The yield stress of nuclear materials is usually increased by radiation-induced defects since these defects act as barriers to the motion of dislocations. In this work, we present a computational approach to estimate the dose dependency of the yield stress of austenitic stainless steels. To make this estimation quantitative, it is necessary to establish the density and size distribution of defects at a certain dose level and the barrier strength of each defect to a dislocation motion.

We computed the increases in the yield strength of austenitic stainless steels by using dislocation dynamics simulations, which simulate the motion of dislocations in a matrix containing radiation-induced defects. We calculated the density and the size distribution of these defects by using a cluster dynamics model. This model takes into account the diffusive encounters between point defects and extended defects. In determining the input parameters for the cluster dynamics calculations, we obtained the primary damage parameters such as the cascade efficiency and the clustering fractions by using molecular dynamics simulations. In the dislocation dynamics simulations, the defects, which are mostly Frank loops, were represented explicitly by planes and the loops were assumed to act as geometrical barriers with a pre-defined strength against dislocation glide. The strength of each loop is dependent on the size of the loop, the dislocation intersection height and the geometrical configuration between the glide plane of a moving dislocation and the habit plane of the loop. We obtained detailed information of these barrier strengths from atomistic simulations.

The computed yield stresses showed a good correspondence with experimentally measured data. The results suggest that the computational methods, by combining the cluster dynamics model and the dislocation dynamics simulation, provide a convenient tool for estimating the amount of a radiation-induced hardening.