Mechanical properties of SiC nanotubes

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ABSTRACT

Mechanical properties of silicon carbide (SiC) nanotubes are investigated by molecular dynamics (MD) simulation with the Tersoff empirical potential. Young's modulus of SiC nanotubes is smaller than that of the other nanotubes considered so far. However, Young's modulus for SiC nanoatubes is larger than that of β–SiC and almost equal to the experimental data for SiC nanorod and SiC whisker. The strain energy of SiC nanotubes is also investigated. The lower strain energy of SiC nanotubes, which is smaller than that of the other nanotubes, shows the possibility of synthesis of SiC nanotubes.

Keywords: SiC nanotube, molecular dynamics, Tersoff, Young's modulus

1 INTRODUCTION

SiC is considered to be a promising material for high–temperature, high–frequency, and in harsh environment because of its outstanding physical, chemical, and thermal properties [1]. Among many polytypes of SiC, 3C and 6H–SiC have been extensively investigated. However, nanostructures of SiC, such as nanotubes, nanowires, nanorods, and whiskers, have been wide spread interest [2] since the discovery of carbon nanotubes (CNT's) [3]. These nanoscale materials show physical and chemical properties different from the bulk. Wong *et al* investigated that the elasticity and strength of SiC nanorods are greater than those of SiC whiskers and bulk SiC [4]. For nanostructures of SiC, a few methods have been proposed so far. But the study of SiC nanotubes has been rarely reported.

Today, aside from CNT's, [5], CN [6], BC_2 [7], BC_2N [8], WS_2 [9], and MoS_2 [10] nanotubes have been synthesized. In addition, theoretical calculations of the structure and properties of Si [11], GaN [12], and GaSe [13] nanotubes have been reported in the literatures. In particular, BN nanotubes were first predicted by the theoretical predictions and subsequently synthesized. Recently, Miyamoto *et al* investigated, theoretically, the possibility of SiC nanotubes using density functional theory (DFT) with the local density approximation and using the nonlocal pseudopotentials [14]. SiC has an enormous energy barrier (~1.25 eV) for transition between sp^2 and sp^3 structures. This means that the synthesis of SiC nanotubes is restricted due to this energy difference. However, they demonstrated that the strain energy of SiC nanotubes is lower than that of CNT's. The lower strain energy suggest the possibility of SiC nanotubes.

In this paper, we investigate mechanical properties of SiC nanotubes using MD simulations based on the Tersoff empirical potential. These theoretical calculations provide considerable information about the possibility of forming SiC nanotubes.

2 SIMULATION DETAILS

For simulations of SiC nanotubes, we use a classical MD method based on the Tersoff empirical potential, where the atomic interactions are described by the potential energy function in the form of an interactive empirical bond-order potential, formulated by Tersoff. For β–SiC, many parameters have been proposed. But Tersoff parameters related graphitic SiC forms have been not reported hitherto due to the absence of these structures. However, Tersoff parameters for carbon have been applied to both diamond and graphite in the literatures. For SiC nanotubes, we thus use the same parameters as those modified by Tang *et al*, which were well optimized for β–SiC. As the result of MD simulations based on the Tersoff potential, the Si–C bond distance (~1.783 Å) of graphitic SiC sheet is almost equal to that (~1.78 Å) of DFT calculation [14]. Therefore, we think that the Tersoff potential can be effectively applied to the investigation of SiC nanotubes. However, the empirical potential has a drawback which is not sufficiently describe properties of structure, as compared with DFT and tight binding theory. This is due to reflect the effects of change in the curvature of nanotubes.

We have carried out MD simulations within the canonical NVT ensemble. To integrate the Newtonian equations of motion, we use the fifth-order predictor-corrector algorithm with a neighbour list technique. Periodic boundary condition is also applied to the axial direction.

For MD simulations of SiC nanotubes, the structure of nanotubes was first constructed from graphitic SiC sheet. By analogy with CNT's, single-wall SiC nan-

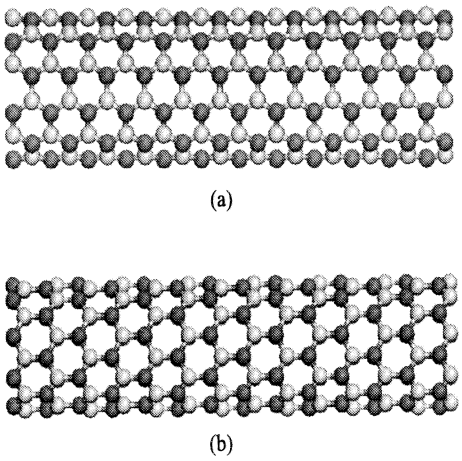

Figure 1: The structure of SiC nanotubes (a) (6,6) SiC nanotube (b) (9,0) SiC nanotube

otubes are characterized by the pair of indices n and m which correspond to the circumference of the nanotube onto the sheet: (n, m=n) armchair, (n, m=0) zigzag and chiral. We have considered both armchair nanotubes ($n \in 6 \sim 9$) and zigzag nanotubes ($n \in 6 \sim 9$). An example of SiC nanotubes is shown in Figure 1.

3 RESULTS AND DISCUSSION

We first investigated the structure and equilibrium properties of SiC nantoutbes. The Si–C bond distance for SiC nanotubes is 1.79 $\pm$ 0.017Å. We find that the bond distance of small diameter SiC nanotutbes decrease as the nanobube diameter is decreased. Figure 2 shows the Si–C bond distance as a function of the nanotube diameter. We think that this behaviour of bond distance is a consequence of the effect of change in the curvature of the nanotube surface with decreasing the nanotube diameter.

We next investigated the mechanical properties of SiC nanotubes. In particular, it is important to determine the Young's modulus Y for nanotubes along the axial direction. The conventional definition of Young's modulus involves the second derivative of the strain energy with respect to strain. Y is given by the following expression.

$$Y = \frac{1}{V_0}\left(\frac{\partial^2 E}{\partial \epsilon^2}\right)_{\epsilon=0} \qquad (1)$$

where E is the strain energy, ϵ is the axial strain and V_0 is the equilibrium volume. In nanotubes, it is difficult to accurately define the thickness for the volume calculation, because of the discrete nature of nanotube structures. Thus, it is physically hard to get an exact volume for the nanotube-like structures. However, the effective thickness of CNT's has been reported on the basis of various assumptions [15–16]. In this paper,

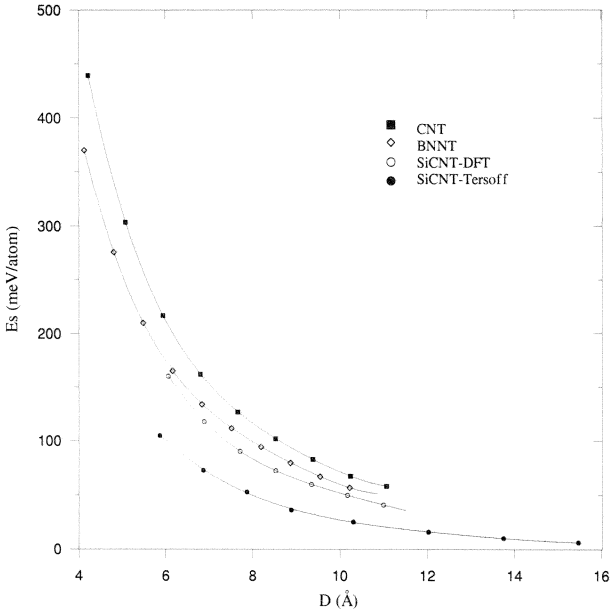

Figure 2: Si–C bond distance as a function of the nanotube diameter for armchair (A6∼A9) and zigzag (Z6∼Z9) SiC nanotubes

we use a different method to obtain the Young's modulus of single-wall BN nanotubes, which is proposed by Hernández *et al* [17]. This method, which is independent of any wall thickness, is defined by the following expression.

$$Y_s = \frac{1}{S_0}\left(\frac{\partial^2 E}{\partial \epsilon^2}\right)_{\epsilon=0} \qquad (2)$$

where S_0 is the surface area of the nanotube in equilibrium. As an approximation, we use the interlayer-distance of graphite ($\sim$ 3.4 Å) for the wall thickness of SiC nanotubes, which is used for the conventional Young's modulus. The value of the Young's modulus is given by $Y = Y_s \ / \ \delta R$. The values of Y are listed in Table 1. The values of Young's modulus for C and BN nanotubes is obtained from Reference [17]. We note that Young's modulus of SiC nanotubes is smaller than that of the other nanotubes considered so far, such as BN or C nanotubes. However, Young's modulus of SiC nanotubes is larger than that of β-SiC ($Y_{100} \sim 0.367$ TPa) and almost equal to the experimental value for SiC nanorods ($Y \sim 0.61$ TPa) [20]. Figure 3 shows Young's modulus Y as a function of the nanotube diameter.

We finally calculated the strain energy E_s for SiC nanotubes. This is defined by the difference between the energy per atom in the nanotube and that in a graphitic sheet. Figure 4 shows the strain energy as a function of the nanotube diameter. The strain energies of carbon [17], BN [17] and SiC [14] (by DFT calculation) nanotubes are shown for comparison. Note, that for a given diameter, the strain energy of the SiC nanotubes is lower

Table 1: Cohesive energy and Young's modulus of SiC nanotubes

	D (Å)	E (eV)	Y (GPa)
SiCNT			
(6,6)	10.31	-5.6556	0.615
(7,7)	12.03	-5.6649	0.621
(8,8)	13.75	-5.6708	0.621
(9,9)	15.47	-5.6747	0.626
(6,0)	5.87	-5.5762	0.524
(7,0)	6.87	-5.6083	0.547
(8,0)	7.87	-5.6281	0.568
(9,0)	8.89	-5.6448	0.591
SiC sheet			
(∞, ∞)		-5.6811	
CNT[a]			
(6,6)	8.20		1.22
(10,0)	7.91		1.22
BNNT[a]			
(6,6)	8.38		0.870
(10,0	8.11		0.837
β–SiC[b]			
			0.367 [100]
SiC nanorod[c]			
			0.610
SiC whisker[d]			
			0.581($\pm$10%)

[a] Reference [17].
[b] Reference [18].
[c] Reference [19].
[d] Reference [20].

than that of the other nanotubes. The lower strain energy of SiC nanotubes ensures the possibility for their synthesis.

4 CONCLUSIONS

We investigated the mechanical properties of SiC nanotubes using molecular dynamics (MD) simulation based on the Tersoff potential. We investigated the bond distance of Si–C, cohesive energy, Young's modulus and strain energy of SiC nanotubes. We used the method proposed by Hernández *et al* for the calculation of Young's modulus, which is independent of the nanotube thickness. We find that Young's modulus of SiC nanotubes is smaller than that of the other nanotubes considered so far, such as BN or C nanotubes. However, Young's modulus for SiC nanotubes is larger than that of β–SiC and almost equal to the experimental value for SiC nanorod and SiC whisker. The strain energy of SiC nanotubes is lower than that of the other nanotubes. In spite of the large energy cost between SiC nanotube and β–SiC, our calculations suggest the possibility for

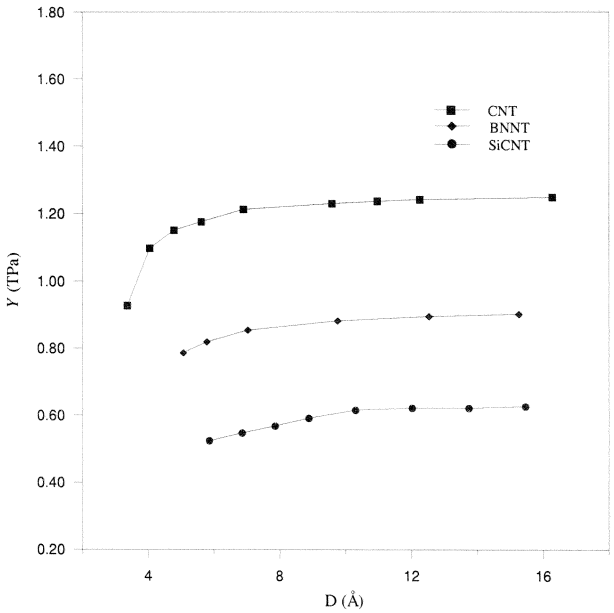

Figure 3: Young's modulus as a function of the nanotube diameter. The value of carbon and BN nanotubes is adapted from Reference 17.

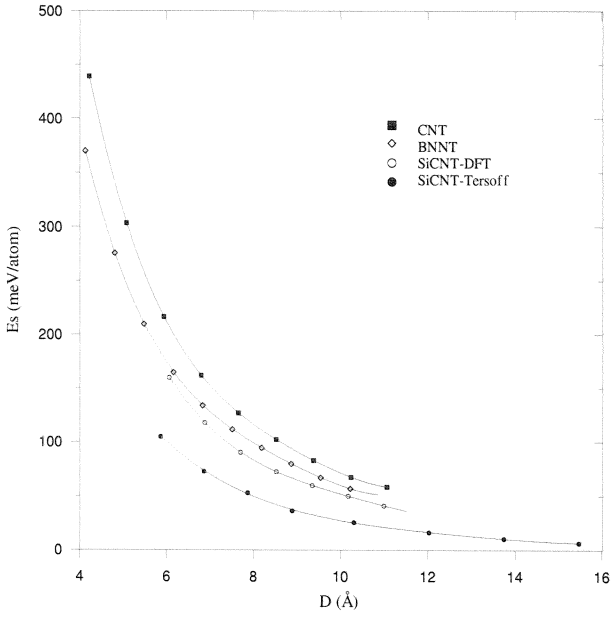

Figure 4: Strain energy as a function of the nanotube diameter. The strain energies of carbon [17], BN [17] and SiC [14] (by DFT calculation) are shown for comparison. The curve is fitted by the least-squares method.

the synthesis of SiC nanotubes.

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