Ab initio molecular dynamics study of U-Mo alloys: structural, mechanical, vibrational and defect properties

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Uranium-molybdenum (U-Mo) alloys are under investigation as candidate fuels for future high-performance research reactors with low-enriched uranium (LEU). U-Mo alloys are characterized by high uranium density, high thermal conductivity and enhanced radiation resistance as compared to other aluminide and silicide fuels. Uranium metal exists in three crystal structures, i.e., a low-temperature orthorhombic α phase, a high-temperature tetragonal β phase, and a body-centered cubic (BCC) γ phase, which is the most stable phase before melting. The BCC γ phase exhibits the most useful properties for nuclear fuel application, however, it is unstable at room temperature. Alloying U with Mo has been shown to stabilize BCC γ phase to low temperatures. Despite the numerous experimental and theoretical investigation of U-Mo alloys, the structural and mechanical behaviors of the metallic fuel under irradiation are still not fully understood. One issue with *ab initio* simulations of BCC γ-U or its U-Mo alloy is their mechanical instability at zero temperature, which prevents the calculation of mechanical and defect properties using first-principles method. Recent studies show that *ab initio* molecular dynamics (AIMD) simulations can overcome this problem by including anharmonic temperature effect to stabilize the BCC γ-U and U-Mo alloy at high temperatures. To this end, we used AIMD simulations to investigate the stabilization of BCC γ-U due to alloying with Mo elements. The structural properties of γ U-Mo alloys are compared with the α and body-centered tetragonal (BCT) phases using radial distribution and bond-angle distribution functions. Mechanical and vibrational properties of U-Mo alloys are predicted from interatomic force constants determined from AIMD trajectories and forces. Finally, the defect formation and fission gas atom incorporation energies in U-Mo alloy were also studied. The currently predicted material properties U-Mo alloys can be used to model the U-Mo fuel behavior under radiation conditions.