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First-principles study of the structure properties of Al(111)/6H-SiC(0001) interfaces

Qingjie Wu[a], Jingpei Xie[b,*], Changqing Wang[b], Liben Li[c], Aiqin Wang[b], Aixia Mao[a]

[a] School of Physics and Engineering, Zhengzhou University, Zhengzhou 450052, China
[b] College of Materials Science and Engineering, Henan University of Science and Technology, Luoyang 471023, China
[c] School of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China

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ABSTRACT

This paper presents a systematic study on the energetic and electronic structure of the Al(111)/6H-SiC(0001) interfaces by using first-principles calculation with density functional theory (DFT). There are all three situations for no-vacuum layer of Al/SiC superlattics, and two cases of C-terminated and Si-terminated interfaces are compared and analyzed. Through the density of states analysis, the initial information of interface combination is obtained. Then the supercells are stretched vertically along the z-axis, and the fracture of the interface is obtained, and it is pointed out that C-terminated SiC and Al interfaces have a better binding property. And, the fracture positions of C-terminated and Si-terminated interfaces are different in the process of stretching. Then, the distance variation in the process of stretching, the charge density differences, and the distribution of the electrons near the interface are analyzed. Al these work makes the specific reasons for the interface fracture are obtained at last.

1. Introduction

Silicon carbide particles reinforced aluminum metal matrix composite (SiC_p/Al) is a kind of materials of aluminum or aluminum alloy as the matrix with SiC particles as enhanced phase. The composite is considered as promising structural material due to its excellent physical and chemical properties, such as low density, high specific modulus, low expansion and high thermal conductivity and etc. It represents the development direction of new lightweight and low-expansion materials for its low manufacturing costing and physical performance design by changing the components [1–4]. By the development of industry and technology, SiCp/Al composite show great potential of application in aviation industry, military field, automobile, electronic packaging and other industries, and get more and more attention [5,6]. By adjusting the composite substrate composition, grain type, content, heat treatment, it is able to design the thermal physical and mechanical properties which are satisfied with the space engineering material and electronic packaging applications requirements and etc. [7–10]

The interface of materials directly influences the properties of composite materials, and the simulation of metal and ceramic materials with the first principles is getting more and more attention. Metal and ceramic interface is a kind of common heterogeneous interface, which has great influence on the service life and performance of materials. In recent years, based on the first principles calculation with density functional theory (DFT), there has been a lot of progress in material design, synthesis and simulation calculation, which is a powerful method to provide fundamental information of interfaces between two solids at atomic level or even at electronic level. In this paper, the Al (111)/6H-SiC(0001) interfaces by first principles are studied to gain an in-depth understanding of the interface combination of the composite materials, thus accumulating necessary cognition for the in-depth study of the mechanical properties.

2. Methodology

In this work, energy and electronic structure are calculated using the Vienna ab initio Simulation Package (VASP) [11,12] code within the framework of DFT theory [13,14]. The projector augmented-waves (PAW) [15,16] method is employed to deal with the interactions between ionic core and valence electrons, and the generalized gradient approximation (GGA) [17] of Perdew–Burke–Ernzerhof (PBE) [18] approach is utilized to describe the exchange-correlation energy functional. The Brillouin zone is sampled with a Γ-centered $[9\times9\times1]$ Monkhorst-Pack mesh [19]. The plane-wave energy cutoff of 600 eV is used in the calculations. Meanwhile, the ground state of electrons can be found, by solving the Kohn–Sham equation [20] with the self-consistent field (SCF) procedure to achieve the electronic minimization. The SCF convergence criteria are set as 10^{-5}eV/atom, and the Hellman-Feynman forces [21] are relaxed to less than 0.001 eV/Å. For C, Si and

* Corresponding author.
E-mail addresses: wuqingjie610@163.com (Q. Wu), xiejp@haust.edu.cn (J. Xie).

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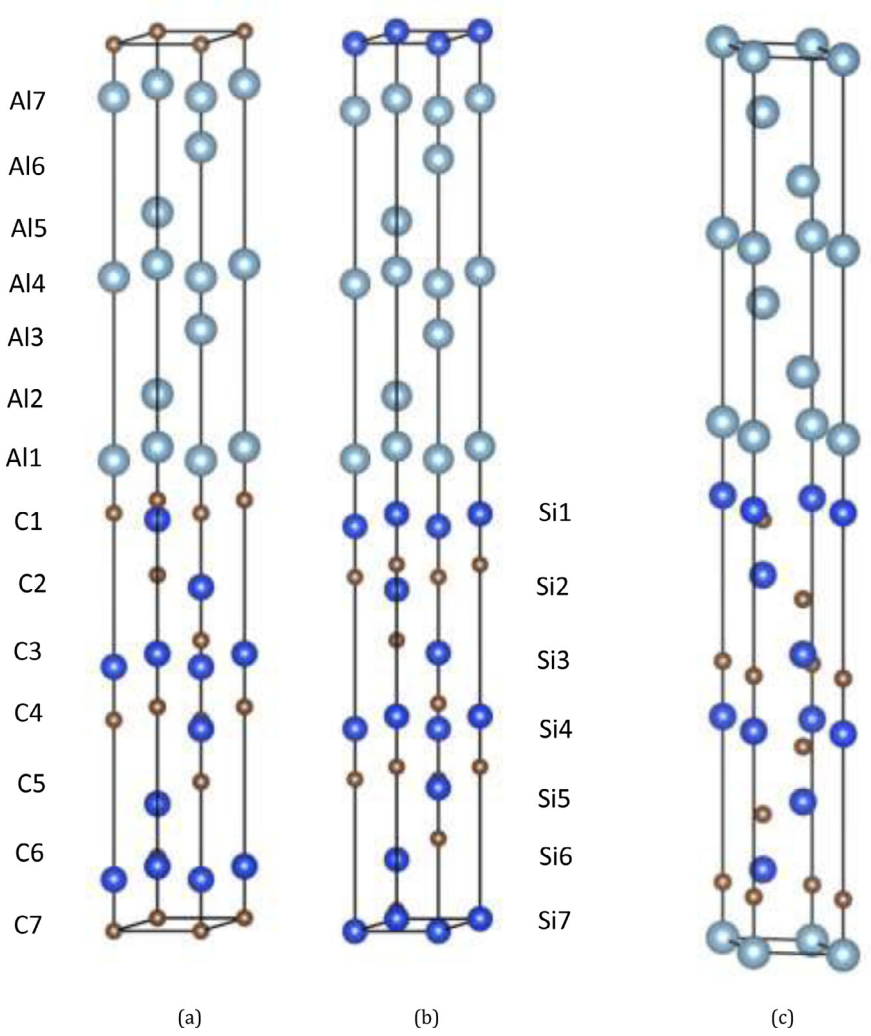

Fig. 1. The structures of Al(111)/6H-SiC(0001) interfaces of (a) C- terminated, (b) Si terminated and (c) both terminated at each side. (Al slabs are named Al1-Al7 from the bottom to top, C slabs are named C1-C7 from top to bottom, and Si slabs are named Si1-Si7 from top to bottom).

Al atoms, the valence electrons considered for their pseudopotential are C $2s^2 2p^2$, Si $3s^2 3p^2$ and Al $3s^2 3p^1$, respectively. The interfaces models are built by using supercell approach with periodic boundary conditions and all simulations are performed at the temperature of 0 K.

3. Simulation model and adhesion

For our system, we build model cells from a 6H-SiC slab at the bottom and a fcc Al slab above, as shown Fig. 1 For the Al slab, the low-index surface orientation (111) is considered having the lowest surface energy of 0.936 J/m^2 comparing with 1.024 J/m^2 of (100) and 1.073 J/m^2 of (110) in our calculation. So we choose the (111) orientation for the Al slab and (0001) orientation for the 6H-SiC slab. For this work, we focus on no vacuum layers models. So, for the SiC slabs, there are three situations about C-terminated (Fig. 1(a)), Si-terminated (Fig. 1(b)) and both terminated at each side(Fig. 1(C)) with Al slabs. 7 layers of Al(111) are placed above 13or 12 layers SiC(0001) as showed in Fig. 1 For the convenience of discussion, we focus on the first two situations about C-terminated (Fig. 1(a)) and Si-terminated (Fig. 1(b)) superlattics.

For bulk Al, we select the FCC structure with space group of FM-3M(NO.225), and with the lattice constants of 4.044 Å after geometric optimization. Bulk 6H-SiC has the HCP structure of P63MC (NO.186) space group. The lattice constants are a = b = 3.078 Å, c = 15.114 Å, respectively, after geometric optimization. Al/6H-SiC interfaces are simulated by building up the hetero-structures consisting of Al (111) with a lattice constant of 2.860 Å and monolayer SiC (1000) with a lattice constant of 3.078 Å, resulting in a lattice mismatch of 7.6%. So we make a geometric optimization about the model, and get the proper lattice constant of 3.068 Å and 3.056 Å for C-terminated and Si-terminated interfaces, respectively.

Calculation for the work of separation decides the most stable structure among the superlattices. The adhesion energy, W_{ad}, is a basic and fundamental quantity to predict adhesion of an interface. W_{ad} can be given by the difference in total energy between the interface and its isolated slabs [12]:

$$W_{ad} = \frac{E_{Al(111)} + E_{SiC(0001)} - E_{total}}{2S}$$

Here, $E_{Al(111)}$ and $E_{SiC(0001)}$ are the total energy of the relaxed, isolates Al and SiC slabs in the supercell when the one of the slabs is kept and the other one is replaced by vacuum, respectively. E_{total} is the total energy of the interface system. S is the interface area of the unit supercell.

For the C-terminated superlattice, the W_{ad} is 2.689 J/ m^2, and for Si-terminated, the result is 1.649 J/ m^2. So the C- terminated superlattice has the stronger banding adhesion comparing with Si-end system.

Fig. 2 shows the density of state (DOS) of C- and Si-terminated interfaces. It can be seen that, SiC obtains some metallic characteristics, because the bands of SiC across Fermi levels for the combination of Al and SiC for both superlattices. The difference is, for the Si-terminated