§26. Development of Binary-Collision-Approximation-Based Simulation Code Applicable to Any Structured Target Material

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We have investigated interactions between hydrogen atoms and carbon materials such as graphite by molecular dynamics (MD) simulations in order to contribute understanding the divertor physics and designing an appropriate configuration. MD simulation is time-consuming, and thus, is limited to about nanometer order and the energy range to about keV order.

In order to investigate plasma-wall interactions (PWI) by numerical simulation, we have to overcome the limitations imposed by MD simulation. A complementary model based on binary collision approximation (BCA) can be established. There have been a number of PWI-related works on BCA-based simulations. 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 an MD model. It, however, can only be applied in a high energy range where multi-body interactions can be neglected.

We employ the BCA-based simulation code ACAT[1], which was developed to simulate atomic collisions in an amorphous target within the framework of the BCA. Projectile particles are traced through binary collisions. Target particles, with which projectiles collide, are randomly distributed in each unit cell whose size is $R_0 = N^{-1/3}$, where N is the number density of the target material. In terms of randomly distributed target particles, this code employs the Monte Carlo method and focuses on atomic collisions in an amorphous target.

In each interaction between the projectile and the collision pair of the target material, we employ the Moliere approximation to the Thomas-Fermi potential as the interatomic potential $V(r)$. The scattering angle is analytically given as a function of the impact parameter and the kinetic energy of the projectile. The trajectories of particles are approximated as their asymptotes. Thus, they consist of linked straight-line segments. The detailed expressions for particle trajectories are given in references[1, 2].

Three parameters are defined: bulk binding energy E_B, displacement energy E_d, and minimum energy E_c. Let us consider a collision from which the original projectile emerges with kinetic energy E_1 after transferring kinetic energy T to the target (collision pair) atom. The target atom is displaced when its kinetic energy exceeds the displacement energy E_d. If $T > E_d$ is satisfied, the target atom is added to the collision cascade with kinetic energy $E_2 = T - E_B$. Each projectile is traced while its kinetic energy exceeds a given minimum energy E_c.

We have extended the ACAT code described above as follows: While a target atom is produced randomly within a cubic collision cell in the original code, our extended version employs rectangular parallelepiped cells, and the positions of target atoms are given as the initial condition. The positions of projectile and target atoms are stored in computer memory, which enables us to treat structured target materials as well as amorphous ones. In the present version, it is assumed that each cell contains zero or one target atom. Thus, we can obtain the position of the target (collision pair) atom from the stored data when the collision cell is specified. We call the extended version "AC∀T" code[2], which stands for atomic collisions in any structured target. The notation ∀ implies that the code can handle any structure including crystalline and amorphous structures.

If the kinetic energy of each projectile T becomes less than a predetermined minimum energy E_c, tracing of the projectile is stopped and its location and velocity are stored, which can be used for the initial condition of a subsequent MD simulation. Here, E_c is determined by the validity condition of the BCA.

We simulate the injection of a hydrogen atom with energy 1.0 keV into a target graphite as an example problem. The incident angle is fixed to $0°$, that is, normal to the target surface, and the incident point is varied for each trial. We find the region where the trajectory is almost straight. This may be caused by a type of channeling. This type of trajectory is not realized in the original ACAT code because it assumes an amorphous target. We observe that the projectile trajectory immediately before stopping is horizontal with fluctuations. In this region, the projectile travels between graphene layers. This type of trajectory is also newly reproduced by our extension of the ACAT code. Thus we expect that the AC∀T code will be useful for the evaluation of channeling effects. 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 are currently developing a hybrid code based on our MD simulation code and our BCA-based code "AC∀T". As the BCA-based code has a relatively small computational load, the resultant hybrid simulation code is expected to simulate carbon materials of submicron order. The AC∀T code itself exhibits new features and is promising for the evaluation of channeling effects. Evaluations of channeling effects and the effects of target material crystallite states on the sputtering yield remain as future works.

1) Yamamura,Y., Mizuno,Y.: IPPJ-AM-40, Inst. Plasma Phys., Nagoya University (1985).

2) Takayama,A., Saito,S., Ito,A.M., Kenmotsu,T., Nakamura,H.: Jpn. J. Appl. Phys. **50** (2011) 01AB03.