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Simulation Study of Hydrogen Injection into Graphite

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Abstract: We have been developing a molecular dynamics (MD) simulation code, a binary collision approximation (BCA) based simulation code, and a BCA-MD hybrid simulation code. In this paper, an overview of the codes is presented. BCA-based simulation results of hydrogen isotopes injection into graphite target are also shown.

Keywords: plasma-surface interaction, binary collision approximation, molecular dynamics, channeling.

1 Introduction

In nuclear fusion devices, plasmas of hydrogen isotopes exist and come in contact with material surfaces. The "divertor configuration" is employed in order to control impurities produced by the impact of plasmas on the surface and to reduce the heat load of plasma-facing materials. Divertor plates, whose potential constituents include carbon and tungsten, are installed in the configuration. Understanding of the divertor physics and designing an appropriate configuration are essential for the establishment of a nuclear fusion reactor. These require knowledge on plasma-surface interactions (PSI). In this context, we have investigated interactions between hydrogen atoms and carbon materials such as graphite by performing molecular dynamics (MD) simulations [Ito, Nakamura and Takayama (2008); Ito and Nakamura (2008)].

The MD simulation code solves equations of motion for all particles under the modified Brenner's reactive empirical bond order (REBO) potential [Brenner, Shenderova, Harrison, Stuart, Ni and Sinnott (2002); Ito, Nakamura and Takayama (2008); Ito and Nakamura (2008)]. The computation of the MD simulation, however, generally has a high cost, which limits the applicable material scale length of the MD simulations to about nanometer order and the energy range to about keV order.

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In order to investigate PSI by numerical simulation, we have to overcome the limitations imposed by MD simulation. A complementary model based on binary collision approximation (BCA) is promising and a number of PSI-related works on BCA-based simulations have been performed. The BCA simplifies interactions between material elements and reduces them to a sequence of binary collisions. A benefit of the model is that it is rather simple and requires less computing resources than the MD model. It, however, can only be applied in a high energy range where multi-body interactions can be neglected.

Existing codes employ the Monte Carlo method, which implies that the target material is assumed to have an amorphous structure. This assumption may be justified for polycrystalline solids, which are formed by many of the materials of interest, since polycrystalline solids with randomly oriented crystallites can be approximated to the first order by an amorphous solid. Verifying the validity of the assumption is another problem.

Another type of BCA-based simulation code is for crystalline targets. They assume that the target material is crystalline, and thus reproduce crystallographic effects including channeling and dechanneling [Robinson and Oen (1963)]. Channeling is a phenomenon where a projectile ion injected parallel to the crystallographic axis or the face of a target material undergoes small-angle scattering without collision and penetrates deeply into the material. Channeling generally increases a range of a projectile.

We have extended the existing BCA-based simulation code ACAT [Yamamura and Mizuno (1985)] so that it can be applied to any structure of target material, including monocrystals, polycrystals, crystals with defects, and amorphous crystals. The extended simulation code AC∀T (atomic collisions in any structured target) [Takayama, Saito, Ito, Kenmotsu and Nakamura (2011)] stores the locations of all the particles and the velocities of recoil atoms in a simulation domain into computer memory so that it can be combined with an MD simulation code.

We have also combined the AC∀T code with the MD code. In the integrated simulation code [Saito, Ito, Takayama, Kenmotsu and Nakamura (2011)] the BCA part covers a higher energy range and a wider spatial region, and the MD part governs a lower energy range and solves equations of motion only in the vicinity of the projectile and recoil atoms. The hybrid simulation code can handle polycrystals or crystals with defects of submicron order more precisely. The threshold energy between the two ranges of energy should be determined in accordance with the validity condition of the BCA.

2 Simulation Models

2.1 Molecular Dynamics (MD) Simulation Model

In our classical MD simulation model, the equations of motion given by the Hamiltonian,

$$H = \sum_i \frac{p_i^2}{2m_i} + U, \tag{1}$$

are solved numerically. Here U is a potential energy, and p_i and m_i are the momentum and the mass of the ith particle, respectively. In our MD simulation, the modified Brenner's REBO potential are employed [Ito, Nakamura and Takayama (2008)]. The potential U contains multi-body part as well as repulsion and attraction part by 2-body interaction. Evaluation of the potential is time-consuming. For the time evolution, the second-order symplectic integration is employed. The typical time step of our simulation is 5×10^{-18}s.

2.2 Binary Collision Approximation (BCA) Simulation Model

In BCA simulation model, interactions between a projectile and/or target material atoms are reduced to a sequence of binary collisions. The asymptotic orbits of the projectile and the target atom at each collision are obtained analytically in a two-body interatomic potential $V(r)$, where r is the distance between the projectile and the target atom. The Moliere approximation to the Thomas-Fermi potential [Molière (1947)] is employed in our BCA simulation code.

The kinetic energy of the projectile is transferred to the target atom at each collision. In addition, a part of the energy is expended for electron excitation. If the kinetic energy of the projectile becomes lower than a given threshold energy, the particle is considered to be seized in the target material. When the kinetic energy of the target atom transferred from the collision pair particle exceeds a given threshold energy, for example, the binding energy of target material, the target atom is considered to recoil and its trajectory and collisions are followed until its kinetic energy is below the given threshold energy.

Conventional BCA based simulation codes employ random number to determine locations of target atoms or symmetry of crystalline target. This means that the conventional simulation codes can treat either amorphous target or crystalline target. In order to overcome the limitation, we have extended a BCA based simulation code. The new BCA based simulation code, named AC∀T (atomic collisions in any structured target), is applicable to any structured target [Takayama, Saito, Ito, Kenmotsu and Nakamura (2011)]. It should be noted that the BCA model ignores multi-body interaction, and thus, it is adequate only for a high energy range.

2.3 BCA-MD Hybrid Simulation Model

The BCA simulation has a typical advantage for availability of collision with high kinetic energy. On the other hand, the MD simulation is more accurate for lower kinetic energy range. The combination of the two kinds of simulation codes compensates each weak point and is applicable to wider spatiotemporal region as well as wider energy range.

In our hybrid simulation code, a projectile and recoiled target atoms are followed by the AC∀T code when their kinetic energies are higher than a given threshold energy. If the kinetic energy of a noticing particle is lower than the threshold energy, the simulation model is switched to the MD.

The threshold energy, at which simulation model is switched, should be determined in accordance with the validity condition of the BCA. It is estimated as about 200eV in our hydrogen-carbon interaction case.

It should be noted that the potential of a simulation model is different from each other, which cause unphysical jumps of kinetic energies. In order to avoid them, we have to consider the energy conservation. That is to say, the energy difference of potential energies between the BCA and the MD is distributed to particles in the simulation domain. A possible model is described in [Saito, Takayama, Ito, Kenmotsu and Nakamura (2011)].

3 Simulation of Hydrogen Injection into Graphite

Comparison between results obtained by AC∀T-MD hybrid simulations and ones by stand-alone AC∀T for a hydrogen atom injection into an graphite shows that the stand-alone AC∀T code is still valid for the first order description of physics in carbon material exposed to energetic hydrogen isotopes [Saito, Ito, Takayama, Kenmotsu and Nakamura (2011)]. Thus we apply the BCA code AC∀T to the injection of energetic hydrogen isotopes into graphite target in this paper.

We set a semi-infinite body of A-B stacking graphite as the target material into the simulation domain. Hydrogen isotopes are injected into the target material and interaction of a projectile and target materials are simulated by the BCA model.

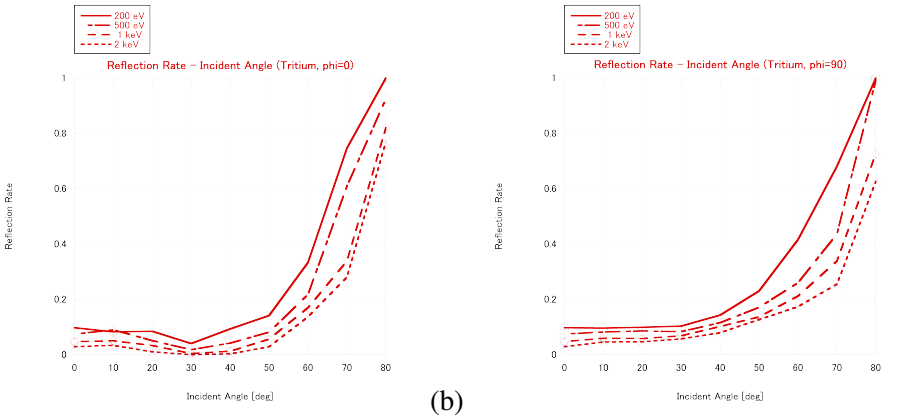
Parameters of simulations are the incident energy, the nuclear species, and the injection and the azimuthal angles of projectiles. In order to obtain statistics we take 10000 trials for each set of parameters. The injection point of each trial is randomly distributed within the periodicity unit of the target material.

Fig. 1 show the reflection rate for tritium injection into graphite target, where the injection energy of tritium atom is varied from 200 eV to 2 keV, the incident angle is varied from 0° to 80° and the azimuthal angle is (a) 0° and (b) 90°, respectively.

The reflection rates in Fig. 1(a) have local minimum at around 30° of the incident angle, while ones in Fig. 1(b) are monotonic increasing function of the incident angle. The monotonic increasing tendency is similar to the case of amorphous carbon target obtained by the original ACAT code. Our simulation shows that the number of recoiled carbons has also local minimum at around 30° of the incident angle, which implies that channeling effect causes such result.

Fig. 2 show the distribution of recoiled carbon atoms, where the injection energy of tritium atom is 1 keV, the incident angle is 60°, and the azimuthal angle is (a) 0° and (b) 90°, respectively. For other nother incident angles, recoiled carbon atoms are distributed along the same slope line on x-z projection. The line is considered a channeling path of the graphite.

The incident x-velocity in the case of Fig. 2(a) is finite, which causes asymmetric distribution of recoiled particles on x-z projection. On the other hand, the incident x-velocity in the case of Fig. 2(b) is zero and the velocity in the x-direction arises via scattering process. Thus the distribution of recoiled particles on x-z projection becomes symmetric in this case.



(a) (b)

Figure 1: Reflection rate for tritium injection into graphite target. Injection energy of tritium atom is varied from 200 eV to 2 keV. Incident angle is varied from 0° to 80° and azimuthal angle is (a) 0° and (b) 90°, respectively.

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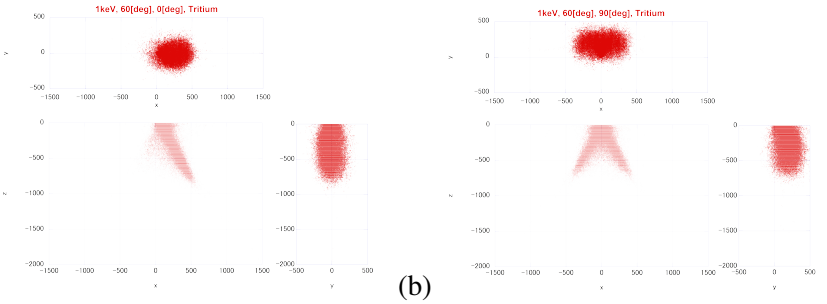

(a) (b)

Figure 2: Distribution of recoiled carbon atoms. Injection energy of tritium atom is 1 keV, incident angle is 60°, and azimuthal angle is (a) 0° and (b) 90°, respectively.

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