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Molecular Dynamics Study of Self-Interstitial Atoms in BCC Metals: Crystallization in Mo and ferromagnetic Fe DANIEL FINKENSTADT, DIMITRIOS PAPACONSTANTOPOULOS, MICHAEL MEHL, Naval Research Laboratory — Among point defects, the self-interstitial atom (SIA) is less well investigated than its relative, the atomic vacancy. Experimentally, the SIA is important for understanding of embrittlement in irradiated materials, however there are other processes in which the SIA may also be important, namely, the solidification and crystallization, at the atomic scale, of matter from the amorphous state. Amorphous structure may be treated within the context of density functional theory as a network of SIA and vacancies. We will present tight-binding molecular dynamics (TBMD) studies of interactions between SIA, vacancies, surfaces and interfaces, within bcc-based metals, with focus on Mo and ferromagnetic Fe. We will show, via TBMD simulation, that structural transformation and mass transfer are facilitated and made rapid by the presence of a SIA. Results are compared, as a benchmark, to previous plane-wave pseudopotential results for SIA formation energies.

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