Effects of rhenium alloying on adhesion of Mo/HfC and Mo/ZrC interfaces: A first-principles study

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Abstract :

Adhesion and electronic structure of Mo/HfC and Mo/ZrC interfaces with and without Re impurity are investigated using first-principles density functional calculations. For Re free interface, results show that Mo atoms bind preferentially on top of C atoms, forming covalent bonds. The presence of Re alloying at the interface improves the adhesion, but does not affect the nature of interfacial Mo-C bonds.

Keywords : ab initio calculations, adhesion, ceramics, density functional theory, electronic density of states,Fermi level, hafnium compounds, metal-insulator boundaries, molybdenum, molybdenum alloys,rhenium alloys.

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