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Theoretical investigation of the interface structure of θ-Al_2O_3/NiAl(001). JYH-PIN CHOU, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan — The atomic structure of θc-Al_2O_3/NiAl(001) interfaces has been investigated by using *ab initio* pseudopotential method based on the density functional theory. Knowledge on physical origin of adhesion on oxide and metal interface is essential for the development of various industrial applications. However, the atomic structure of the interface has not been fully clarified yet. In this study, surface energies of the Al-terminate and Ni-terminate NiAl(001) are calculated. Geometry configurations and bond adhesion strength betweenθc-Al_2O_3 and NiAl(001) are determined..

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