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Stress dependent defect energetics in Tungsten from first-principles MD. HOSSAIN, California Institute of Technology, JAIME MARIAN, Lawrence Livermore National Laboratory — Tungsten (W) is an important material for high temperature applications due to its refractory nature. However, like all transition metals from the VI-A group, W suffers from low-temperature brittleness and lack of ductility, which poses serious questions for its use as a structural material. Tungsten's mechanical properties can be enhanced by alloying with elements with d-electrons, such as Re, which has resulted in successful commercial alloys. In this work, we obtain the formation and migration energetics of Re solute atoms in terms of their interaction with vacancies and dislocations. To explore the influence of external stresses on Re transport properties, we examine the role of hydrostatic and shear deformation on the vacancy formation energy (VFE) and migration energy barrier (Em) in BCC W from first-principles calculations by developing a pseudopotential with 6s2, 6p0, 5d4, and 5f0 electronic states for the valence electrons. We find that under hydrostatic deformation, increase or decrease of vacancy formation energy depends on the type of deformation – tensile or compressive, while for shear deformation it decreases irrespective of the magnitude of applied deformation. On the other hand, migration energy barrier always decreases under hydrostatic deformation, but shows path-length dependent behavior under shear deformation. This talk will discuss the underlying principles and possible routes for enhancing mechanical strength from a physics perspective.

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