. Figure 2 depicts initial condition and Figure 3 after 4ps. Growth to spread carbon net can be seen in the figure.

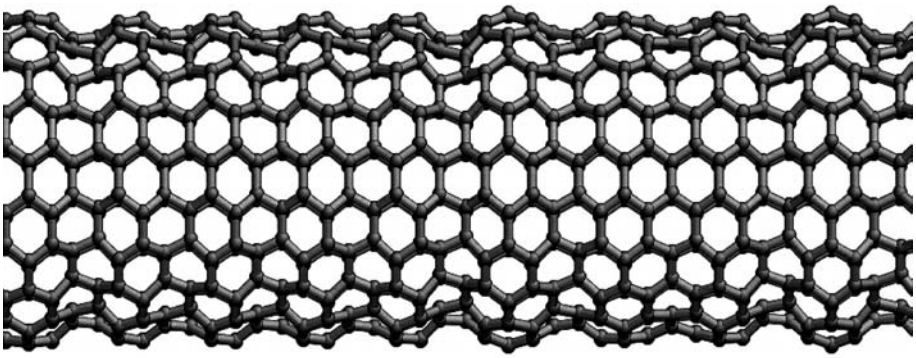

Fig. 1 Structure of nanotube by 92% compression.

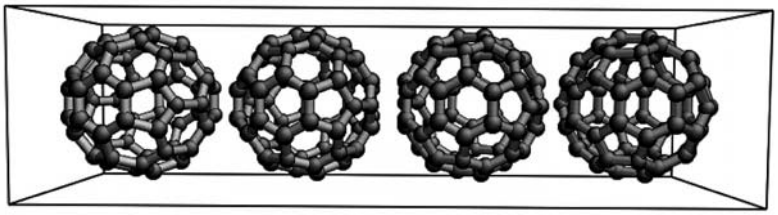

Fig. 2 Initial condition of fullerens inside a nanotube.

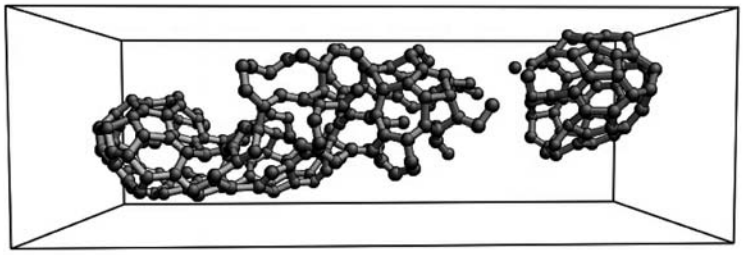

Fig. 3 Structure of fullerens inside a nanotube after 4ps at 3500k.

2.3. The Carrier Lifetime in CNT

As for device application of carbon nanotubes, the lifetime of excited carriers in nanotubes is very important information since the lifetime is a key factor for switching speed and quantum efficiency of the devices. We have investigated the carrier lifetime in carbon nanotube by performing the time-dependent density functional theory (TDDFT) being coupled with the molecular dynamics (MD). This kind of simulation can include both electron-electron and electron-phonon interaction without any adjustable parameters. Figure 4 shows the energy gap reduction of hot-hole and electron in (3,3) carbon nanotube. The decay time-constant is extremely fast, the initiation of the decay is observed at 70 fs while significant gap reduction is observed around 200 fs. We will search temperature dependence of this decay process to highlight the electron-phonon coupling in this decay process.

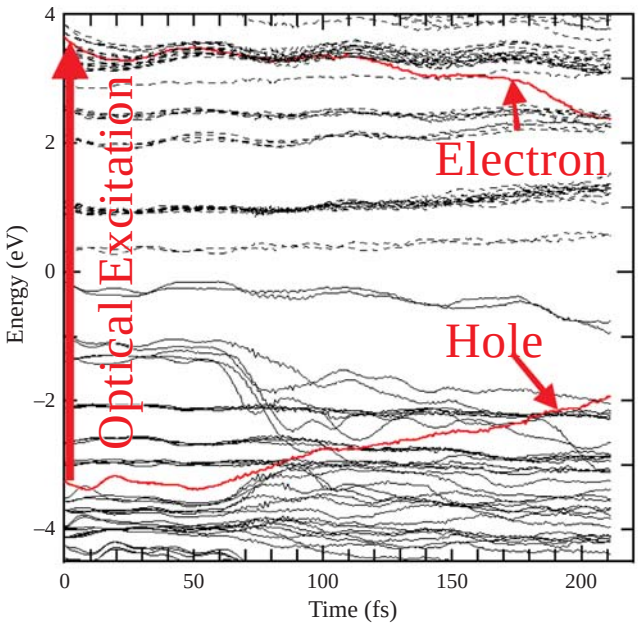

Fig. 4 The energy gap reduction of hot-hole and electron in (3,3) carbon nanotube.

References

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