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The effects of one-dimensional migration of self-interstitial clusters on the formation of void lattices

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Abstract

A series of kinetic Monte Carlo computer experiments performed on idealized systems clearly reveals the dramatic effects of 1-D migration of self-interstitial atom (SIA) crowdion clusters on the stability of void lattices. In the presence of migrating SIA, void lattices are shown to be unstable under pure 3-D SIA migration, but they are extremely stable, relative to random arrays of voids, under 1-D SIA migration. Void lattices remain stable even under the condition of fairly frequent changes in the Burgers vectors of the 1-D migrating SIA clusters. Clusters with average 1-D path segments having lengths on the order of the nearest neighbor distance in the void lattice can maintain the stability of void lattices.

1. Introduction

Void lattices in irradiated metals were first observed about 30 years ago [1], and while they have been the subject of many theoretical and experimental studies since then, no definitive theory of void lattice formation exists. Reviews of some earlier theoretical ideas are given in Refs. [2,3], and they are primarily based on some form of anisotropic mass transport as outlined by Foreman [4]. Other theories based on elastic interactions of voids or spatial fluctuation of defects have been generally discounted because they cannot explicitly predict the formation of the void super-lattice, i.e. that the void lattice has the same lattice structure of the metal and is aligned with the crystal lattice. Theories based on anisotropic diffusion of defects can account for the requisite super-lattice, but, so far, their premises are founded on unproven defect migration properties, usually associated with the migration of single self-interstitial atoms (SIA). A mechanism proposed by Evans [5] requires planar anisotropy of dumbbell interstitial diffusion, while the theory of Woo and Frank [3] is based on 1-D migration of single crowdions over distances on the order of the void lattice spacing. Experimental evidence of these anisotropies in the diffusion of SIA defects is circumstantial at best, and recent molecular dynamics (MD) simulations offer no proof that single SIA have such migration properties [6]. On the other hand, recent MD simulations do show that stable clusters of crowdions are produced directly in cascades and that they can migrate one-dimensionally as highly glissile dislocation loops for significant distances [7,8]. Furthermore, there is evidence that one-dimensionally migrating SIA (crowdion) clusters can be made to occasionally change direction (change Burgers vector) by thermal activation or by interactions with other microstructural elements [7].

1-D diffusion of crowdion clusters was adopted as a major premise of the production bias model (PBM) of void swelling [9], while subsequent inclusion in the PBM of the effects of the changes in Burgers vectors on the defect reaction kinetics of crowdion clusters has been shown to be quite successful in describing many aspects of microstructure evolution under cascade-producing irradiation [10]. Thus, one-dimensionally migrating crowdion clusters with Burgers vector changes have become central to the PBM. The rationale for the present investigation is that, since the PBM provides a reasonable

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explanation of void swelling, then its basic premises should also be compatible with the formation of void lattices. Thus, the 1-D migration of crowdion clusters with occasional Burgers vector changes is examined here as a necessary condition for the formation of a void lattice.

2. Kinetic Monte Carlo experiments

Kinetic Monte Carlo computer thought experiments were performed with a simple model for the interactions of vacancy and SIA defects with voids in which the average length of the 1-D migration path segments of SIA clusters is the variable quantity. A cubic test cell containing an atomic-scale, face-centered cubic lattice was used. The cell contained spherical voids and mobile defect clusters, each defect being associated with a lattice site of the underlying crystal structure. The mobile clusters consisted of identically sized crowdion and vacancy clusters. Each crowdion cluster migrated in a 1-D random walk along a randomly chosen close-packed direction ($\langle 1\,1\,0\rangle$) on the fcc crystal lattice for exactly n_{dc} jumps before randomly choosing the close-packed direction for its next 1-D random walk of n_{dc} jumps. The vacancy clusters migrated by 3-D random walks on the fcc crystal lattice. The vacancy and SIA clusters did not interact among themselves, i.e., there was no clustering or annihilation. The SIA and vacancy clusters represent the defects that interact with the voids and do not interact with each other or other sinks (except 'grain boundaries', see below). A mobile defect was absorbed into a void if their separation was less than or equal to the sum of their radii. Voids increased or decreased in size depending on their interactions with the vacancy and SIA clusters. An additional feature of the interaction of SIA clusters with the voids was that, upon interaction, the center of gravity of the void was moved according to an algorithm depending on the positions of the void and the SIA cluster at contact. It was assumed that vacancies arrived at the void uniformly from all directions and made no net change in the void's center of gravity. For the studies reported on here, the movement of the center of gravity of voids was not an important effect.

The test cell contained about 7×10^6 crystal lattice sites. The void lattices studied in this volume typically consisted of 256 voids having an fcc lattice constant $A = 30a_0$, where a_0 is the crystal lattice parameter. The initial void radii were equal and of size $R = 3.5a_0$, giving a ratio $A/R = 8.6$, which is within the range 5–15 of observed values [2]. Tens of thousands of mobile defect clusters were introduced into the volume at random positions, and each was jumped sequentially until a reaction occurred.

Periodic boundaries were applied to the test cell such that a mobile defect jumping out of the cell was assumed to reenter the cell at the same position on the opposite face. The boundaries were not 'infinitely periodic'. That is, any defect that traversed the complete cell a given number of times without interacting with a void was assumed to be absorbed in some 'other' sink and was removed from the system. Because of the geometry of this condition, the other sink is most representative of a grain boundary. Periodicity was required so that voids near the edges of the cell would see a flux of defects from all directions. However, allowing infinitely periodic boundaries, especially when n_{dc} is very large, can result in extremely long computer runs. The limit of four complete traverses was found to give a reasonable balance between convenient running times and sufficient sampling of the volume by defects. Undoubtedly, the results are sensitive to the number of traverses allowed, and this parameter should be studied rigorously in future computer experiments.

The KMC modeling was used to investigate the role of 1-D migration and the effects of Burgers vector changes on the 'shadow effect', whereby voids aligned along close-packed directions shield each other from 1-D migrating SIA defects, as postulated by Foreman [4] as a mechanism to select or preserve a void lattice. Consider voids aligned in a lattice having the same symmetry as the crystal (as depicted in two dimensions in Fig. 1) and the imaginary cylindrical volumes connecting the voids along the close-packed directions. Because each void is in the 'shadow' of the voids on either side of it along the close-packed directions, only the

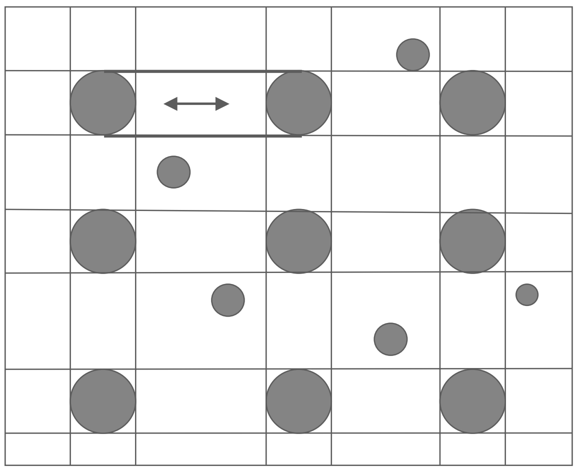

Fig. 1. 2-D schematic diagram of a void lattice depicting the cylindrical volumes lying along close-packed directions between voids that contain the only 1-D migrating crowdion clusters that can interact with the voids (e.g. the cylinder at the upper left containing the double headed arrow). The shadowing effect preserves the voids at the intersection of the cylinders, while the voids not in the shadows of the lattice voids are exposed to a much higher flux of SIA crowdions and eventually disappear.

crowdion clusters within the cylinders and traveling in the directions of the cylinder axes can interact with the voids in the lattice. Any voids not at a void lattice site will be subjected to much larger fluxes of crowdion clusters and have much lower probability of survival.

The strength of the shadow effect was investigated in a series of KMC experiments. A lattice of 256 uniform-sized voids in the test cell described above was supplemented by 256 additional voids of the same size placed at random positions within the cell. The cell was then 'irradiated' with 50 000 crowdion clusters placed randomly in the cell and executing 1-D random walks along the close-packed directions, each for n_{dc} jumps before selecting a new Burgers vector direction. Each void contains vacancies equivalent to the SIAs in 100 crowdion clusters. There were no mobile vacancy clusters in this experiment. Runs were done with different values of n_{dc}. Fig. 2 shows the initial configuration looking down the [0 0 1] direction of the cubic volume. Fig. 3 shows the same view after irradiation by the crowdion clusters with $n_{dc} = 1$ jump, the condition for 'pure 3-D' migration. The lattice voids and random voids were attacked equally by the crowdion clusters.

Figs. 4–6 show the results of the shadowing experiments for $n_{dc} = 500$ jumps ($L = 0.85$), $n_{dc} = 1000$ jumps ($L = 1.2$), and $n_{dc} = 5000$ jumps ($L = 2.7$), respectively, where L is the average 1-D path length for n_{dc} jumps of the crowdion clusters in units of the nearest neighbor distance in the void lattice. For the average 1-D path length of $L = 2.7$ nearest neighbor distances the random voids were annihilated and the lattice voids survived nearly intact. For $L = 1.2$ nearest neighbor distances the shadowing effect was strong, but somewhat diminished relative to the case with larger L. Even when L was less

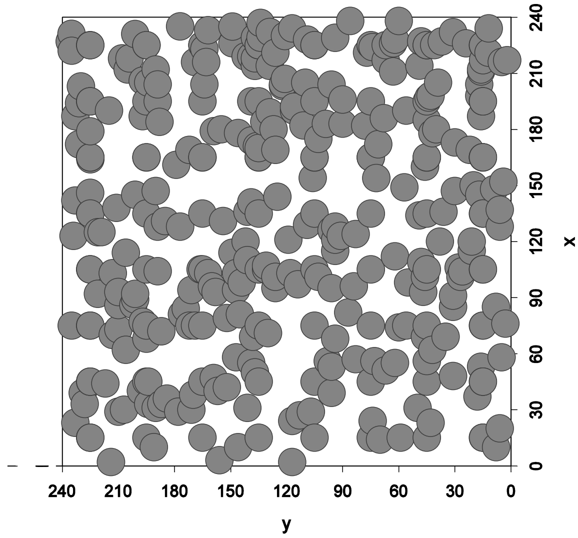

Fig. 2. Looking down the [0 0 1] axis of a cubic cell containing 256 voids in a lattice plus 256 randomly placed voids.

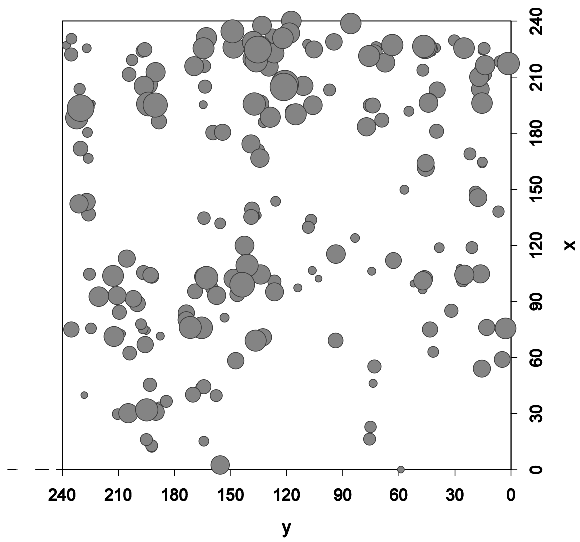

Fig. 3. Looking down the [0 0 1] axis of a cubic cell containing 256 voids in a lattice plus 256 randomly placed voids after irradiation by 50 000 interstitial clusters migrating in 3-D ($n_{dc} = 1$) on the crystal lattice. The sizes of the dots are scaled to the sizes of the remaining voids.

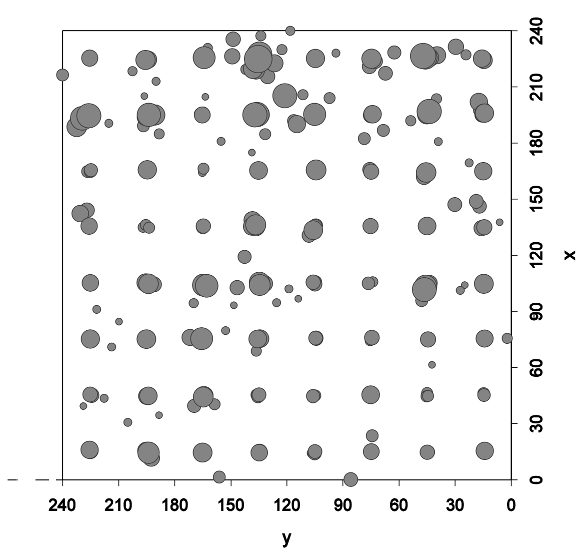

Fig. 4. Looking down the [0 0 1] axis of a cubic cell containing 256 voids in a lattice plus 256 randomly placed voids after irradiation by 50 000 interstitial clusters migrating on the crystal lattice in 1-D segments of average length $L = 0.85$ nearest neighbor distance of the void lattice ($n_{dc} = 500$). The sizes of the dots are scaled to the sizes of the remaining voids.

than the void lattice nearest neighbor distance, $L = 0.85$, the lattice voids overwhelmingly survived relative to the random voids, although many of the lattice voids became quite small. In the more realistic situation where vacancies are constantly replenishing the voids, it is clear

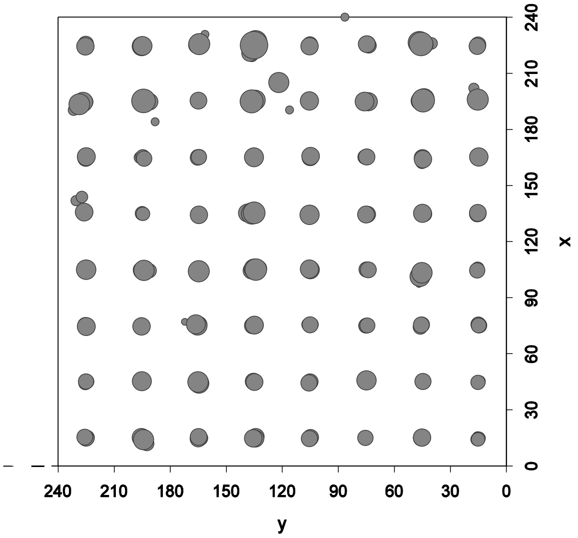

Fig. 5. Looking down the [0 0 1] axis of a cubic cell containing 256 voids in a lattice plus 256 randomly placed voids after irradiation by 50 000 interstitial clusters migrating on the crystal lattice in 1-D segments of average length $L = 1.2$ nearest neighbor distance of the void lattice ($n_{dc} = 1000$). The sizes of the dots are scaled to the sizes of the remaining voids.

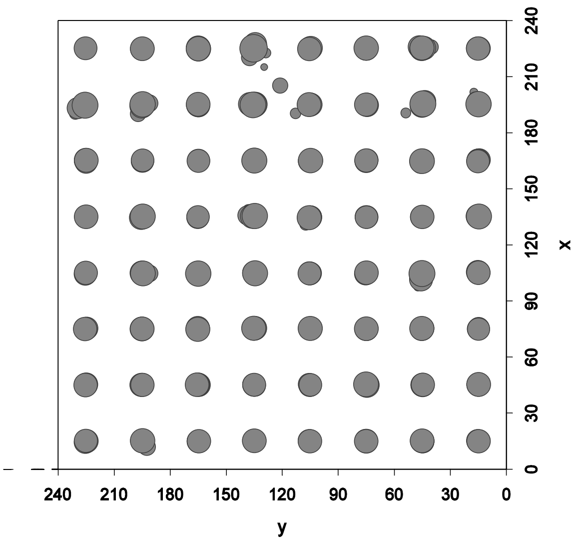

Fig. 6. Looking down the [0 0 1] axis of a cubic cell containing 256 voids in a lattice plus 256 randomly placed voids after irradiation by 50 000 interstitial clusters migrating on the crystal lattice in 1-D segments of average length $L = 2.7$ nearest neighbor distance of the void lattice ($n_{dc} = 5000$). The sizes of the dots are scaled to the sizes of the remaining voids.

that the void lattice voids will survive relative to the random voids even at L values on the order of the void lattice spacing.

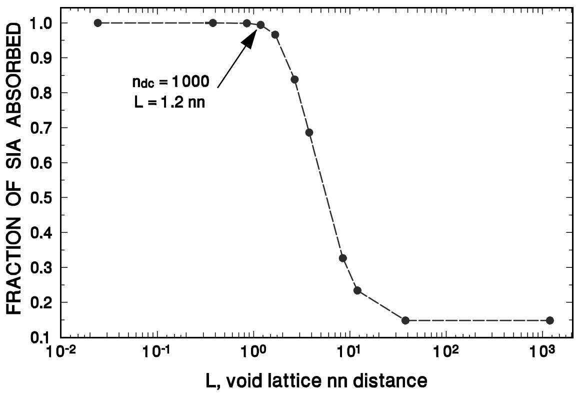

Fig. 7. Crowdion cluster absorption into lattice voids as a function of the average length L of their 1-D path segments given in units of the void lattice spacing.

Experiments were also performed to test the size stability, whether the voids grow or shrink, as a function of the value of L. A lattice of 256 voids in a cell, as described above, was irradiated with crowdion clusters and an equal number of vacancies. If, on average, equal numbers of vacancies and SIA interact with the voids in the lattice, then, on average, the void size will remain stable. Thus, for an established void lattice, irradiation by equal concentrations of vacancies and SIA crowdions, both migrating in 3-D ($n_{dc} = 1$ for the crowdions), will result in maintaining a stable void size. When L increases, the fraction of SIA going to voids decreases, as shown in Fig. 7. For $L = 1.2$ nearest neighbor distances ($n_{dc} = 1000$ jumps), about 99.4% of the crowdions go to voids, while at $L = 1.7$ ($n_{dc} = 2000$ jumps) the fraction of crowdions absorbed is about 96.5%. The fraction of crowdions absorbed into voids drops to the pure 1-D limit, 14.8% for this void lattice, at about $L = 20$. This limiting value corresponds to the fraction of crowdions contained in the cylinders connecting the voids along close-packed directions that can interact with voids, as determined simply by geometry.

3. Conclusions

Based on the results of these studies, the shadow effect is very strong, and it does not require 1-D path lengths significantly greater than the void lattice spacing for crowdion clusters to be effective in selecting a void lattice, relative to random voids. Of course, the shadow effect is much stronger if the crowdion clusters have longer 1-D path lengths, but under those conditions the fraction of crowdions available for interacting with the voids becomes much smaller. To maintain the void size under the long 1-D path length conditions requires that the available SIA in crowdion clusters must outnumber the available 3-D migrating vacancies by a large factor (up to a factor of 7 in the example here). Also, under the actual conditions in real materials, crowdion clusters with very long 1-D path lengths may be rare. Thus, it should be possible to maintain a void lattice when the average 1-D path lengths of a significant fraction of crowdion clusters is on the order of the void lattice spacing. However, the range of 1-D path lengths required for void lattice formation have not yet been determined.

Acknowledgements

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