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Influence of stacking fault energies on the size distribution and character of defect clusters formed by collision cascades in face-centered cubic metals

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ABSTRACT

Molecular dynamics simulations are performed to evaluate the influence of the stacking fault energy (SFE) as a single variable parameter on defect formation by collision cascades in face-centered cubic metals. The simulations are performed for energies of a primary knock-on atom (E_{PKA}) up to 50 keV at 100 K by using six sets of the recently developed embedded atom method–type potentials. Neither the number of residual defects nor their clustering behavior is found to be affected by the SFE, except for the mean size of the vacancy clusters at $E_{PKA}=50$ keV. The mean size increases as the SFE decreases because of the enhanced formation of large vacancy clusters, which prefer to have stacking faults inside them. On the other hand, the ratio of glissile self-interstitial atom (SIA) clusters decreases as the SFE increases. At higher SFEs, both the number of Frank loops and number of perfect loops tend to decrease; instead, three-dimensional irregular clusters with higher densities appear, most of which are sessile. The effect of SFE on the number of Frank loops becomes apparent only at a high E_{PKA} of 50 keV, where comparably large SIA clusters can be formed with a higher density.

1. Introduction

Molecular dynamics (MD) simulations have revealed that collision cascades directly produce clusters of vacancies and self-interstitial atoms (SIAs) as well as mono-defects when the energy of a primary knock-on atom (E_{PKA}) is higher than several kiloelectronvolts (keV) [1–3]. The stable configurations of clusters and their character—either glissile or sessile—are important parameters to be quantified by MD simulations because they strongly affect subsequent microstructural evolutions and mechanical property changes [4,5]. For face-centered cubic (FCC) metals, these defect clusters can have several possible configurations [6]. Static energy calculations based on the dislocation theory have revealed that the stable configuration depends on the stacking fault energy (SFE) as well as the cluster size. For SIA clusters, the formation energy of a Frank loop at a certain size increases with the SFE. A higher SFE decreases the critical radius of an SIA loop, with which the stable configuration changes from a Frank loop to a perfect loop; concurrently, the character changes from sessile to glissile. On the other hand, for vacancy clusters, the configurations with stacking faults inside them—namely, a stacking fault tetrahedron (SFT) or Frank loop—can be stable in low-SFE metals, whereas a microvoid or perfect loop appears more preferentially in high-SFE metals [7]. One would expect that the character of defect clusters directly formed by collision cascades would reflect that evaluated by static energy calculations. However, a previous study of MD simulations at $E_{PKA}=10$ and 20 keV indicated that the number of SIA-type perfect loops tends to increase at low SFEs and that of SIA-type Frank loops seems to be independent of the SFE. The previous study also indicated that the SFE seems to have little influence on vacancy clusters just after collision cascades with these E_{PKA}. The influence becomes apparent by annealing at 1100 K for 100 ps, where large clusters are formed at a sufficiently high density [8]. Both of these observations are different from predictions based on the dislocation theory [9]. The difference may arise from the fact that comparably large clusters are formed with an extremely low number density under the low E_{PKA} conditions employed in the previous

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Table 1
Material properties for six sets of the interatomic potentials.

Intrinsic SFE (mJ/m^2)	14.6	24.8	44.1	61.6	94.6	186.5
Lattice constant (Å)	3.639	3.639	3.639	3.639	3.639	3.638
Cohesive energy (eV/atom)	−3.425	−3.416	−3.423	−3.429	−3.428	−3.427
Vacancy migration energy (eV/atom)	0.91	0.91	0.92	0.93	0.95	1.00
Vacancy formation volume ($\Omega_f/\ \Omega_0$)	0.703	0.705	0.708	0.710	0.717	0.731
<100> dumbbell distance (Å)	2.079	2.077	2.076	2.081	2.081	2.080
Formation energy (eV/atom)						
Vacancy	1.11	1.12	1.11	1.10	1.07	1.03
Interstitial	2.82	2.81	2.81	2.82	2.82	2.81
Elastic constant (GPa)						
C_{11}	173	174	174	175	175	178
C_{12}	128	127	127	127	127	125
C_{44}	84	84	84	84	84	83
Melting point (K)	1349	1352	1353	1355	1356	1351

Table 2
Cell size and number of simulation runs at each E_{PKA}.

E_{PKA}, keV	Number of atoms	Number of calculations
1	60,480	40
5	311,040	40
10	586,080	40
20	1,157,328	40
50	10,976,000	20

study. In the real environment of nuclear reactors, collision cascades with higher E_{PKA} are more likely to occur, which will generate large clusters at high densities. Hence, the effects of SFE on the configurations and character of clusters may become significant with higher E_{PKA}. Austenitic stainless steel, which is widely used as an in-core structural material in light water reactors, is an FCC metal with one of the lowest SFEs. To clarify the characteristic features of the defect formation process in austenitic stainless steel, it is necessary to elucidate the effects of the SFE on this process.

In this study, we performed MD simulations for FCC metals to investigate the influence of the SFE on defect formation by collision cascades with a wide E_{PKA} range of 1–50 keV, with particular focus on higher E_{PKA} values. In Section 2, simulation and visualization methods are described. Then, in Section 3, the analyses of the size distributions and character of the clusters as well as the number of residual defects in terms of the SFE influence are presented. Conclusions are drawn in Section 4.

2. Methods

The LAMMPS code, which is developed by Sandia National Laboratories for classical MD simulations [10], was used in this study. We chose the six sets of embedded atom method (EAM)-type interatomic potentials developed by V. Borovikov et al. [11]. The original potential was developed for pure Cu at an SFE of 44.1 mJ/m^2 [12], and the other five potentials were derived by changing the SFE. Table 1 presents the material properties for the six EAM-type potentials used in this study. The SFEs ranged from 14.6 to 186.5 mJ/m^2, whereas the other material properties unrelated to the SFEs were kept almost identical (maximum variation of less than ~10%). These EAM-type potentials were smoothly joined to the ZBL potential [13] at short-distance regions by using fifth-order spline functions. With these potentials, we could evaluate the influence of the SFE as a single variable parameter on defect formation by collision cascades.

Table 2 lists the cell size and number of simulation runs at each E_{PKA} value. Periodic boundary conditions were applied in all axis directions. The cell size for each condition was selected such that it was large enough to prevent the cascade from overlapping with itself because of periodic boundaries. Before the initiation of a collision cascade, an equilibrium configuration at a pressure close to zero was obtained by MD runs at 100 K for approximately 10 ps. E_{PKA} was given to the atom near the center of the cell in a high-index direction, namely [1 3 5]. The time step for the simulation was set to be variable so that the displacement of the fastest atom was less than 1% of the lattice constant within one time step. Neither electron excitation nor energy damping at the boundaries was incorporated in any of the simulations. The collision cascade was followed by microcanonical ensemble evaluation. The temperature increase in the cell because of the collision cascade event did not exceed 70 K. The calculations were finalized approximately 50 ps after the initiation of the collision cascade. For some cases at E_{PKA} = 50 keV, if the motion of clustering changed dramatically even after 50 ps, calculations were performed for an additional 50 ps.

Defect identification and visualization were carried out by using the procedure described in a previous study [14]. In each atom, the nearest neighbor site was searched. Then, a site with no atoms was defined as a vacancy site. When a site with more than two atoms was found, an SIA was considered to exist there. In this analysis, a point defect was defined as belonging to a cluster if it was within the first-nearest-neighbor distance from another point defect. The total number of defects was evaluated by counting all the defects included in mono-defects and defect clusters. The defect configuration was identified by using the common neighbor analysis (CNA) method [15,16]. Structures other than FCC or hexagonal-closed-pack (HCP) were colored in red, whereas HCP structures were colored in blue.

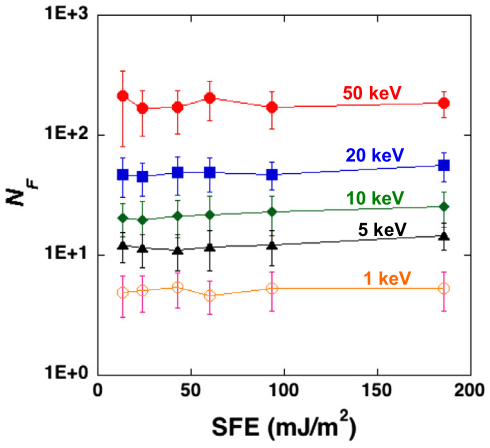

Fig. 1. Number of residual defects as a function of the SFE.

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