§15. Erosion of Single-Crystalline Graphite under Hydrogen Plasma Irradiation

Saito, S. (Nagoya Univ.),
Ito, A.M., Takayama, A., Nakamura, H.

Divertor plates of a nuclear fusion reactor are bombarded with hydrogen plasmas. Under bombardment of plasmas whose thermal energies are higher than the binding energy of target material, it is expected that the structure of target materials will dynamically change. For example, when a single-crystalline graphite is bombarded by hydrogen plasmas, the surface of the graphite turns into hydrogenated amorphous carbon via the chemical and physical reactions with incident hydrogen atoms. This structural change affects the processes of retention, reflection, and sputtering, which is an interesting issue of plasma-surface interaction (PSI).

There have been a number of works related to PSI in binary-collision-approximation-based (BCA) simulations. However, BCA simulation is not appropriate for low-energy collisions because it ignores the interaction between surrounding atoms, although it is applicable to high energy collisions. In order to expand the computable energy range, we have been developing a hybrid simulation[1] of molecular dynamics (MD) and BCA simulations. In this paper, therefore, BCA-MD hybrid simulation is performed to investigate the erosion process of single-crystalline graphite under hydrogen plasma irradiation.

Hydrogen atom injection into single-crystalline graphite is performed by pure BCA and BCA-MD hybrid simulation. The graphite is set to 50 Å in length, 43 Å in width, and 1005 Å in depth. The z-axis of the simulation box is set parallel to the edge of the target material whose length is 1005 Å. Periodic boundary conditions are used in the x- and y-directions. The temperature of the target material is set to 0 K. 1,000 hydrogen atoms are injected one by one into the target material. The incident energy is set to 1 keV. The incident angle is set parallel to the z-axis, i.e., perpendicular to the (0001) surface. In the case of BCA-MD hybrid simulation, the simulation method switches from BCA to MD when the kinetic energy of the projectile and recoil atoms becomes the threshold energy E_{th} = 200 eV.

Figure 1 shows the target material after 1,000 hydrogen atom injections. Figure 1 (a) and (b) shows the results by pure BCA and BCA-MD hybrid simulation, respectively. In this figure, bonds are drawn between two atoms that are within a distance less than the cut-off length of Brenner's REBO potential. The hydrogen and carbon atoms are drawn in colors corresponding to their bonding state. sp, sp^2, and sp^3 carbons are drawn in yellow, green, and red, respectively. Gray, blue, purple, and white represent atoms that have zero, one, five, and six bonds, respectively.

From Fig. 1(a), it is found that there are atoms that have more than 4 bonds in the result of pure BCA simulation. A carbon atom has, at maximum, only four covalent bonds. The atoms that have more than 4 bonds are unstable. By contrast, the simulation result of BCA-MD hybrid simulation does not include such an unstable structure. BCA-MD hybrid simulation is more appropriate than pure BCA simulation in the case where chemical reaction plays a dominant role.

From Fig. 1(b), it is also found that the structure of the target material in the result of BCA-MD hybrid simulation changes dynamically, while the result of pure BCA simulation indicates that the structure almost completely remains a graphene sheet. This is because the surrounding atoms near the projectile and recoil atoms move to minimize their potential energy at each collision in the case of BCA-MD hybrid simulation, whereas only the projectile and target atoms move at each collision in the case of pure BCA simulation.

Figure 2 shows the depth profile of the ratio of the bonding states and hydrogen density at 1,000 injections. The solid and dashed lines are the results obtained by BCA-MD hybrid and pure BCA simulations, respectively. From this figure, it is found that the ratio of sp to sp^3 also has the same two peaks at z = 200 Å and z = 500 Å as the hydrogen density. The result calculated by BCA-MD hybrid simulation has a lower density at the peak at z = 500 Å, which is generated by the channeling effect, than that calculated by pure BCA simulation. This is because the speed of amorphousization of the target material calculated by BCA-MD hybrid simulation is higher than that calculated by pure BCA simulation.

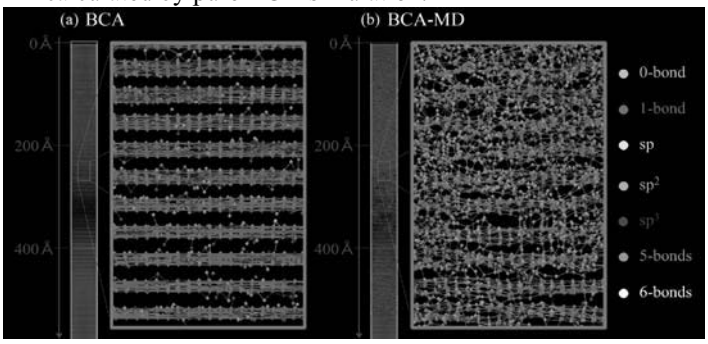

Fig. 1 Target material after 1,000 hydrogen atom injections in (a) BCA and (b) BCA-MD hybrid simulations.

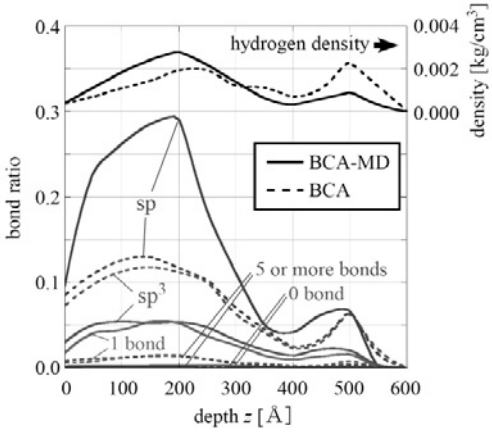

Fig. 2 Depth profile of hydrogen density and the proportion of bonding states.

1) S. Saito, A. M. Ito, A. Takayama and H. Nakamura: Jpn. J. Appl. Phys. **52** (2013) 01AL02 (6 pages).