

STOCHASTIC ANNEALING SIMULATION OF CASCADES IN METALS - H. L. Heinisch (Pacific Northwest National Laboratory¹)

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 stochastic annealing simulation code ALSOME is used to investigate quantitatively the differential production of mobile vacancy and SIA defects as a function of temperature for isolated 25 keV cascades in copper generated by MD simulations. The ALSOME code and cascade annealing simulations are described. The annealing simulations indicate that above Stage V, where the cascade vacancy clusters are unstable, nearly 80% of the post-quench vacancies escape the cascade volume, while about half of the post-quench SIAs remain in clusters. The results are sensitive to the relative fractions of SIAs that occur in small, highly mobile clusters and large stable clusters, respectively, which may depend on the cascade energy.

PROGRESS AND STATUS

Recent molecular dynamics (MD) studies have confirmed that significant clustering of both vacancies and self-interstitial atoms (SIAs) takes place by the end of the quenching stage of a cascade, and that small interstitial clusters can form glissile loops with migration energies on the order of 0.1 eV. The segregation of the vacancy and SIA distributions and the clustering give rise to a differential production of mobile vacancies and SIAs that has a strong temperature dependence. At temperatures above recovery Stage V, vacancies can evaporate from clusters, while large SIA clusters produced in the cascade remain stable, leading to a differential increase of mobile vacancies that represents a "production bias" that may be responsible for void swelling.

The creation of defects, their migration through the material, and their influence on microstructure evolution take place over time and distance scales that span up to twenty orders of magnitude. In practice, multiple models are required to study radiation damage over the entire range of scales. Molecular dynamics (MD) is effective in describing the defect creation at the atomic scale in the sub-nanosecond time frame, and reaction rate theory is necessary for describing the microstructure evolution over macroscopic distances and reactor lifetimes. Stochastic annealing simulation helps bridge the gap between MD and rate theory. It preserves the identity and position of individual defects, and it is practical at scales of up to microns and seconds. Stochastic annealing simulation is being used in two primary applications: 1.) to study the short term annealing of defects in the vicinity of an individual cascade, essentially extending the MD description of a cascade through the diffusional phase, and 2.) to study the interactions of defects in a volume of material subjected to a flux of cascades, essentially a molecular scale simulation of microstructure evolution.

Stochastic annealing simulations are being performed with the ALSOME computer code. In ALSOME defects are the interacting entities. Each defect is associated with a lattice site and is characterized as a

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

sphere with a radius determined by the number of point defects it contains. Defects that are mobile (single point defects and small clusters) jump stochastically according to relative jump probabilities based on their type (vacancy or interstitial) and size and weighted by their concentration. Two defects interact, becoming a single defect, when they are within a critical reaction distance that depends on their types and sizes. Defects may dissolve stochastically, one point defect at a time, depending on their relative stability. Defects may also be absorbed at sinks depending on either spatial location or statistical criteria. Input to ALSOME consists of a list of defects with positions, types and sizes; activation energies for migration and dissolution; critical reaction distances; rates of defect production or annihilation at sinks when appropriate; and temperature. In practice, defect distributions are taken from MD simulations and most activation energies are from atomistic simulations or measured values where available.

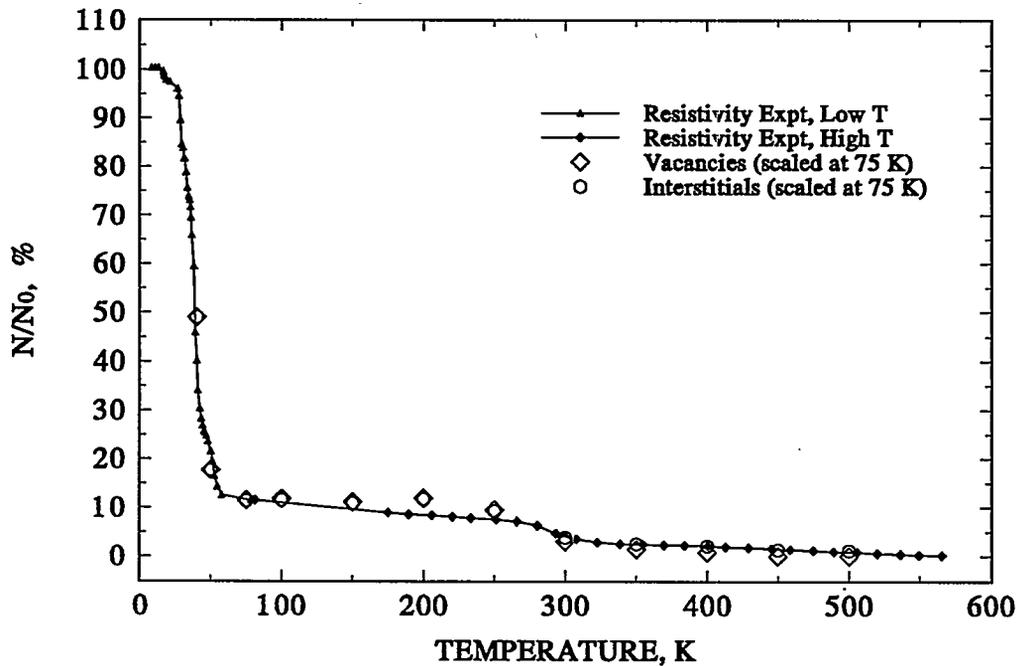


Figure 1. ALSOME Simulations of Isochronal Annealing of Copper Irradiated by Electrons to 100 ppm Frenkel Pairs.

One way to test the annealing model is to simulate the resistivity recovery experiments on material irradiated with electrons at low temperatures. Figure 1 shows the ALSOME results and experimental results[1] for isochronal annealing of electron-irradiated copper. The general shape of the recovery curve is well matched. The ALSOME simulation did not include effects of the sink structure and impurities in the experiments, which are unknown.

Figure 2 shows the results of ALSOME simulations[2] of short-term annealing of two quenched MD cascades in copper[3]. The cascades, both 25 keV, are at the threshold energy of subcascade formation, and they are the most energetic cascades simulated by MD to date. The fractions of initial defects escaping

the cascade region as a function of temperature demonstrate the concept of production bias[4] in cascade-producing irradiations. Above $0.3T_m$, which is the beginning of the void swelling regime, the fraction of escaping vacancies is almost double that of escaping interstitials. The interstitials remaining in the cascade volume reside in large, stable interstitial clusters, and about half of the escaping interstitials are in the form of rapidly moving (in one dimension) small glissile loops.

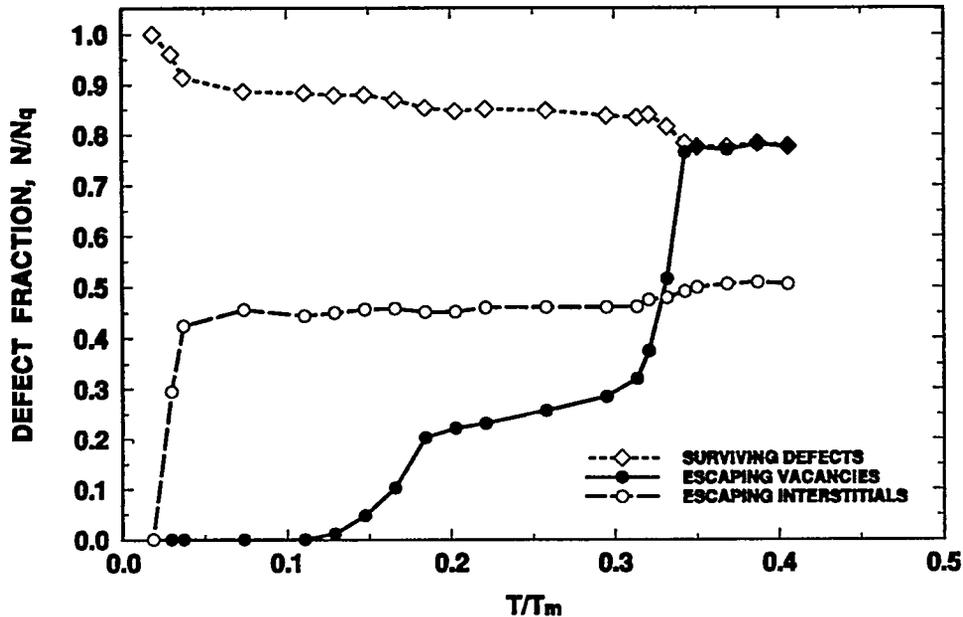


Figure 2. Short-term Annealing of Isolated 25 keV Cascades in Copper. The fractions of total surviving defects and escaping defects are relative to the number of defects present after the quenching of the cascade.

As in rate theory (but unlike MD), stochastic annealing simulations must explicitly contain the provisions for all important phenomena to occur. One should maintain a healthy skepticism of results of these simulations. On the other hand, such simulations by their nature, allow one to explore the effects of various mechanisms, conditions and phenomena in a controlled, totally observable system.

FUTURE WORK

A regular journal article on the work summarized here has been written and will be submitted to the *Journal of Nuclear Materials*. ALSOME simulations of irradiations by both high energy electrons and neutrons are in progress. For these simulations, larger volumes with periodic boundaries are used. Methods of simulating sink distributions are being investigated. Methods for investigating the annealing stage of high

energy cascades that have multiple subcascades are also being studied. A comparison of annealing stage behavior of cascades in fcc and bcc metals is being planned.

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