

**A KINETIC MONTE CARLO STUDY OF MIXED 1-D/3-D DEFECT MIGRATION** - H.L. Heinisch (Pacific Northwest National Laboratory)\*, B.N. Singh (Risø National Laboratory, Denmark), S.I. Golubov (Institute of Physics and Power Engineering, Russia)

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#### EXTENDED ABSTRACT

Kinetic Monte Carlo (kMC) techniques are being used to study a key element of microstructure evolution under irradiation: diffusion of defects by migration that has characteristics of both one-dimensional (1-D) and three-dimensional (3-D) random walks.

It has been shown in virtually all MD simulations of displacement cascades in metals that self-interstitial atoms (SIA) readily form clusters that are, or can become, glissile dislocation loops. In MD simulations of collision cascades in pure metals it has been observed that clusters of coupled crowdions can form directly during the production of cascades [1]. Such clusters are crystallographically equivalent to small, perfect interstitial dislocation loops that are glissile. Like single crowdions, the crowdion clusters can move one-dimensionally by thermal activation, having extremely small migration energies [2]. In general, cascade-producing damage events in metals introduce localized damage regions containing a mix of SIA and vacancy defects that include (depending on the material and the temperature) immobile clusters, mobile defects moving by three-dimensional random walks and mobile defects moving by one-dimensional random walks. Analytical theories describing the evolution of the defect population and the microstructure under irradiation must be able to address the disposition of all these types of defects. It has also been observed in recent MD simulations of glissile SIA cluster motion that the 1-D gliding clusters can change the direction of their 1-D motion by thermal activation [3,4] or by interaction with another defect [5]. The result is that a gliding SIA cluster effectively moves in three dimensions by a series of segments of 1-D random walks along different directions, we call this "mixed 1-D/3-D" migration.

The production bias model of void swelling (PBM) is an analytical theory that has been developed to explicitly address the issues arising from cascade damage, including the formation and transport of glissile SIA clusters [6]. In the current PBM model defect reaction kinetics of both 1-D and 3-D migration can be accommodated using different functional forms for the dependence of 1-D and 3-D reaction kinetics on the size and number densities of the microstructural features. However, a functional form for the reaction kinetics of mixed 1-D/3-D migration is not known.

To gain insight into the reaction kinetics for mixed 1-D/3-D migration, kMC simulations of simple idealized problems can be performed and analyzed to determine the functional relationships of relevant variables to the degree of mixed 1-D/3-D migration. For example, the probability of absorption into a concentration of stationary absorbers of spherical capture radius  $R$  varies as  $1/R$  for pure 3-D migration and as  $1/R^2$  for pure 1-D migration [7]. It is of interest to examine the dependence on the absorber radius for mixed 1-D/3-D migration.

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In the kMC model, the locations of defects are monitored as they hop on a face-centered cubic lattice. The defects can execute 1-D, 3-D or mixed 1-D/3-D random walks of various 1-D segment lengths simply by choosing a value for the variable NJDC, the number of jumps between direction changes, for 1-D migrating defects. The basic concepts of the kMC method for studying defect kinetics under mixed 1-D/3-D migration are described further in earlier publications [8,9]. In these idealized studies all defects have the same properties and there is no recombination or clustering. The migrating defects interact with stationary spherical absorbers of uniform absorption radius  $R$ . The absorbers are unsaturable and do not change size upon absorbing a migrating defect.

Simulations were done by placing a mobile defect at a random initial position near the center of a random array of absorbers of radius  $R$  in a computational cell of fixed volume and following it until it was either absorbed by a spherical absorber or escaped from the cell (or equivalently, was absorbed by the boundary of the cell). Simulations were done with 1000 defects for each set of conditions, i.e., each data point on the following figures represents the average results for 1000 defects.

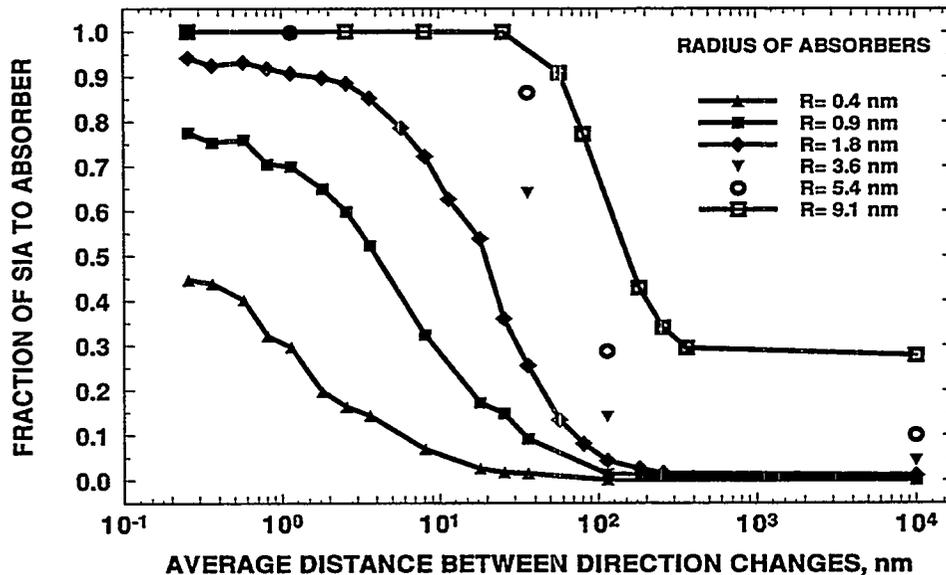


Figure 1. The fractions of mobile defects absorbed by a periodic array of absorbers of radius  $R$  as a function of the average distance traveled between direction changes,  $L$ , in nm for various values of  $R$ .

Figure 1 shows the fraction of defects absorbed in absorbers as a function of the average distance traveled between direction changes  $L = a (NJDC/2)^{1/2}$ , where  $a$  is the FCC lattice parameter. Data are plotted for various values of absorber radius,  $R$ , illustrating how the

fraction absorbed varies with both  $R$  and  $L$ . The curves clearly illustrate the difference in reaction kinetics of defects that are transported by 1-D, 3-D and mixed 1-D/3-D migration.

Figure 2 shows the mean free path (the average distance traveled by a defect before being absorbed) as a function of the absorber radius. Data are plotted for different constant values of NJDC. These log-log plots are essentially straight lines of different slope, depending on the value of NJDC. For pure 3-D migration (NJDC=1) the mean free path should vary as  $1/R$ , while for pure 1-D migration it should vary as  $1/R^2$ . In general, we might expect that for mixed 1-D/3-D migration the mean free path should vary as  $1/R^M$ , where  $M$  depends on the value of NJDC.

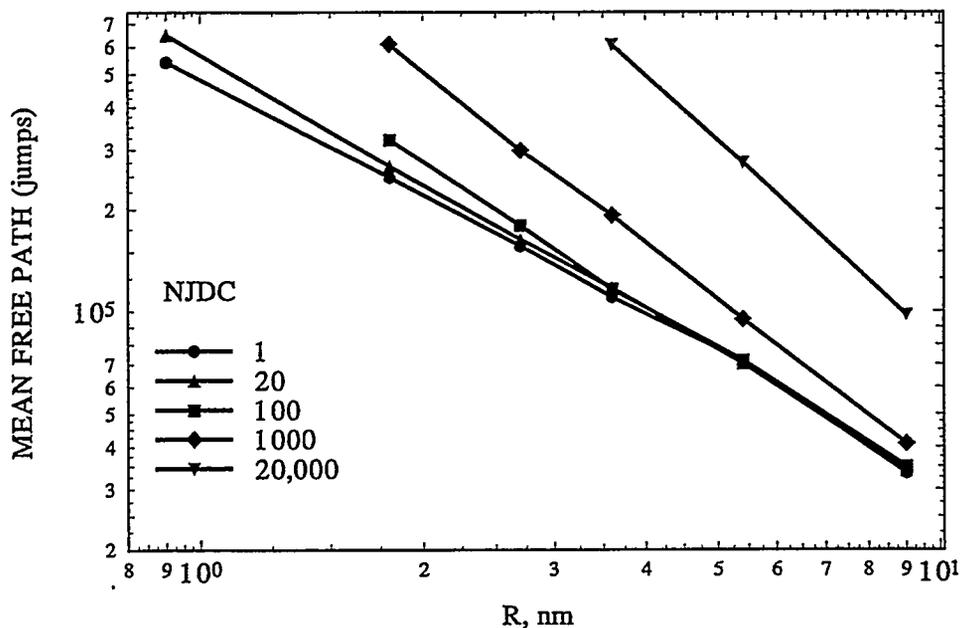


Figure 2. The mean free path (average distance traveled by a defect to an absorber) in units of defect jumps on a FCC Cu lattice as a function of the absorber radius  $R$  in nm for various values of the number of jumps between direction changes NJDC for mixed 1-D/3-D migration.

In Figure 3 a plot of the negative slope  $M$  of the lines in Figure 2 as a function of  $L$  reveals that  $M$  varies from  $M=1.1$  for NJDC=1 (pure 3-D migration) to  $M=2$  for NJDC=20,000 (near pure 1-D migration). Thus, the dependence of mean free path on absorber radius varies approximately from  $1/R$  to  $1/R^2$  as expected, as the dimensionality of the migration changes from pure 3-D to mixed 1-D/3-D to pure 1-D.

The values of  $M$  in Fig. 3 for pure 1-D and pure 3-D migration are somewhat higher than the ideal values because of the finite size of the computational cell and the fixed length of time used in the kMC simulations. In essence, the entire distribution of diffusion paths is not

being sufficiently sampled by the simulation. Thus, it is premature to determine the functional dependence of  $M$  on  $L$  from data such as presented in Fig. 3. However, these results illustrate the power of kMC simulations to explore phenomena and display relationships between variables that would be very difficult or impossible to obtain through analytical methods or results of experiments. Establishing such functional relationships is important because, as an irradiation proceeds, the scale of the microstructure changes, so the reaction kinetics for defects under mixed 1-D/3-D migration change continuously as the size and concentration of reaction partners changes. Also, the value of  $L$  that determines the nature of the mixed 1-D/3-D reaction kinetics may well depend on the changing microstructure as well as on the temperature.

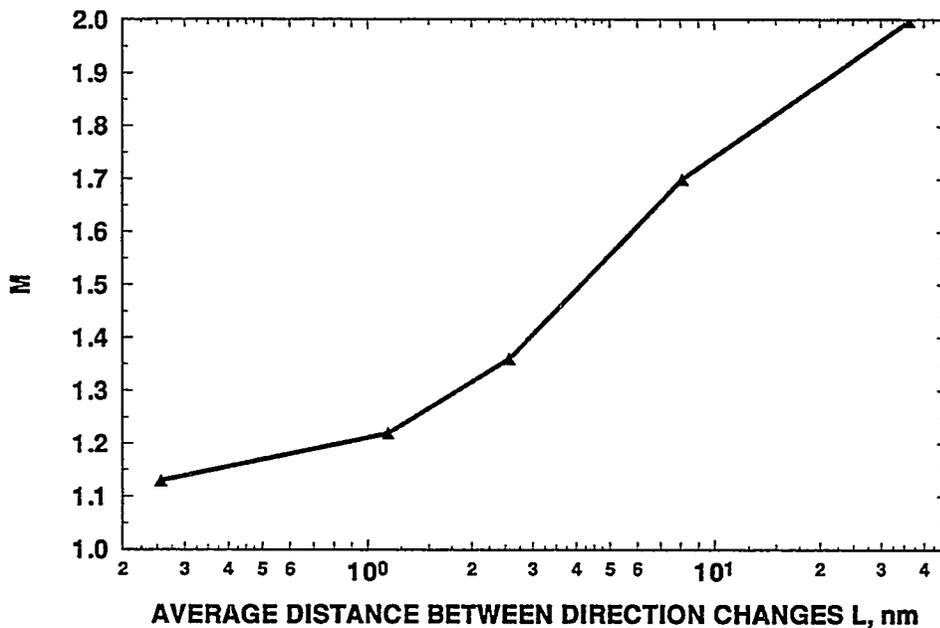


Figure 3. Values of the exponent  $M$ , where the mean free path of defects to absorbers varies as  $1/R^M$ , as a function of  $L$ , the average distance between direction changers for mixed 1-D/3-D migration.

Future work will include revising the kMC simulation technique for extraction of complete mean free path information, followed by subsequent analysis of the functional relationships involved in the reaction kinetics of mixed 1-D/3-D migration and the scale of microstructural features, e.g. the size and concentration of absorbers.

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