§22. Destructions of Layered Structure of Graphite by First-principle Calculations

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The sputtering and erosion of atoms from surfaces by particle bombardment is significant process in a wide range of materials physics and applications, such as microfabrications of semiconductor processes[1] or plasma-wall interaction in a magnetic confinement fusion device[2]. Especially chemical erosion/sputtering processes[3] are important to determine etching characteristics, such as species of desorbed clusters.

Previously, the first-principle calculations of hydrogen adsorption in graphite was performed[4, 6] determining the energetically most stable configuration of the system consisted of graphite and hydrogen atoms with the conjugate gradient (CG) method. They employed SIESTA code developed by Spanish atomic physicists[5].

We have continued our work[7] which extend the previous calculation so as to include the spin polarization e ect of atoms. We employ the graphite consisting of five graphene sheets with 108 hydrogen atoms as the initial state. Hydrogen atoms placed at the 1st, 2nd, and 3rd inter-layer space and there are 36 hydrogen atoms for each inter-layer. All of the other conditions are

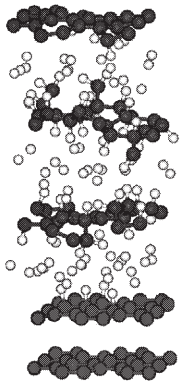

Fig. 1: The initial configuration of graphite with 108 hydrogen atoms.

same with those of Ref.4). Figure 1 shows the hydrogenated graphite after energetically stabilization calculation (however, it is not most stable state). It can be easily seen that 2 dimensional structure is collapsed into 3 dimensional, i.e., the bond structure between carbon atoms has been changed from sp2 like to sp3 like.

Figures 2 and 3 show the first and third layer of the graphite shown in Fig.1. First of all, the equivalent existence of hydrogen atoms on both sides of a graphene sheet is important[8] for modifications of the sheet, because the 3rd layer in Fig.3 is clearly well modified rather

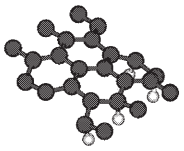

Fig. 2: The 1st layer of the graphite shown in Fig.1.

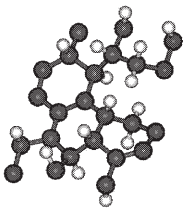

Fig. 3: The 3rd layer of the graphite shown in Fig.1.

than the 1st layer in Fig.2. Moreover, we can not find clear evidence that each CH_2 site tends to break and leave from a graphene sheet. In Fig.3, one bond between carbon atoms is broken, but all CH_2 sites still connecting each other. Then, we speculate that main desorbed products are consisited of not only CH_x type but many of C_yH_x ($y, x \neq 0$ or 1) type. Indeed, by classical molecular dynamics simulations[9], it has been obtained that most frequently observed etching product species has the form C_2H_x and next one is CH_x. Then, we can also speculate that adjacent two CH_2 sites is one of the most in uential seed of chemically etched byproducts.

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