

Molecular Dynamics Simulation of Wall Damage by Energetic Ions in Inertial Fusion Reactor

慣性核融合炉での高エネルギーイオンによる炉壁損傷の
分子動力学シミュレーション

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In an inertial fusion reactor, energetic ions are generated by implosion process of a fusion fuel. They irradiate reactor wall with high flux and energy up to several MeV. Lattice defects caused by the ion irradiation affect mechanical strength of the wall material. We developed molecular dynamics code to simulate lattice defects due to knocking on atoms by energetic ions. An energetic ion loses its energy by inelastic collisions that excite electrons in the material. In order to include electron-lattice interaction, we introduce langevin dynamics. We reveal the process of generation and disappearance of the lattice defects using the simulation.

1. Introduction

In the inertial fusion reactor, energetic ions are generated by nuclear fusion reaction or fuel implosion process. Alpha particles are caused by fusion reaction and other ions are debris from fusion fuel. Energetic ions irradiate first wall of the reactor with high energy up to several MeV and interact with wall material. The ions collide with atoms in the material and can knock on the atoms. Knocked-on atoms cause lattice defects such as vacancy or interstitial. Lattice defects affect mechanical strength of the wall material. It could be a serious issue for long-term operation of the reactor. Therefore, it is important to understand the dynamics of lattice defects. In this study, we have developed a molecular dynamics code to simulate lattice defects caused by energetic ions.

2. Molecular dynamics simulation

We use classical molecular dynamics (MD) to calculate ion-material collision and moving of atoms in the wall material. Using MD simulation, we can deal with motions of each atom and observe microphysics such as the lattice defect. In the MD simulation, the trajectories of atoms are determined by solving equation of motion.

Equation of motion of energetic ion is given as

$$m_{ion} \frac{\partial \mathbf{v}_{ion}}{\partial t} = \mathbf{F}_{ZBL} + \mathbf{F}_{elec} \quad (1)$$

where m_{ion} and \mathbf{v}_{ion} are mass and velocity of an

energetic ion. \mathbf{F}_{ZBL} and \mathbf{F}_{elec} are forces by ZBL potential and electronic stopping power. ZBL potential means coulomb collision between the ion and atoms including effect of ZBL screening function [1]. Electronic stopping power means inelastic collision that an energetic ion excites electron in the material [2,3].

We use langevin equation to describe motion of atoms that compose wall material.

$$m \frac{\partial \mathbf{v}_i}{\partial t} = \mathbf{F}_{EAM} + \mathbf{F}_{ZBL} - \gamma \mathbf{v}_i + \mathbf{R} \quad (2)$$

where m and \mathbf{v}_i are mass and velocity of atoms in the material. \mathbf{F}_{EAM} is force by EAM potential. γ and \mathbf{R} are friction coefficient and random force for electron-lattice interaction. Metallic bond potential is estimated by EAM (Embedded Atom Method). EAM potential is given by the sum of the pair potential among nuclei and the energy to embed an atom, which determined by the electron density at the position [4]. Langevin dynamics describes electron-lattice interaction [5]. Energy loss ($-\gamma \mathbf{v}_i$) or gain (\mathbf{R}) of the lattice is equal to energy gain or loss of the electronic system. In our simulation code, simulation box is divided into cells and electronic temperature is defined in each cell.

For electronic system calculation, heat diffusion equation of electron in the material is given as

$$\rho_e c_e \frac{\partial T_e}{\partial t} = \nabla \cdot (\kappa \nabla T_e) - G(T_e - T_l) + S_{ion} \quad (3)$$

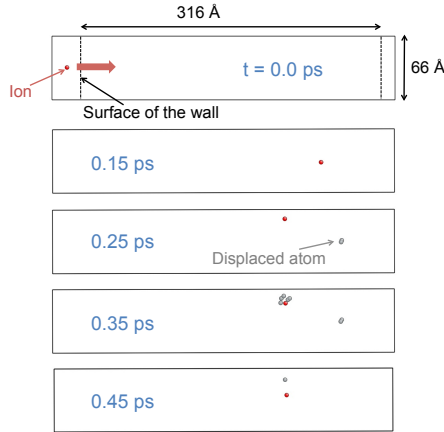


Fig.1. Visualization of displaced atoms

where T_e and T_l are electron and lattice temperature. ρ_e is electron density. c_e and κ_e are electronic specific heat and thermal conductivity. G is electron-lattice coupling factor. S_{ion} is heating term by energy deposition of an energetic ion.

3. Simulation of an energetic ion irradiation

In the present study, we simulate the irradiation of an alpha particle (He^{2+}). Injection energy of the alpha particle is 1 keV. We assume tungsten for first wall material. Initial temperature of tungsten is 300 K. The simulation box size is $66 \text{ \AA} \times 316 \text{ \AA} \times 66 \text{ \AA}$, which is divided into $3 \times 10 \times 3$ cells to define electron temperature. Periodic boundary conditions are used in x and y directions. The boundary in z direction is a free boundary. For time integration, we use velocity verlet method. In order to perform the simulation efficiently, we use variable time step so that the maximum displacement is 0.063 \AA in a time step.

We perform the simulation until 1.6 ps and study the displacement of atoms. The displaced atom is defined as an atom displaced from original position more than 1 \AA . Figure 1 shows visualization image of injected ion and displaced atoms. First, an injected ion penetrates straight into tungsten because of its high velocity. Then, slowed down ion knocks on atoms and is scattered. Number of displaced atoms increases by knocking on atoms, but later, it decreases as moving atoms being stabilized. Figure 2 shows the time evolution of the number of displaced atoms. The number of displaced atoms reaches the maximum of 7 at around 0.35 ps. After that, it is reduced due to the atom motion. The displaced atoms totally disappear at 0.46 ps. Figure 3 shows the time evolution of lattice and electron temperature. Simulation box is divided into cells that contain about 690 atoms. Temperature is defined in each cell. In Fig. 3, maximum temperature in the

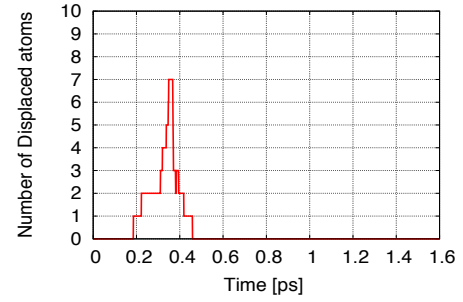


Fig.2. Time evolution of the number of displaced atoms

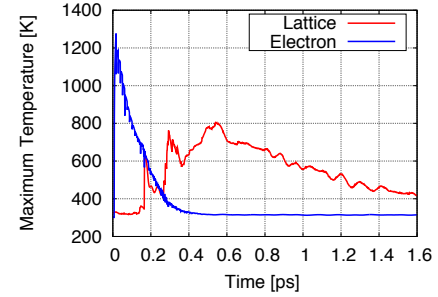


Fig.3. Time evolution of two temperature

simulation box is plotted. First, electrons have maximum temperature due to electrons excited by an energetic ion. After that, electron temperature decreases by electronic heat diffusion and electron-lattice energy relaxation. Since 0.2 ps, maximum lattice temperature increases because atoms receive due to elastic collision with ions.

4. Summary

We have developed MD code to simulate lattice defect caused by energetic ions including effect of electron excitation. The number of displaced atoms due to knocking on atoms by 1 keV α particle reached 7 at 0.35 ps. However, lattice defects decrease with moving atoms being stabilized. Finally they disappear at 0.46 ps.

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