Contribution ID: **56**   Type: **Contributed Focus Session Oral Presentation**

Modified Moliere's Screening Parameter and its Impact on Calculation of Radiation Damage

Wednesday, 21 May 2014 14:10 (25 minutes)

The Moliere approximation of elastic Coulomb scattering cross sections plays an important role in accurate description of non-ionization energy, DPA radiation damage etc. The cross section depends only on a single parameter that describes the atomic screening. Moliere calculated the screening angle for the Tomas-Fermi distribution of electrons in atoms. In this report, the screening parameter was recalculated using a more accurate atomic form-factor obtained from the self-consistent Dirac-Hartree-Fock-Slater computations. For relativistic particles, the new screening angle can differ from the Moliere approximation by up to 50%. At the same time it is rather close to other independent calculations. A simple parameterization of the updated atomic screening parameters is proposed. DPA and non-ionization energy-loss calculated using the Hartree-Fock atomic form-factor is compared against results based on the other atomic screening models. The sensitivity of radiation damage calculation on parameters of the Coulomb elastic scattering cross section is discussed.

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Session Classification: Focus Session 3: Target Facility Simulation Challenges

Track Classification: Target Facility Simulation Challenges