

THE EFFECTS OF ONE-DIMENSIONAL GLIDE ON THE REACTION KINETICS OF INTERSTITIAL CLUSTERS - H. L. Heinisch (Pacific Northwest National Laboratory), B. N. Singh (Risø National Laboratory, Denmark) and S. I. Golubov (Institute of Physics and Power Engineering, Russia)

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EXTENDED 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 both 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 being 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 theory. Earlier studies using kMC simulations [1,2] have demonstrated the significant effects of 1D and mixed 1D/3D migration on defect reaction kinetics. The present work seeks to determine the functional dependence of defect reaction kinetics on the variables affecting the defect-sink interactions under mixed 1D/3D migration.

In the kMC simulations, defects migrate one at a time through the crystal by random hopping from one fcc lattice site to an adjacent lattice site in pure 3D or mixed 1D/3D migration, depending on the nature of the defect, until they are absorbed in randomly distributed unsaturable spherical absorbers of equal radius R and number density N . The "sink strength" of defect sinks in 3D is defined as $k_{3D}^2 = 6/(a_0^2 \langle n \rangle)$, where a_0 is the (fcc) lattice constant and $\langle n \rangle$ is the average number of hops to absorption determined from the simulations. For mixed 1D/3D migration we define the sink strength to be $k_M^2 = 4/(a_0^2 \langle n \rangle)$ to reflect the 1D nature of the hops. The usual formula used in analytical rate theories to describe the sink strength in terms of the characteristics of the sink population (3D) is

$$k^2 = 4\pi RN, \quad (1)$$

which is valid for small R , representing volume fractions of absorbers less than a few percent. The simulation results for pure 3D are well-represented by the form of eq (1), modified to take into account the discrete hopping nature of the diffusion process (see the full paper). For pure 1D migration in the analytical theory, the sink strength varies as R^4 . Figure 1 is a log-log plot of the sink strength as a function of R for various values of L , the average distance between direction changes for mixed 1D/3D migration. The straight lines are fits of a power law function to the simulation results, with the power $m=1$ for pure 3D and with values that vary up to about $m=2$ as L increases.

Thus, the existence of mixed 1D/3D migration introduces a new variable into the reaction kinetics: the average distance between direction changes, L . So, in the analytical theory, the concept of "sink strength" is determined not only by the concentration and properties of

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the sinks, but also by the kinetic properties of the migrating defects. Simulation results demonstrate that the dependence of sink strength on the size and concentration of sinks under mixed 1D/3D migration lies between those for pure 1D and pure 3D migration and varies with L .

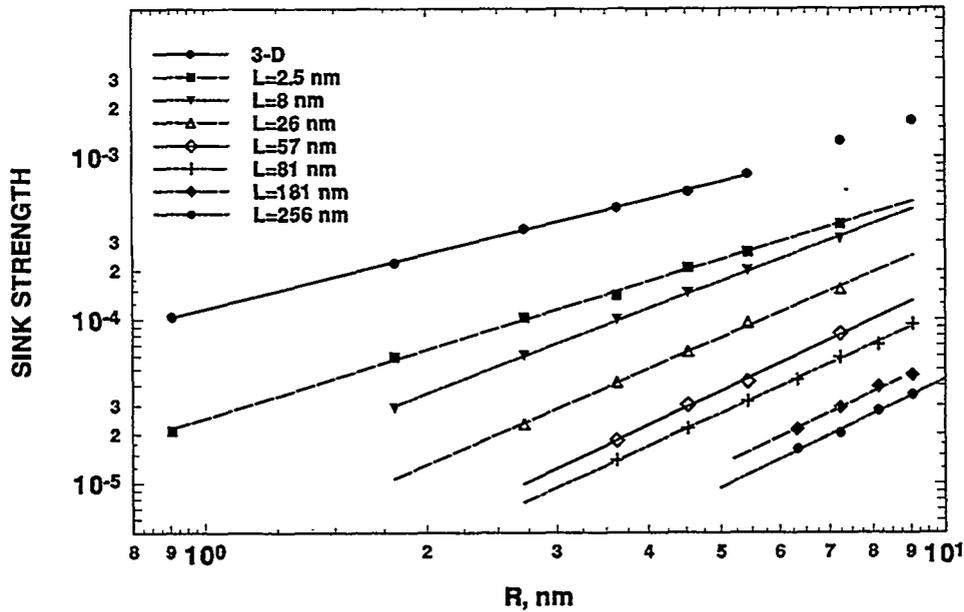


Figure 2. The points are the sink strengths measured in kMC simulations ($k^2 = 4/(a_0^2 \langle n \rangle)$) plotted versus the absorber radius R for various values of L , the distance between direction changes for mixed 1-D/3-D migration. The straight lines are fits of the power law function $k_M^2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

Recent theoretical developments by Barashev, Golubov and Trinkaus [3,4] have, by two different approaches, identified the relationship between the sink strength k_M^2 and L and R for mixed 1D/3D reaction kinetics to be

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

This expression is consistent with the behavior of the exponent m as a function of L in Fig. 1, i.e. that k_M^2 varies directly as R^2 (at least approximately), but it is true only for values of L greater than the absorber radii. This is illustrated in Fig. 2, where simulation results are compared with eq. (2). While there is good agreement between the simulations and the analytical theory at values of L larger than the absorber size, the theory still needs to be developed to fully describe the transition between mixed 1D/3D and pure 3D.

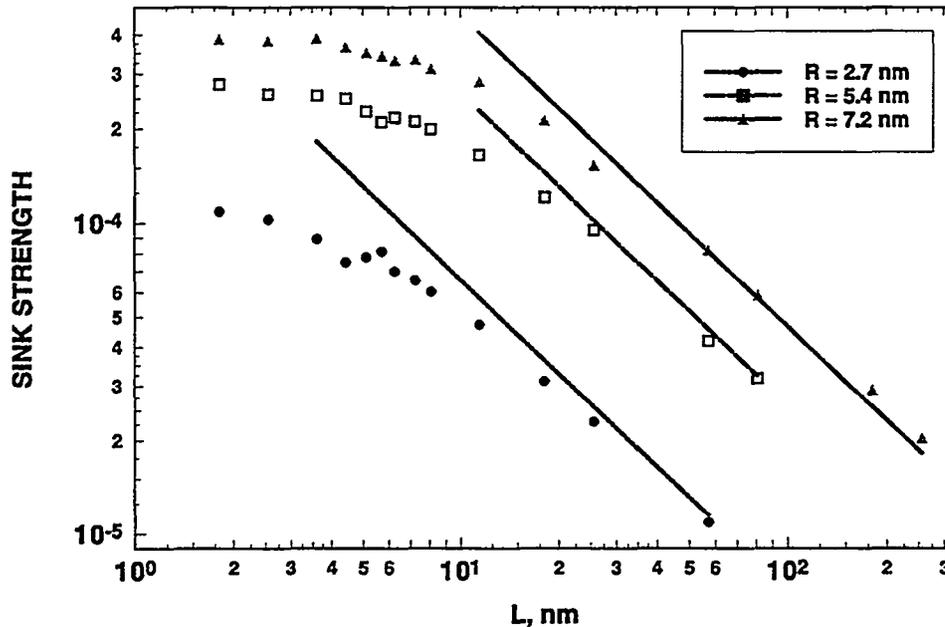


Figure 4. Comparison of kMC simulation results with the analytical expression for the sink strength under mixed 1D/3D migration, eq. (2). The sink strengths are plotted as a function of L , the average distance between direction changes, for several values of R , the absorber radius. All length dimensions are in nm.

Future work will aim at further elucidating the ramifications of mixed 1-D/3-D migration on defect reaction kinetics, especially the transition to pure 3D migration, through additional kinetic Monte Carlo simulations and analytical theory development.

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