Effects of transition element additions on the mechanical and electronic structure properties of Al (111)/6H-SiC (0001) interface: A first principles study

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Abstract

In this work, effects of 20 transition element additives on the interfacial adhesion energy and electronic structure of Al (111)/6H-SiC (0001) interfaces have been studied by first principles method. For clean Al (111)/6H–SiC (0001) interfaces, both Si-terminated and C-terminated interfaces have covalent bond characteristics. The C-terminated interface has stronger binding energy, which is mainly due to the stronger covalent bond formed by the larger charge transfer between C and Al. The results show that the introduction of many transition elements, such as 3d transitional group Mn, Fe, Co, Ni, Cu, Zn and 4d transitional group Tc, Ru, Rh, Pd, Ag, can improve the interfacial adhesion energy of the Si-terminated Al (111)/6H-SiC (0001) interface. However, for the C-terminated Al (111)/6H-SiC (0001) interface, only the addition of Co element can improve the interfacial adhesion energy. Bader charge analysis shows that the increase of interfacial binding energy is mainly attributed to more charge transfer.

1. Introduction

Due to their good physical and chemical properties, SiC particle reinforced aluminum matrix composites have been widely used in aerospace, automobile and other industries [1-3]. As a bridge between SiC particle and Al matrix, the SiC/Al interface structure plays an important role in the properties of the composites [4]. In order to improve the interfacial wettability and adhesion of Al/SiC interfaces, elements additive in Al matrix has become one of the most extensively used techniques to fabricate composites with excellent performance [5].

In the experiment, many researchers have studied the wetting and bonding behavior of the interface between Al and SiC [6-7]. By the sessile drop technique in high vacuum, Laurent et.al. have researched the wetting kinetics in the A1-SiC system [8]. They found that the addition of Sn can improve wetting of the A1-SiC interface owing to the decrease in surface tension of Al, while Cu additions deteriorate wetting due to the decrease in A1 interactions with the SiC. The wettability of Al-SiC system can be enhanced by adding a small amount of Mg in Al matrix [9]. Moreover, the experimental results showed that Cu, Si and Mg all can reduce the amount of Al_4C_3 formed on the interface to varying degrees and improve the Al-SiC interfacial reaction [10-11]. The role of the Si addition in molten Al on the wetting was presumably attributed to its segregation at the interface and the formation of strong chemical bonds with the SiC surface [11].

In recent decades, the first-principles calculation based on density functional theory (DFT) has become one of the most extensively powerful tool to study the metal–ceramic interface information at atomic and even electronic levels [12-15]. It can accurately estimate atomic and electronic structures at the interface and the influence of alloying element on the stability of the interface [16-18]. The results show that strong covalent bonds can be formed at the metal-ceramic interface and the bonding strength of the interface can be improved by adding alloying elements to the metal matrix. In earlier years, the Al-SiC interfaces have been investigated by quantum chemistry methods [19] and ab-initio calculations [20,21]. Recently, the structural and mechanical properties of the Al(111)/6H-SiC(0001) [22-24] and Al (100)/6H–SiC(0001) [25] interfaces have been researched by first-principles method. All these studies suggest that the strong bonding of SiC / Al interface is attributed to the formation of covalent bonds. Apart from these, effects of alloying element additions on interfacial adhesion properties of Al(111)/4H-SiC(0001) [26] and Al(111)/3C-SiC(111) [27] interfaces have been studied by the first-principles method. However, a systematic theoretical study on effects of transition metal additives on the Al(111)/6H-SiC(0001) interfacial properties have been rarely reported.

In this paper, first-principles calculations were performed to investigate effects of twenty transition element additions on the mechanical and electronic structure properties of Al(111)/6H-SiC(0001) interface. The results show that the interfacial bonding energy of the Si-terminated Al(111)/6H-SiC(0001) interface can be improved by introducing 3d transition group elements, such as Mn, Fe, Co, Ni, Cu, Zn, and 4d transition group elements, such as Tc, Ru, Rh, Pd, Ag. However, for the C-terminal one, only adding Co element can improve the interfacial bonding energy. Bader charge analysis shows that the interfacial binding energy is closely related to atomic charge transfer. Our calculated results can give a profound understanding of the mechanism of alloying elements that improve the adhesive strength of Al (111)/ 6H-SiC (0001) interfaces.

2. Details of Calculation Methods

In this work, first-principles calculations were carried out by the Vienna ab-initio simulation package (VASP) code [28, 29]. Total energy and electronic structure calculations were performed with the projector augmented-wave (PAW) [30, 31] method. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) [32] approach was used to describe the exchange correlation functional. The cut-off energy value of wave functions was set to 600 eV. The energy calculations were conducted in the first irreducible Brillouin zone with a Γ-centered $15\times15\times1$ Monkhorst–Pack (MP) grid [33]. The convergence criteria for electron and ion relaxation are 10^{-5} and 10^{-4} eV, respectively. Meanwhile, for interface calculations, the force tolerance of each atom was set to 10^{-2} eV/Å.

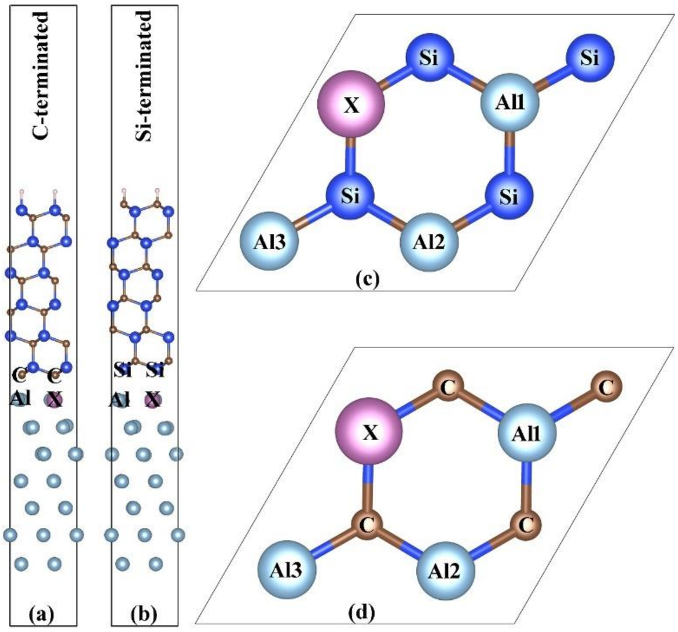

Figure 1. The 2×2×1 supercell model of Al(111)/6H-SiC(0001) interface. (a) Side view of the C-terminated interface. (b) Side view of the Si-terminated interface. (c) Top view of the C-terminated interface. (d) Top view of the Si-terminated interface. Light-blue, brown, blue and violet spheres represent Al, C, Si and impurity atoms, respectively.

According to previous studies [19-23, 27], the binding energy of the Al(111)/6H-SiC(0001) is the highest when the C (Si) atom is directly above the Al atom. Therefore, we only study this configuration here. As shown in Figure 1, a 2×2×1 supercell is used to do all calculations in this research. The supercell consists of seven Al atomic layers and six SiC atomic layers. A 2×2 Al slab along the [-110] and [-101] base vectors matches a 2×2 SiC slab. The lattice constants of Al and SiC are 2.859 Å and 3.095 Å, respectively. Thus, the lattice mismatch is about 7.6%. The softer aluminum matrix is stretched along two basis vectors to form a coherent interface with the harder SiC. In order to eliminate the influence between adjacent supercells, a vacuum layer of no less than 20 Å is left in the z direction. The whole supercell is relaxed to release the internal stress. One of the interfacial Al atoms is replaced by a transition metal atom X. In this way, the interface doping concentration is 25%, while the bulk doping is only 3.57%.

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3. Results and Discussion

3.1 Clean Al (111)/6H-SiC (0001) interfaces

The atomic and electronic structures of Al (111) / 6H-SiC (0001) interface have been given in detail our in previous studies [22, 23]. In order to compare with the results of the following doping interfaces, we further study the interface charge transfer. Figure 2 shows the charge density difference of the Al (111) / 6H-SiC (0001) interfaces. The charge density difference is defined as

$$\rho_{diff} = \rho_{Al(111)/SiC(0001)} - \rho_{Al(111)} \text{ - } \rho_{SiC(0001)} \qquad (1)$$

Where $\rho_{Al(111)/SiC(0001)}$, $\rho_{Al(111)}$ and $\rho_{SiC(0001)}$ are the charge density of the Al (111) / SiC (0001) interface system, the isolated Al(111) and SiC(0001) slabs, respectively. According to this definition, a positive value represents charge enrichment and a negative value represents charge dissipation. It can be seen from the figure 2 (a) and (b) that the atomic charges at the interface are rearranged regardless of Si- or C-terminated interface. Charge transfer occurs between Al matrix and SiC. Some charges from Al matrix and SiC are accumulated at the interface. At the C-terminated interface, a covalent bond is formed between C and Al atoms. In the same way, covalent bonds are formed between Si and Al atoms at the Si-terminated interface. Moreover, the length of C-Al bond is about 1.99 Å, which is much smaller than that of Si-Al bond about 2.53 Å. The shorter the bond length is, the greater the binding energy is, and there should be more charge transfer. The adhesion energy of C-terminated interface is about 3.90 J/m^2, which is indeed larger than that of Si-terminated interface, 2.93 J/m^2. The interfacial adhesion energy is defined as the energy required to form the interface per unit area. It is expressed by the formula:

$$E_{ad} = \frac{E_{Al(111)} + E_{SiC(0001)} - E_{Al(111)/SiC(0001)}}{A} \qquad (2)$$

Where $E_{Al(111)}$, $E_{SiC(0001)}$ and $E_{Al(111)/SiC(0001)}$ represent the energy of the Al(111) slab, the SiC(0001) slab and the Al(111)/6H-SiC(0001) interface, respectively. A is the area of the interface.

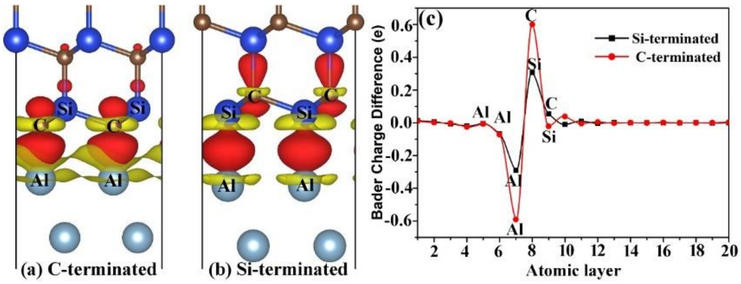

Figure 2. Charge density difference of the Al(111)/6H-SiC(0001) interfaces. Red and yellow denote charge enrichment and deficiency, respectively. The isosurfaces are set to 0.003 e/Å^3 (a) the C-terminated interface. (b) the Si-terminated interface. (c) Bader charge difference diagram of different atomic layers of the Al(111)/6H-SiC(0001) interfaces. The positive and negative values represent the gain and loss charges, respectively.

Detailed analysis of atomic charges may help to understand bonding properties such as bond strength. In this paper, we will focus on the atomic net charge distributions according to Bader analysis [34, 35]. The Bader charge difference of each atom in the interface system is defined as

$$Q_{diff} = Q_{Al(111)/SiC(0001)} - Q_{Al(111)} - \mathrm{Q}_{SiC(0001)} \qquad (3)$$

Where $Q_{Al(111)/SiC(0001)}$, $Q_{Al(111)}$ and $Q_{SiC(0001)}$ represent the Bader charge of the corresponding atom in the Al(111)/SiC(0001) interface, the Al(111) and the SiC(0001) slab. Thus, $Q_{diff} > 0$ indicates that the charge of the atom increases and $Q_{diff} < 0$ indicates that the charge of the atom decreases. The Bader charge difference of each atom in each atomic layer is shown in Figure 2 (c). It can be seen from the figure that only the atomic charge at the interface changes significantly. For the C-terminated Al(111)/SiC(0001) interface, Al atom loses charge and C atom gains charge. Similarly, for the Si-terminated interface, the Al atom loses the charge and the Si atom gains the charge. Therefore, it can be seen that when SiC and Al form the interface, the electrons in Al matrix transfer to SiC. More importantly, there are more transferred charges, about 0.6e/atom, at the C-terminated Al(111)/SiC(0001) interface than the Si-terminated one, about 0.3e/atom. Is is the reason why the adhesion energy of the C-terminated Al(111)/SiC(0001) interface is larger than that of the Si-terminated one.

3.2 Al-X (111)/6H-SiC (0001) interfaces

The effects of alloying elements on the mechanical properties of the interface have been systematically studied by replacing an Al atom with a transition metal atom. For all 3d and 4d transition families, a total of 20 transition metal elements are considered in this work. The adhesion energy is a very important mechanical parameter to describe the interface bonding characteristics. Similar to the clean interface, it can be defined as

$$E_{ad} = \frac{E_{Al-X(111)} + E_{SiC(0001)} - E_{Al-X(111)/SiC(0001)}}{A} \qquad (4)$$

Where $E_{Al-X(111)}$, $E_{SiC(0001)}$ and $E_{Al-X(111)/SiC(0001)}$ denote the energy of the Al-X(111) slab, the SiC(0001) slab and the Al-X(111)/6H-SiC(0001) interface, respectively. A is the area of the interface. X stands for a doping element. Adhesion energies of the Al-X(111)/SiC(0001) interface with different doping elements has been shown in Figure 3. For comparison, the adhesion work of the clean Al(111)/SiC(0001) interface is also shown in the figure. The red dotted line represents the adhesion work of the C-terminated Al(111)/SiC(0001) interface, and the black dotted line represents the adhesive work of the Si-terminated Al(111)/SiC(0001) interface. It can be seen from the figure that, similar to the clean interface, the adhesion work of C-terminated interface is greater than that of Si- terminated interface for the same doping element. For the C-terminated interface, only Co element doped in the Al matrix can significantly improve the interfacial adhesion energy. It is mainly because the bond strength of C-Co is greater than that of C-Al. However, for the Si-terminated interface, many elements, such as Mn, Fe, Co, Ni, Cu, Zn 3d transition elements and Tc, Ru, Rh, Pd, Ag 4d transition elements, can improve the interfacial adhesion energy. It is mainly due to the greater bonding strength of these elements with Si than that of Al and Si. It can be concluded that the introduction of transition metal elements into Al matrix is mainly to improve the binding energy of the Si-terminated interface. The same conclusion is obtained for Cu doped at the Al(111)/4H-SiC(0001) interface [26] and Mg doped at the Al(111)/3C-SiC(111) interface [27]. That is to say the doping of Cu and Mg into the Al matrix can increase the bonding of the Si-terminated interface, but decrease the binding of the C-terminated interface.

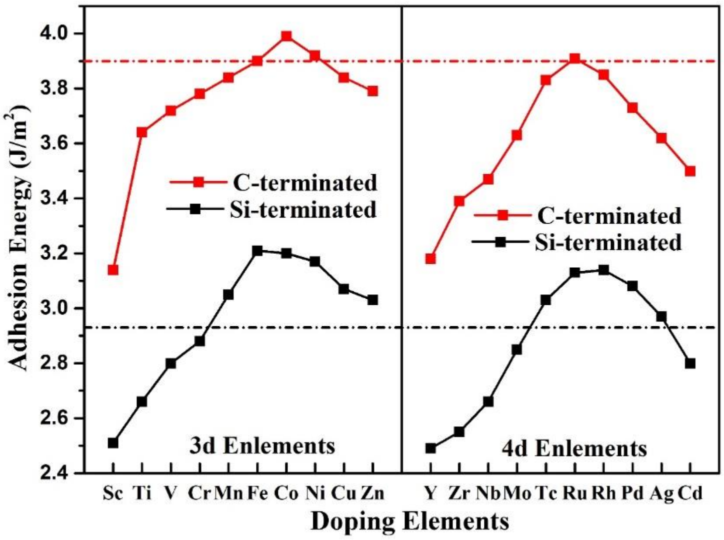

Figure 3. Adhesion energies of the Al-X(111)/SiC(0001) interface with different doping elements.

Figure 4 shows bond lengths at the Al-X/SiC(0001) interface with different doping elements. For comparison, the bond lengths of the clean Al(111)/SiC(0001) interface is also shown in the figure. The red dotted line represents the C-Al bond length at the C-terminated Al(111)/SiC(0001) interface, and the black dotted line represents the Si-Al bond length at the Si-terminated Al(111)/SiC(0001) interface. The black solid circles and squares represent the bond lengths of Si-X and Si-Al at the Si-terminated Al-X(111)/SiC(0001) interface, respectively. And the red solid circles and squares represent the bond lengths of C-X and C-Al at the C-terminated Al-X(111)/SiC(0001) interface, respectively. X stands for a doping element. As can be seen from Figure 4, the bond length at the C-terminated interface, whether C-Al or C-X, is shorter than that at the Si-terminated interface, just like that at the clean interface. It shows again that the bonding strength of C-terminated interface is higher than that of Si-terminated interface. For all transition elements X, the length of C-X bond is longer than that of C-Al bond at the C-terminated interface. The same is true for the Si-terminated interface. This is mainly because the atomic radius of the transition metal element X is longer than that of Al. Due to the introduction of transition elements, such as Mn, Fe, Co, Ni, Cu, Zn, Tc, Ru, Rh, Pd, Ag, the length of Si-Al bond at the Si-terminated Al-X(111)/6H-SiC(0001) interface is shorter than that of clean Al (111)/6H-SiC(0001) interface. The shorter the bond length, the stronger the bond. In order to facilitate researchers to access the relevant data, all results of bond lengths and adhesion energies at the Al-X(111)/6H-SiC (0001) interface are summarized in Table 1 and Table 2.

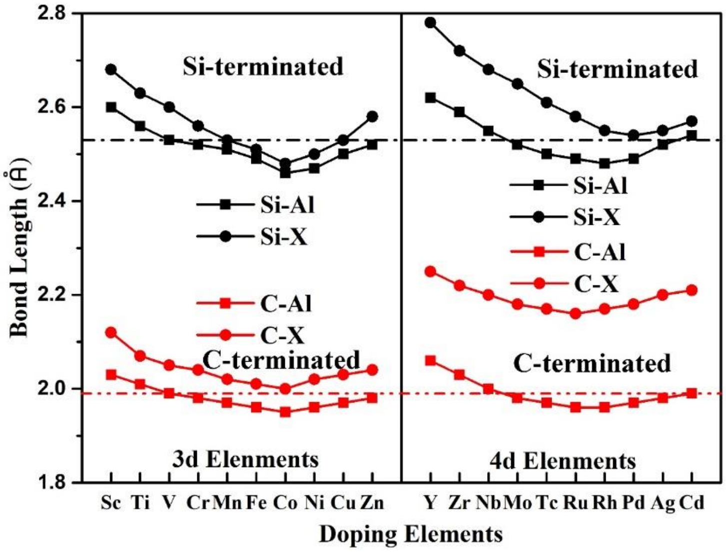

Figure 4. Bond lengths at the Al-X/SiC(0001) interface with different doping elements.

Table 1. Bond length (Å) and adhesion energy E_{ad} (J/m^2) at the C-terminated Al-X (111)/6H-SiC (0001) interface.

Interfaces	Doping Elements	C-Al (Å)	C-X (Å)	E_{ad} (J/m^2)	Doping Elements	C-Al (Å)	C-X (Å)	E_{ad} (J/m^2)
C-terminated	Sc	2.03	2.12	3.14	Y	2.06	2.25	3.18
	Ti	2.01	2.07	3.64	Zr	2.03	2.22	3.39
	V	1.99	2.05	3.72	Nb	2.00	2.20	3.47
	Cr	1.98	2.04	3.78	Mo	1.98	2.18	3.63
	Mn	1.97	2.02	3.84	Tc	1.97	2.17	3.83
	Fe	1.96	2.01	3.90	Ru	1.96	2.16	3.91
	Co	1.95	2.00	3.99	Rh	1.96	2.17	3.85
	Ni	1.96	2.02	3.92	Pd	1.97	2.18	3.73
	Cu	1.97	2.03	3.84	Ag	1.98	2.20	3.62
	Zn	1.98	2.04	3.79	Cd	1.99	2.21	3.50
	Free	1.99	-	3.90	-	-	-	-

Table 2. Bond length (Å) and adhesion energy E_{ad} (J/m^2) at the Si-terminated Al-X (111)/6H-SiC (0001) interface.

Interfaces	Doping Elements	Si-Al (Å)	Si-X (Å)	E_{ad} (J/m^2)	Doping Elements	Si-Al (Å)	Si-X (Å)	E_{ad} (J/m^2)
Si-terminated	Sc	2.60	2.68	2.51	Y	2.62	2.78	2.49
	Ti	2.56	2.63	2.66	Zr	2.59	2.72	2.55
	V	2.53	2.60	2.80	Nb	2.55	2.68	2.66
	Cr	2.52	2.56	2.88	Mo	2.52	2.65	2.85
	Mn	2.51	2.53	3.05	Tc	2.50	2.61	3.03
	Fe	2.49	2.51	3.21	Ru	2.49	2.58	3.13
	Co	2.46	2.48	3.20	Rh	2.48	2.55	3.14
	Ni	2.47	2.50	3.17	Pd	2.49	2.54	3.08
	Cu	2.50	2.53	3.07	Ag	2.52	2.55	2.97
	Zn	2.52	2.58	3.03	Cd	2.54	2.57	2.80
	Free	2.53	-	2.93	-	-	-	-

The charge of each atom at the interface has been calculated by Bader analysis. By analyzing the charge of atom, we can know the transfer of charge. Bader charge difference of each atom at the Al-X(111) /6H-SiC(0001) interface has been shown in Figure 5. The positive and negative values represent the gain and loss of charges, respectively. The serial numbers of the eight atoms at the interface are the same as those in Figure 1. Al1, Al2, Al3 and X denote three Al and doping atoms, respectively. C1, C2, C3, C4 and Si1, Si2, Si3, Si4 represent four C and Si atoms, respectively. As can be seen from the Figure 5, the Bader charge difference of each nonmetal atom (whether C1, C2, C3, C4 atom of the C-terminated interface or Si1, Si2, Si3, Si4 atom of the Si-terminated interface) at the interface is positive. And the Bader charge difference of each Al atom at the interface is negative. These results show that nonmetal atoms gain charges and Al atoms lose charges. Consequently, covalent bonds are formed between metal and nonmetal atoms at the interface. Whether 3d or 4d transition elements are introduced at the Al-X(111)/6H-SiC(0001) interface, as shown in Figure 5, the Bader charge difference of C1, C2, C3 carbon atoms has no obvious change. Only the Bader charge difference of the C4 atom, which is above the doping atom X, decreases slightly with the increase of atomic number (from Sc to Zn 3d elements and from Y to Cd 4d elements). It is very interesting that Bader charge difference of metal atom changes with atomic number. When Sc, Ti, V, Y or Zr is added into the Al(111) /SiC(0001) interface, it loses charges just like the Al atom, but when Mn, Fe, Co, Ni, Cu, Zn, Mo, Tc, Ru, Rh, Pd, Ag or Cd atom is added to the interface, it gains electrons. These results indicate that the transition metal atoms not only form covalent bonds with nonmetallic C (Si) atoms at the interface, but also form metal bonds with Al atoms.

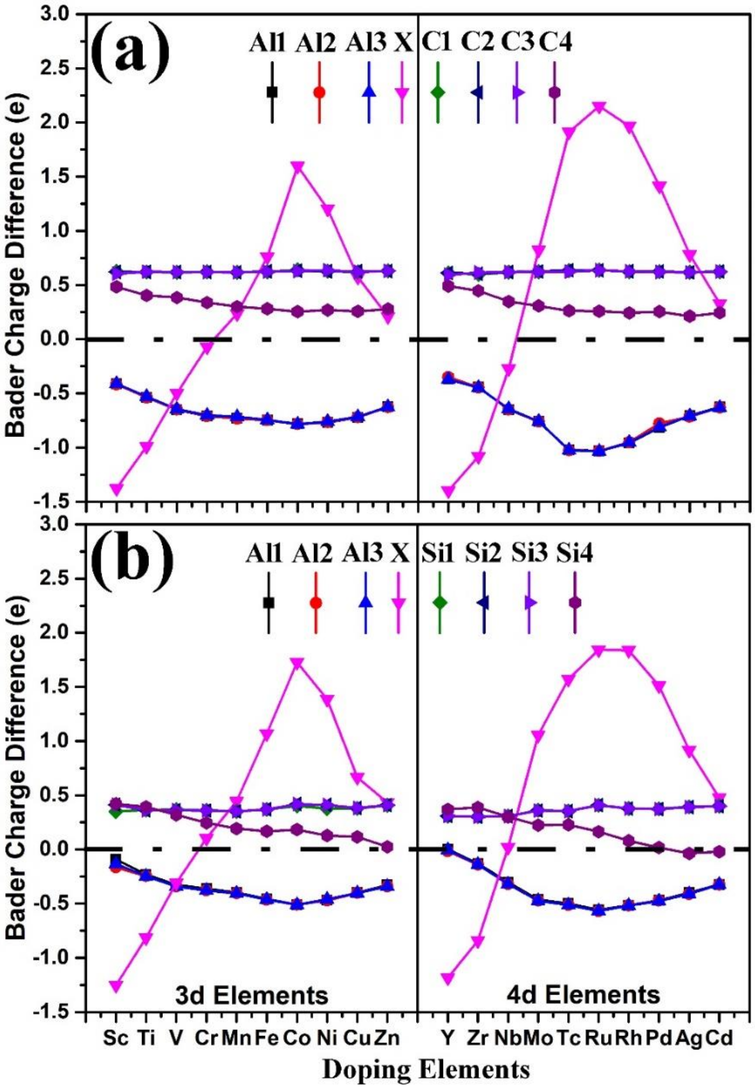

Figure 5. Bader charge difference of each atom at the Al-X(111)/6H-SiC(0001) interface. The positive and negative values represent the gain and loss of charges, respectively. The serial numbers of the eight atoms at the interface are the same as those in Figure 1. (a) the C-terminated interface, (b) the Si-terminated interface.

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Especially, when a Co atom is doped into the C-terminated Al(111) /SiC(0001) interface, it obtain electrons not only from the C atom, but also from the Al atom. In this way, the introduction of Co atoms promotes the formation of not only strong Co-C bonds, but also stronger Al-C bonds at the interface. Therefore, the adhesion energy of the C-terminated Al-Co (111) / SiC (0001) interface is higher than that of the clean C-terminated Al (111) / SiC (0001) interface. Although there is more charge transfer at the C-terminated interface of Tc-Al(111)/SiC(0001), Ru-Al(111)/SiC(0001) and Rh-Al(111)/SiC(0001), the radius of Tc, Ru, Rh is too large to form stronger covalent bonds. Thus, the introduction of Tc, Ru or Rh into the C-terminated Al(111)/SiC(0001) interface cannot improve the interfacial adhesion energy.

The strength of Si-Al bond is smaller than that of C-Al bond. When Mn, Fe, Co, Ni, Cu, Zn, Tc, Ru, Rh, Pd or Ag is added into the Si-terminated Al(111) /SiC(0001) interface, more charge transfer occurs between the doping atom and other atoms. And a stronger covalent bond is formed between the Si atom and the doping atom. Therefore, the introduction of Mn, Fe, Co, Ni, Cu, Zn, Tc, Ru, Rh, Pd or Ag into the Si-terminated Al(111)/SiC(0001) interface can improve the interfacial adhesion energy. Because of lower surface energy of the Si-terminated SiC(0001), the Si-terminated Al(111)/SiC(0001) interface is more prone to existing. Therefore, adding transition metal elements into SiC particle reinforced aluminum matrix composites is mainly used to improve the adhesion energy of Si-terminated interface, and then improve the mechanical properties of the composites.

4. Conclusions

Effects of 20 transition elements doping on the interfacial adhesion and electronic structure of Al (111) / 6H-SiC (0001) have been studied by first principles calculations in this paper. The main conclusions are summarized as follows:

(1) For the clean Al (111) / 6H-SiC (0001) interface, covalent bonds are formed at both C-terminated and Si-terminated interfaces. According to Bader's charge analysis, there is more charge transfer between C and Al at the C-terminated interface, which leads to higher adhesion energy.

(2) For the C-terminated Al (111) / 6H-SiC (0001) interface, the adhesion energy of the interface can be improved only when Co is doped at the interface. The strength of covalent bond between transition metal atom and C atom is weaker than that of C-Al bond. This may be attributed to the larger atomic radius of transition metal atoms.

(3) For the Si-terminated Al (111) / 6H-SiC (0001) interface, when Mn, Fe, Co, Ni, Cu, Zn, Tc, Ru, Rh, Pd or Ag is doped at the interface, the adhesion energy of the interface can be improved. It is mainly due to the formation of stronger Si-X bonds at the interface. The doped transition metal atom not only forms a strong covalent bond with the Si atom, but also promote more charge transfer between Al atoms and Si atoms, forming stronger Si-Al bonds.

Acknowledgments

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