

**STOCHASTIC ANNEALING SIMULATIONS OF DEFECT INTERACTIONS AMONG SUBCASCADES-** H. L. Heinisch (Pacific Northwest National Laboratory<sup>1</sup>) and B.N. Singh (Risø National Laboratory)

### 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 effects of the subcascade structure of high energy cascades on the temperature dependencies of annihilation, clustering and free defect production are investigated. The subcascade structure is simulated by closely spaced groups of lower energy MD cascades. The simulation results illustrate the strong influence of the defect configuration existing in the primary damage state on subsequent intracascade evolution. Other significant factors affecting the evolution of the defect distribution are the large differences in mobility and stability of vacancy and interstitial defects and the rapid one-dimensional diffusion of small, glissile interstitial loops produced directly in cascades. Annealing simulations are also performed on high-energy, subcascade-producing cascades generated with the binary collision approximation and calibrated to MD results.

### PROGRESS AND STATUS

Even after the longest practical MD simulation, the defect clusters of a single cascade remain spatially localized in a "metastable" state far from the spatial and temporal uniformity required for the global picture to which rate theory may be applied. Atomic scale stochastic annealing simulation provides the necessary link between the localized, short-term, atomistic view of individual MD cascades and the spatially averaged global view required for the application of rate theory.

**SUBCASCADE INTERACTIONS.** Irradiations by high energy sources such as fusion neutrons, spallation neutrons, high energy protons and heavy ions produce a significant amount of damage in the form of high energy cascades that have multiple subcascades. It is important to know how the defect evolution within the high energy cascade is affected by the presence of subcascades in close proximity. Present computational resources are not capable of routinely generating high energy cascades by MD in the large numbers and arbitrary orientations required for good statistics. However, it should be possible to study the effects of subcascades on the annealing stage of high energy cascades by simply "constructing" multiple-subcascade cascades from a set of lower energy cascades, i.e., by placing individual cascades in close proximity and annealing them simultaneously. This procedure does not address the possible interactions among subcascades during the thermal spike or quenching stages.

Multiple-subcascade cascades in copper were approximated by replicating two 25 keV copper cascades [1] in several randomly chosen positions at a fixed separation distance to produce cascades with 2-5 "subcascades." The center-to-center separation of subcascades in this pseudo-cascade is 35 lattice parameters, slightly less than the average subcascade spacing determined in binary collision simulations of

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<sup>1</sup>Pacific Northwest National Laboratory is operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830.

copper cascades[2]. The pseudo-cascade also has been given a more compact configuration than the average cascade in copper to maximize possible effects of intersubcascade defect interactions. The results of annealing 100 such pseudo-cascades as a function of temperature are shown in Fig. 1. The fractions of surviving pairs and escaping defects are about 10% less than for the average of 100 anneals of the two individual 25 keV cascades (i.e. infinite separation), which is on the order of the standard deviation of the average values. Thus, there is only a minor effect of subcascade interaction during the annealing stage. There is a small systematic decrease in surviving and escaping defect fractions as a function of the number of subcascades per cascade, but there is essentially no effect of subcascade interaction on the average SIA and vacancy cluster sizes.

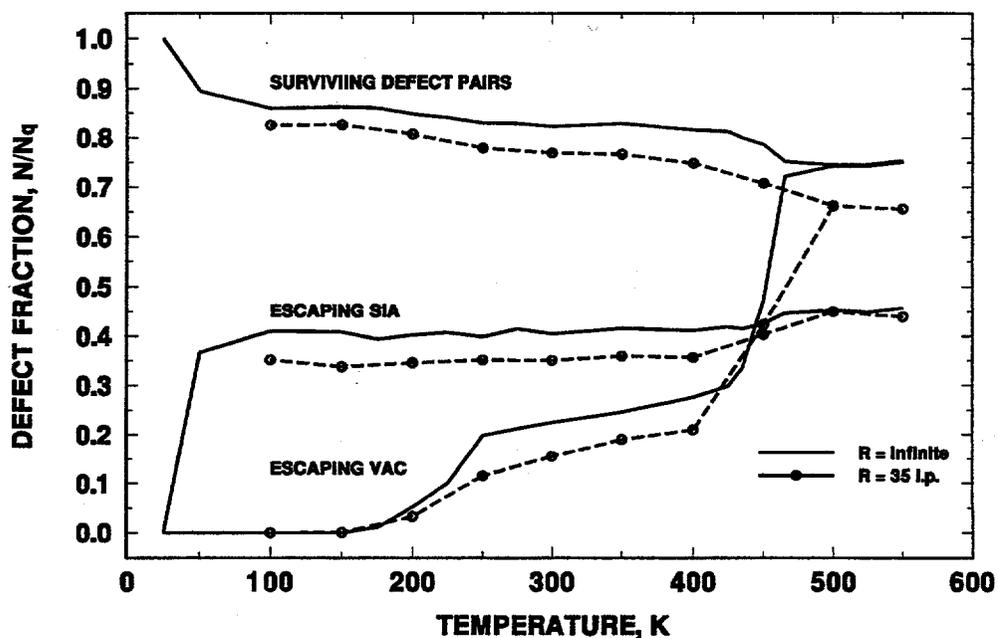


Figure 1. The fractions of point defects surviving recombination and of vacancies and interstitials escaping from 25 keV cascades in copper during the annealing stage, as a function of cascade annealing temperature. A comparison is made of annealing results for individual 25 keV copper cascades ( $R = \text{infinite}$ ) and pseudo-cascades consisting of sets of five 25 keV "subcascades" having an average center-to-center separation of 35 lattice parameters ( $R = 35 \text{ l.p.}$ ). Each data point represents the average of anneals of 100 different arrangements of the five cascades.

**APPROXIMATING HIGH ENERGY CASCADES.** In light of the small amount of interaction observed among subcascades, it might be possible to estimate defect production and evolution in high energy, subcascade-producing cascades by linearly extrapolating from results at cascade energies near the subcascade threshold. However, even though MD has been used successfully to simulate cascades near threshold energies, those simulations are at the limit of computational capabilities, and only a small number of cascades can be produced at those energies. Also, at energies above the threshold, the size distribution of

subcascades may have significant influence on defect production and should be studied. Thus, it is of interest to develop easily-calculated approximations to high-energy cascades for such studies, especially for input to annealing simulations. A reasonable starting point is to use the binary collision approximation to simulate the collisional stage of the cascade. Variations of this approach have been employed, of necessity, several times in the history of radiation effects simulations [3,4,5].

A major advantage over the earlier attempts is that MD simulations now exist to which the binary collision calculations can be calibrated. A series of individual time steps of the two 25 keV cascades in copper discussed above have been analyzed to extract the collisional stage information that would be calculated in a binary collision approximation to this cascade. Thus, both the collisional stage configuration of displaced atoms and the post-quench defect configuration are known for the MD cascade. The ideal calibration would consist of a general algorithm for the transformation of the collisional stage displacement configuration to the quenched stage defect distribution. As a first attempt, the method of Ref. [5] was used. That is, exaggerated parameter values for defect mobility and interaction distances were applied to the binary collision results for a simulated time of about 10 ps, the typical duration of cascade evolution through the quenching stage. It is possible to choose "quenching" parameter values that give correct numbers of post-quench defects, but the cluster size distributions and the compactness of the post-quench vacancy distribution observed in the MD simulations cannot be achieved by this approach.

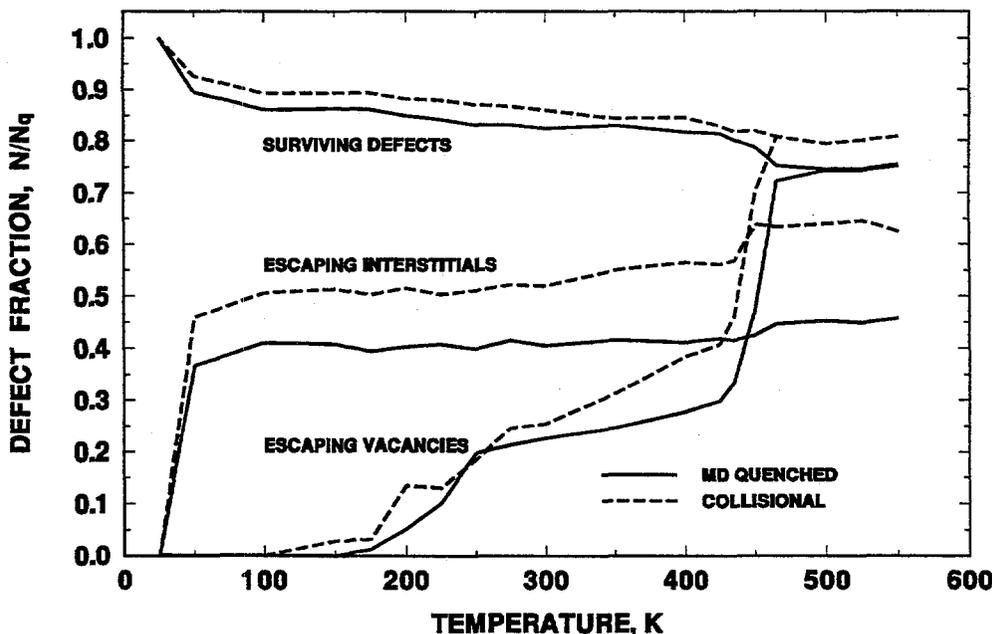


Figure 2. The fractions of point defects surviving recombination and of vacancies and interstitials escaping from 25 keV cascades in copper during the annealing stage, as a function of cascade annealing temperature. The solid lines are for the annealing of cascades fully quenched by MD, while the dashed lines are for the annealing of the same cascades that were artificially quenched from the collisional stage.

Obtaining the correct defect configuration after the artificial quenching stage may not be so important if the defect configuration following the subsequent annealing stage is well described. Thus, annealing simulations were performed for the 25 keV cascades artificially quenched from the collisional stage. Fig. 2 shows the results as a function of annealing temperature. These results are encouraging, being qualitatively similar to those obtained for the quenched MD cascades. The largest discrepancy is in the numbers of escaping SIAs, because fewer large, immobile SIA clusters form during the artificial quench. Because of the importance of the SIA and vacancy clusters and their stability and diffusion characteristics to the results of the annealing stage, a more realistic artificial quenching scheme is required, especially one that more specifically deals with the energy and particle transport properties of the material.

#### FUTURE WORK

The results discussed here were included in 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. Refinements of the model for high energy cascades are in progress, and annealing simulations of defect accumulation under ongoing irradiations are being developed.

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