Simulated irradiation in the high dose limit

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Modelling highly damaged materials – exposed to over 0.1 displacements per atom (dpa) – where saturation of damage is often observed, is difficult because a microstructure containing high density of defects evolves non-linearly as a function of dose. In this study we show how to determine both hydrogen retention and thermal diffusivity changes in tungsten exposed to high irradiation dose, using no adjustable parameters.

First, we generated converged high dose (>1 dpa) microstructures, using a combination of the creation-relaxation algorithm (CRA) and massively overlapping collision cascade molecular dynamics (MD) simulations. We make robust estimates of vacancy and void regions using a modified Wigner-Seitz decomposition. The resulting estimates of the void surface area is used to predict the deuterium retention capacity of tungsten as a function of radiation exposure. The predictions were compared to deuterium retention measured by nuclear reaction analysis.

The theory gives an excellent match to the experimental data, with both model and experiment showing that 1.5-2.0 at.% deuterium is retained in tungsten in the limit of high dose. We then make robust estimates of the total defect content by statistically comparing the atomic potential energy distribution to the expected thermal distribution. With the defect count identified, and a simple model relating electronic scattering rate to excess energy with a single parameter- the resistivity per Frenkel pair- we compute conductivity changes as a function of dose. These were compared to thermal diffusivity measurements made at low temperature using transient grating spectroscopy, and found to give an excellent match over the range of doses studied.

We conclude that combining CRA and MD generates high quality microstructures, and that from these we can make forward predictions for low-temperature engineering properties as a function of elastic boundary conditions and dose, without needing user reparameterization.