International Journal of Fluid Mechanics & Thermal Sciences
2019; 5(4): 91-95
http://www.sciencepublishinggroup.com/j/ijfmts
doi: 10.11648/j.ijfmts.20190504.11
ISSN: 2469-8105 (Print); ISSN: 2469-8113 (Online)

First-principles Analysis of SiC/Al Composites Interface

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To cite this article:
Qipeng Wang, Junlei Shi. First-principles Analysis of SiC/Al Composites Interface. *International Journal of Fluid Mechanics & Thermal Sciences*. Vol. 5, No. 4, 2019, pp. 91-95. doi: 10.11648/j.ijfmts.20190504.11

Received: August 30, 2019; **Accepted**: October 7, 2019; **Published**: October 17, 2019

Abstract: The interface of SiCp/Al composites is an important factor affecting the properties of materials, Different interface layers have different interface bonding strengths, which have different effects on the properties of SiCp/Al composites. In this paper, the possible binding energy of interface in SiCp/Al composites is studied, then the influence of the interfacial binding energy on the SiCp/Al composites is analyzed, and the method of controlling the interface of SiCp/Al composites is proposed. Firstly, three interface models that may exist in SiCp/Al composites were constructed in Material Studio software, and the model structure was optimized, then the first-principles simulation of the optimized interfaces model of SiCp/Al composites was carried out, and the interfacial bonding energy of SiC-Al, SiC-SiO_2-Al and SiC-Al_2O_3-Al was calculated respectively. The order of the interfacial binding energy was: SiC(100)-Al(100) < SiC(100)-SiO_2(100)-Al(100) < SiC(100)-Al_2O_3(100)-Al(100). It can be known from the simulation results that the interfacial bonding energy of the interface layer containing the oxide is large, since the oxide can improve the wettability between the matrix and the reinforcement. Therefore, in order to obtain a well-bonded SiCp/Al composite, the SiC particles are usually surface-modified to regulate the interface of the SiCp/Al composite. Thereby, the SiCp/Al composite material with high interface bonding strength and excellent performance is obtained.

Keywords: SiCp/Al Composite, First Principle, Interface, Simulation

1. Introduction

SiCp/Al composite material is a kind of material with high specific strength, large specific modulus, good thermal conductivity, good electrical conductivity, small thermal expansion coefficient, good dimensional stability, good wear resistance [1-6] etc. It has a wide range of applications in aerospace, electronic packaging, marine, automotive, precision instruments [7-13] etc. The properties of the composite material are mainly determined by the properties of the matrix and the reinforcement and the interface formed between the two, where in the interface plays an important role in the performance of the composite. The interface properties of metal matrix composites mainly include interface bonding strength, thermal conductivity etc. The interface bonding strength is an important index to characterize the mechanical properties of the interface. It can be regarded as the critical stress acting on the interface when the metal matrix and the reinforcing phase are separated along the interface. The interface bonding strength of different interface layers is also different.

In SiCp/Al composites, interfacial layers such as SiC-Al, SiC-SiO_2-Al, SiC-Al_2O_3-Al etc are usually formed. A good interfacial layer is beneficial to improve the performance of SiCp/Al composites, so we hope to obtain good interface. The greater the interface bonding energy, the more stable the interface structure, but it is very difficult to measure the interface bonding energy by experimental methods. Therefore, researchers have widely used Materials Studio (MS) software to simulate interface bonding energy. In the SiCp/Al composite interface simulation, the Visualizer, Castep and Forcite modules in the MS software are mainly used, and the Visualizer module can be used to build interface structure models; the Castep module can optimize the structure and the first-principles energy calculation; the Forcite module enables energy calculation, geometric optimization, dynamics simulation [14-18]. The results calculated by the first-principles method can be consistent

with the experimental values, and this method is economical and simple. The first-principles calculation is a method based on density functional theory to determine the properties of materials such as geometry, electronic structure, thermodynamic properties and optical properties by self-consistent calculation. In the calculation, the basic physical constants that are completely independent of experience can be used to calculate the properties of the material in the ground state. It is also called the ab-initio calculation method [18].

Li [19] et al calculated the adhesion, stability, and electronic structure of the Fe/WC interface by first-principles. The adhesion work of the best Fe/WC interface was found to be C-terminal 9.7Jm^{-2} and W-termination 5.1Jm^{-2}. Luo [20] et al carried out molecular dynamics simulation of the interface of Al-SiC formed by three kinds of low-index surfaces of SiC/Al composites (100), (110) and (111), and calculated bonding energy and the experimental values are consistent. Donald [21] et al calculated the adhesion and stability of the Al(111)/WC(0001) interface, and found that the most geometric structure of the WC(0001) surface is W-terminally connected. Guo [22] et al simulated the Ni coating on SiCp/Al composites. They used the molecular dynamics simulation in MS software to calculate the interfacial binding energy between Ni and SiCp/Al composites. The calculation results are consistent with the experiment.

Based on the predecessors, the interface of SiC-Al, SiC-SiO_2-Al, SiC-Al_2O_3-Al in SiCp/Al composites was established by MS software, and the first-principles simulation was carried out. The bonding energy of various interface layers was calculated. The interface of the maximum bonding energy of SiCp/Al composites can be found.

2. Materials Studio Simulation

2.1. Model Construction

In this study, the interface structure of SiCp/Al composites such as SiC-Al, SiC-SiO_2-Al and SiC-Al_2O_3-Al was established by MS software. Firstly, the crystal structures of SiC, Al, SiO_2, Al_2O_3 are found in the MS software material library as shown in Figure 1 (see Table 1 for the parameters of each crystal structure).

Table 1. *Crystal structure parameters.*

Materials	Space group	Space group code	Lattice parameter
SiC	P63MC	186	3.078×3.078×10.046
SiO_2	P6222	180	5.01×5.01×5.47
Al_2O_3	R-3C	167	4.759×4.759×12.991
Al	FM-3M	225	4.0495×4.0495×4.0495

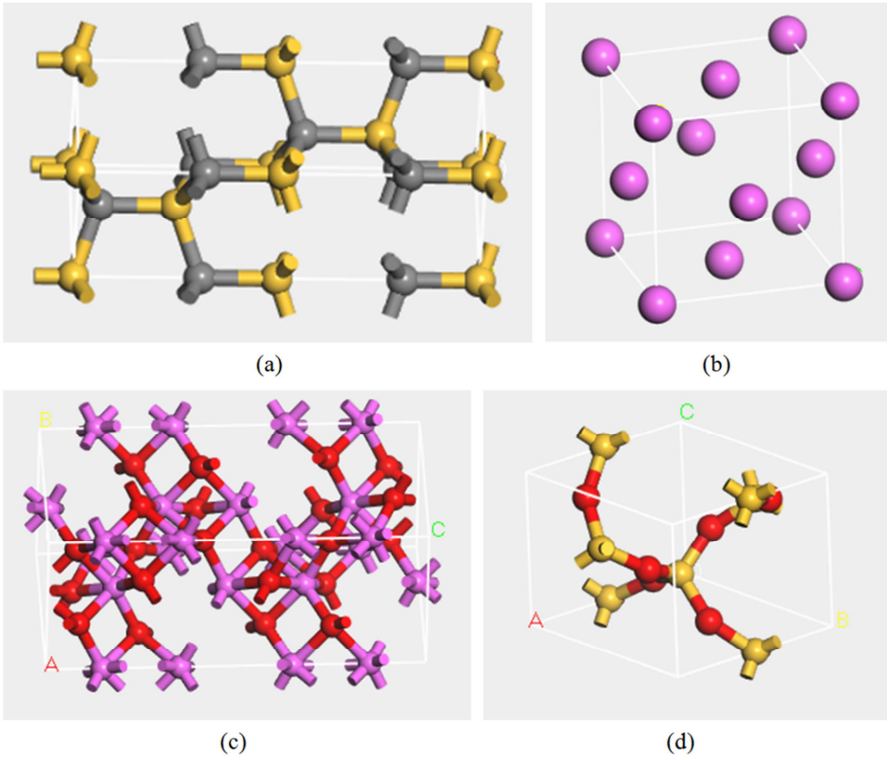

Figure 1. *Different crystal structure models: (a) SiC; (b) Al; (c) Al_2O_3; (d) SiO_2 (In the figure, the purple atom is Al, the red atom is O, the yellow atom is Si, and the gray atom For C).*

Then select the (100) crystal plane of each crystal structure through the Surfaces tool in the MS software, and then use the Build Layers tool to build three interface models of SiCp/Al composites, interface model shown in Figure 2.

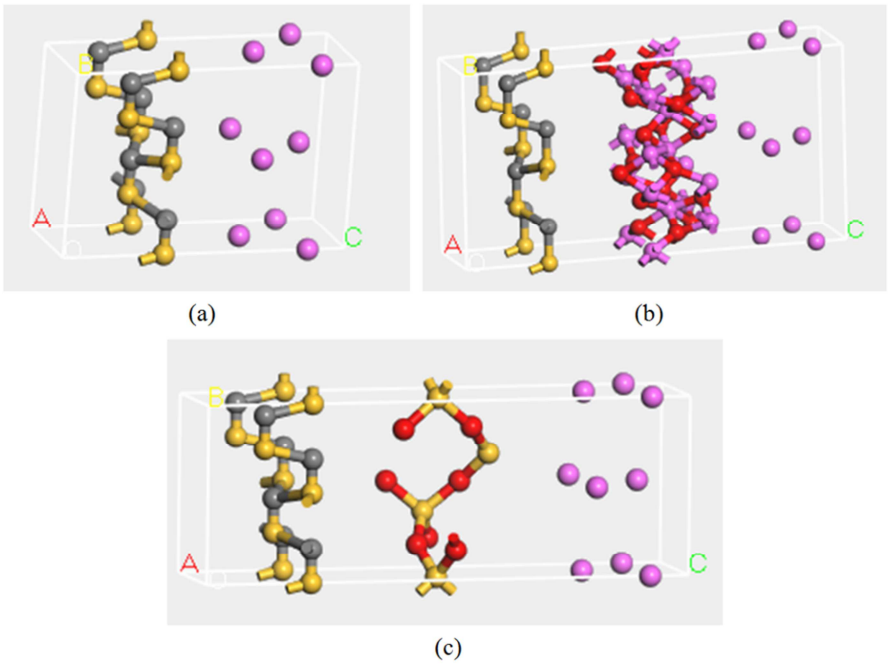

Figure 2. *SiC/Al Composite Interface Model:(a) SiC-Al; (b) SiC-Al_2O_3-Al; (c) SiC-SiO_2-Al.*

2.2. Model Optimization and Calculation

The structure of the established model is optimized by the Castep module in the MS software to make it closer to the real state. The optimized structure is shown in Figure 3. It can be seen from the figure that the Al atoms have different degrees of diffusion.

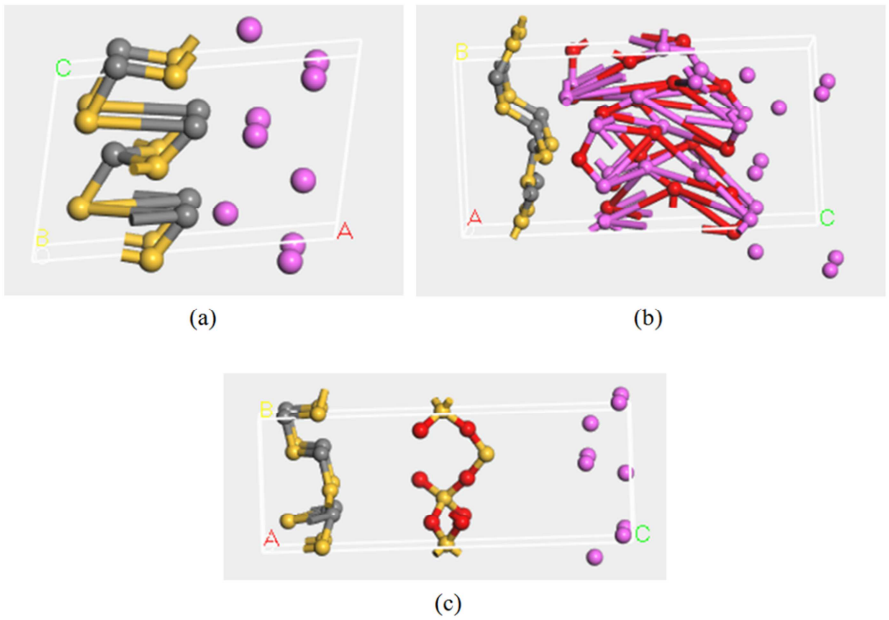

Figure 3. *The optimized interface model of SiC/Al composites: (a) SiC-Al; (b) SiC-Al_2O_3-Al; (c) SiC-SiO_2-Al.*

The optimized structure and each layer of its structure are subjected to first-principles simulation, and the total energy of each layer can be obtained to calculate the energy of the interface layer. The calculation equation is shown in (1).

$$E_{12} = E_1 + E_2 - E \tag{1}$$

Where E_{12} and E are the interface layer energy and the total energy, respectively. E_1 and E_2 are the energy of each layer structure. The interface bonding energy can be calculated [21] by equation (2).

$$W = \frac{E_{12}}{A} \tag{2}$$

Where W is the interface binding energy and A is the

interface area.

3. Results and Analysis

In SiCp/Al composites, the interface is a major factor affecting its performance. If a good interfacial layer is formed between the SiC reinforcement and the Al matrix, it will help to improve the performance of the SiCp/Al composite. This requires us to research and control the interface. From the simulation results in Tables 2-4, we can see that the interfacial bonding energy of SiCp/Al composite is: SiC-Al < SiC-SiO_2-Al < SiC-Al_2O_3-Al. Since the Oxides promote good wetting bonding at the interface between SiC and Al, and also avoid SiC and Al to form Al_4C_3, This brittle substance deteriorates the interface bonding strength.

Table 2. *Interface Interfacial Energy of SiC-Al Composites.*

Interface	Energy (ev)	Interface area (Å^2)	Binding energy (ev/Å^2)
SiC-Al	-1271		
SiC	-1039	25.12	0.36
Al	-223		

Table 3. *Interface Interfacial Energy of SiC-SiO_2-Al System.*

Interface	Energy (ev)	Interface area (Å^2)	Binding energy (ev/Å^2)
Al-SiO_2-SiC	-4222		
SiC	-1038	35.77	0.56
SiO_2	-2944		
Al	-220		

Table 4. *Interface Interfacial Energy of SiC-Al_2O_3-Al System.*

Interface	Energy (ev)	Interface area (Å^2)	Binding energy (ev/Å^2)
Al-Al_2O_3-SiC	-9844		
SiC	-1038	26.39	0.72
Al_2O_3	-8569		
Al	-218		

In order to obtain a large interface binding energy, SiC particles are usually surface-modified and coated to improve wettability and prevent reaction, thereby improving interface structure stability. Surface modification of SiC particles is a common method, including coating modification and high temperature oxidation [23-25]. High temperature oxidation is the most widely used surface modification method. It is beneficial to the formation of SiC-SiO_2-Al interface in SiCp/Al composites and improves the performance of SiCp/Al composites.

4. Conclusion

In this paper, The interface layer structure with three possible existences of SiC(100)-Al_2O_3(100)-Al(100), SiC(100)-SiO_2(100)-Al(100), SiC(100)-Al(100) are established by MS software. Then using the Castep module to optimize the three structures and first-principles calculations, the three possible interface bonding energies are as follows:

SiC(100)-Al_2O_3(100)-Al(100)>SiC(100)-SiO_2(100)-Al(100)> SiC(100)-Al(100).

SiC-SiO_2-Al interface can be obtained by surface modification of SiC particles, which is beneficial to the formation of good interface of SiCp/Al composites and improve the performance of SiCp/Al composites.

Acknowledgements

This work was financially supported by Anhui Province Postdoctoral Science Foundation (2017B213).

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