

Monte Carlo simulations based on the binary collision approximation (BCA) have been widely used to predict the depth profile of primary radiation defects in materials due to ion beam irradiation. The most representative code of those is the Stopping and Range of Ions in Matter (SRIM), where two modes, full-cascade (FC) and quick calculation (QC), are offered in the modeling of primary radiation damage. However, because of the low computational efficiency of SRIM, previously only a limited number of cases can be computed to provide insights into this issue. Here, we used IM3D, a SRIM-like code but 1000 times faster, to reveal the discrepancy between FC and QC over the periodic table for five ion energies, including more than 33,586 ion-target combinations. We show that the ratio of vacancy creation by FC/QC based on the direct-output method ranges from 1 to 3, with a fitted normal distribution centered near 1.8 to 2. Surprisingly, this ratio is very weakly dependent on the ion element, suggesting that the intrinsic discrepancy between FC and QC may originate from the different consideration of target effect. By visualizing the results for a selected ion on the periodic table, we further discover that the targets with a high FC/QC vacancy ratio appear to be localized at the right half of the transition metal region. Also, we quantitatively unravel the relative error of vacancy depth by QC due to the neglected “forward scattering” effect. The maximum relative error is up to 80% for 1 keV ions, while it decreases rapidly as the ion energy increases. Finally, we show that both the displacement threshold energy and the binding energy can impact the FC/QC vacancy ratio significantly.