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Section 6. Modeling radiation effects in materials

The effects of one-dimensional glide on the reaction kinetics of interstitial clusters

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Abstract

Collision cascades in metals produce small interstitial clusters and perfect dislocation loops that glide in thermally activated one-dimensional (1D) random walks. These gliding defects can change their Burgers vectors by thermal activation or by interactions with other defects. Their migration is therefore 'mixed 1D/3D migration' along a 3D path consisting of 1D segments. The defect reaction kinetics under mixed 1D/3D diffusion are different from pure 1D diffusion and pure 3D diffusion, both of which can be formulated within analytical rate theory models of microstructure evolution under irradiation. Atomic-scale kinetic Monte Carlo (kMC) defect migration simulations are used to investigate the effects of mixed 1D/3D migration on defect reaction kinetics as a guide for implementing mixed 1D/3D migration into the analytical rate theory. The functional dependence of the sink strength on the size and concentration of sinks under mixed 1D/3D migration is shown to lie between that for pure 1D and pure 3D migration and varies with L, the average distance between direction changes of the gliding defects. It is shown that the sink strength in simulations for spherical sinks of radius R under mixed 1D/3D migration for values of L greater than R can be approximated by an expression that varies directly as R^2. For small L, the form of the transition from mixed 1D/3D to pure 3D diffusion as L decreases is demonstrated in the simulations, the results of which can be used in the future development of an analytical expression describing this transition region.

1. Introduction

In the first wall or blanket of a fusion reactor, self-interstitial atoms (SIA) created in the collision cascades of energetic recoil atoms in metals can form as crowdions and clusters of coupled crowdions along close-packed directions. These crowdions and clusters (essentially small, perfect dislocation loops) can migrate in one-dimensional (1D) random walks by thermally activated glide (activation energy < 0.1 eV) [1]. Compared to defects migrating in 3D, the SIA and SIA clusters migrating in 1D have a much smaller probability of interacting with other defects within the cascade region. It has been shown that clusters migrating by 1D glide can change their Burgers vectors by thermal activation [2,3] or interaction with another defect [4] and continue their 1D glide along another close-packed direction. The result is a 3D diffusion path that is made up of segments of 1D glide, which we refer to as 'mixed 1D/3D' defect migration (Fig. 1). Previously we have shown [5] that the effects of mixed 1D/3D migration can be characterized in terms of the average distance between Burgers vector direction changes, L, and that the defect reaction kinetics vary significantly and smoothly between pure 3D and pure 1D as a function of L. We have also shown [6] how atomic-scale kinetic Monte Carlo (kMC) computer simulations of idealized defect interaction experiments can be used to study the effects of mixed 1D/3D migration and directly guide the development of analytical theories of the global

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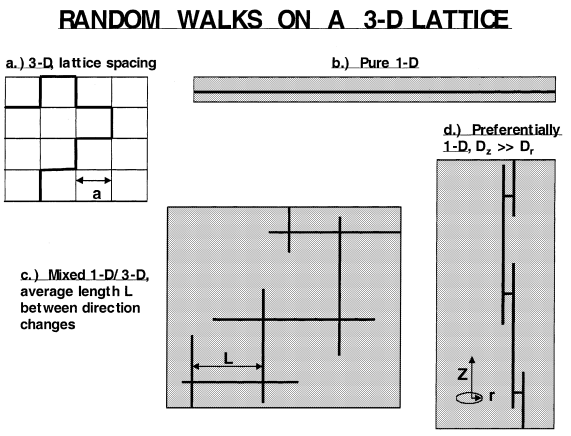

Fig. 1. Schematic illustration of defect migration paths by: (a) 3D random walk on the crystal lattice; (b) 1D random walk; (c) mixed 1D/3D migration consisting of a 3D path made up of segments of 1D random walks in different random close-packed directions; (d) preferentially 1D migration consisting of segments of 1D random walks in the same direction broken by occasional hops to adjacent atom rows.

evolution of irradiated microstructure under mixed 1D/3D migration. Analytical descriptions of defect reaction kinetics involving pure 3D or pure 1D migration are well known. However, analytical descriptions for mixed 1D/3D migration and the transitions from mixed 1D/3D to pure 1D or pure 3D are just now being developed [7]. Some analytical solutions have been found, but descriptions of the transition from mixed 1D/3D to pure 3D are still under development. Earlier theoretical studies of the effects of deviations from pure 1D diffusion on the reaction kinetics of SIAs in metals were performed by Seeger et al. See for example the 1976 paper by Gösele and Seeger [8]. Their work examined the effects of 'preferentially 1D' migration in which defects continue migrating in the same direction but make occasional hops to adjacent planes (Fig. 1(d)). Our current body of work [5–7] is, to our knowledge, the first study of reaction kinetics under mixed 1D/3D migration. In the present paper, we use kMC simulations to investigate the quantitative relationships between the sink strength, sink size, sink concentration and L.

2. Simulation results

A kMC computer code was used to perform simulations of idealized defect interaction experiments on a 3D face-centered cubic (fcc) lattice. In the simulations a mobile SIA cluster executes a random walk (by 1D, 3D or mixed 1D/3D migration) through a random 3D array of stationary spherical absorbers. The defect migrates by discrete hops to nearest neighbor lattice sites. The hop direction is chosen by random selection from the set of allowable directions – either forward or back along a particular $\langle 1\,1\,0\rangle$ direction for a 1D hop or in any of the 12 $\langle 1\,1\,0\rangle$ directions in the fcc lattice for a 3D hop. The center of each absorber is associated with an fcc lattice point, as is the center of the migrating SIA. The absorbers have uniform constant absorption radii R; when a migrating SIA hops to a lattice site within R of the center of an absorber, it is assumed absorbed. Since we are interested in understanding defect kinetics, and not the simulation of defect accumulation, the absorbers remain unchanged in size and position after absorbing a defect. For mixed 1D/3D migration, the defect executes v random 1D hops, then it chooses any one of the 12 $\langle 1\,1\,0\rangle$ directions along which to continue with its next 1D segment of v hops. The average net distance travelled between direction changes is $L = \sqrt{v}\,a_0/\sqrt{2}$, where a_0 is the fcc lattice parameter.

The computational cell is a cube of size 2790 fcc lattice parameters on edge, which is 1 μm in Cu, and it contains 10 000 absorbers, resulting in a number density $N = 10^{22}$ absorbers/m^3. In the simulations a migrating SIA is initially placed in a random position near the center of the cell, and it hops in the specified manner until it is absorbed. The number of hops to absorption is recorded for each defect. Every data point in the following figures represents the average result for at least 1000 migrating SIAs. To assure the absorption of each defect, periodic boundaries are assumed for the cell. The periodicity should have little effect on the results as long as the migrating defect makes at least several direction changes within the cell before reaching the boundary.

Computer experiments were generally performed for various values of R, holding the number density of absorbers fixed. Thus, as R increases, the volume fraction of absorbers increases. A spherical absorber of radius $R = 5a_0$ in Cu has a diameter of about 3.6 nm and contains about 500 lattice sites. At a number density of $N = 10^{22}$ m^{-3}, the volume fraction is 0.00024, and the absorbers are, on average, about 50 nm from each other.

Fig. 2 is a plot of the sink strength as a function of R for pure 3D migration. The sink strength for 3D migration is defined as $k^2_{3D} = 12/(a_0^2\langle n\rangle)$, where $\langle n\rangle$ is the average number of hops to absorption determined from the simulations. The curve, a third-order polynomial in R fitted to the entire range of the data, is not intended to have any particular physical significance at this time other than to demonstrate the curvature in the plot. Note, however, that the data points are also well-fit by the dashed straight line up to about $R = 15a_0$ (volume fraction of absorbers 0.65%). At $R = 25a_0$ (volume fraction 3%) the linear relationship under-predicts the sink strength determined from the simulations in this example by about 25%. At the largest radius in the figure, $R = 50a_0$ (volume fraction 24%), the linear model under-predicts the sink strength by a factor of 3. The

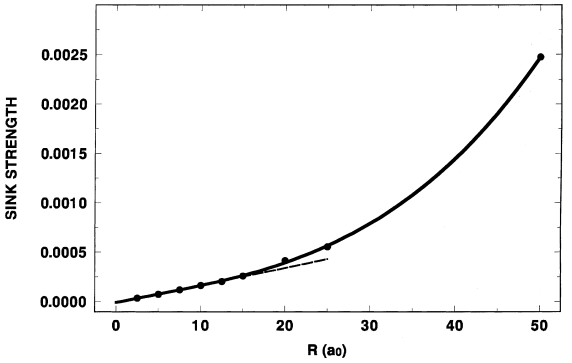

Fig. 2. The points are the values of the sink strength measured in kMC simulations ($k^2 = 12/(a_0^2\langle n\rangle)$) plotted vs the absorber radius R in lattice parameters for pure 3D migration. The curve is a fit of a third degree polynomial in R to all the points. The dashed line is a straight line fitted to the points in $0 < R < 15a_0$.

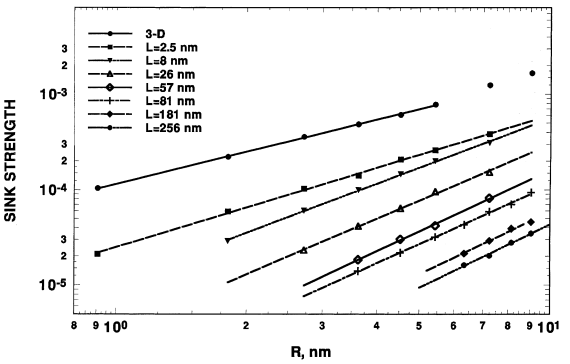

Fig. 3. The points are the sink strengths measured in kMC simulations ($k^2 = 4/(a_0^2\langle n\rangle)$) plotted vs the absorber radius R for various values of L, the distance between direction changes for mixed 1D/3D migration. The straight lines are fits of the power-law function $k_M^2 = \alpha(R - a_0/\sqrt{2})^m$, where α and m are fitting constants that vary with L.

approximately linear dependence at small R is compatible with the usual formula used in analytical rate theories for sink strength

$$k^2 = 4\pi RN, \tag{1}$$

which is valid for small volume fractions of absorbers. Further discussion of the simulations in this paper will be limited to values of R corresponding to volume fractions below about 3%, where, for pure 3D migration, the sink strength is linear in R.

When a straight line is fitted to the data in Fig. 2 for $R < 15a_0$, the line does not pass through the origin, i.e., the sink strength is not zero when $R = 0$. This is likely a result of the discrete nature of the diffusion mechanism, in which each defect hop is a fixed distance of $a_0/\sqrt{2}$ on the lattice along the $\langle 1\,1\,0\rangle$ direction. In the expression for the sink strength in pure 3D, Eq. (1), if R is translated by $a_0/\sqrt{2}$, i.e.,

$$k_{3D}^2 = 4\pi\left(R - a_0/\sqrt{2}\right)N, \tag{2}$$

then the plot of k_{3D}^2 vs $(R - a_0/\sqrt{2})$ is more nearly a straight line through the origin.

To determine the functional dependence of sink strength on R for mixed 1D/3D migration at small volume fractions the process above was carried out for mixed 1D/3D simulations for various values of L, and the results were plotted in log–log plots. Fig. 3 contains plots of sink strength as a function of R for values of L (in copper) from 2.56 to 256 nm, where now the sink strength for mixed 1D/3D migration is defined as $k_M^2 = 4/(a_0^2\langle n\rangle)$, the factor of 4 reflecting the 1D nature of the hops. The 3D sink strength is also plotted. These log–log plots are each fitted with straight lines representing the power-law expression:

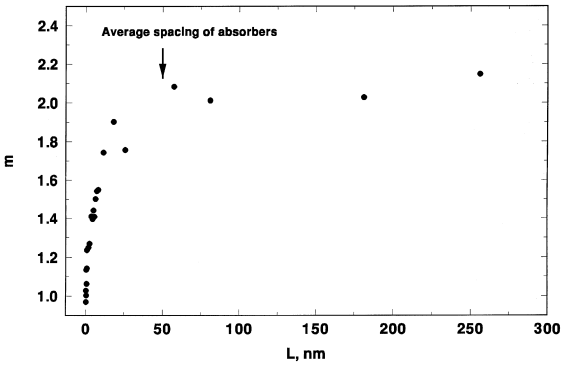

Fig. 4. Values of the power law exponent m, where the sink strength varies as R^m, plotted as a function of L, the average distance between direction changes for mixed 1D/3D migration. The arrow indicates the value of L that is equal in length to the average spacing of the absorbers.

$$k_M^2 = \alpha(R - a_0/\sqrt{2})^m, \tag{3}$$

where α and m are fitting constants that vary with L.

In Fig. 4 the exponents $m(L)$ determined for each L value in Fig. 3 are plotted vs L to show how the sink strength's dependence on R varies with L. At small L, the value of m increases rapidly from $m = 1$ for pure 3D to $m \cong 2$, then m gradually increases over the range of L values in this plot.

3. Discussion and conclusions

Recent theoretical developments by Trinkaus et al. [7] have identified the relationship between the sink

strength k_M^2 and L and R for mixed 1D/3D reaction kinetics to be

$$k_M^2 = 4\pi R^2 N/\sqrt{2}L, \quad L \gg R. \tag{4}$$

This expression is consistent with the behavior of the exponent m as a function of L in Fig. 4, i.e., k_M^2 varies directly as R^2 (at least approximately) for values of L greater than the absorber radii. It is interesting to note that the largest value of L on this plot is more than five times the average spacing between absorbers at this concentration, and the value of the exponent m is still near 2. For pure 1D the sink strength should vary as R^4. Thus, the defect reaction kinetics are of decidedly mixed 1D/3D character for values of L much larger than the average spacing of the absorbers. The transition from mixed 1D/3D reaction kinetics with $m = 2$ to 1D reaction kinetics having $m = 4$ is not apparent at these values of L. Meaningful kMC simulations for very large values of L require an extremely large computational cell; so it may be somewhat difficult to investigate the smooth transition from mixed 1D/3D kinetics ($m = 2$) to pure 1D kinetics ($m = 4$) by computer simulations. The analytical theory may offer the best way to investigate the mixed 1D/3D to pure 1D transition [7].

It may well be more important to understand the transition from mixed 1D/3D kinetics to pure 3D kinetics, since it is likely that effects of temperature, alloying and radiation damage will tend to shorten the distance between Burgers vector changes. Figs. 3 and 4 illustrate that significant information about this transition can be obtained from kMC simulations. Fig. 5 shows a comparison of sink strengths determined in the simulations with sink strengths calculated using Eq. (4). The sink strengths are plotted as a function of L for several values of R. Eq. (4) predicts the sink strength quite well for values of L above about 30 nm. The log–log plot in Fig. 5 emphasizes the differences between the simulations and the theory at the small values of L. Nevertheless, it is apparent that at small values of L, the functional dependence of the sink strength on L and R is significantly different from Eq. (4). At present, the challenge of determining how to incorporate the behavior at small L into a smooth transition over all values of L and R (within the small volume-fraction approximation) in the analytical rate theory still remains.

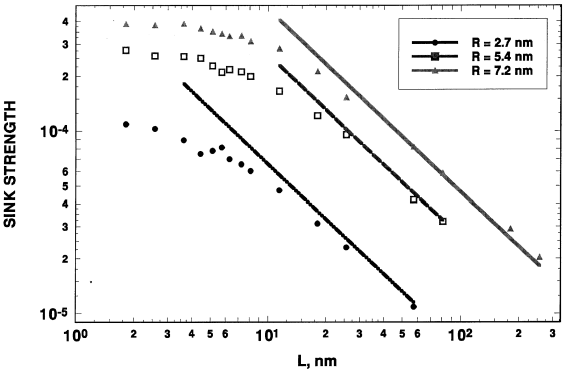

Fig. 5. Comparison of kMC simulation results with the analytical expression for the sink strength under mixed 1D/3D migration, Eq. (4). The sink strengths are plotted as a function of L, the average distance between direction changes, for several values of R, the absorber radius. All length dimensions are in nm.

Acknowledgements

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