KINETIC MONTE CARLO STUDIES OF THE REACTION KINETICS OF CRYSTAL DEFECTS THAT DIFFUSE ONE-DIMENSIONALLY WITH OCCASIONAL TRANSVERSE MIGRATION—H. L. Heinisch (Pacific Northwest National Laboratory),* H. Trinkaus (Institute für Festkörperforshung), and B. N. Singh (Risø National Laboratory)

EXTENDED ABSTRACT

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SUMMARY

The reaction kinetics of the various species of mobile defects in irradiated materials are crucially dependent on the dimensionality of their diffusion processes. Sink strengths for one-dimensionally (1D) gliding interstitial loops undergoing occasional direction changes have been described analytically and confirmed by kinetic Monte Carlo (KMC) simulations. Here we report on KMC simulations investigating the transition from 1D to 3D diffusion for 1D gliding loops whose 1D migration is interrupted by occasional 2D migration due to conservative climb by dislocation core diffusion within a plane transverse to their 1D glide direction. Their transition from 1D to 3D kinetics is significantly different from that due to direction changes. The KMC results are compared to an analytical description of this diffusion mode in the form of a master curve relating the 1D normalized sink strength to the frequency of disturbance of 1D migration.

PROGRESS AND STATUS

Introduction

There are experimental observations of features in irradiated materials that cannot be rationalized in terms of the 3D diffusion kinetics of vacancy and SIA defects assumed in conventional rate theory [1,2]. Moreover, in it has been recognized that some deviation of the reaction kinetics of SIA clusters from that for pure 1D diffusion are necessary for proper representation of phenomena described by the theory of radiation damage [3]. Computer modeling has shown that energetic displacement cascades in metals produce clusters of self-interstitial crowdion defects (actually small glissile dislocation loops) that diffuse by one-dimensional (1D) glide along close packed directions with migration energies less than 0.1 eV [4,5]. Under certain conditions, the 1D migrating loops can individually undergo a thermally-activated change in the direction of their 1D migration (i.e., a change in the direction of the Burgers vector of the dislocation loop) to a different close-packed direction [6,7].

An analytical treatment of defect interactions for defects following the reaction kinetics for 1D to 3D via the changing of Burgers vectors was developed for use in reaction rate theories of microstructure evolution under irradiation [8]. As part of that work, KMC simulations of the 1D to 3D transition for defects interacting with a variety of sizes and densities of sinks were also performed that corroborated the analytical theory. In the present work, we examine a different type of 1D/3D reaction kinetics in which the 1D paths of gliding loops are occasionally interrupted by excursions due to conservative climb by dislocation core diffusion . The 2D climb excursion is in a plane, normal to the direction of glide, after which glide is resumed along the original glide direction. This mode of defect migration was considered some time ago, for example by Gösele and Seeger [9], who referred to this mode as “preferential 1D migration,” especially in the case where the climb excursions are small and infrequent. An analytic theory similar to that for 1D/3D “direction change” reaction kinetics has been developed that describes the effects of the frequency of climb excursions on sink strengths throughout the range from pure 1D to pure 3D. This paper reports on KMC simulations performed in support and corroboration of the analytical theory, the development of which will be described in detail elsewhere.

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Computer Simulations

The KMC model consists of immobile spherical “absorbers” that are unsaturable, maintaining a constant radius R and number density N throughout the simulations. The absorbers are randomly arranged in a large test volume, and migrating “defects” are introduced into the volume one at a time, starting at random positions near the center of the volume and hopping on a face-centered cubic lattice until being absorbed by an absorber. During the migration of each defect, its deviations from pure 1-D hopping occur regularly according to the conditions under investigation. All hops of a defect are chosen randomly from the possible hops permitted by the restrictions on its motion. The “lifetime” of each defect is defined as the total number of hops it makes before being absorbed by one of the absorbers. Each data point in the KMC results reported in Figs. 1 and 2 represents the average behavior of at least 1000 migrating defects.

In Fig. 1, the values of the sink strengths determined from the KMC simulations are plotted as a function of the average distance traveled by the defects in each 1D migration segment, i.e., the distance traveled between the occurrences of the non-1D events. In this paper, the non-1D events studied are either a change in the direction of the 1D migration (1D/3D) or a 2D climb excursion transverse to the 1D migration direction (preferential 1D). In both cases the average length of the 1D segments is proportional to the average of the square root of the number of 1D hops in each 1D segment. For 1D/3D migration, the 1D (glide) migration of each defect is regularly interrupted by a change in direction of the 1D migration. In both cases less frequent interruption of the 1D glide results in greater distance traveled during each individual 1D glide migration path segment. The two sets of data points plotted between the preferential 1D and 1D/3D data sets are results for the preferential 1D mode when the defects make multiple 2D climb hops during each excursion from 1D migration. The addition of larger climb excursions during each interruption of 1D pushes the sink strengths for preferential 1D toward the 1D/3D values.

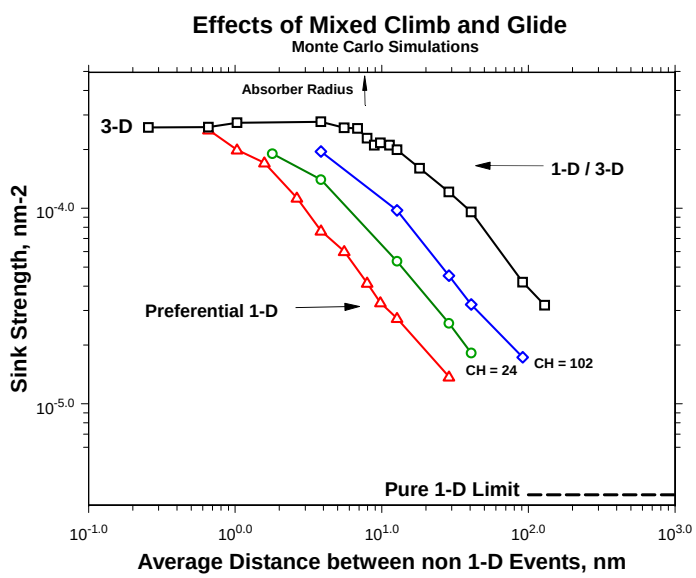

Fig. 1. Sink strength as a function of the average length of 1D migration path between disturbances of the 1D migration by diffusive climb events (Preferential 1D) compared to effects of the disturbance by change of glide direction (1D/3D). Data lying between the “1D/3D” and “Preferential” curves are for cases of Preferential 1D in which more “climb hops” (CH=24,102) are performed during each climb excursion of the preferential 1D migration.

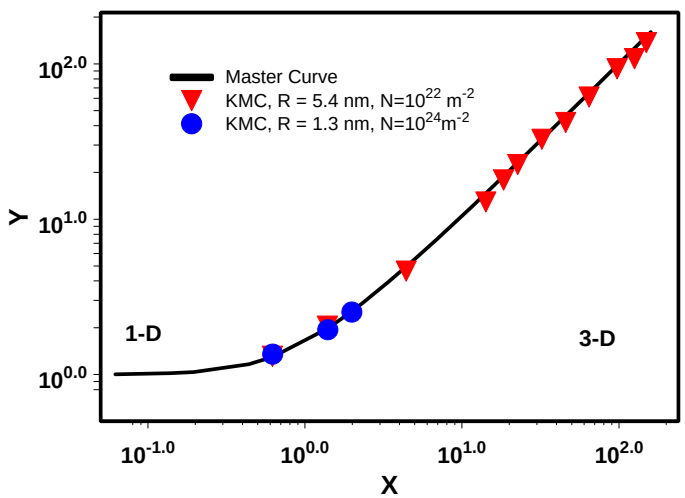

Fig. 2. Comparison of the analytical expression of the "Preferential 1D Master Curve," to the KMC results for two different conditions involving absorbers of different radius R and number density N.

Analytical Master Curve

A master curve relating sink strength to the "disturbance of 1D diffusion" for 1D/3D defect migration was developed earlier by Trinkaus et al. [10], and it was shown to match very well with sink strength data generated in KMC simulations for 1D/3D migration. This master curve concept has subsequently been reconfigured and extended to describe preferential 1D migration as well. The new master curve is presented here for comparison with results of the KMC simulations. Details of the derivation of the new master curve and discussion of its implications will be presented in another publication.

The master curve has the form

$$Y = 0.5\{1 + [1 + 4X^2]^{1/2}\} \quad (1)$$

where Y is the sink strength normalized to its value for pure 1-D

$$Y = k^2/k_1^2 \quad (2)$$

and X is a measure of the "disturbance of 1-D diffusion." The "disturbance of 1-D diffusion" for disturbance by Burgers vector changes (1D/3D) is represented as

$$X = (L^2k_1^2/12+k_1^4/k_3^4)^{-1/2} \quad (3)$$

where L is the 1-D path length between direction changes. For preferential 1D, the disturbance of 1D diffusion by conservative climb is given as

$$X = (\delta^{1/2}\, f(\delta)\, k_3^2/k_1^2) \quad (4)$$

where $\delta = D_{tr}/D_{lo}$, the ratio of the transverse and longitudinal diffusivities, and

$$f(\delta) = 3[1-\delta]^{1/2} /\{(1 + 2\delta) \arccos(\delta^{1/2})\}\,. \quad (5)$$

In Fig. 2, the KMC results for Preferential 1D migration are compared to the analytical master curve, Equation 1. For Fig. 2, simulations were also performed for a system of absorbers having a smaller size, R = 1.8 nm, and a higher number density, N = 10^{24} m^{-3}, especially to achieve results closer to the pure 1D

limit, as well as to test the master curve over a range of conditions. The agreement of the master curve with the KMC results for both sets of absorbers is excellent.

Conclusions

The KMC simulations confirm the 1-D to 3-D behavior predicted by the analytical expressions for both the loop glide direction change mechanism (1D/3D) and the glide-climb (preferential 1-D) mechanism. The master curve relating the normalized sink strength to the disturbance of 1-D diffusion, corroborated by KMC modeling, illustrates the validity of the comprehensive analytical representation of these phenomena. Furthermore, the analytical representation of 1D to 3D diffusion reaction kinetics utilized to form the master curve is well-suited for modeling damage accumulation under the locally anisotropic diffusion conditions of defects in materials where such 1D-migrating defects are formed.

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