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Secondary Electron Yield of Elemental Metals: First Principles Parameterization of Monte Carlo Simulations[1] MACIEJ POLAK, DANE MORGAN, University of Wisconsin, Madison, RAVINDRA JOSHI, MADHI SANATI, XIAOLI QIU, Texas Tech University, Lubbock, IVANA GONZALES, RYAN JOHNSON, RAUL GUTIERREZ, University of New Mexico, Albuquerque, MULTIPACTOR MURI COLLABORATION — Suppressing multipactor is crucial in designing efficient radio frequency (RF) systems. The use of low secondary electron yield (SEY) materials helps mitigate multipactor, hence, accurate SEY data is needed. In this work, the SEY of 25 elemental metals in face-centered cubic (FCC) and body-centered cubic (BCC) lattices was calculated using Monte Carlo (MC) simulations. The inelastic electron scattering was described by differential inverse inelastic mean free paths obtained with the use of the Penn approximation applied to dielectric functions obtained through full-potential and pseudopotential density functional theory (DFT) calculations, which was also used to calculate work functions. Comparison with the available experimental data shows high predictive capability of using first-principle data in MC simulations of SEY. This study is the first step in building a larger SEY database, which in turn will aid in high-throughput search for low SEY materials through machine learning.

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