STOCHASTIC ANNEALING SIMULATION OF COPPER UNDER CONTINUOUS NEUTRON IRRADIATION - H.L. Heinisch (Pacific Northwest National Laboratory)* and B.N. Singh (Risø National Laboratory)

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SUMMARY

This report is a summary of a presentation made at ICFRM-8 on computer simulations of defect accumulation during irradiation of copper to low doses at room temperature. The simulation results are in good agreement with experimental data on defect cluster densities in copper irradiated in RTNS-II.

EXTENDED ABSTRACT

Stochastic annealing simulation provides a bridge between the atomistic and macroscopic scales that enables the direct effects of cascade production on the microstructure to be investigated. We report here on the simulation of damage accumulation under low doses of cascade-producing irradiation in copper at room temperature. The computer simulations were performed using the stochastic annealing code ALSOME, which is described in detail in earlier publications [1,2]. For defect accumulation simulations, the same model for annealing is used as for individual cascades, along with the same defect parameter values. The annealing volume for the accumulation simulations is significantly larger than for individual cascades, and new cascades are introduced into the volume as the annealing progresses to simulate the conditions of an ongoing irradiation. To make the computation tractable with respect to computer time, a relatively small cubic volume 54 nm on edge was chosen, and periodic boundaries were applied. Room temperature irradiation of copper by 14 MeV neutrons, as with RTNS-II, was simulated with a flux of 5, 10, and 25 keV cascades generated in MD simulations by Diaz de la Rubia and Guinan [3] and by Foreman et al. [4]. Fusion neutrons produce recoil atoms with an average energy of about 300 keV, but cascades produced by those high energy recoils are formed as a series of subcascades [5]. Thus, the flux of 5-25 keV MD cascades introduced into the simulation annealing volume should be a reasonable first approximation to the individual subcascades formed in irradiations by 14 MeV neutrons. A dose of slightly more than 0.1 DPA was obtained by introducing approximately 12,000 cascades into the annealing simulation volume. This large set of cascades was produced by repeated use of the 13 available MD cascades. Although periodic boundaries were used, the existence of a finite grain size (or a density of other intrinsic sinks) was simulated by imposing a limit on the number of times a mobile defect could traverse the simulation volume. Defects reaching the equivalent of 380 nm on average are considered to have reached a grain boundary or other intrinsic sink, and they are removed.

Doses up to 0.1 DPA were simulated at various damage rates, and the damage accumulation was observed as a function of dose. Figure 1 shows the defect cluster density as a function of dose for a simulated irradiation at a dose rate of 10^{-10} DPA/s, as in RTNS-II. The simulation results are compared to experimental cluster densities obtained from three different irradiation experiments on annealed copper in RTNS-II [6-8]. The RTNS-II test specimens were irradiated at dose rates varying from about 10^{-11} to 10^{-9} DPA/s. The

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vacancy and SIA cluster densities are shown separately, as well as their total. The simulated total density of clusters is in very good agreement with the experimentally reported cluster density, being within about a factor of 2 throughout the range of doses.

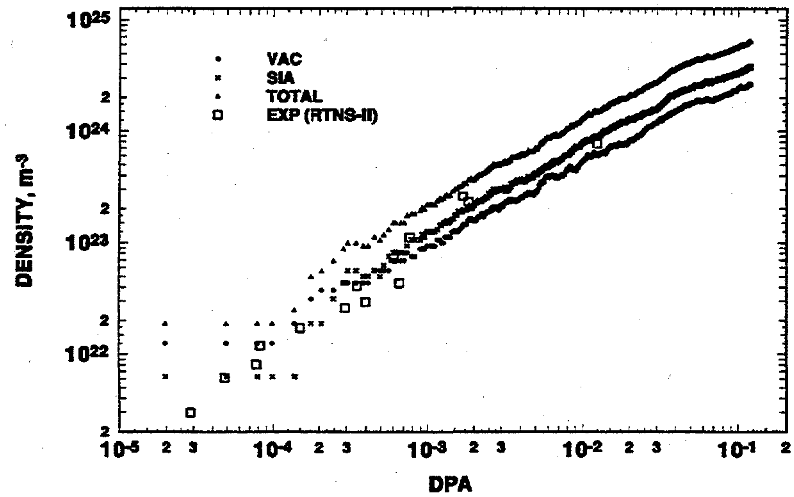

Figure 1. Vacancy, SIA and total cluster densities as a function of accumulated dose for copper irradiated at 300K under cascade-producing irradiation (as by 14 MeV neutrons) at 10^{-10} DPA/s. Simulation results are compared to experimental data from TEM observations of copper irradiated in RTNS-II [6,7,8]

The effects of dose, dose rate, cascade overlap and interstitial cluster mobilities on damage accumulation were investigated in further simulations. The surviving defect fraction is 1-2% of the calculated DPA value, with the vacancy clusters showing the greater variation with dose rate. Other investigations demonstrate the small, but noticeable, effects of cascade overlap at doses up to 0.1 dpa and the considerable sensitivity of defect accumulation to the allowable maximum size of glissile SIA loops in the model. The knowledge of SIA cluster and loop migration and stability are critical to continued development of stochastic annealing simulations of defect accumulation.

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