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Growth and Dissolve of Defects in Boron Nitride Nanotube

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ABSTRACT

The defect formation energy of boron nitride (BN) nanotubes is investigated using molecular-dynamics simulation. Although the defect with tetragon-octagon pairs (4-88-4) is favored in the flat cap of BN nanotubes, BN clusters, and the growth of BN nanotubes, the formation energy of the 4-88-4 defect is significantly higher than that of the pentagon-heptagon pairs (5-77-5) defect in BN nanotubes. The 5-77-5 defect reduces the effect of the structural distortion caused by the 4-88-4 defect, in spite of homoelemental bonds.

Key Words : Boron Nitride, Defect, Simulation, Dynamics

1. Introduction

Boron nitride (BN) nanotubes, together with carbon nanotubes, have been considered as promising materials for the electronic industry due to their unique structures and physical properties. The pentagon-heptagon pairs (5-77-5) defect in BN systems generates the less favorable homoelemental bonds such as B-B and N-N bonds. The high energy cost of the frustrated B-B and N-N bonds makes BN systems structurally unstable. Blase *et al.* suggested that the cost of the six frustrated bonds in the $B_{12}N_{12}$ isomer is 9.3 eV, that is 1.6 eV per frustrated bond [1]. Because of this frustration effect, it is known that it is not possible to make the odd numbered ring defects such as pentagons or heptagons in BN systems. Therefore, the even numbered rings with only B-N bonds, such as octagons or tetragons, are considered. The investigations of the topological defect with even numbered rings have been reported by many theoretical calculations and experiment [2, 3]. However, it has been recently proposed that the 5-77-5 defect may appear in BN nanotubes to reduce high stress caused by the geometrical strain. Bettinger et al proposed that the 5-77-5 defect appears to be more favorable in spite of its homoelemental B-B and N-N bonds, as it is associated with less geometrical strain [4].

In this study, we investigate the formation energy of topological defects in BN nanotubes using molecular-dynamics (MD) simulations. The MD simulations are based on the Tersoff-like potential. We also investigate the structural transformation of BN nanotubes with the tetragon-octagon pairs (4-88-4) defect.

2. Modeling Method and Procedure

We use a classical MD method for BN nanotubes, based on the Tersoff-like potential, where the atomic interactions are described by the potential energy function in the form of an interactive empirical bond order potential [5]. For MD simulations of BN nanotubes, we use the same parameters as those proposed by Albe *et al.* [6]. Albe *et al.* proposed the Tersoff-like potential for BN, which describes the structure and the energy of BN polymorphs including sp^2 structures and BN clusters as well as pure B and N bonds. We perform the MD simulations within the canonical NVT ensemble. We also use the fifth-order predictor-corrector algorithm with a neighbour list technique to integrate the Newtonian equations of motion. The MD simulation is calculated for 2×10^5 iterations (100 ps) with a time step of 0.5×10^{-15} s.

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3. Simulation Results

We consider both (n, n) and (n, 0) nanotubes ($n \in 5 \sim 10$) to investigate the defect formation energy of BN nanotubes. For (n, n) nanotubes, the supercell has 30 unit cells with a supercell length of 75.35 Å. For (n, 0) nanotubes, the supercell contains 15 unit cells, and the supercell length is 65.25 Å. The 4-88-4 defect makes a distorted structure in spite of only B-N bonds. This is due to high stress caused by the structural deformation. We find that the formation energies of the 4-88-4 defect are 12.54 eV and 13.44 eV in (5, 5) and (10, 0) BN nanotubes, respectively.

The recent investigations have reported that the formation energy of defect in (5, 5) BN nanotubes is 10.6 eV using ab *initio* gradient-corrected density functional theory [4, 7]. Fig. 1 shows the formation energy of the 4-88-4 defect as a function of diameter. It is found that the formation energy increases with increasing diameter. This is caused by the reduced strain as the diameter increase, although the 4-88-4 defect makes the distorted structure. We also investigate the defect formation energy and structures of BN nanotubes with the 5-77-5 or SW (Single Wall) defect. It is investigated that the formation energies of the 5-77-5 defect are 4.02 eV and 4.62 eV corresponding to (5, 5) and (10, 0) BN nanotubes, respectively. This result is much smaller than that of the 4-88-4 defect. This indicates that the 5-77-5 defect is energetically favored, as compared to the 4-88-4 defect, in spite of its B-B and N-N bonds. Therefore, while the even numbered ring including the 4-88-4 is favored in the flat cap of BN nanotubes, BN clusters, and the growth of BN nanotubes, it is thermodynamically possible to generate the 5-77-5 for the defect of BN nanotubes. The 5-77-5 defect reduces the effect of the geometrical distortion caused by the 4-88-4 defect. It has been reported by Bettinger *et al.* [4] that the SW formation energies of (5, 5) and (10, 0) BN nanotubes are 5.6 eV and 5.3 eV using ab initio method, and 2.6 eV and 2.8 eV using tight-binding method, respectively. As shown in Fig. 2, the formation energy of the 5-77-5 defect also increases with increasing diameter. These results agree well with the trend of carbon nanotubes, investigated by Pan *et al.* [8].

4. Results and Discussions

In BN systems, the high energy cost of defects with frustrated B-B or N-N bonds makes energetically unstable. However, although the 4-88-4 defect is favored in the flat cap of BN nanotubes, BN clusters, and the growth of BN nanotubes, the formation energy of the 4-88-4 defect is significantly higher by 7-10 eV

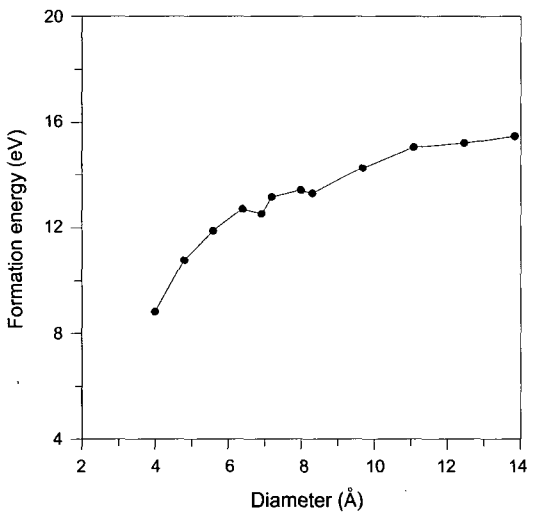

Fig. 1. Formation energy of the 4-88-4 defect as a function of diameter of BN nanotubes.

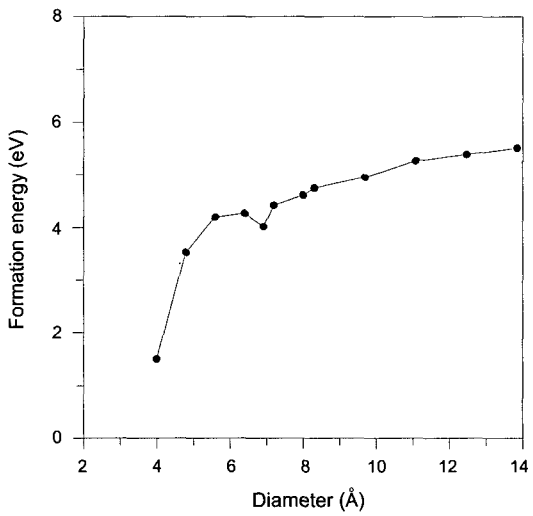

Fig. 2. Formation energy of the 5-77-5 defect as a function of diameter of BN nanotubes.

than that of the 5-77-5 defect for BN nanotubes. The 4-88-4 defect in BN nanotubes makes a distorted structure in spite of only B-N bonds. The 5-77-5 defect reduces the effect of the geometrical distortion caused by the 4-88-4 defect. Therefore, the 5-77-5 defect is energetically more favorable than the 4-88-4 defect for BN nanotubes.

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