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Atomistic Simulations of Energetic Particle Interactions with the First Wall.[1] ROGER STOLLER, Oak Ridge National Laboratory — Atomistic simulations of the interactions between energetic particles and a fusion reactor first wall have been carried out using molecular dynamics to investigate both primary damage formation in the structural first wall material and the sputtering of surface atoms which can lead to contamination of the plasma. In the case of damage formation in the structural material, the results provide a quantitative measure of the effect of a nearby free surface on the evolution of atomic displacement cascades, and the nature of the residual damage produced. This damage is characterized by the total number of point defects (vacancies and interstitials), as well as the number and size distribution of point defect clusters produced. A sufficient number of simulations have been completed to statistically evaluate variations between surface-influenced and bulk cascades. Surface sputtering from the molecular dynamics simulations is compared to the results obtained with a more simple, and widely-used Monte Carlo model (SRIM).

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