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The impact of short-range forces on high-energy atom collisions in displacement cascades.[1] GERMAN SAMOLYUK, ROGER STOLLER, Oak Ridge National Lab, USA, ARTUR TAMM, Institute of Technology, University of Tartu, Estonia, LAURENT BELAND, G. MALCOLM STOCKS, Oak Ridge National Lab, USA, ALFREDO CARO, Los Alamos National Laboratory, USA, LYUDMILA SLIPCHENKO4, Purdue University, USA, YURY OSETSKIY, Oak Ridge National Lab, USA, ALVO AABLOO, Institute of Technology, University of Tartu, Estonia, MATTIAS KLINTENBERG, Uppsala University, Sweden, YANG WANG, Pittsburgh Supercomputer Center, Carnegie-Mellon University, US — Simulation of primary radiation damage formation in solid materials involves collisions between atoms with a few hundred keV of kinetic energy. As a result, during these collisions, the distance between two colliding atoms can approach 0.05 nm. For such small atomic separations, interatomic potentials significantly underestimate the potential energy. The common practice involves using a screened Coulomb pair potential to describe the high-energy interactions and to smoothly join this to the equilibrium potential. However, there is no standard method for choosing the joining parameters and defect production during cascade evolution has been shown to be sensitive to how the joining is done. We developed a new procedure, which includes the use of ab initio, calculations to determine the pair interactions at intermediate distances, together with systematic criteria for choosing the joining parameters. Results are presented for the case of nickel.

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