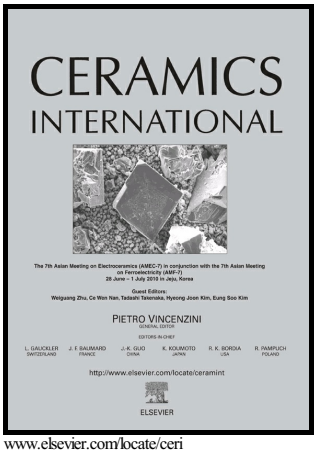

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First-Principles Study of Adhesion Strength and Stability of the TiB_2/TiC Interface in Composite Materials

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Abstract:

The properties of a TiC(0 1 0) surface, a TiB_2(0 1 $\bar{1}$ 0) surface, and TiC(0 1 0)/TiB_2(0 1 $\bar{1}$ 0) interfaces were investigated by first-principles calculations. The work of adhesion (W_{ad}), the interface energy (γ_{int}), and the electronic structure of the interfaces were determined. The results show that the C-BS1-B1, C-TS-B2, and Ti-BS1-B1 interfaces are the most stable interfaces. Among all models, the C-TS-B2 interface is most stable and exhibits the highest W_{ad} value (4.77 J/m^2) and the lowest γ_{int} value (1.12 J/m^2). All three stable interfaces exhibit strong covalent bonding due to the interfacial C-sp and B-sp orbital hybridization; the stable interfaces investigated in this study are as stable as the TiC(1 1 1)/TiB_2(0 0 0 1) interface reported in a previous study.

Keywords: First-principles calculation; TiC/TiB_2 interface; Adhesion strength; Interfacial energy

1. Introduction

Titanium carbide (TiC) ceramics have been widely investigated for industrial applications due to their excellent physical and chemical properties, such as high hardness and melting point, low density, high corrosion resistance, and wear-resistance [1-4]. Titanium diboride (TiB_2) has received considerable attention due to its properties of high strength, hardness, and ductility of the matrix/TiB_2 coherent interfaces[4-7]. For example, Xiao[8] showed that Ti/TiC coatings possessed not only good frictional properties and corrosion resistance but also had good tin-repelling and hydrophobic characteristics. A Ti/TiC coating provides excellent protection against corrosion of lead-free solder in wave soldering. Miao[9] studied the mechanical properties and thermal stability of rolled W-0.5 wt% TiC alloys and demonstrated that the good thermal stability was attributed to the

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