§27. Particle Simulation of Hydrogen Injection into Single-Crystal Graphite in Submicrometer Scale

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

To understand a mechanism of chemical and physical interactions between hydrogen plasmas and divertor plates in a nuclear fusion device, it is necessary to study elementary processes of the reactions. In molecular dynamics (MD) simulations, the equations of motion of atoms are solved numerically. We investigated plasma–wall interaction on the divertor plates made of carbon materials by the MD simulation with modified Brenner's reactive empirical bond order (REBO) potential in the previous works [1]. A typical scale length of the MD simulation box in these works is several nm.

In order to expand the simulation box to more realistic scale length, i.e., several μm, we develop a hybrid simulation code between the MD simulation code with the REBO potential and atomic collision in any structured target (ACΔT) code [2]. In the ACΔT code, where binary collision approximation (BCA) is used, a two-body interaction is calculated instead of computing all particles for every step in the MD simulation. Therefore computation time is saved. As the partner of the MD simulation, we choose the ACΔT code for its fast calculation of a location and a velocity of the particle.

We demonstrate an ACΔT-MD hybrid simulation for a hydrogen atom injection into an ideal graphite which is 321 Å long, 347 Å wide and 1005 Å deep. The graphite consists of 300 graphene sheets. Periodic boundary conditions are imposed on the horizontal direction. The initial temperature of the graphite is set to 0 K. The hydrogen atom with the kinetic energy 1 keV is injected vertically into the graphite.

Thousand simulations with the same initial graphite and randomly changed injection position of hydrogen have been performed. To compare the trajectories, pure ACΔT simulations have also been performed. Fig. 1 shows the histograms of the depth $d_\perp$ and the horizontal distance $d_\parallel$ from the injection point at the surface to the final positions in the result of both the ACΔT-MD hybrid and pure ACΔT simulation. The histogram of the depth $d_\perp$ by ACΔT-MD has lower average and standard deviation than those by pure ACΔT. This behavior is caused by the difference of the interaction potentials between ACΔT and MD. In ACΔT, the two-body interaction potential is used to calculate the force between particles. On the other hand, the multi-body interaction is treated in the MD simulation. Therefore, the kinetic energy of the moving particle is dissipated to the surrounding particle more easily in the MD simulation than in the ACΔT simulation. This fact derives the shorter average of depth $d_\perp$ in ACΔT-MD.

A comparison between the averages of $d_\parallel$ in both simulations shows an agreement except one difference, that is, the standard deviation by ACΔT-MD is larger than that by pure ACΔT. This difference is driven by the fact that the histogram by ACΔT-MD has a long tail. The long tail appears in the histogram of $d_\parallel$ by the ACΔT-MD simulation, because hydrogen atoms horizontally move for a long distance in the interlayer region of the graphite.

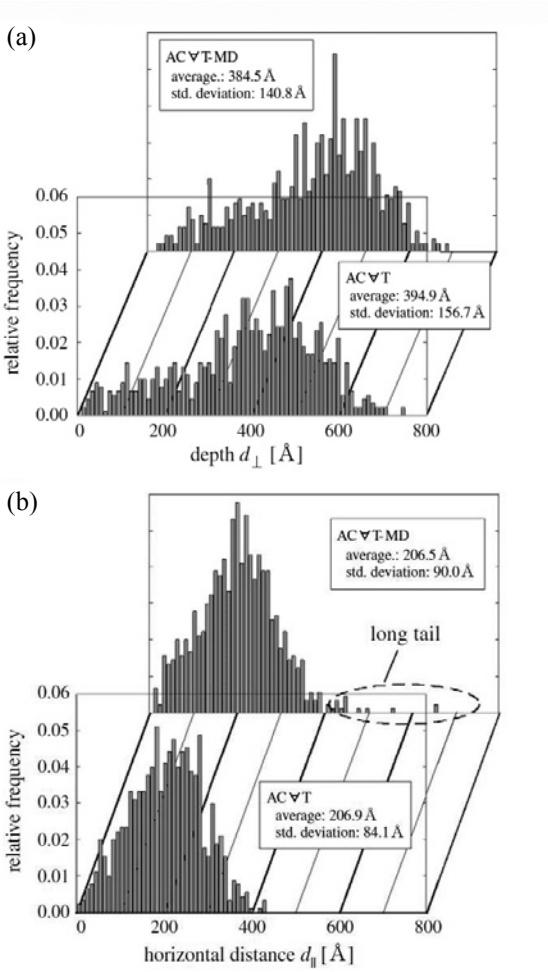

Fig. 1. Histograms of the depth $d_\perp$ and the horizontal distance $d_\parallel$ of 902 injections which were retained in the simulation box as the result of both the pure ACΔT and ACΔT-MD hybrid simulation. Ninety eight trajectories went out of the simulation box. [3]

[1] S. Saito, A. Ito and H. Nakamura, Plasma Fusion Res. **5** (2010) S2076.
[2] A. Takayama, S. Saito, A.M. Ito, T. Kenmotsu and H. Nakamura, Jpn. J. Appl. Phys. **50** (2011) 01AB03.
[3] S. Saito, A.M. Ito, A. Takayama, T. Kenmotsu, and H. Nakamura, J. Nucl. Mater., doi:10.1016/j.jnucmat.2010.12.233, (2011).