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First-principles molecular dynamics simulations of high-concentration deuterium implantation in liquid lithium MOHAN CHEN, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, 08544, USA, TYLER ABRAMS, MICHAEL JAWORSKI, Princeton Plasma Physics Laboratory, Princeton, NJ, 08543, USA, EMILY CARTER, Department of Mechanical and Aerospace Engineering, Program in Applied and Computational Mathematics, and the Andlinger Center for Energy and the Envi —
First-principles molecular dynamics (FPMD) is performed to study liquid lithium (Li) samples with high-concentration deuterium (D) implantation. First, we validate FPMD against experimental properties of solid and liquid Li and LiD. The calculated properties of both Li and LiD include relative stabilities and bulk moduli of several solid phases, melting temperatures, pair distribution functions, and bond angle distribution functions. Excellent agreement is obtained between FPMD and available experimental data. Next, we randomly implant D atoms at four different concentrations into liquid Li at different temperatures. Specifically, the ratios of D:Li atoms studied are 0.25, 0.50, 0.75 and 1.00, and the temperatures range from 400 to 1143 K. FPMD reveals several interesting properties of these liquid Li samples with implanted D atoms. For example, we observe fast nucleation of rock-salt structures of LiD for samples at temperatures lower than the melting point of LiD (960 K). We find that the pure Li component is quickly suppressed with increased concentration of D atoms, and that no D clusters form. Finally, because measured diffusivities of D in liquid Li vary by several orders of magnitude, we predict the diffusivities of both Li and D atoms in all samples.

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