Modeling the primary damage in nickel and nickel-based alloys: influence of cascade energies and morphologies in displacement cascades.

The interaction between high energetic particles and metals causing primary radiation damage has been studied for a long time using molecular dynamics. Five interatomic potentials for nickel differing either by their equilibrium part or by the hardening procedure have been included in this study. A characterization based on static non-equilibrium properties and threshold displacement energy (TDE) was done to look for correlations between the potential characteristics and the cascade properties. The dominating feature of this work is to explore extensive statistics of more than 7000 cascades for each interatomic potential with cascade energies ranging from 0.5 keV to 120 keV in pure nickel. The total number of defects, the number of SIA and vacancy clusters, and the size distributions are analyzed using multivariate multiple linear regression analysis based on seven primary damage descriptors and three morphology descriptors.