Molecular Dynamics and Density Functional Simulations for Classification of Hydrogenated Amorphous Carbon

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As is well-known, the simple way to classify amorphous carbon materials is the classification by hydrogen content and the ratio of numbers of sp^3/sp^2 carbon atoms[1]. However, this classification is not enough to classify in atomic scale. The atomic configuration of the amorphous carbon material depends strongly on the path of its formation process. Actually, by the molecular dynamics (MD) simulation, we predicted that the hydrogen free amorphous carbon materials which are created by different processes has same ratio of numbers of sp^3/sp^2 carbon atoms and same radial distribution function, and but they differ in orientation of C-C bonds[2]. Moreover, from the density functional theory (DFT) simulation, we suggest that the number density of sp^3 carbon atoms is an appropriate parameter than the ratio of numbers of sp^3/sp^2 carbon atoms in the comparison between tetrahedral amorphous carbon (ta-C) and a pure diamond[3]. Thus, more detailed classification way is required to advance the control of amorphous carbon formation in plasma experiments. The purpose of our simulation study is is to find new classification parameters for amorphous carbon materials.

Recently, we can evaluate the physical properties of amorphous carbon materials, such as elastic modulus, electronic band structure and so on, by using the DFT simulation. The evaluated elastic modulus of ta-C agrees well with experimental values[3]. To perform the DFT simulation, we first need to know the atomic configuration of the amorphous carbon. In principle, from the MD simulating realistic experimental condition, we can obtain the similar atomic configuration of the amorphous carbon. For example, the thin films of amorphous carbon should be obtained by the simulation of plasma chemical vapor deposition (PCVD) process. However, to reproduce the ta-C created by PCVD process in the MD simulation, the potential model to represent interatomic interaction was newly developed[4].

We, previously focusing on hydrogen free amorphous carbon (a-C:H), advance to hydrogenated amorphous carbon. In this paper, the elastic modulus of a-C:H are evaluated from the DFT calculation, and then these calculation results are also used for the development of new potential model of carbon-hydrogen systems for MD. The purpose of this study is to find new classification parameter for a-C:H.

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