ANGULAR DEPENDENCE OF PEELING A CARBON NANOTUBE FROM SILICON SUBSTRATE: STEERED MOLECULAR DYNAMICS SIMULATION AND THEORETICAL ANALYSIS

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Summary Steered molecular dynamics (SMD) simulations are performed to study adhesion and peeling of a single wall carbon nanotube (SWCNT) from a silicon substrate. The critical peel-off force is found to depend on the peeling angle. For the SWCNT under investigation, we find that the simulation results can be explained by a continuum model of an adhesive elastic band on substrate. The analysis suggests that the theoretical analytical results show a good agreement with the SMD results when the peeling angle is larger than 90º.

INTRODUCTION

With the decreasing feature size of very large scale integrated circuits (VLSI), current process technology has entered the nano stage. The feature size of interconnecting wires decreased to nano stage will face many problems including scale effect and stable reliability. Carbon nanotubes (CNTs) have huge potential superiority and applying prospect. CNTs which replace copper wire as interconnect wire in high density three-dimensional micro-electronic packaging through silicon via (TSV) technology [1]. Therefore, study on adsorption performance of the CNT/Si interface structure appears to be especially important.

As a new advanced material, carbon nanotube with its superior mechanical and electrical properties, found by Iijima [2] since 1991, already aroused wide concern of the researchers. The experimental method is difficult to study the mechanical characters of atomic-scale structures in real time due to the limitation of experiment condition. Alternatively, molecular dynamics (MD) method is now widely used for nanostructure systems. Shi et al. [3] investigated the relation between the stripping angle and the biggest stripping force by simulating the process of drawing DNA molecular from substrate with MD method. The Steered molecular dynamics (SMD) [4] is a latest atomic-scale computer modeling technique, which simulates atomic force microscopy (AFM) [5] or Single Molecule Force Spectroscopy (SMFS) [6] technique by using a virtual ideal spring to replace common loading, and record real-time parameter based on traditional molecular dynamics. Büyüköztürk et al. [7] used the SMD method to simulate the process of peeling and shearing a single molecular chain of epoxy resin on silica substrate, and they found that the relation between the maximum peel force and the peel distance appears to be linear. To the authors' knowledge, little work has been conducted on peeling a CNT on a silicon substrate.

The purpose of this article is lying in exploring adsorption properties of the CNT/Si interface in atomic scales. SMD simulations are performed to simulate the whole process of peeling single carbon nanotube on silicon substrate by combining statistical average thoughts. The influence of the peeling angle on the critical peel-off force is investigated by comparing the calculated results from the theoretical model with the SMD simulated results.

MODEL FOR PEELING

Peeling of a thin film or an elastic band from substrate has been traditionally treated by a linear elastic continuum model [8]. Here we apply such a model to interpret the simulation of peeling a single wall carbon nanotube (SWCNT) on silicon substrate.

Imagine a CNT with radius r and Young's modulus E peeling at an angle θ from a silicon substrate under a peel force increased to maximum from zero gradually (Fig. 1). Considering the energy changes of virtual peeling distance δl of the CNT, there are three aspects of the energy changes: adhesive energy change $-v_w\pi r^2\delta l$ (v_W being the unit volume of the adhesive energy); potential energy change $F(1-\cos\theta)\delta l$ (assuming the CNT to be inextensible); elastic energy change $F^2\delta l/2\pi r^2E$ (consisting of two components: A component $F^2\delta l/\pi r^2E$ which is the work done at constant force in peeling the region δl, and a component $-F^2\delta l/2\pi r^2E$ which is the amount of recoverable strain energy stored in the peeled carbons. Adding up all these energy changes, irrespective of kinetic energy and other energies, the critical peel-off force can be determined by the energy conservation:

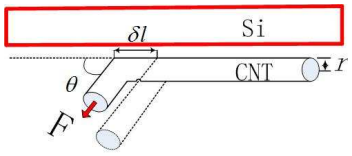

Figure 1 Schematic representation of peeling a CNT from a Si substrate.

$$-v_w\pi r^2\delta l+F(1-\cos\theta)\delta l+F^2\delta l/2\pi r^2E=0. \quad (1)$$

Eliminating δl, Equation (1) yields,

$$F^2/2\pi r^2E+(1-\cos\theta)F-v_w\pi r^2=0. \quad (2)$$

This equation shows how the three terms, adhesive, potential, elastic, interact. In general situation, the first elastic term may be neglected because the Young's modulus E is usually much larger than the stress F.

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EXPERIMENTAL DETAILS

We perform Isothermal-Isobaric(NVT) SMD simulations at the 293 K temperature for 6.0 picoseconds (ps) with a time step of 0.0005 ps to let the system reach its equilibrium configuration, and then study the interface behaviour between CNT and Si, as shown in Fig. 2. The initial distance between the bottom of the CNT and the top (1 0 0) surface of Si of is set up to 5.0 Å. The distance between the bottom of the CNT and the top of Si substrate becomes to be 2.25Å after relaxation. The sizes L_x, L_y and L_z of the Si substrate along the *x*, *y* and *z* directions (shown in Fig. 2), are 6.789 Å, 117.767 Å and 324.503 Å respectively, and consists of 15660 atoms. The CNT (8 8) has a length of L=121.75 Å and radius r=5.416 Å, and consists of 1600 atoms.

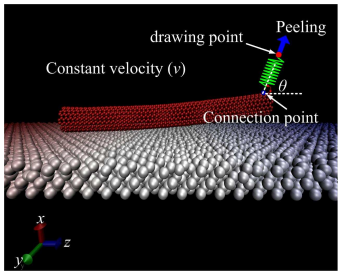

Figure 2 Peeling a SWCNT on a silicon substrate in SMD simulation.

The Tersoff potential is adopted to show the interaction of C-C and Si-Si, which is widely used currently when considering the interaction between atoms of carbon and between atoms of silicon [9]. For non-bond interaction, the atoms of carbon and silicon were treated as uncharged Lennard−Jones particles with ε=0.003466 eV (ε-potential well depth) and σ=2.86 Å (σ-nuclear radius) [10]. The following computation experiments are carried out in an existing MD code called LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [11] where velocity scaling method is adopted to keep the temperature of system constant with the non−periodic boundary conditions in all dimensions.

RESULTS

It is first necessary to find the value of v_W, the unit volume of the adhesive energy for the CNT-Si interface. It can be achieved by using the peeling test at an angle of θ=90º. The CNT radius r is 5.416 Å and its Young's modulus E measured in tensile tests is 1.0 TPa. $\cos\theta=0$ as θ=90º. The first term is neglected because the Young's modulus E is usually much larger than the stress F. With the critical peel-off force (F_{max}=822 pN) being considered, v_W is estimated to be about 8.925 pN/Å. Equation (2) can be written as,

$$5.429\times10^{-5}F_{\max}^2+(1-\cos\theta)F_{\max}-822=0\cdot \quad (3)$$

Figure 3 shows the comparison of the critical peel-off force F simulated by the SMD simulations with the theoretical predictions calculated from equation (3). A good agreement between theory and experiment is found when the peeling angle is larger than 90º.

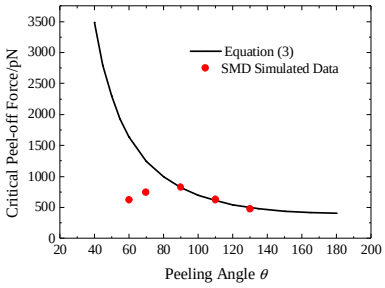

Figure 3 Dependence of peeling angle on critical peel-off force.

CONCLUSIONS

We have used steered molecular dynamics simulations to study the adsorption and peeling of SWCNT on a silicon surface. The critical peel-off force depends on the peeling angle, and the SMD simulated results agree well with the theoretical predictions for peeling angles larger than 90º.

ACKNOWLEDGEMENTS

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