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Interstitial cluster motion in displacement cascades

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Abstract

Displacement cascades of energies up to 30 keV were investigated by molecular dynamics simulations in α-iron, nickel and in ordered intermetallic compounds Ni_3Al. Different models of embedded-atom potentials were used in conjunction with a modification of the short-range repulsive interaction. Interstitial clusters were found to be very mobile at any size. The direction of the dumbbells in a cluster configuration was different as compared to that in an isolated configuration. A glide mechanism and a one-dimensional motion of these clusters were observed in different systems under investigation. Several types of cluster–cluster interactions have been observed: coalescence of two clusters with distinct glide cylinders assisted by the flip of the Burgers vector of one of the clusters, growth of a cluster by the absorption of isolated interstitials and elimination of vacancies swept by a large interstitial cluster. The migration trajectories and the diffusion coefficients of some clusters were investigated. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

Defect production by displacement cascades is the primary source of damage and microstructural modifications in materials under irradiation by neutrons or ions. A fundamental understanding of the defect production and of the atomistic mechanism involved in the disorder state is therefore of great help for macroscopic models to predict the aging behaviour of these materials.

In the present study, molecular dynamics simulations were used to investigate various dynamical features of the cascades and particularly the motion of interstitial clusters in nickel, α-iron and ordered intermetallic compound Ni_3Al.

2. Models

The computational cell was a parallelepipedic microcrystallite bounded by periodic conditions and containing approximately 60 000 to 2 million of atoms. The initial velocities of the atoms were determined from a Maxwellian distribution, so that the desired lattice temperature was reached before the introduction of the cascade. A modified link-cell method [1] was used to update partially the neighbour tables.

The EAM potentials derived by Haftel et al. [2] and by Rubini and Ballone [3,4] were used for simulations in α-iron and nickel or Ni_3Al, respectively. At short separations, they were jointed to a fitted Born–Mayer potential and to the universal Ziegler and Biersack function [5]. The parameters are given in a previous paper [6]. In our simulations, a vacancy is defined as the lattice site where there is no atom inside a sphere of radius equal to half the next nearest neighbour distance. A dumbell interstitial or a replaced atom is defined at this site, if the sphere contains two atoms or a 'non-original' atom, respectively.

3. Results

Displacement cascades from 1 to 30 keV were generated by primary knock-on atoms ejected from their site with an initial velocity near the ⟨4 1 1⟩ direction. Most of the PKA in Ni_3Al were nickel. For each run, the number of Frenkel pairs as well as the number of defect clusters and the number of replaced atoms were measured. When the PKA energy E is expressed in keV, these Frenkel pair and replacement numbers can be

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Table 1
Values of A and m in the power-law fits for the numbers of Frenkel pairs and replacements

System	Frenkel pairs		Replacements	
	A	m	A	m
α-Fe	~8.25	0.967		
Ni	~4.49	0.643		
Ni_3Al	~3.68	0.655	~152.69	1.243

represented by the power-law fits as proposed by Bacon et al. [7]:

$$N = AE^m, \tag{1}$$

where the results were obtained from an average of at least four runs for each cascade energy. The values of the constants A and the exponents m for cascades in α-iron, nickel and in Ni_3Al are given in Table 1. Similar simulations have been performed with different potentials in α-iron [8,9] and in Ni_3Al [10,11].

In Ni_3Al, clusters of $n_v \geqslant 12$ vacancies and $n_d \geqslant 18$ dumbbells were observed in cascades of energy higher than 6 keV. Large clusters exhibit a three-dimensional morphology. While the stable configuration of an isolated interstitial in nickel and in Ni_3Al is the $\langle 1\,0\,0\rangle$ dumbbell or mixed-dumbbell, the configuration of clusters of three or more interstitials were found to be formed by parallel $\langle 1\,1\,0\rangle$ dumbbells centered at two or three adjacent (1 1 1) planes. In α-iron, the configuration of clusters of four or more interstitials was found to consist of parallel $\langle 1\,1\,1\rangle$ dumbbells, whose centers were located at different (1 1 0) planes.

4. Migration mechanism of interstitial clusters

In nickel and α-iron, interstitial clusters of any size formed in displacement cascades were found to be very mobile, while in Ni_3Al, their mobility was considerably reduced. During their motion, the cluster configuration was changing continually very much like an amoeba. The mechanism consists of an elementary glide of any one dumbbell of the cluster towards a neighbouring site in the direction of its axis. The motion is similar to the well-known motion of a crowdion. The next step consists of a similar glide of the rest or of only a part of the cluster, so as to restore a new cluster in the adjacent plane [12]. The mechanism results in a one-dimensional motion of the cluster along its glide cylinder and gives rise to a complex and continually changing morphology during the evolution of displacement cascades.

Several types of cluster–cluster interactions or events between a cluster and other point defects have been observed (Fig. 1): coalescence of two clusters with distinct glide cylinders assisted by the flip of the Burgers vector of one of the clusters, growth of a cluster by the absorption of isolated dumbbell interstitials and elimination of single or di-vacancies swept by a large interstitials cluster. These different events observed after 30 ps in a 10 keV cascade in nickel, i.e., after the usually assumed final phase of the cascade evolution are relevant and must be taken into consideration when modelling the microstructural evolution of materials under irradiation as done in Refs. [13–16].

To eliminate the possible influence of stress or subthreshold effects of the cascade on the mobility of the interstitial clusters, we also performed simulations with the following conditions. Starting from the defect configuration obtained after a 10 keV cascade of nickel, we forced a partial defect recombination, so as to keep only one cluster of n dumbbells and a same number of single vacancies which are well separated from the interstitial cluster. Quenching of 0 K were performed by putting the velocity of each atom to be zero whenever its sign is opposite to that of its acceleration. Then, the crystal is set again to a given temperature by usual applications on the atom velocities from a maxwellian distribution. Simulations were performed in nickel for clusters with 3–6 dumbbells and at three temperatures 600, 800 and 1000 K for each cluster size. Figs. 2(a)–(c) show the trajectories of the center of mass of the 3-dumbbells cluster at 600, 800 and 1000 K, respectively, and Figs. 3(a)–(c) those of the 5-dumbbells cluster at the three same temperatures, respectively. From these figures, we can see that the clusters performed mostly an one-dimensional motion along the $\langle 1\,1\,0\rangle$ direction, with more or less frequent changes in direction to another $\langle 1\,1\,0\rangle$. For the 5-dumbbells cluster, the direction changes increase with the temperature (Fig. 3) while this tendency is not established for the 3-dumbbells cluster (Fig. 2), perhaps owing to unsufficient simulation times. Note that, the trajectory of the center of mass is not always a regular straight line segment, even if during this period the cluster is executing a one-dimensional motion, because on the one hand the axes of all of its dumbbells are not exactly parallel to the $\langle 1\,1\,0\rangle$ direction in the same time, and on the other hand one or more dumbbells are making a rotation and attempting to escape the cluster. For each of the cluster under investigation, the migration was taking place by collective glide along the $\langle 1\,1\,0\rangle$ direction by a dissociation and reassociation mechanism of the dumbbells to the cluster in different adjacent (1 1 1) planes [17]. Owing to this particular migration, we have calculated the diffusion coefficient of the clusters defined as

$$D = \frac{\langle R^2\rangle}{2\Delta t},$$

where $\langle R^2\rangle$ is the mean value of the square of the displacement R of the center of mass measured in segments of equal time duration Δt determined in a particular chosen one-dimensional migration. The results obtained

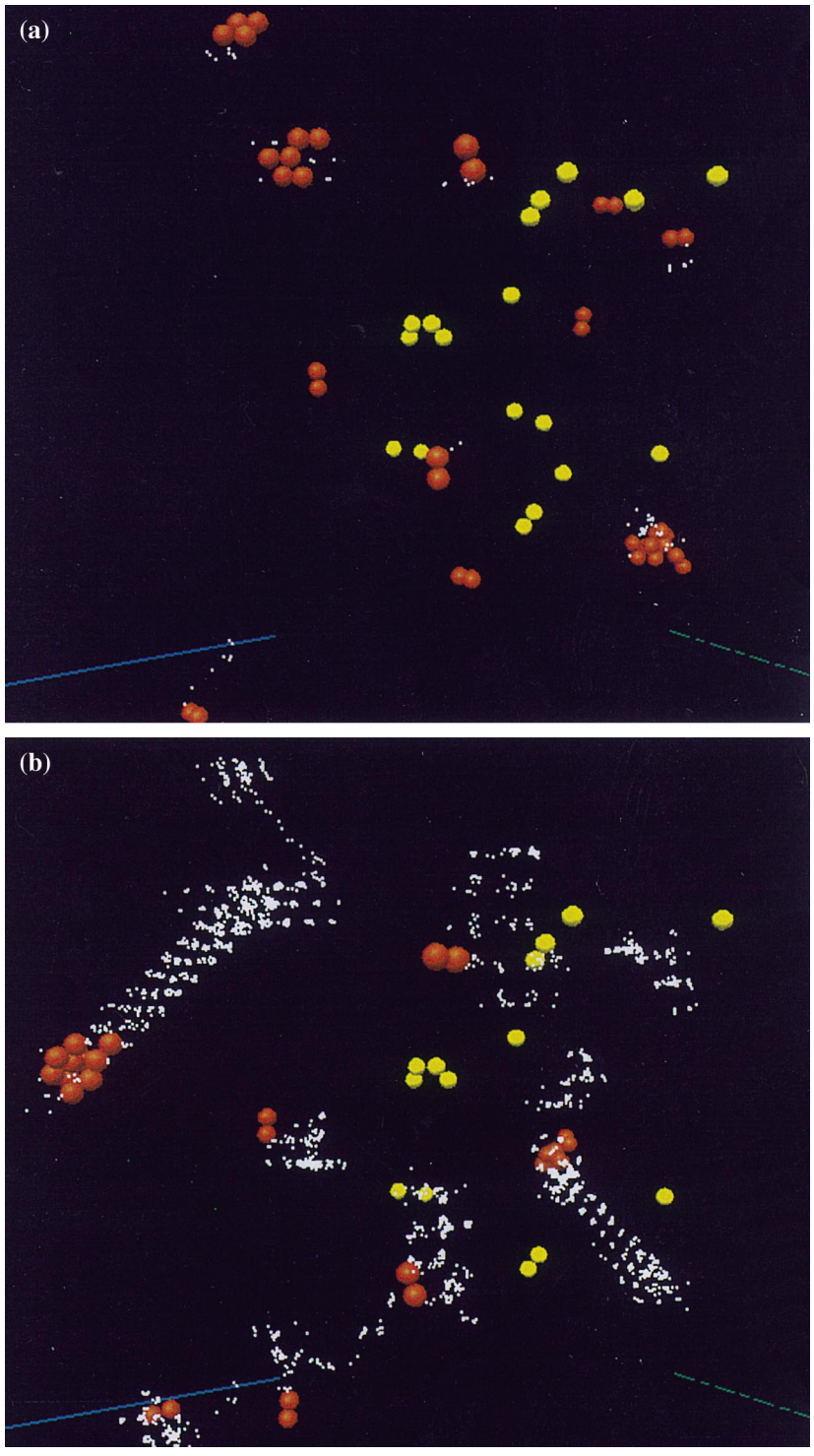

Fig. 1. Point defects and interstitial clusters observed in a 10 keV cascade in nickel: (a) at 30 ps (interstitial atoms and vacancies are represented by red yellow spheres, respectively); (b) at 70 ps. Note the interaction between two small clusters 2-d and 3-d resulting in a larger cluster 5-d assisted by the flip of the Burgers vectors and in a new direction of motion of the latter. Three single vacancies and one di-vacancy were eliminated by the glide motion of interstitial clusters.

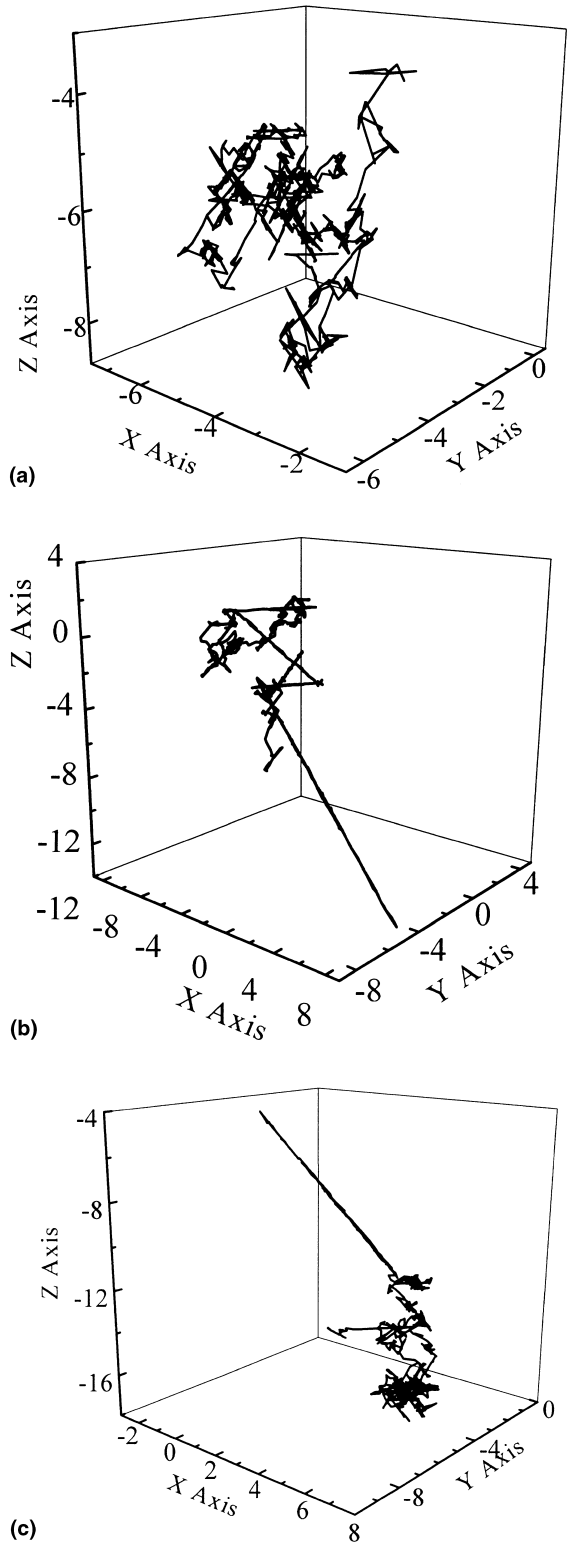

Fig. 2. Center-of-mass trajectories of the cluster of 3-dumbbells (during 230 ps): (a) at 600 K; (b) at 800 K and (c) at 1000 K.

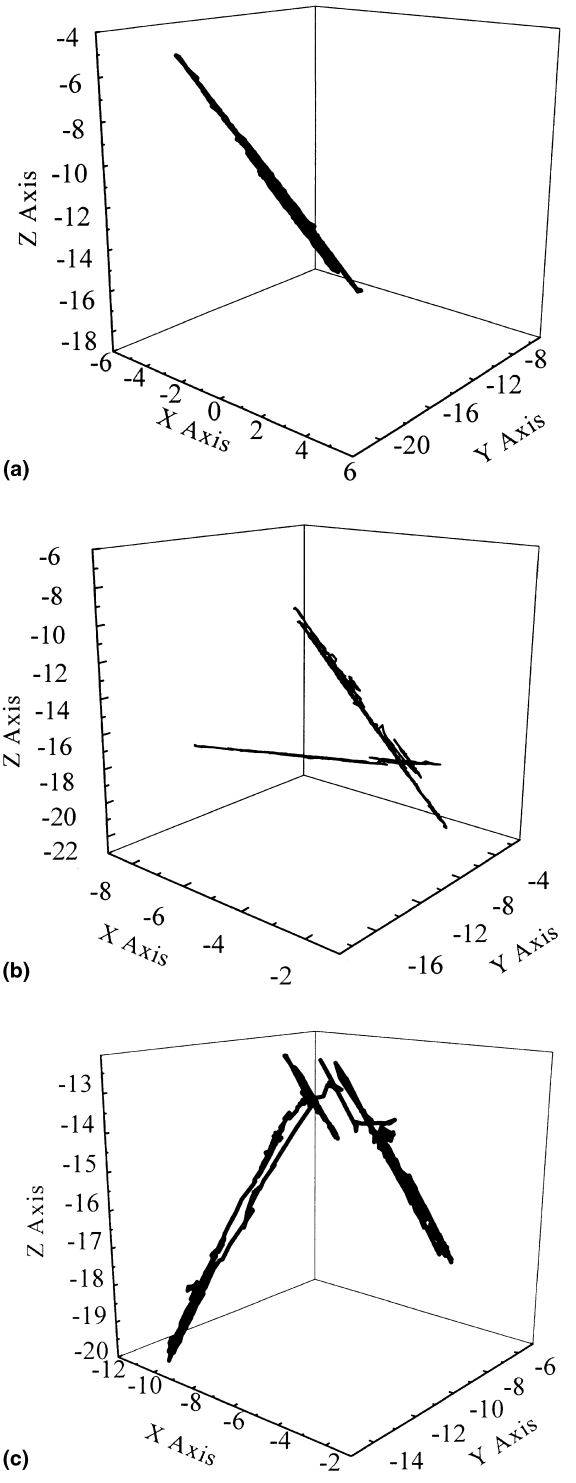

Fig. 3. Center-of-mass trajectories of the cluster of 5-dumbbells: (a) at 600 K (during 300 ps); (b) at 800 K (300 ps) and (c) at 1000 K (260 ps).

for D with the 3-d cluster depend strongly on the value of Δt and on the origin of the segment, from 0.4 to 2.5×10^{-3} cm^2 s^{-1} at 800 K. The same scatter was obtained at 600 and 1000 K. The results of D for the 5-d cluster were also scattered in the range of 0.2 and 1.5×10^{-3} cm^2 s^{-1} at the same temperatures. The migration energy for these clusters cannot be deduced from the present data, contrary to the results on the 3-d cluster of Soneda and Diaz [18] in α-iron.

Studies on dislocation pinning by small interstitial loops, as those performed by Rodney and Martin [19], have been performed but the results will be presented elsewhere.

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