Monte Carlo Simulation of Ion Implantation, Sputtering and Primary Damage in Complex Nuclear Materials

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In fusion devices, ion retention, sputtering and radiation damage of materials during plasma-material interaction (PMI) are major concerns in the selection of compatible plasma-facing materials (PFMs). A universal, open-source and computationally efficient 3D Monte Carlo code, IM3D, has been developed to study ion implantation, sputtering and primary damage in complex nuclear materials. IM3D is based on fast indexing of scattering integrals and the SRIM stopping power database, and allows the user a choice of Constructive Solid Geometry (CSG) or Finite Element Triangular Mesh (FETM) method for constructing 3D shapes and microstructures. The influence of surface roughness on ion implantation and sputtering of materials as well as the developing of an efficient primary radiation damage model have been systematically performed: 1) The restrictive relationship between ion retention/sputtering of materials and surface roughness has been investigated by coupling a Gaussian-type rough surface model into IM3D. It shows that in fusion engineering the radiation albedo effect cased by surface roughness could be deleterious as it enhances primary ion implantation, but is beneficial as it reduces ion sputtering for PFMs. 2) Based on the quasi-free diffusion approximation of point defects, a cascade-annealing model has been developed to eliminate the spatial-correlation effect of primary irradiation defects. Primary radiation damage in arbitrary complex materials under energetic particle irradiation can thus be estimated quantitatively and rapidly, which shows that the althermal and diffusion-recombination by spatial-correlation are the two key processes in the evolution of primary defects. The results are much helpful for understanding the practical problems like H/He retention, surface erosion and neutron radiation damage of materials in nuclear fusion.

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