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Atomic modeling of stability and thermal characteristics of metastable tungsten as a plasma-facing fusion material[1] ANNA WOLZ, University of Virginia, JEROME GUTERL, Oak Ridge Associated Universities, STEFAN BRINGUIER, General Atomics — Plasma-facing materials must be able to sustain large heat and particle fluxes in future fusion reactors. Recent experiments have suggested the existence of a metastable W-B phase at room temperature [1] which may be a suitable plasma-facing material. Exploring the influence of implanted species on lattice stability and thermal properties therefore provides additional insight. First, the stability of W phases BCC and FCC is analyzed by solving the phonon dispersion relation at various temperatures (0-4000K) and pressures (100-105 atm). The phonon spectra are deduced from the eigenvalues of the dynamical matrix obtained from molecular dynamics simulations (LAMMPS) [2], and compared to existing calculations for pure W [3] to assess the validity of the phonon calculation and interatomic potential. The effects of impurities on the stability of W phases are examined from the phonon spectra when H, He, and B impurities are introduced into a W lattice. [1] Y. Raitses, 60th APS-DPP conference 2018 [2] Zhang, H. Y (2018). Computational Materials Science, 144, 32-35 [3] Kong, L. T. (2011). Computer Physics Communications, 182(10)

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