

# A multiscale and multiphysics framework to simulate radiation damage in nano-crystalline materials

This work presents a multiscale and multiphysics framework to investigate the radiation-induced damage in nano-crystalline materials. The framework combines two methodologies, including molecular dynamics simulations with electronic effects and long-term atomistic diffusion simulations in nano-crystalline materials. Using this framework, we investigated nano-crystalline materials' self-healing behavior under radiation events. We found that the number of defects generated in nano-crystals during the cascade simulations was less than in single crystals. This behavior was due to the fast absorption of interstitial atoms in the grain boundary network during the cascade simulations, while vacancies migrated to the boundaries in a much longer time scale than interstitial atoms. Thus, nano-crystalline materials showed a self-healing behavior where the number and size of the defects are drastically reduced with time.