KINETIC MONTE CARLO STUDIES OF 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)

(Summary of a paper presented at the International Workshop on Basic Aspects of Differences in Irradiation Effects between FCC, BCC and HCP Metals and Alloys, Cangas de Onis, Spain, October 15-20, 1998. The paper will appear in the workshop proceedings in J. Nucl. Mater.)

EXTENDED ABSTRACT

A comparison of the available experimental results on cluster density and void swelling clearly demonstrates that there are very significant differences in the defect accumulation behavior between fcc and bcc metals irradiated under cascade damage conditions over a wide temperature range [1]. In an attempt to understand the mechanisms responsible for causing these large differences in the swelling behavior between fcc and bcc metals, Golubov, Singh and Trinkaus [2] have analyzed the experimental results on void swelling within the framework of the production bias model (PBM) with the assumption of one-dimensional (1-D) diffusional transport of self-interstitial atom (SIA) clusters. Molecular dynamics (MD) studies have demonstrated that the structure, stability, and the fraction of glissile SIA clusters (migrating one-dimensionally) that are produced in cascades in bcc iron are different from that in fcc copper [3,4].

The concept of "pure" 1-D diffusional transport implies that the gliding SIA clusters (essentially small glissile dislocation loops) are assumed to maintain the same Burgers vector throughout their lifetime (until they interact with a sink). It was found that incorporating the assumption of pure 1-D diffusional transport of SIA clusters into the PBM does not provide an adequate explanation for the observed large differences in the swelling behavior between fcc and bcc metals [2]. Rather, Golubov et al. [2] have proposed that the treatment of the damage accumulation in the PBM should include the effects of changes in the Burgers vector of SIA clusters during their 1-D diffusional transport. MD simulation studies have shown that such changes can occur either by thermal activation [5,6] or by interaction with another SIA cluster [7]. The net effect of this kind of migration is a defect migration path that is 3-D but consists of segments of 1-D random walks. The reaction kinetics of this mixed 1-D/3-D type of migration will depend on the average length of 1-D segments relative to the size and concentration of other defects and microstructural features the SIAs can interact with.

Unfortunately, at present, there exists no mathematical description of the reaction kinetics for 1-D glide with random Burgers vector changes. Some guidance can be found from earlier work by Gösele and Seeger [8], who analytically described the reaction kinetics of single crowdions involved in defect recovery during annealing experiments. Their work demonstrated that even a very small deviation from the pure 1-D diffusion (which in their case involved infrequent jumps of crowdions from one row of atoms to another, continuing in the same direction in "preferentially " 1-D migration) leads to a decisive change in the reaction kinetics. While this conclusion has been taken to be the central argument in the treatment of defect accumulation and void lattice formation in fcc and bcc metals by Golubov

* Pacific Northwest National Laboratory is operated for the U.S. Department of Energy by Battelle Memorial Institute under contract DE-AC06-76RLO 1830.

et al. [2], there still remains the difficulty of analytically describing the effects of random Burgers vector changes and mixed 1-D/3-D migration.

In order to gain insight on these processes, we began investigating the changes in reaction kinetics as a function of changes in the Burgers vector of one-dimensionally diffusing SIA clusters, and the size and density of randomly or periodically distributed sinks using kinetic Monte Carlo simulations.

When the frequency of changes in the Burgers vector is so high that the mean transport distance between Burgers vector changes becomes of the order of the lattice parameter of the crystal, the reaction kinetics under these conditions can be assumed to be the same as in the case of "pure" 3-D diffusional transport. Thus, the Monte Carlo simulations are used to study the reaction kinetics of the two limiting cases of "pure" 1-D (i.e. when there is no change in Burgers vector) and "pure" 3-D diffusional transport, as well as when the diffusional transport occurs as a mixture of 1-D and 3-D.

Empirical computational studies of the effects of scale and Burgers vector change were performed using a simple kinetic Monte Carlo computer code, following the basic concepts of the ALSOME kinetic Monte Carlo code used for annealing studies of cascades [9] and simulations of defect accumulation under irradiation.[10] Studies were performed to determine the effects on absorption of defects into a static array of unsaturable absorbers as a function of the number of jumps N between direction changes, varying from N=0 for "pure" 3-D migration with equally probable jumps along any of the twelve <110> directions to N=∞ for pure 1-D migration. These were done for different absorber sizes and concentrations, and were plotted in terms of the average distance between direction changes, $L = a\,(N/2)^{1/2}$, where a is the FCC lattice parameter.

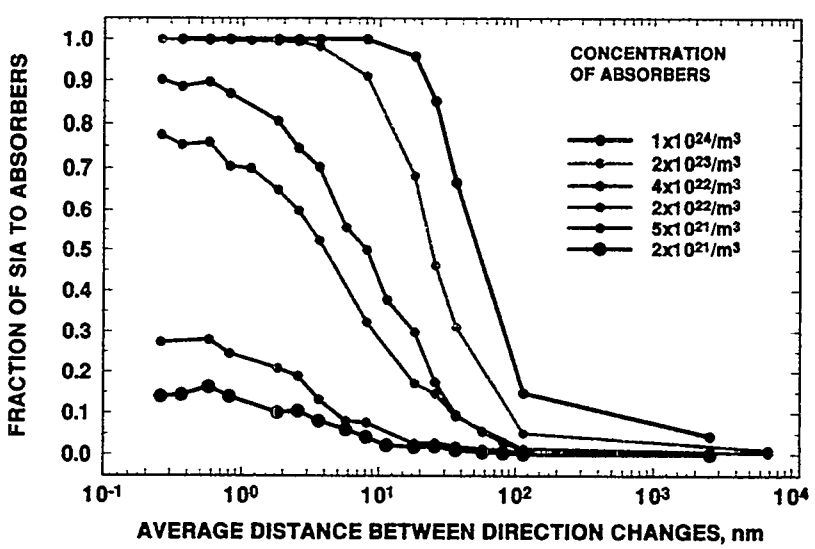

Figure 1. The fractions of mobile SIAs absorbed by a periodic array of absorbers of radius 0.9 nm as a function of the average distance traveled between direction changes for various concentrations.

As an example, Figure 1 shows the fraction of defects absorbed as a function of L for six different levels of concentration of a periodic array of absorbers of radius R=0.9 nm. Every data point represents the average value for the individual trajectories of 1000 mobile defects, initiated one at a time at random positions and with randomly chosen initial migration directions within the computational cell. When the probability of meeting an absorber increases at higher concentration, the transition from 1-D to 3-D behavior as a function of L becomes much sharper. This illustrates how defect reaction kinetics in a global sense will change differently during defect accumulation, depending on the value of L.

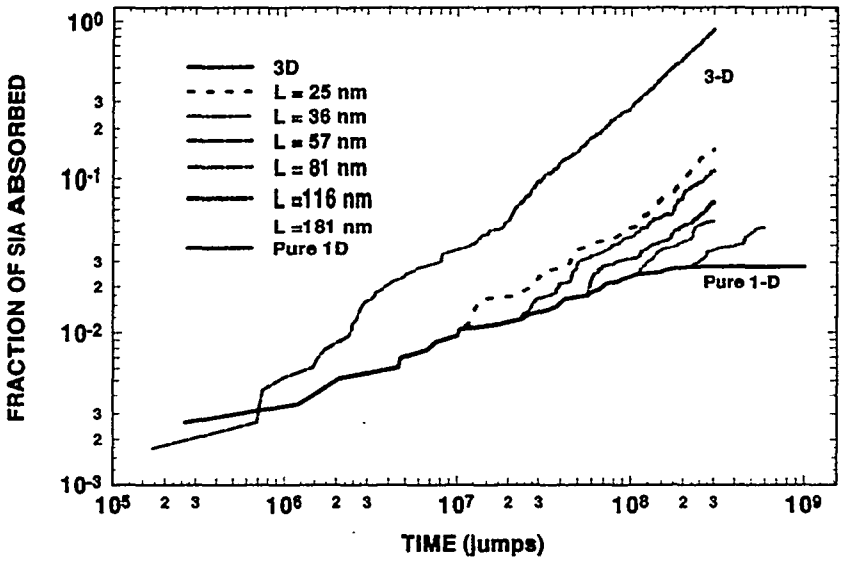

Figure 2. The fraction of 1000 initial SIAs absorbed in a random array of absorbers as a function of time (in units of defect jumps) for various values of L, the average distance between direction changes

In another example, Fig. 2 shows results of a simulation of recovery (or decay of a defect population) as a function of time. In this case 1000 mobile SIAs were placed randomly in a cell containing a random array of stationary absorbers. The SIAs did not interact with each other. Figure 2 shows the number of mobile SIAs absorbed in the absorbers as a function of time, which is measured in units of defect jumps, for runs using various values of L and the same set of random numbers. The upper curve is for 3-D migration with $L=a/\sqrt{2}$, and it shows essentially linear absorption with time. The lower curve is for pure 1-D ($L=\infty$), and it tends toward a saturation value reflecting the finite size of the cell. In every intermediate case, there is a transition from 1-D behavior to near 3-D behavior once the defects have migrated distances comparable to the distances between direction changes. In all cases here about 3% or less of the defects are absorbed under pure 1-D kinetics; significant absorption occurs only in the regime where the defects display near 3-D kinetics.

Figure 2 illustrates that even if the distance L between direction changes is large, there is a regime in which 3-D reaction kinetics takes place. The importance of the onset of 3-D behavior is directly related to the scale, relative to L, of the microstructural features with which the SIAs can interact.

Future work will aim at further elucidating the ramifications of mixed 1-D/3-D migration on defect reaction kinetics through additional kinetic Monte Carlo simulations and incorporating them analytically into the PBM.

ACKNOWLEDGEMENTS

This work was partly supported by the European Fusion Technology Programme and partly supported by the U.S. Department of Energy under contract DE-AC06-76RLO 1830 with Battelle Memorial Institute a the Pacific Northwest National Laboratory.

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