THE EFFECTS OF ONE-DIMENSIONAL MIGRATION OF SELF-INTERSTITIAL CLUSTERS ON THE FORMATION OF VOID LATTICES - H. L. Heinisch (Pacific Northwest National Laboratory)* and B. N. Singh (Risø National Laboratory, Denmark)

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EXTENDED ABSTRACT

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. Crowdion clusters having the property of three-dimensional diffusion in the material along paths consisting of segments of one-dimensional random walks are central to the Production Bias Model of void swelling [2], which has been shown to be quite successful in describing many aspects of microstructure evolution under cascade-producing irradiation. The rationale for the present investigation is that if a theory can explain void swelling, then it should also be compatible with the formation of void lattices. Thus, a key element of the Production Bias Model, the one-dimensional migration of crowdion clusters with occasional Burgers vector changes, was examined as a necessary condition for the formation of a void lattice.

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 (<110>) on the fcc crystal lattice for exactly n_{dc} jumps before randomly choosing the close-packed direction for its next random walk of n_{dc} jumps. The vacancy clusters migrated by 3-D random walks on the fcc crystal lattice. 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 [3] as a mechanism to select or preserve a void lattice. 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. There were no mobile vacancy clusters in this experiment. Runs were done with different values of n_{dc}. Figure 1a shows the initial configuration looking down the [001] direction of the cubic volume. Figure 1b 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. Figures 1c and 1d show the results for n_{dc} = 500 jumps and n_{dc} = 5000 jumps, respectively. The average 1-D path length for 500 jumps is about 0.85 times the nearest neighbor distance of voids in the lattice, while that for 5000 jumps is 2.7 times. The effect of shadowing is quite strong, even when the 1-D path length is of modest size.

KMC computer experiments were also performed to test the size stability, whether the voids grow or shrink, as a function of the value of n_{dc}. A lattice of 256 voids in a cell, as described above, was irradiated with equal numbers of crowdion clusters and vacancies. It was found that, under

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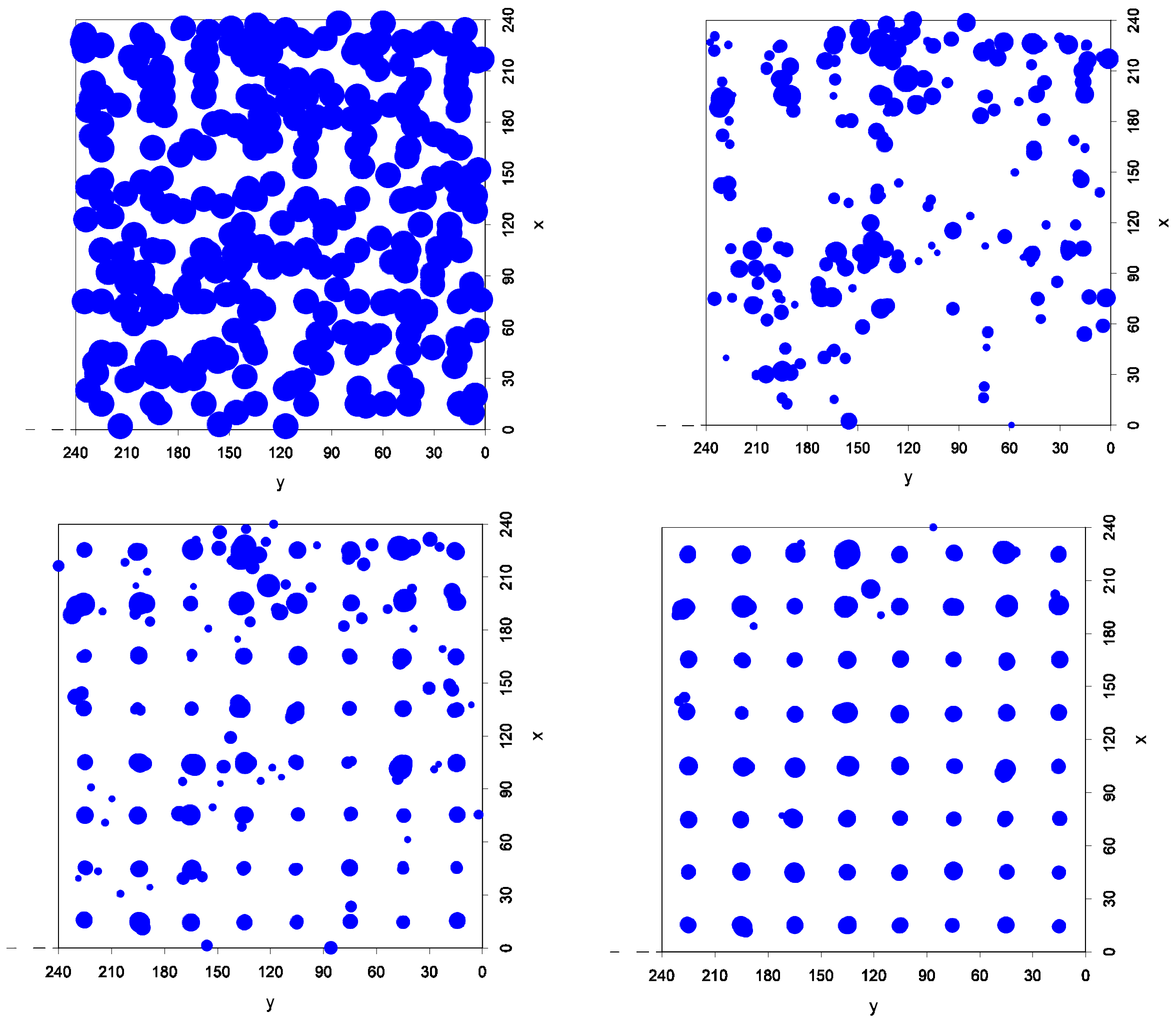

Figure 1. Looking down the [001] axis of a cubic cell a.) containing 256 voids in a lattice plus 256 randomly placed voids. b.) after "irradiation" by 50,000 interstitial clusters migrating on the crystal lattice with n_{dc} = 1 (3-D) c.) after "irradiation" by 50,000 interstitial clusters migrating on the crystal lattice with n_{dc} = 500 (1-D segments of average length L = 0.85 nearest neighbor distance of the void lattice) d.) after "irradiation" by 50,000 interstitial clusters migrating on the crystal lattice with n_{dc} = 5000 (1-D segments of average length L = 2.7 nearest neighbor distance of the void lattice). The sizes of the dots are scaled to the sizes of the remaining voids.

the condition of equal numbers of vacancies and interstitials available to interact with the voids, the size stability of voids in the lattice could be maintained when SIA clusters have 1-D path lengths on the order of the void lattice spacing.

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 (about a factor of

7 in the example here). However, under the actual conditions in real materials, crowdion clusters with very long 1-D path lengths are probably 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. Further KMC computer experiments will be aimed at determining the conditions for void lattice formation.

REFERENCES

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