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First-principles investigations of structural properties and energies stabilities of W-Re alloy for fusion reactor application

Tungsten (w) is considered as the potential plasma facing material for fusion reactor application due to its exceptional mechanical and thermal properties. The notable properties of tungsten are its high melting point, high thermal conductivity, hardness, and low sputtering yield. However, tungsten also presents a very low fracture toughness limiting its application as plasma coating material. To enhance the ductility of W material, in this study, we investigate the structural, mechanical and energetic properties of Tungsten-Rhenium (W-Re) alloys at various rhenium (Re) concentrations ranging from 6% to 37%, using first-principles density functional theory (DFT) calculations. The energies stabilities and equilibrium volumes of W-Re alloyed material were calculated following full volume-cell relaxation (V-C relax) procedures. Our results reveal systematic trends in lattice constant contraction leading to volume reduction (249.79Å3 to 244.47Å3) as the concentration increases. The increase in W-Re alloy concentration leads to different lattice constant sizes a≠b≠c leading to anisotropic geometry, suggesting the symmetry change from BCC counterparts. Energetic stability based on mixing enthalpies shows that Re alloy further stabilizes the structure with concentrations increment. These findings provide a go ahead for further intensive and extensive investigations of W-Re alloys material for ductility.

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