



Full Length Article

First-principles calculations on wetting interface between Ag-Cu-Ti filler metal and SiC ceramic: Ag (1 1 1)/SiC (1 1 1) interface and Ag (1 1 1)/TiC (1 1 1) interface



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ABSTRACT

Interfacial properties of Ag (1 1 1)/SiC (1 1 1) interface and Ag (1 1 1)/TiC (1 1 1) interface were researched by first-principles calculations to investigate the reason that Ag-Cu-Ti filler metal shows the superior reactive wettability on SiC ceramic. The calculated results show that, 7 atom-layers Ag (1 1 1) surface, 11 atom-layer SiC (1 1 1) surface and 9 atom-layer TiC (1 1 1) surface can represent the Ag bulk, SiC bulk and TiC bulk, effectively. Ag (1 1 1)/SiC (1 1 1) interface and Ag (1 1 1)/TiC (1 1 1) interface with C-terminated structure and TL stacking sequence show the highest interfacial stability. Chemical bonds at Ag (1 1 1)/SiC (1 1 1) interface and Ag (1 1 1)/TiC (1 1 1) interface are mainly formed by the interaction between 1st layer C atoms in SiC (or TiC) slab and 1st layer Ag atoms in Ag slab. Interfacial energy of Ag (1 1 1)/SiC (1 1 1) interface is much larger than that of Ag (1 1 1)/TiC (1 1 1) interface, which indicates that the formed TiC reaction layer between Ag-Cu-Ti filler metal and SiC ceramic indeed plays the positive role on improving the wettability of Ag-Cu-Ti filler metal on SiC ceramic.

1. Introduction

Because of the low melting-point, excellent joint performance and remarkable reactive wettability on ceramic materials, Ag-Cu-Ti filler metal has been widely used to braze SiC ceramic and SiC ceramic matrix composites [1–3]. Actually, in all of the advantages above mentioned, the major reason that Ag-Cu-Ti filler metal getting the widely recognized is the superior reactive wettability on SiC ceramic, and the corresponding mechanism has been investigated [4].

$$\cos \theta_{\min} = \cos \theta_0 - \frac{\Delta G_r}{\delta_{lv}} - \frac{\Delta \delta_r}{\delta_{lv}} \quad (1)$$

Because that Ag-Cu-Ti filler metal/SiC ceramic is a typical reactive wetting system, so the wetting behavior must be followed by Laurent's law, as given in Eq. (1) [5]. In which, θ_{\min} is the minimal contact angle, the larger θ_{\min} means the more excellent reactive wettability; θ_0 is the equilibrium contact angle for the wetting system before interface reaction; δ_{lv} is the surface tension of the liquid filler metal; ΔG_r and $\Delta \delta_r$ are the released free energy and change of interfacial energy caused by interface chemical reaction, respectively.

Tillmann et al [6] studied the reactive wettability of Ag-Cu-Ti filler

metal on SiC ceramic, and found that the TiC layer formed by interface chemical reaction can decrease the interfacial energy (leading to $\Delta \delta_r < 0$), therefore improving the wettability of Ag-Cu-Ti filler metal. However, Boadi et al [7] took the negative attitude and believed that free energy releasing (leading to $\Delta G_r < 0$) caused by interface chemical reaction is the essential reason that Ag-Cu-Ti filler metal shows the superior wettability on SiC ceramic.

Because that is very hard to measure or calculate the released free energy ΔG_r during the interface chemical reaction, the only method to research this problem is calculating and comparing the interfacial energy between Ag-Cu-Ti/SiC interface and Ag-Cu-Ti/TiC interface ($\Delta \delta_r$). There are two possible conclusions: (i) if interfacial energy of Ag-Cu-Ti/TiC interface is larger than that of Ag-Cu-Ti/SiC interface ($\Delta \delta_r > 0$), it can be concluded that the free energy releasing caused by interface chemical reaction is the essential reason that Ag-Cu-Ti filler metal shows the superior reactive wettability on SiC ceramic. (ii) if interfacial energy of Ag-Cu-Ti/TiC interface is smaller than that of Ag-Cu-Ti/SiC interface ($\Delta \delta_r < 0$), it indicates that the formed TiC reaction layer indeed play the positive role on improving the wettability of Ag-Cu-Ti filler metal on SiC ceramic.

As well known, Ag-Cu-Ti filler metal is mainly composed of Ag base,

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dotted with small amounts of Cu-Ti and Ag-Cu intermetallic compounds [8–10]. So, it is no doubt that the interface energies of Ag-Cu-Ti/TiC interface and Ag-Cu-Ti/SiC interface are almost completely controlled by Ag/TiC interface and Ag/SiC interface, respectively. Therefore, it is feasible to employ interface energies of Ag/TiC interface and Ag/SiC interface to replace those of Ag-Cu-Ti/TiC interface and Ag-Cu-Ti/SiC interface in this work.

First-principles calculation based on density functional theory (DFT) is an important and recognized method for investigating the microscopic surface and interface [11–13]. Yang et al [14] studied the structural and energy properties of NbC/NbN interfaces by first-principles calculation, and found that C-terminated NbC is more inclined to join with the Nb-terminated NbN, and the interfacial energy reaches 5.89 J/m². Kumar et al [15] investigated the effect of γ/γ' interface on the tensile and shear strengths of nickel-based superalloys by first-principles study, and found that the shear strength of the cubic plane of the γ/γ' interface is marginally lower than those of bulk γ and γ' phases. Li et al [16] established the twin boundary interfaces of TiN (ZrN) and normal interfaces of TiN/ZrN using first-principles methods, and showed that the adhesion energies for the twin interface structures and the normal interface structures are both 3.52 J/m², indicating that they have the similar stability.

In this work, the most representative Ag/TiC and Ag/SiC interfaces were selected and established. Subsequently, interfacial atomic structure, interfacial ideal adhesion energy, charge distribution, especially interfacial energy of the two interfaces were calculated and compared using a first-principles density functional plane-wave ultrasoft pseudopotential method. The investigation can research the interfacial properties of Ag/TiC and Ag/SiC interfaces effectively, and then provides the physical basis for investigating the essential reason that the Ag-Cu-Ti filler metal shows the excellent reactive wettability on SiC ceramic.

2. Methods

This work is a typical computational investigation. At first, planar misfits of the low index Ag/SiC interface and Ag/TiC interface were calculated according to Bramfitt's two dimensional lattice misfit theory for choosing the most representative Ag/SiC interface and Ag/TiC interface [17].

After the specific interfaces have been determined, the interfacial properties were researched using first-principles calculations. During this processing, all calculations were carried based on the pseudo-potential plane-wave within the DFT (density functional theory) [18,19] using CASTEP code (Cambridge Sequential Total Energy Pack-age) [20]. GGA (generalized gradient approximation) with PBE (Perdew-Burke-Ernzerhof) functional was employed as the exchange-correlation functional [21].

The single-particle Kohn-Sham wave functions were expanded using plane waves with a cutoff energy of 380 eV, whatever the calculation system is a bulk, a surface, or an interface [22]. Because that the calculation needs a three-dimensional periodic system as an input, a 12 Å vacuum space along the c-axis was used to eliminate the long interactions from periodic boundary condition calculations. The k-points number, which does the sampling of the irreducible wedge of the Brillouin zone, keeps increasing until the calculated energy converges within the required tolerance and was set to 8 × 8 × 8 for the bulk, and 8 × 8 × 1 for the surface and interface [23]. The Broyden-Fletcher-Goldfarb-Shanno optimization method was employed in order to converge the energy with the setting convergence tolerance of energy of 1.0 × 10⁻⁵ eV/atom, maximum force of 0.03 eV/Å, and maximum displacement of 1.0 × 10⁻³ Å [24,25].

3. Interface selection

Ag/SiC and Ag/TiC interfaces both contain a large number of

possible combinations, such as Ag(1 0 0)/SiC(1 0 0) interface, Ag(1 0 0)/SiC(1 1 0) interface, Ag(1 1 1)/SiC(1 1 0) interface, Ag(1 0 0)/TiC(1 0 0) interface, Ag(1 0 0)/TiC(1 0 1) interface, Ag(1 1 1)/TiC(1 1 1) interface, et al. Because that it is impossible to calculate all of them, it is very important to choose the most representative Ag/SiC interface and Ag/TiC interface preferentially.

Bramfitt's [17] lattice misfit theory indicates that the solidification interface usually be influenced by the lattice distortion energy, which is determined by atomic misfit. The interface with small misfit degree shows the great forming tendency and stability. Therefore, it is effective to select the most representative Ag/SiC and Ag/TiC interface by calculating the misfit degree δ of the low index interfaces according to Eqs. (2) and (3):

$$\delta_{(hkl)_{SiC}}^{(hkl)_{Ag}} = \sum_{i=1}^3 [(|d_{[uvw]_{Ag}}^i \cos \theta - d_{[uvw]_{SiC}}^i|/d_{[uvw]_{SiC}}^i)/3] \times 100\% \quad (2)$$

$$\delta_{(hkl)_{TiC}}^{(hkl)_{Ag}} = \sum_{i=1}^3 [(|d_{[uvw]_{Ag}}^i \cos \theta - d_{[uvw]_{TiC}}^i|/d_{[uvw]_{TiC}}^i)/3] \times 100\% \quad (3)$$

in which, $(hkl)_{Ag}$ is a low-index plane of Ag, $[uvw]_{Ag}$ is a low-index direction in $(hkl)_{Ag}$, $(hkl)_{SiC}$ and $(hkl)_{TiC}$ are the low-index planes of SiC and TiC, while $[uvw]_{SiC}$ and $[uvw]_{TiC}$ are the low-index directions in $(hkl)_{SiC}$ and $(hkl)_{TiC}$, respectively. Besides that, $d_{[uvw]_{Ag}}^i$ is the interatomic spacing along $[uvw]_{Ag}$, while $d_{[uvw]_{SiC}}^i$ and $d_{[uvw]_{TiC}}^i$ are those along $[uvw]_{SiC}$ and $[uvw]_{TiC}$, θ is the angle between the $[uvw]_{Ag}$ and $[uvw]_{SiC}$, and that between $[uvw]_{Ag}$ and $[uvw]_{TiC}$.

The calculated planar misfits of Ag/SiC and Ag/TiC low index interfaces are listed in Tables 1 and 2. From them, it can be found that in all of the interfaces, Ag(1 1 1)/SiC(1 1 1) interface and Ag(1 1 1)/TiC(1 1 1) interface show the smallest lattice misfits, which are 3.18% and 4.03%, respectively. The calculated results indicate that the two interfaces above mentioned show the strongest formation tendency and stability, so they can be considered as the most representative Ag/SiC interface and Ag/TiC interface, respectively.

4. Surface property

Crystal structures of SiC bulk, TiC bulk and Ag bulk are shown in Fig. 1. From Fig. 1, it can be found that SiC, TiC and Ag all show face-centered cube structure with FM-3M space group, in which, each (Si, Ti)C cell contains eight atoms and each Ag cell contains four atoms [26–28]. Moreover, from Fig. 1(a) and (b), for SiC, C atom is located at the tetrahedral center, while for TiC, C atom is located at the octahedral center.

Although SiC bulk, TiC bulk and Ag bulk show the same crystal structure, Ag(1 1 1) surface, SiC(1 1 1) surface and TiC(1 1 1) surface show various terminated characteristics. Ag(1 1 1) surface is the typical non-polarized plane, so it shows just one terminated structure. While because that SiC(1 1 1) surface and TiC(1 1 1) surface are the polarized planes, there are both six possible terminated structures, as shown in Figs. 2(a)–(f) and 3(a)–(f).

Before Ag(1 1 1)/SiC(1 1 1) interface and Ag(1 1 1)/TiC(1 1 1) interface be established, the minimum numbers of atom-layers (minimum thickness) of Ag(1 1 1) surface, SiC(1 1 1) surface and TiC(1 1 1) surface must be investigated preferentially. It is important to insure that the slabs at both side of interface are thick enough to show the bulk-like characteristics, as it is known that the property of interface composed by thin films is different significantly from that composed by bulks.

In order to decide the needed minimum numbers of atom-layers, the convergence tendencies of Ag(1 1 1) surface, SiC(1 1 1) surface and TiC(1 1 1) surface were investigated according to their surface energies. Because that Ag(1 1 1) surface is the non-polarized plane, the surface energy can be calculated according to Eq. (4) [29,30]:

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