A MOLECULAR DYNAMICS CALCULATION TO CASCADE DAMAGE PROCESSES

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ABSTRACT

In this work, Molecular dynamics simulation was performed to study the cascade damage evaluation initial from a 250 eV Primary Knock-on Atoms (PKAs) in gold. For this purpose, the simulations were carried out using the molecular dynamics code GRAPE to study the cooling phase of a cascade from the thermodynamic point view. Interatomic interaction of the cascade was investigated by the Morse potential and it is found that during the cooling phase of the cascade local equilibrium was realized.

KEYWORDS: displacement cascade, primary damage, Morse potential, molecular dynamics

1. Introduction

Radiation damage processes from initial defect production to microstructure evolution occur over a wide spectrum of the time and size scale. Atomic collision sequences during the collisional phase continue for a few tenth of picosecond in a small region on nanometer scale. The subsequent cooling phase takes place for nearly $10^{11}$ sec [1, 2].

Molecular dynamics method is a well-defined microscopic description of many-body system [3]. Computing the phase space trajectories of a collection of molecules that individually obey classical laws of motion [4], molecular dynamics computer simulations provide the most realistic description of the primary damage state including the collisional and cooling phase. Binary collision approximation provides a realistic description of the gross features of defect spatial distribution with requisite physical reality in statistically significant numbers, including the size, number and spacing of subcascades [5, 6].

The cascade damage methods are classified into four stages (Thermal phase, collisional phase, diffusional phase and cooling phase). The cooling phase is defined as stage of the dissipation of energies deposited locally during the collisional phase, ending when the cascade region reaches thermal equilibrium with its surroundings. During the cooling phase, average kinetic energy in a cascade core is well above the melting temperature of materials and the significant rearrangement of defects takes place, including recombination and clustering, after the cooling phase, interaction of point defects occurs by normal, thermally activated diffusion [7].

Displacement cascade, in a material, can be visualized as a series of elastic collisions initiated with the lattice atoms, where the lattice atom is hit by a high energy particle. The initially-bombard a target is named PKA. The Norgett-Robinson-Torrens (NRT) model suggested that the number of Frenkel pairs produced by a PKA of energy [8-10]. It is used to calculate radiation damage calculation method exposure unit known as displacement per atom (dpa). Thus, dpa has been used as a standard measure for computing proton-neutron induced radiation damage production from different radiation sources [11-15]. Molecular dynamics simulation of processes in metals have been studied by many research groups including temperature dependence of the processes of cascade damage [16-18].

MDGRAPE code is a series of special-purpose computer system built for particle-based simulations such as molecular dynamics simulation [19, 20]. In this paper, the primary states of cascade damage processes are simulated to study the cooling phase in gold, using the molecular dynamics simulation method.

2. Molecular dynamics simulation methods

A major computer simulation method to analyse development processes of cascade damage is GRAPE code to study the cooling phase of a cascade from the
thermodynamic point view. Molecular dynamics are performed to study a computational cell and to apply many body interatomic potential based on embedded atom method (EAM) [21] to description of atom behaviour. In this paper, 250 eV cascade is simulated in gold. One atom is chosen as 250 eV PKA in the direction of [120], from the computational cell. Computational cell contains 10800 gold atoms corresponding to a rectangular parallelepiped of $15\alpha_0 \times 15\alpha_0 \times 12\alpha_0$, where $\alpha_0$ is the lattice constant. For atoms in the vicinity of the boundary of the cell, periodic boundary conditions are employed. A time step equals to $3 \times 10^{-15}$ s for all the calculations. Since the system is thermally insulated, in the present study, interatomic interaction is described using pair-wise Morse potential [22] which is adjusted by the cohesive energy, elastic constants and compressibility of gold.

3. Results and discussion

In this study, Molecular dynamics measurement was performed to study the cooling phase of a cascade in gold, considering from the thermodynamic point view that the initial lattice temperature is 0 K. Figure 1 shows the time dependence of the number of displaced atoms for 250 eV cascade by using Morse potential where a displaced atom is defined to be displaced by over one-quarter of the lattice constant from nearest lattice site. It is also shown that an initial increase is followed by a decrease due to the spontaneous recombination of unstable defect pairs. Furthermore, durations of relaxation phases and collisional are estimated to be both 0.13 psec. It also observes the migration of a small number of interstitial atoms during the following cooling phase.

Figure 2 shows the time dependence of average kinetic energy. In the collisional phase the average kinetic energy rapidly decreases due to conversion of the kinetic energy to potential energy, establishing approximate equipartition of energy during the subsequent cooling phase, the kinetic energy remains constant due to the thermally insulated system. Furthermore, during the cooling phase, the migration of interstitial atoms with relatively high kinetic energies (0.1 ~ 1 eV) is observed.

Figure 3 shows the velocity distribution at 0.26, 0.52 and 2.0 psec. It is clear that the velocity distribution of moving atoms can change and gradually approaches the Maxwell Boltzmann distribution. It is observed that from the initial stage of the cooling phase, the system is strongly deviated from thermal equilibrium, while, at top stage of the cooling phase, equilibrium velocity distribution has been almost established. The velocity distribution of the central region is almost close to the Maxwell Boltzmann distribution as shown in Figure 4. However, statistics is not enough to give a smooth curve. This result is calculated using the adiabatic molecular dynamics system where electronic contribution to dissipation of thermal energies in cascades is not considered. Since in noble metals as gold, the contribution is small due to weak coupling of the electronic system with the lattice. Thus, Figure 5 does not indicate an equilibration between the electronic and lattice systems. However, this figure seems to imply that at least, local temperature of the lattice system can be described even at such an early stage of the cooling phase of cascade evolution.

![Fig. 1. Number of displaced atoms as a function of time for a 250 eV cascade in gold using the Morse potential](image1)

![Fig. 2. Average kinetic energy as a function of time for a 250 eV cascade in gold using the Morse potential](image2)

![Fig. 3. Velocity distribution at 0.26, 0.52 and 2.0 psec](image3)
distribution of moving atoms can change and gradually approaches the equilibrium distribution. Local equilibrium of the lattice is established, indicating that the simple jump processes of defects may be applied to the simulation of cascade evolution after the collisional phase. Accordingly, more work could be done by using extremely high energy, temperature and more metals.

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4. Conclusions

In this study, the primary states of cascade damage processes are simulated to study the cooling phase, using the molecular dynamics calculation at 250 eV in gold. At early stage in cascade cooling phase, the total kinetic energy remains constant due to the thermally insulated system, the velocity distribution of moving atoms can change and gradually approaches the equilibrium distribution. Local equilibrium of the lattice is established, indicating that the simple jump processes of defects may be applied to the simulation of cascade evolution after the collisional phase. Accordingly, more work could be done by using extremely high energy, temperature and more metals.
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