Kinematic Limits of SRIM Damage Models: Evaluating QDC, FDC, and MCS Algorithms in Carbon Targets

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This study presents a comparative analysis between the three damage calculation models of the SRIM (Stopping Range of Ions in Matter) software package across different ion mass and incident energy regimes. Interactions of helium, nitrogen, and chlorine ions were simulated with the three models across an incident energy range of 1 keV to 10 MeV in a Highly Oriented Pyrolytic Graphite (HOPG) target, modeled as carbon in the software. Stopping power components, relative difference in damage predictions, energy partitioning mechanisms and spatial damage profiling were evaluated to determine where each model can be better applied.

The SRIM software provides three distinct algorithms for calculating target damage. The Quick Damage Calculation (QDC) model prioritizes computational efficiency by employing the analytical Norgett-Robinson-Torrens (NRT) modified Kinchin-Pease method. The Full Damage Cascades (FDC) approach utilizes Free Flight Path (FFP) approximations to execute a detailed tracking of the incident ion trajectories and all subsequent recoil cascades. Finally, the Monolayer Collision Steps (MCS) algorithm bypasses the FFP approximations, forcing the Monte Carlo engine to meticulously evaluate scattering events and energy losses at each atomic monolayer, making it the most accurate model at the expense of longer execution times and higher computational cost.

The results indicate that the NRT-modified Kinchin-Pease analytical model inherent to the QDC algorithm loses accuracy for light ions, such as helium, in low-to-intermediate energy regimes (10 keV to 1 MeV), exhibiting relative differences in vacancies-per-ion predictions as high as 25% when compared to the MCS baseline. Conversely, for heavier projectiles like chlorine, QDC accuracy improves significantly, reducing this relative discrepancy to approximately 5%. This behavior is intrinsically linked to energy partitioning and mass stopping phenomena. For light ions, incident energy is dissipated predominantly via electronic stopping, generating sparse recoil events where continuous analytical approximations fail against the strict event-by-event tracking of MCS. In heavier mass regimes, nuclear stopping dominates the energy-loss spectrum, producing high-density displacement cascades that statistically validate the QDC approximations. Consequently, while the QDC model provides a reliable and resource-efficient alternative for heavy-ion implantations governed by dense cascades, it is inadequate for light-ion regimes.

In contrast to QDC, the Free Flight Path (FFP) approximations employed by the FDC algorithm demonstrate a high degree of convergence with the MCS baseline, reaching relative differences that approach 0% for helium and remain below 1% for chlorine. Nevertheless, interactions involving nitrogen projectiles exhibit a pronounced divergence, peaking at 7.69% for 1 keV incident ions. This phenomenon is dictated by the kinematic

factor Λ for elastic collisions, the fundamental parameter governing non-ionizing energy transfer. Given its atomic mass, nitrogen achieves a near-perfect elastic energy transfer efficiency ($\Lambda \approx 0.994$) with carbon atoms, resulting in the most prolific generation of displacement cascades among the studied ions. While the FDC model provides a highly detailed tracking mechanism, the higher amount of secondary damage cascades induced by optimal Λ values exceeds the spatial resolution of the FFP approximations. Therefore, accurately resolving the damage morphology in kinematically matched regimes necessitates the meticulous monolayer event tracking inherent to the MCS model.