DEFECT INTERACTIONS WITHIN A GROUP OF SUBCASCADES - H. L. Heinisch (Pacific Northwest National Laboratory[1])

OBJECTIVE

The objective of this work is to determine the energy and temperature dependence of defect production and microstructure evolution for the development of fission-fusion correlations.

SUMMARY

The evolution of the defect distributions within high energy cascades that contain multiple subcascades is studied as a function of temperature for cascades in copper. Low energy cascades generated with molecular dynamics are placed in close proximity to simulate the arrangement of subcascades within a high energy event, then the ALSOME code follows the evolution of the cascade damage during short term annealing. The intersubcascade defect interactions during the annealing stage are found to be minimal. However, no conclusions regarding effects of subcascades on defect production should be drawn until intersubcascade defect interactions during the quenching stage are examined.

PROGRESS AND STATUS

Molecular dynamics (MD) studies of cascade-producing radiation damage are limited in the size of cascade that can be simulated and the length of time the simulation can be followed at the atomic scale. MD simulations of cascades at energies capable of producing well defined subcascades ($E > 50$ keV in Cu) are not possible, and simulated cascade evolution times greater than about 100 ps are not practical. To obtain a quantitative understanding of defect production and evolution under fusion irradiation conditions, it is necessary to go beyond the practical size and time restrictions of MD using models that realistically describe the important characteristics of the defects and their interactions.

To go beyond MD in time, stochastic annealing simulations have been used to follow the evolution of cascade damage at an atomic scale[1]. Annealing simulations have demonstrated a differential in the number of mobile vacancies and SIAs escaping the cascade that has a strong temperature dependence and is the basis for the "production bias" that promotes void swelling. This phenomenon is shown to be the result of the production of vacancy and self-interstitial atom (SIA) clusters directly in the collision cascade, the stability of SIA clusters relative to the stability of vacancy clusters, the existence of small, highly mobile SIA loops, and the relative spatial separation of the vacancy and SIA defects. All of these features are modeled explicitly in the ALSOME stochastic annealing code.

To go beyond MD limitations on recoil energy, binary collision approximation (BCA) models have been considered. A BCA model is capable of dealing with the highest energy recoils, but one cannot follow the cascade beyond the collisional stage. Calibrations of BCA to MD results at lower energies have been attempted with limited success[2]. The total numbers of vacancies and SIAs remaining after the quenching stage can be acceptably modeled in the calibration, but the cluster size distributions, which have been found to be extremely important during the subsequent annealing stage[1], are not sufficiently similar by the calibrated BCA and MD models.

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Defect Interactions Among Subcascades. To gain some insight into the effects of defects produced in subcascades interacting with defects within other subcascades, high energy cascades were "constructed" from MD cascades of lower energies. Two 25 keV cascades generated with MD[3] were placed within the same ALSOME annealing volume, separated by a fixed distance, and annealed as a single cascade. Results for three different center-to-center cascade separations R are displayed in each plot here: R=35a (lattice parameters), which is just greater than edge to edge separation of the defect distributions; R=5a , which is near total overlap of the cascades; and R=infinite, which is the sum of the results when the two cascades were annealed separately. Each data point is for the annealing of 100 configurations of randomly-chosen, constant-separation translations of one cascade relative to the other.

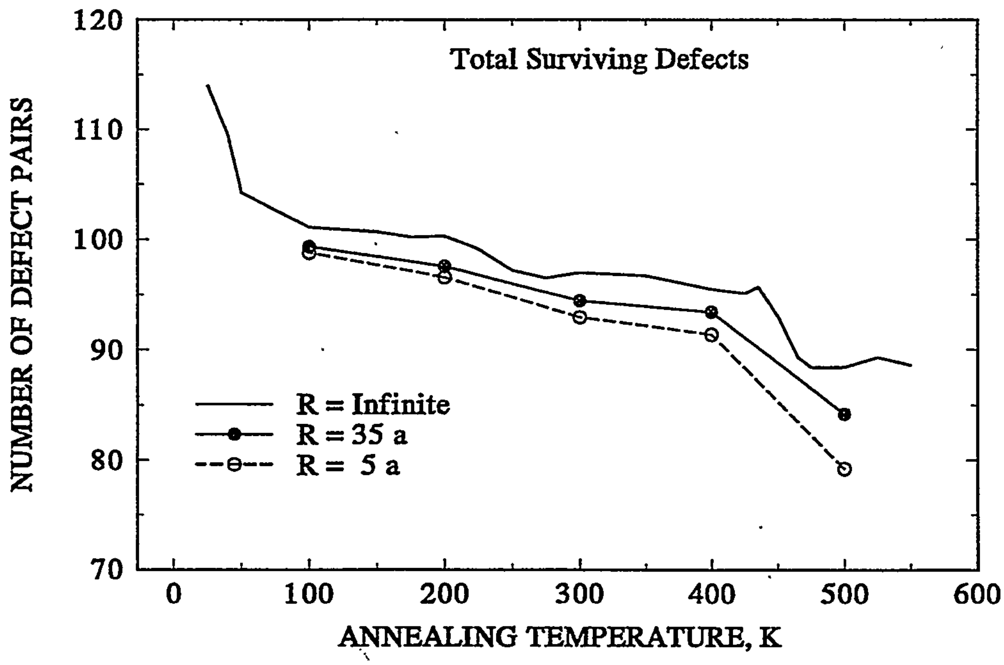

Figure 1. The total number of surviving defect pairs as a function of annealing temperature for subcascade separations of 35a, 5a, and infinite separation.

Figure 1 is for the total number of surviving defect pairs, i.e., the initial (post-quench) number minus the annihilations. The accounting is done in terms of single point defects (a cluster of 6 point defects counts as 6). At any temperature, a fraction of the surviving defects is mobile, and most of the mobile defects leave the cascade region during annealing. The remainder are immobile clusters remaining in the vicinity of the cascade. The longer solid line is the sum of surviving defect pairs for the two individual cascades (R=infinite), which was simulated at about 20 different temperatures. The solid line with filled circles is for R=35a and was done for only 5 temperatures. The lines are to aid the eye in grouping the data for a particular condition. The actual shape of the annealing curve would be similar to the R=infinite curve. The dashed line with open circles is for R=5a. Note the small differences in total defect pair survival as a function of separation. The trend of these small differences is that fewer defects survive as the subcascade separation decreases and that the differences due to subcascade separation are greater with increasing temperature. These trends are also in the data for escaping SIAs and vacancies in Fig. 2 and Fig. 3, respectively.

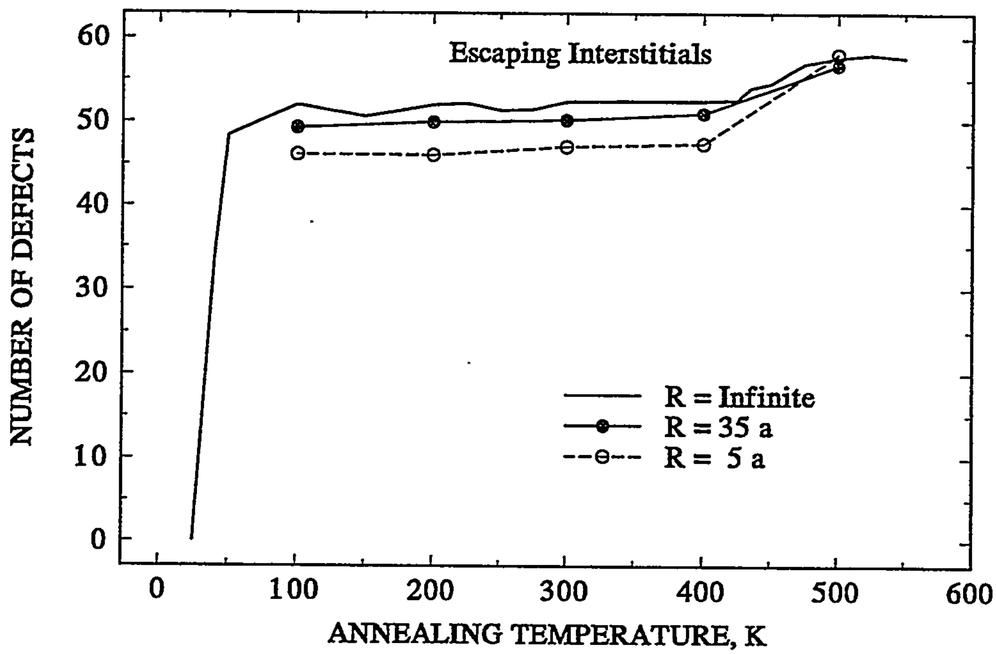

Figure 2. The number of SIAs escaping the cascade as a function of annealing temperature for subcascade separations of 35a, 5a, and infinite separation.

The results of this simulation indicate that during the annealing stage of cascade evolution there is little interaction of defects with other defects in an adjacent subcascade. This is due to the spatial separation of the vacancy and SIA distributions in a single subcascade and the difference in mobilities of vacancy and SIA defects. The SIAs are spread around the periphery of each subcascade and move much more quickly than the vacancies, which are concentrated near the center of each subcascade. When entering the region of another subcascade, the mobile SIAs are more likely to encounter the surrounding SIAs than the vacancies in the center. In this simulation at R=35a there is about 20% recombination within each subcascade, and about 5% additional recombination involving defects from different subcascades. Above about 400 K, where vacancy clusters become unstable, the vacancies stream out from the centers of the subcascades, but only after the mobile SIAs have already escaped the cascade. Some additional recombination occurs as a few vacancies find the remaining larger immobile SIA clusters. The simulation at R=5a is unphysical because two separate subcascades could not form in the same place without affecting each other significantly during the quenching stage. It was simply included to see if additional defect interactions would occur if the two sets of defects were in even closer proximity. There is only slightly more interaction.

This simulation investigated the defect interactions occurring only during the annealing stage, which takes place by thermally activated diffusion of defects after the thermal spikes of each subcascade have quenched.

The effects of the thermal spikes of adjacent subcascades quenching simultaneously have not been considered here, but it is an important issue that needs to be understood before conclusions are drawn.

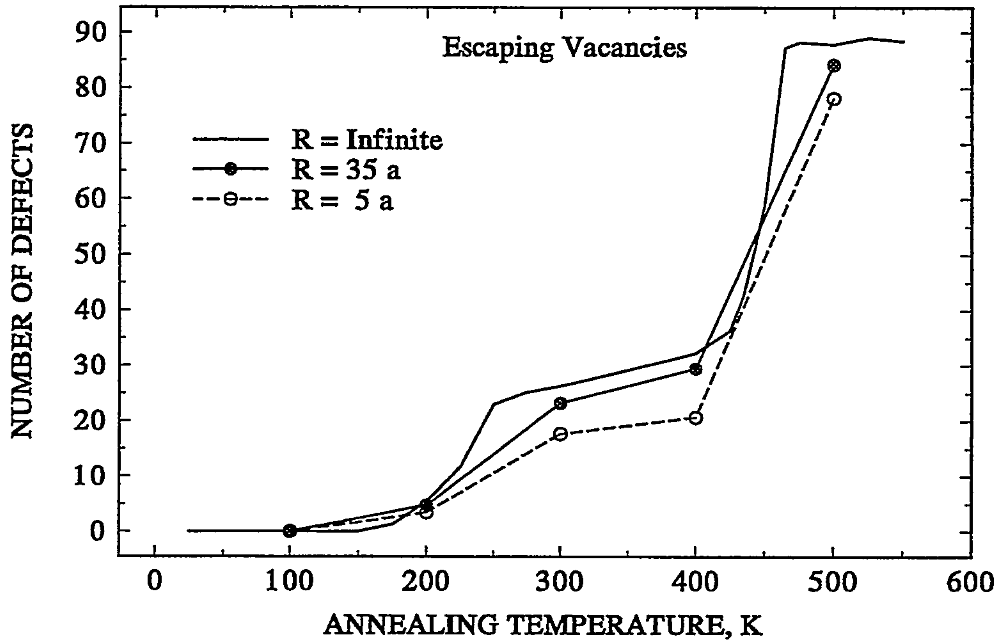

Figure 3. The number of vacancies escaping the cascade as a function of annealing temperature for subcascade separations of 35a, 5a, and infinite separation.

FUTURE WORK

The results here will be part of a presentation at the workshop on Defect Production, Accumulation and Materials Performance in Irradiation Environment, Davos, Switzerland, October 2-8, 1996. Proceedings will be published in the Journal of Nuclear Materials. New methods are being investigated for calibrating the output of the BCA cascade model to MD results to give more realistic cluster size distributions after quenching. MD simulations to determine the characteristics of subcascade interactions during the quenching stage are being considered. The sensitivity of ALSOME annealing results to the characteristics of small glissile loops, which are a key element in the defect evolution, is being tested.

REFERENCES

1. H. L. Heinisch and B. N. Singh, "Stochastic Annealing Simulation of Differential Defect Production in High Energy Cascades," J. Nucl. Mater., in press.

2. H.L. Heinisch, B. N. Singh and T. Diaz de la Rubia, "Calibrating a Multi-model Approach to Defect Production in High Energy Collision Cascades," J. Nucl. Mater. 212-215 (1994) 198.

3. T. Diaz de la Rubia and M.W. Guinan, Mater. Res. Forum 97-99 (1992) 23.