SIMULATION OF THE STRUCTURE OF SCREW DISLOCATIONS IN THE INTER-LAYER OF GRAPHITE

Kei Wako[A], Tatsuki Oda[B], Masaru Tachibana[C], and Kenichi Kojima[A]

[A]Department of Information Science, Yokohama Soei Junior College, Miho-cho 1, Midori-ku, Yokohama, Kanagawa 226-0015, Japan
[B]Graduate School of Integrated Science, Yokohama City University, Seto 22-2, Kanazawa-ku, Yokohama 236-0027, Japan
[C]Graduate School of Natural Science and Technology, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Introduction

Researches on dislocations in graphite have been carried out from the 1950s. For example, edge dislocations [1] and partial dislocations in the basal plane [2] have been observed by transmission electron microscopy (TEM). The spiral growth patterns which originate from the screw dislocation have been observed [3, 4]. Moreover, it was observed by atomic force microscope (AFM) that growth spirals had the height of 6.7 Å (length of double-layer of graphite) or 3.3 A (single-layer) [5]. Although these results indicate that the screw dislocations are formed in the graphites, the direct evidence of screw dislocations has not been obtained. Recently, it has been reported that the screw dislocations were observed in the inter-layer of the multi-walled carbon nanotubes by TEM observation [6]. The screw dislocations in the multi-walled nanotubes were highly mobile as characterized by its glide, climb, and the glide-climb interactions, at temperatures of about 2000 C. However, dynamical process and detailed structure do not yet become clear.

The stable structure of the screw dislocation dipole in the graphite is studied by Suaretz *et al*. with the simulation using local density approximation (LDA) [7]. The LDA calculation is good accuracy, but need a high computational resource. Therefore it is difficult to deal with the dynamical process for the dislocations, the properties in finite temperature, and large scale simulation. Tight-binding method is one of the efficient methods to overcome these difficulties. In the present study, as the first step for the tight-binding calculation, the stable structure of the screw dislocation in the graphite was investigated with the tight-binding method. The detail of the core structure is studied, and compare to the result of LDA calculation. The formation energy by the tight-binding method is lower than that of LDA calculation, but the optimal structure quite similar with each other. It is shown that the optimized structure do not depend on the initial position of the screw dislocation.

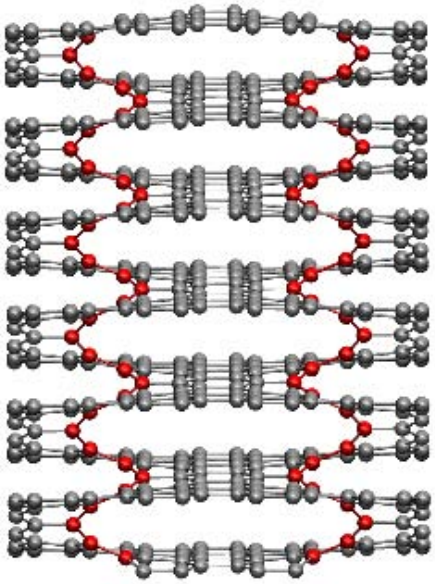

Fig. 1 The stable structure of the screw dislocation dipole in inter-layer graphite. The atoms of the dislocation core are denoted by red. The unit cell for the structural optimization had 6 layers of graphene as shown in this figure.

Method

In the present study, the long-range transferable tight-binding model parameterized by Omata *et al*. [8] was used. Since this model represents inter-layer interaction of graphite, this model was appropriate method for calculation of the screw dislocations of the graphites. Structural optimizations were performed for the AA-stacked graphite which had the unit length 16.9 x 16.7 x 21.3 Å. The unit cell had 672 atoms and 6 layers of graphene. From the stable structure of graphite calculated by Omata's tight-binding model [8], the C-C bond length and inter-layer distance were 1.39 and 3.55 Å respectively in the initial configuration. The structural optimization was performed under the periodic boundary condition. The periodic boundary condition requires an overall Burgers vector of $\mathbf{b} = 0$. Thus the calculation was performed to the dipole with two screw dislocations with opposite Burgers vectors.

Results and Discussion

The structural optimization is performed for the dislocation dipole which two screw dislocations induced at the center of the hexagonal ring of the graphene. Figure 1 shows the stable structure of the dipole of the screw dislocation. The atoms corresponded to the dislocation core are denoted by red in Fig. 1. It is shown that these red atoms form the screw in inter-layer of the graphite. There were no dangling bonds in the optimal structure. This screw link neighboring graphite planes into one helical structure. The optimal structure of the formation energy per dislocation is 0.67 eV/Å. This value is

lower than that of LDA calculation [7] of 2.35 eV/Å. It seems that this discrepancy is caused by the difference of the calculation method.

Figure 2 shows the unit structure of the dislocation core. Two hexagonal rings of perfect crystal are shown and denoted by black. The center of the dislocation is surrounded by the red atoms as shown in the Fig. 2. The distance between atoms denoted by the arrows was estimated. The differences between our results and that of LDA calculation are 0.69 - 3.03 %. Thus the distance is quite similar with each other.

The structural optimizations for the various positions of the dislocation center are performed. Firstly, in the described above, the dislocations are induced to the center of the hexagonal ring. Secondly, the structural optimization is performed for the dislocation which is induced at the center of the C-C bond. As the results of the optimization, the stable structure of the dislocation is same one as shown in Figure 1. Finally the optimization for the dislocation which is induced on the carbon atoms also results in the same structure. The stable structure does not depend on those initial positions.

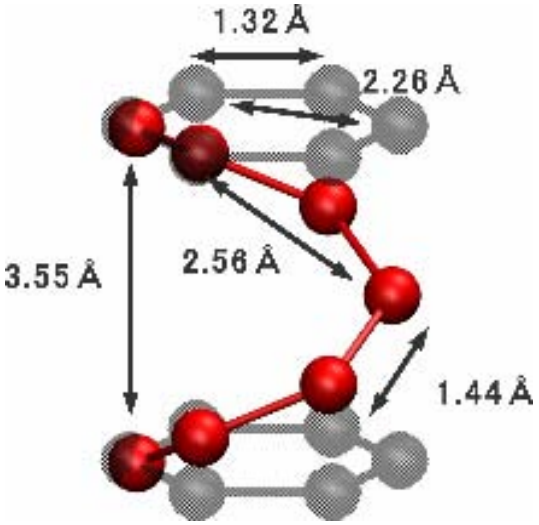

Fig. 2 The unit structure of the dislocation core. Two hexagonal rings of perfect crystal are shown and denoted by black. The length between atoms denoted by the arrows was calculated

References

[1] Dawson IM, Follett EA. An Electron Microscope Study of Synthetic Graphite. Proc. R. Soc A 1959; 253: 390-402.
[2] Amelinckx S, Delavignette P. Electron Optical Study of Basal Dislocations in Graphite. Journal of Applied Physics 1960; 31: 2126.
[3] Hennig GR. Screw Dislocations in Graphite. Science 1965; 147: 733.
[4] Horn FH. Spiral Growth on Graphite. Nature 1952; 170: 581.
[5] Rakovan J, Jaszczak JA. Multiple length scale growth spirals on metamorphic graphite 001 surfaces studied by atomic force microscopy. Am. Mineral. 2002; 87: 17.
[6] Huang JY, Ding F, Yakobson BI. Dislocation Dynamics in Multiwalled Carbon Nanotubes at High Temperatures. Phys. Rev. Lett. 2008; 100: 35503.
[7] Suarez-Martinez I, Savini G, Haffenden G, Campanera J, Heggie MI. Dislocations of Burgers vector c/2 in graphite. Phys. Status Solidi C 2007; 4: 2958-2962.
[8] Omata Y, Yamagami Y, Tadano K, Miyake T, Saito S. Nanotube nanoscience: A molecular-dynamics study. Physica E 2005; 29: 454-468.