Atomistic simulation of primary radiation displacements and damage in multi-atomic target using BCA-based SRIM code

In this study, the vacancy and damage production behaviors for H, He, C and O incident ions on fluorine-doped tin oxide (FTO) thin films were examined by using the full cascade (FC) option of SRIM-2013 code. The quick option was not deployed in this study because many authors have critiqued its applicability in multi-atomic targets. The ion energies were varied from 10 KeV to 10 MeV and the target thickness was adjusted at each ion energy until all the ions are absorbed within the target. The numbers of atomic displacements were evaluated using both the direct computation using the “vacancy.txt” SRIM output file, and the damage energy-based manual manipulation of the Norgett-Robinson-Torrens (NRT) defect production model. We compared the SRIM vacancy.txt results with the ion range and damage in nanostructures” (iradina) code in order to validate the SRIM results. Depth-dependent damage production profile, in unit of displacement per atom (dpa) was calculated using the damage energy approach only. It’s observed that the “FC vacancy.txt” method overestimated vacancy production compared to values calculated using the “FC damage energy” method. Also, good agreements were observed between the SRIM and iradina vacancy productions. The dpa rate for O and C ions were found to be higher than that of He and H.