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Short Communication

Theoretical Study of The Alloying Elements on the Properties of Tib_2 Ceramic Reinforced Fe Matrix Composite

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In recent decades, ceramic particles reinforced iron matrix composites (CPRIMCs) are regarded as the main achievements in wear resistant materials area [1-3]. Among many iron matrix composites, TiB_2 ceramic reinforced Fe matrix composite (TiB_2/Fe) behaves large elastic modulus, high mechanical strength, and advanced hardness and wear resistance [4,5]. Additionally, the high electrical conductivity of TiB2 ceramic [6] enables machining of TiB2/Fe composite easily using electrical discharge machining. Agarwal and Dahotre [7] discussed the reinforcing mechanism of TiB2/Fe composite, the epitaxial growth of iron on TiB2 particles is revealed, and the orientation relationship was found as TiB2 (0001)/Fe (111). However, much less information is available for the effects of alloying elements on the properties of TiB2/Fe interface.

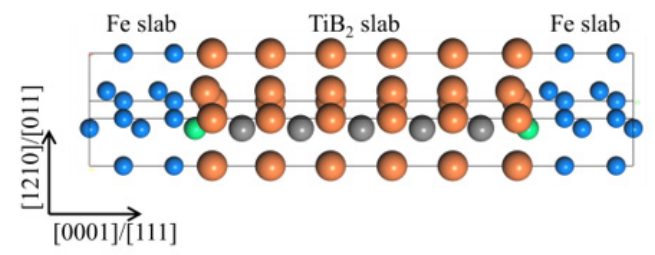

Figure 1: Interfacial atomic structures of the TiB2 (0001)/Fe (111) interface.

We use the method proposed in [8] to investigate the atomic structures, chemical bonding, stability and fracture mechanism of TiB_2/Fe composite. It is found that B-terminated interface with HCP site behaves the most stable nature and belongs to non-diffusive configuration. Based this configuration, the segregation behavior of alloying additives X (X=Si, Al, Cr, Mn, Ni, Mo) on the interface of TiB_2 ceramic reinforced iron matrix composite as well as the effects of these additives on the interfacial adhesion, electronic and magnetic properties were studied. The results indicated that Cr, Mn and Mo may segregate at the TiB_2 (0001)/Fe (111) interface because of their low heat of segregation barrier (Figure 1).

Moreover, compared with the work of adhesion of different alloying doping interfaces, the introduction of Cr, Mn improves the adhesive strength of TiB_2(0001)/Fe (111) interface through strong covalent interactions between Cr/Mn and B atoms. The best strengthening effect on TiB_2 (0001)/Fe (111) interface can be attributed to Mn because of the highest interfacial work of adhesion and critical stress of Mn-doped interface; we also found the interfacial work adhesion energy is high than fracture energy of TiB2 and Fe slabs, indicating the mechanical strength of the interface is more remarkable than both TiB_2 and Fe bulks, and the mechanical failure will initiate at the Fe interior.

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Conflict of Interest

No conflict of interest.

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