Insights Into the Interface Properties of Mg/Ti Via Experiments and First-Principles Calculations

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Abstract： In order to understand in depth the interface characteristics between Ti particles and Mg matrix, and reveal the strengthening mechanism of Ti particles reinforced Mg matrix composites, the interface structure, work of adhesion and the interface electronic structure of the Mg(0001)/Ti(0001) interface have been studied by experiments combined with first-principles methods. The calculation results of the work of adhesion show that the Ti-HCP interface is more stable than the Ti-OT interface. The electronic structure analysis results show that the Ti-Mg bond formed at the Ti-OT interface has a weak covalence and exhibits the characteristics of a Ti-Mg ionic bond. The electronic characteristics of the Ti-HCP interface are metallic bonds.

Keywords: First-principles calculation; Mg/Ti interface; Work of adhesion; Electronic structure

1 Introduction

Compared to conventional Mg alloys, particle reinforced Mg matrix composites (PMMCs) have higher strength, better wear resistance and better fatigue and creep properties, which has attracted a lot of research attention in recent years [1, 2].

Reinforcement particles are divided into ceramic particles and metal particles. Compared to ceramic particles, metal particles such as Cu, Ni, Fe and Ti have high ductility and excellent elastic modulus and can be used as candidate materials for strengthening Mg matrix composites [3, 4]. In particular, Ti particles can improve the strength of composites while maintaining good ductility, and experimental studies have been reported.

For Ti particle reinforced Mg matrix composites, the interface properties between Ti particles and the Mg matrix have an important effect on the ductility, strength and fracture mechanism of the composites, so it is necessary to have a basic understanding of these interface properties. However, it is very limited to systematically investigate the interface properties of composites by experiments alone. In recent years, what is recognised as a first-principles method for the study of microscopic surfaces and interfaces has been widely used. This method can reveal the interfacial properties of Ti/Mg from the atomic scale, such as atomic configuration, interfacial adhesion and interfacial bonding, which will help to understand the strengthening mechanism of Ti particle reinforced Mg matrix composites and improve the overall mechanical properties of the composites. In this work, the interfacial properties of Mg(0001)/Ti(0001) are calculated by the first-principles method in order to clarify the interfacial structure, work of adhesion and interfacial fracture mechanism, and to guide the design of novel Mg/Ti composites.

2 Experimental procedure

In this work, high purity magnesium ingot was used as the matrix material of the composite. Spherical Ti metal particles with a particle size range of 1-20μm were used as the reinforcing phase. The Mg-10wt%Ti composite was prepared by the stirring casting method.

In this work, based on the density functional theory (DFT) plane-wave pseudopotential method, generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) approach was employed to describe the exchange-correlation functional. The plane-wave cutoff energy was set as 400eV. The k-point sampling meshes obtained by using the Monkhorst-Pack scheme were set to 9×9×9 for bulk Mg and bulk Ti, and 9×9×1 for all the surfaces and interfaces.

3 Result and discussion

1.Microstructure of Ti/Mg composites

Fig.1 shows the microstructure of Ti/Mg composites, and it can be seen that the particles are uniformly dispersed.

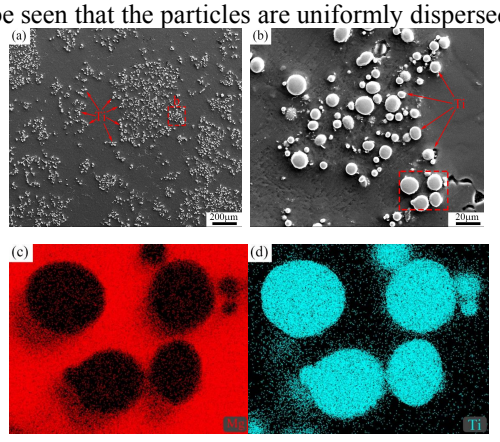

Fig. 1. Microstructure of Ti/Mg composites

2. Surface properties of Mg and Ti

In order to ensure the accuracy of the calculation, 7-layer Mg(0001) and Ti(0001) slabs were selected to establish the Interface model for the subsequent calculations in this work.

3. Interface properties of Mg and Ti

Two different Mg(0001)/Ti(0001) interface models were established, as shown in Fig. 2. Two different stacking sequences are "OT" and "HCP".

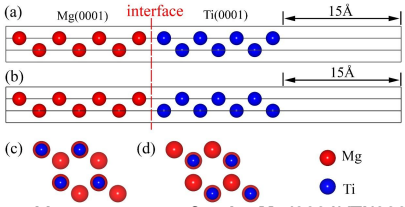

Fig. 2. Two stacking sequences for the Mg(0001)/Ti(0001) interface. (a) (c): "OT", (b) (d): "HCP"

The Work of adhesion (W_{ad}) of the Ti-HCP interface after relaxation is the largest, increasing from 0.961J/m^2 before relaxation to 1.430J/m^2 after relaxation. The W_{ad} at the Ti-OT interface is 0.107J/m^2 before relaxation and 0.673J/m^2 after relaxation.

Table 1 The calculated Wad and interfacial distance and that after relaxation

Stacking sites	Unrelaxed		Relaxed	
	d_0(Å)	W_{ad}(J/m^2)	d_{int}(Å)	W_{ad}(J/m^2)
Ti-OT	2.8	0.107	2.904	0.673
Ti-HCP	2.4	0.961	2.520	1.430

4. Electronic structure and bonding

Fig. 3 shows the charge density of the Mg(0001)/Ti(0001) interface. A change in color represents a change in charge concentration, with blue indicating less charge and red indicating more charge. The formation of charge sharing regions at the interface can be clearly observed (see red arrows). However, the distribution of charge sharing region on the Ti-HCP interface is large, which indicates that the interface interaction is strong and the interface bonding strength is high.

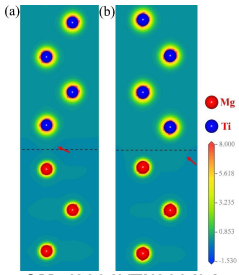

Fig. 3. Charge density of Mg(0001)/Ti(0001) interfaces: (a) OT model, (b) HCP model.

Fig. 4 shows the charge density difference of the Mg(0001)/Ti(0001) interface. The red regions represent charge accumulation and the blue regions represent charge dissipation. For the Ti-OT interface, the charge distribution between the Ti atom and the Mg atom has some directionality, but the amount of charge is relatively small, indicating that the Ti-Mg bond formed at the interface has a weak covalence. For the Ti-HCP interface, the interfacial Ti atom and Mg atom form an charge accumulation region at the interface, showing the characteristics of non-directional metal bonding. It is also observed that the charge aggregation on the Ti atom side of the interface is significant, showing the characteristics of Ti-Mg ionic bonding.

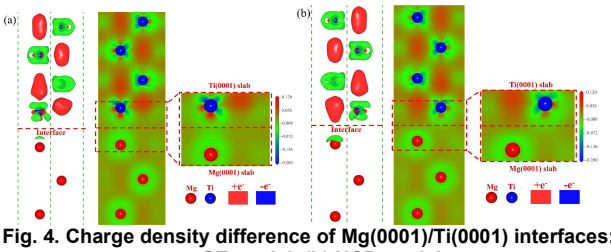

Fig. 4. Charge density difference of Mg(0001)/Ti(0001) interfaces: (a) OT model, (b) HCP model.

Fig. 5a shows the PDOS of the Ti-OT interface. Comparing the electron orbital curve of the interfacial atoms, it can be seen that the trough of the 2p electron orbital curve of the interfacial Mg atoms near the Fermi level is lower than that of the inner layer, indicating that the metallic property of the interfacial Mg atoms is reduced and the covalence is improved. Fig. 5b shows the PDOS of the Ti-HCP interface. The interface Mg atom shows a new DOS peak at -2.26 eV compared to the internal Mg atom, while the peak at 0.258 eV is significantly enhanced.

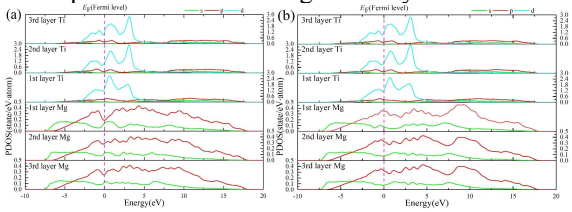

Fig. 5. The partial density of states for Mg(0001)/Ti(0001) interfaces: (a) OT model, (b) HCP model.

4 Conclusion

(1) In the Ti/Mg interface, the Wad of the Ti-HCP interface is 1.430J/m^2, and that of the Ti-OT interface is 0.673J/m2, which indicates that the binding strength of the Ti-HCP interface is higher.

(2) For the Ti-OT interface, the Ti-Mg bond formed at the interface has weak covalency. At the Ti-HCP interface, Ti atoms and Mg atoms form an electron accumulation region on the interface, showing the characteristics of non-directional metal bonding.

References

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