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Ab-initio calculation of (101) and (100) surface for β-FeSi₂

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Abstract

We study the atomic and electric structure on the (101) and (100) surface of β-FeSi₂ by ab-initio calculation using the projector augmented wave method (PAW). The cohesive energy calculated with the slab model show that the structure Si layer biased in the surface is stable. The simulated STM image indicate that the charge in the neighborhood of Fermi level concentrated on Fe-Si bonding.

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1. Introduction

β-Iron disilicide, β-FeSi₂, has been attracting much attention as one of environmentally semiconductor [1]. Thin films and nanoparticles of β-FeSi₂ have been well studied in silicon-based optoelectronic and thermoelectric applications [1-3]. Large-sized and high-purity single crystalline and flat surface of β-FeSi₂ were successfully obtained in recent years[4-7]. Also scanning tunneling microscope (STM) and low-energy electron diffraction (LEED) images of clean (100), (101) and (110) surfaces of β-FeSi₂ revealed the absence of long-ranged surface reconstruction for the homoepitaxy [8]. It is necessary that the atomic structure of the surface be understand for applications of β-FeSi₂. However, it is difficult to distinguish a kind of atom on surface with STM image. In this paper we report the most stable structures of the (101) and (100) surface and charge density distributions with the conditions. We also shown the STM image of (101) and (100) surface by ab-initio calculation.

2. Calculation method

We used a periodic calculation with the Vienna Ab-initio Simulation Package code (VASP 4.6) [9-11]. In the VASP program, the Kohn-Sham equations are solved with Generalized Gradient Approximation (GGA) proposed by Perdew and Wang [12] and Perdew et al. [13]. Projector augmented Wave (PAW)[14, 15] approach has been used with plane wave basis sets. The PAW potential is constructed in such a way that for Fe the 3s²3p⁶ core states are treated as valence states, which was also done for the 3s²3p⁶ valence states of Si. It approximated by using slab
model to treat interfaces. $\beta$-FeSi$_2$ has the structure of six type (101) surface and five type (100) surface in Fig.1. Fig.2a shows a triclinic cell containing four Fe and eight Si layers as slab model.

Fig.1 The structure patterns of (a) (101) and (b) (100) surface.

Fig.2 Slab model unit cell of $\beta$-FeSi$_2$
(a) (101) (a=15.24, b=7.79, c=14.00), (b) (100) (a=23.54, b=7.79, c=7.83)

The integrations in the Brillouin zone are performed using a 1 x 2 x 2 Monkhorst-Pack sampling in the Brillouin zone. For the geometry optimizations, the upper part of the slab (three layers) has been optimized while the lower has been frozen.

3. Results and Discussion

The stability of the (101) and (100) surface is compared with each cohesive energy. Fig.3a shows the cohesive energy calculated the six type of (101) surface structure as a function of super cell size. The layer type (I) consisted of only Si is most stable in the six type layers. In (100) surface, it’s necessary to consider five type structure in (100) surface. The cohesive energy calculated the five type of (100) surface structure as a function of super cell
size in Fig.3b. The layer type (II) is most stable in the five type layers. This layer consists of both Fe and Si atoms. These calculation results show that the distinction of surface is impossible by the atom kind included in the surface.

Fig.3 Cohesive energy in the layer of (a) (101) and (b) (100) surface as a function of the number of atom in super cell.

Fig.4 shows the surface that is the same structure in bulk and the optimized structure. The structure of Fig.4b also is the layer type (II) in Fig.2b. The structure optimization in Fig.4b is almost the Si migration along with the (100) surface. However, both Fe and Si migration on (101) surface is slightly. The difference of these movements is understood the number of bonding between Fe and Si. It is quite likely that the number of bonding between Fe and Si causes the difference of these movements.

The bonding on (100) and (101) surface is two and three, respectively. Hence, The Si atom on the (101) surface is restrained because the bonding on (101) surface is more than that on (100) surface. Fe-Si-Fe angle on (100) surface optimized from 114° to 111°, this angle approaches 109° consisted of positive tetrahedral.
Fig. 5 shows the simulated STM image surface calculated with ab-initio method. The image is integrated over the energy of 1 eV below the Fermi level and are correspond approximately to the experimental STM images impressed voltage 1.0eV [8]. The charge concentration on (101) and (100) surface has the diffraction like Zig-Zag and checked pattern, respectively. This image pattern also is almost corresponding to the reference experimental data[8].

The result means that the charge in the neighborhood of Fermi level has not necessarily concentrated on the atom position. The charge concentration of calculated $\beta$-FeSi$_2$ has the possibility of shifting from the atom position and is located on the Fe-Si bonds. Hence, It is possible that the electron activated between Fe and Si takes part in the adhesion on the surface.

Conclusions

We calculated the cohesive energy of $\beta$-FeSi$_2$ as slab model with ab initio method. The result indicated that Si Layer surface is most stable. Moreover, the simulated STM image calculated with ab-initio method means the charge distribution neighbor. The calculated result means that the charge in the neighborhood of Fermi level concentrated on Fe-Si bonding.

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