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First-principles investigation of Wsingle bondV and Wsingle bondMo alloys as potential plasma facing materials (PFMs) for nuclear application

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Abstract

Density-functional theory (DFT) based first-principles calculations were used to investigate the crystal structure, binding energy, phase stability and elastic properties of body-centered cubic (BCC) W-based binary solid solutions. The effect of alloying up to 50 atomic percent (at.%) concentration range is determined from the virtual-crystal approximation (VCA) approach. Resulting BCC solid solutions are assessed in comparison to the ideal Vegard's law. Solubility of the alloying elements is characterized by the negative enthalpy of mixing. The values of elastic constants computed for the ground state structures are used to assess the effect of alloying on the ductility and hardness. Based on current results, it seems key to strike a tricky balance between moderate Pugh's modulus ratio (B/G) between bulk and shear moduli (B,G) and elastic anisotropy (A) such that high hardness is not completely compromised at the expense of ductility. The predicted property trends are in agreement with existing theoretical and experimental data, which is indicative that the VCA approach is reliable in development of such alloys.