§12. Material Temperature Dependence of Hydrogen Retention in Single Crystalline Graphite by BCA Simulation

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Divertor plates of a nuclear fusion reactor are bombarded with hydrogen plasmas. Under hydrogen plasma irradiation, surface erosion and hydrogen retention are caused on the surface of the divertor plates. For the steady-state operation of nuclear fusion device, it is required to understand deeply the elementary processes of erosion of the divertor plates and hydrogen retention under plasma irradiation in atomic scale. Carbon material is still one of candidates for divertor plates although tungsten material is in the focus of attention in recent years. To investigate the erosion and hydrogen retention in graphite material in atomic scale, we perform molecular simulation in this study.

There have been a number of works related to PSI in binary-collision-approximation-based (BCA) simulations. In our previous research, we extended ACAT to AC∀T (Atomic Collision in Any structured Target) code which handles any structure of target materials, including monocrystals, polycrystals, crystals with defects, and amorphous [1]. AC∀T code also has the ability to treat the time evolution of target materials by plasma irradiation [2], thermal vibration of the target atoms [3], diffusion process and of incident atoms in target materials, and structural relaxation process of target materials [4]. In this study, we perform BCA simulation of hydrogen injection into single crystalline graphite by AC∀T code to investigate the surface erosion and the hydrogen retention in the graphite under hydrogen plasma irradiation. The erosion and retention strongly depends on the material temperature, therefore, material temperature dependence of those processes is investigated in detail.

Simulation of hydrogen injection into single crystalline graphite is performed by AC∀T code. The size of target material is set to 30.1 Å ×26.0 Å ×334.8 Å. The *z*-axis of the simulation box is set parallel to the edge of the target material whose length is 334.8 Å. Periodic boundary conditions are used in *x*- and *y*-directions. The temperature of the target material is set to 800 K, 1600 K, and 2400 K. 10,000 hydrogen atoms are injected one by one into the target material. The incident energy of hydrogen atom is fixed to 100 eV. The incident angle is set to parallel to *z*-axis, i.e., perpendicular to (0001) surface. The *x*- and *y*-coordinates of the starting position of the hydrogen atom are set randomly. Diffusion coefficient D is set to 1.29×10^{-8} $Å^2$/ns, 1.54×10^{-6} $Å^2$/ns, and 7.61×10^{-6} $Å^2$/ns, for the case of T=800 K, 1600 K, and 2400 K, respectively. Incident flux F is set to 1.0×10^{-10} $Å^{-2}ns^{-1}$. Therefore, interval between injections is 12.8 ms.

Figure 1 shows the target material when the fluence is equal to 2.56 $Å^{-2}$. Clearly the crystalline structure of graphite is destroyed by the plasma irradiation. Compared to the result of the material temperature T =1600 K or 2400 K, significant hydrogen atoms are retained near the material surface when T=800 K because the diffusion coefficient at T=800 K is low. Figure 2 shows the time evolution of hydrogen density. The density quickly saturates with low value when T is large.

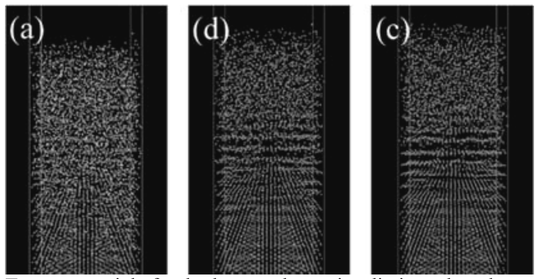

Fig. 1 Target material after hydrogen plasma irradiation when the material temperature is set to (a) 800K, (b) 1600K, and (c) 2400 K. The fluence is 2.56 $Å^{-2}$.The incident energy is 100 eV. White and green dots denote hydrogen and carbon atoms, respectively.

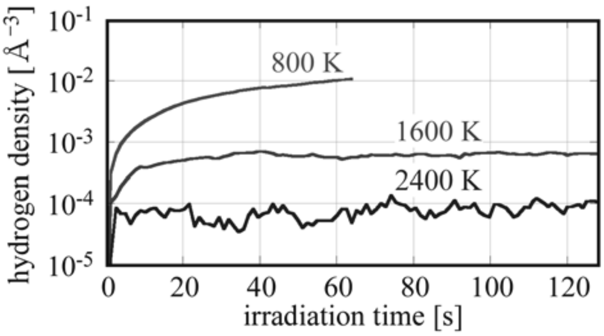

Fig. 2 Time evolution of hydrogen density.

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3) S. Saito, A. Takayama, A. M. Ito and H. Nakamura, Proc. 31st JSST Annual Conference (2012) 46.
4) S. Saito, M. Tokitani and H. Nakamura, Comm. Computer Info. Sci. 474 (2014) 176.