Ab initio investigation of Al/Mo_2B interfacial adhesion

H. Si Abdelkader, H.I. Faraoun

Abstract :

First-principles calculations were performed to study the adhesion and the interfacial electronic structure of aluminum/molybdenum semi-boride (Al/Mo_2B) interface. The work of adhesion (W_{ad}) was calculated for both terminations of the Mo_2B surface and it was found that Mo-terminated has larger W_{ad} than the B-terminated one. It was shown that interfacial Al and B atoms form polar covalent bonds, while bonding of interfacial Al and Mo atoms mainly presents metallic character.

Keywords : Ab initio calculations; Adhesion; Surface and interface; Aluminum; Molybdenum borides.

Journal Title / Revue : Computational Materials Science, ISSN : 0927-0256, DOI : 10.1016/j.commatsci.2010.10.025, Issue : 3, Volume : 50, pp. 880–885, January 2011.