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Non-Ionizing Energy Loss in Silicon: Geant4 and TRIM simulations and defect cluster studies towards more advanced NIEL concept for radiation damage modelling and prediction

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The concept of Non-Ionizing Energy Loss (NIEL) is used to compare and quantify the damage caused to semiconductor devices in various radiation environments. However, the current NIEL concept has a limitation in predicting the formation rates of cluster and point defects in silicon crystals for different particles and particle energies. Experimental observations have revealed differences in radiation damage produced by neutrons and protons with the same displacement energies (i.e., damage parameters normalized to NIEL).

In previous contributions for the RD50 workshop Geant4 simulations of high-energy particles (neutrons, protons, and electrons) were reported and Primary Knocked-on atoms (PKA) were analyzed. Additionally, a specific Geant4 physics module ScreenedNuclearRecoil was employed to track the subsequent creation of silicon cascades. The OPTICS (Ordering points to identify the clustering structure) algorithm was utilized as a tool to differentiate between isolated and clustered defects.

In this study, the ScreenedNuclear module in Geant4 is replaced by the more widely accepted SRIM/TRIM(Stopping Range in Matter/ Transport Range in Matter) simulation framework. Furthermore, this work combines Geant4, SRIM/TRIM, and the OPTICS algorithm. Neutrons, protons, and electrons are defined as the initial beam in Geant4. The resulting Primary Knocked-on atoms (PKA) are compared with FLUKA simulations and saved for further analysis. Separate studies are conducted on low-energy recoils using the TRIM framework and the OPTICS algorithm, and the results are also saved. By combining the results obtained from Geant4 and TRIM+OPTICS, it becomes possible to estimate the NIEL specifically relevant to vacancy creation, rather than the total NIEL. This revised approach allows for a more accurate prediction of damage and estimation of clustered and isolated defects for different incident particle energies.

Authors: GARUTTI, Erika (Hamburg University (DE)); DAWSON, Ian (University of London (GB)); MOLL, Michael (CERN); SUBERT, Vendula (Hamburg University (DE))

Presenter: SUBERT, Vendula (Hamburg University (DE))

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