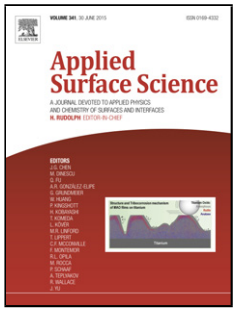

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A first principles study of adhesion and electronic structure at Fe (110)/graphite (0001) interface

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Highlights

1. The surface energy of graphite (0001) and Fe (110) have been calculated and the number of layers of graphite slab and Fe slab has been estimated.

2. The work of adhesion of Fe (110)/graphite (0001) interface with different interfacial separation d_0 (1.7–3Å) have been systematically discussed.

3. The total electron density and electron density difference of Fe (110)/graphite (0001) are used to study the bonding characteristics.

4. The Interfacial energy and fracture toughness of Fe (110)/graphite (0001) are estimated.

Abstract

Using first–principles calculations, we discuss the bulk properties of bcc Fe and graphite and that of the surface, the work of adhesion, and the electronic structure of Fe (110)/graphite (0001) interface. In this study, the experimental results of the bulk properties of bcc Fe and graphite reveal that our adopted parameters are reliable. Moreover, the results of surface energy demonstrate that nine atomic layers of graphite (0001) and five atomic layers of Fe