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CALCULATION OF ELECTRONIC STATES OF Si(337) SURFACE*

Jia Yu(贾 瑜), Ma Bing-xian(马丙现), Shen San-guo(申三国), and Yang Shi-e(杨仕娥)

Laboratory of Materials Physics, Zhengzhou University, Zhengzhou, 450052, China

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Using the scattering-theoretic method and employing the nearest-neighbor tight-binding formalism to describe the bulk electronic structure, we have studied the electronic structure of Si(337) surface. The wave-vector-resolved layer densities of states are presented. The results show that there are six surface bound states in the range from -12.0 to 2.0 eV. Some properties of these surface states are discussed.

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I. INTRODUCTION

With the rapid development of various epitaxial growth methods such as molecular beam epitaxy (MBE) and their applications in optoelectronic devices, some high-index surfaces of semiconductors were noted and put into application increasingly.

For some semiconductor such as Si, Ge or GaAs, which has diamond or zincblende structure, some of their high-index surfaces (for example, (103), (112), (113), (115) and (337)) are stable surface and have stepped structures with $m(100) \times n(111)$. Since heteroepitaxial growth along these directions can restrain from forming some defects, for example, the antiphase domain, the quality of thin films can be improved. So the high-index surfaces are very important for heteroepitaxial growth. Theoretically, it is thought that the Si(112) surface is an ideal substrate for this purpose.[1,2]

Xing *et al.*[3−5] have studied the geometrical structure of Si(337) surface by low-energy electron diffraction (LEED) method, the results showed that in the area adjacent to Si(112), the best and the stable surface for epitaxial growth is not the Si(112) surface, but the Si(337) surface. For Si(337) surface, Xing and his co-workers have found 1×1 stable surface structure by LEED measurement. In addition to a strong Si(337)1×1 surface, they also observed for the first time a 2×1 reconstruction LEED pattern along the direction of $[1\bar{1}0]$ in their further study recently.[5] Besides this, they have also studied the relation between the change of electronic affinity potential and crystallographic directions in his earlier study; according to it, they found a minimum value of potential on the Si(337) surface as well as on the three low-index surfaces and the Si(113) high-index surface. Since electronic affinity potential can show the relative amplitude of the surface dipole moment, the minimum of it also proves that Si(337) surface is a stable high-index one.[3]

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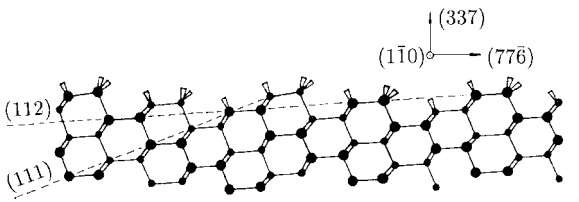
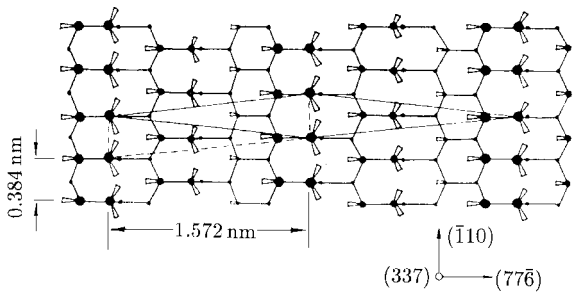
Up to now, to our knowledge, there has been no report on the electronic states of Si(337) surface in the theoretical or experimental study. So the study of the electronic states of Si(337) surface will be of significance. In this paper, we adopt the nearest neighbour tight-binding model sp^3s^* proposed by Vogl *et al.*[6] to describe the bulk electronic structure, then we produce the ideal Si(337) surface by removing layers method, the electronic structure of Si(337) surface is presented by the Green function method in the frame of the scattering theory. The wave-vector-resolved layer densities of states (LDOS) are presented. In addition, some properties of these surface states are discussed.

II. METHOD

The lattice constant of Si is a=0.540 nm. The side view and the top view of the bulk truncated Si(337) ideal surface and primitive cell of Si(337) are shown in Figs.1(a) and 1(b). There are two kinds of Si atoms in each surface primitive cell, which is on the site of two different crystal lattices, respectively. For the bulk truncated bulk Si(337) surface, three atom-layers are needed to be removed. Therefore, there are seven dangling bonds in every primitive cell, in which there are three bonds both in the first layer and the second layer, respectively, the other one is in the third layer. Comparison with other high-index surfaces, there are 3.4 dangling bonds on every square lattice constant, which is larger than both (112) and (113) surface in the density of dangling bonds, which have 3.3 and 1.8 dangling bonds, respectively.



(a) Side view



(b) Top view

Fig.1. Schematic diagram of the surface geometry for Si(337).

In this paper, we perform calculations for the surface electronic structure of Si(337) by using the scattering theory method proposed by Pollmann *et al.*[7,8] who used this method to calculate the electronic structure of low-index planes, such as(100), (110) and (111) in

Si, Ge and GaAs. Their results are in good agreement with the experimental data. In addition, we also present the calculated results of the electronic structure of CdTe(110), ZnTe(110) and ZnS(110) relaxed surfaces.[9,10] Since it is a semi-empirical method, its results are less accurate in comparison with that of the first principle calculations, but it can give more distinct properties in some aspects, such as orbital or local characters of electronic states. In this paper, we generalize this method to high-index (337) surface. We limit our consideration to a nearest-neighbor tight-binding theory, to produce infinite free Si(337) surfaces, three atom-layers should be removed so as to decouple two infinite surfaces. In our calculation, we employ 2s, 2p and s* of Si atoms as basis to expand the Bloch functions. We adopt Vogl's sp^3s^* model to describe the bulk electronic structure, the empirical matrix elements parameters are taken from Ref.[6]. Considering the Si(337) surface has 1×1 stable structure, the influence on the electronic states of the surface atoms relaxation is neglected in our calculation.

Ⅲ. RESULTS AND DISCUSSION

A. The wave-vector-resolved LDOS

In order to discuss the surface electronic property, we first present the LDOS of the special point in the surface Brillouin zone. Figures 2(a)–2(c) are the LDOS of the X, Γ, Y points on the edge of surface Brillouin zone, respectively. In Fig 2, m is the layer index which indicates the number of layers below the surface, bulk indicates the bulk layer density of states. Here we will discuss the electronic states in the valence band and the fundamental gap in the range we most care for. As a representative result, we only give the LDOS analysis of X point in the surface Brillouin zone.

In Fig.2(a), five diagrams labeled by m=1, m=2, m=3, m=4 and bulk stand for the first, the second, the third, the fourth and the bulk layer densities of states. From the bulk layer density of states, we can see that there are two regions, namely from -11.0 to -5.0 eV and from -3.3 to -1.20 eV, in which the electronic states occupy below the valence band top. For an ideal surface, we can find six sharp peaks in the range of -12 to $+2$ eV which we call bound surface states in these surface layers. we label them by S_1, S_2, S_2', S_4, S_3' and S_3 respectively. They are located at -5.5, -0.4, -0.39, 0.5, 0.79 and 0.8 eV below the top of the valence bands respectively. By analyzing the amplitude of these surface states in each layer, we can determine in which layer these states are localized and then we can conclude the relation between these surface states and chemical bonds between different layers. Firstly, S_1 is located in the deep level below the top of the valence band and electron states occupy each of the first four layers; in the first two layers the amplitudes of LDOS of the surface states are the same, and they have a large occupations of electronic states; in the third layer the occupation becomes smaller, but in the fourth layer it becomes bigger. So S_1 is mainly related to the change of bonds formed by the atoms between the surface layer and the second layer, which we call back-bond states. Secondly, S_2 and S_3 have a large occupation in the first layer. As the number of layers below the surface increases, the amplitude of the LDOS in them reduces quickly. This shows that they are localized in the

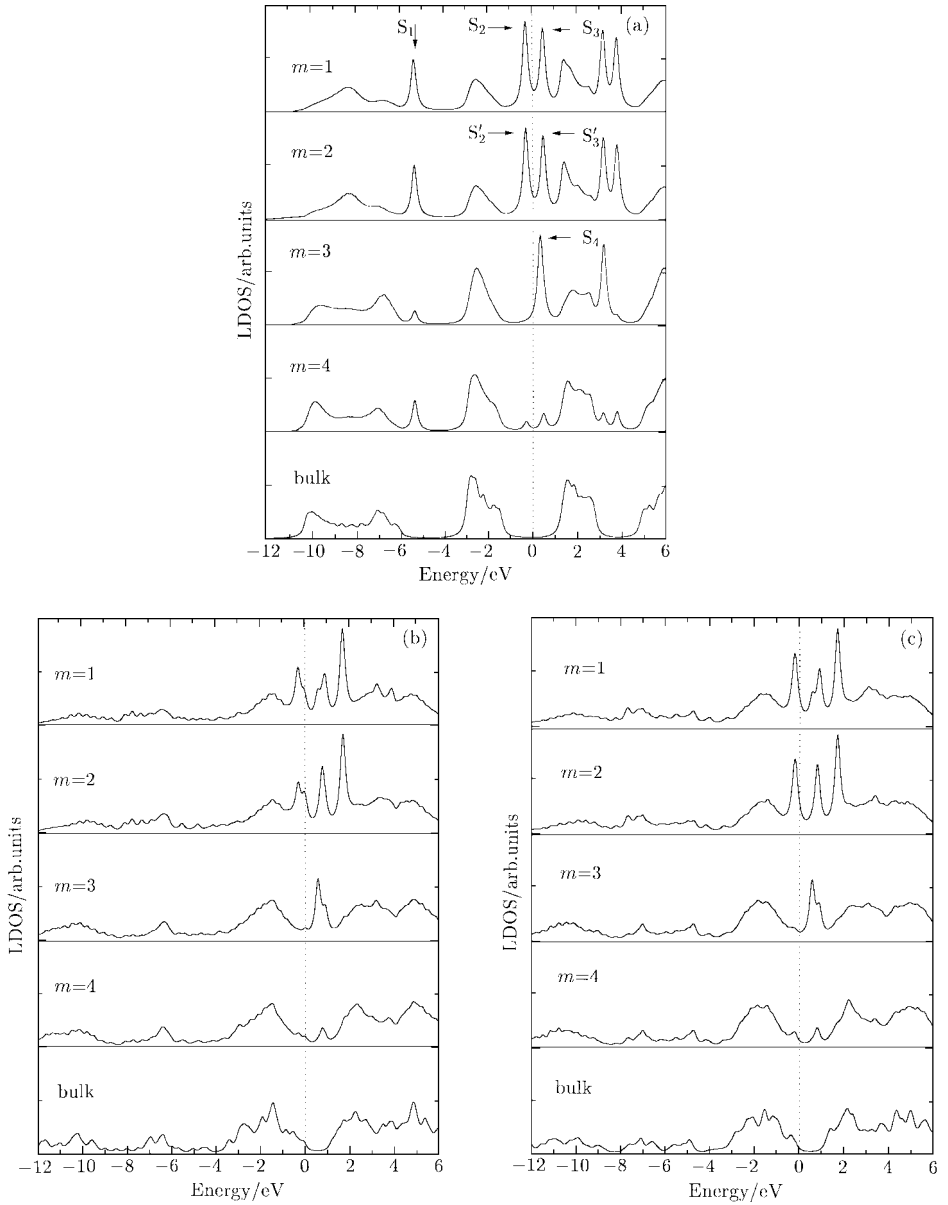


Fig.2. The wave-vector-resolved LDOS of Si(337) surface; (a), (b) and (c) correspond, respectively, to those at X, Γ, and Y in the surface Brillouin zone.

first layer and originate mainly from the three dangling bonds at the surface layer. Similarly, S'_2 and S'_3 have a large occupation in the second layer and have small occupation in other layers, so we conclude that they originate mainly from the three dangling bonds at the second layer. Compared with S_2 and S_3, respectively, S'_2 and S'_3 have a small energy level shift since the atoms in the second layer are closer to the bulk environment than that in the first layer. Finally, the surface state S_4 has a large amplitude of layer density states in third layer, but has little amplitude in the other layers. This shows that S_4 arises from the one dangling bond in the third layer. From the orbital-resolved LDOS, we can see that S_1

shows mainly s orbital characteristic, while S_2 and S_2' show mainly p orbital characteristic; S_3, S_3' and S_4 show s and p orbital characteristic.

Figures 2(b) and 2(c) illustrate the LDOS at Γ and Y points in the surface Brillouin zone respectively. Compared with Fig.2(a), the amplitude of LDOS and the energy levels in which these states are located have changed, but the orbital characteristic and local properties have not. The difference is that the surface state S_1 has disappeared at Γ and Y.

B. The change of LDOS and dispersion along Γ-X line

In order to understand the dispersion characters of these surface states, the wave-vector-resolved densities of states of ten wave-vector point along the high-symmetry line Γ-X in equivalent intervals are shown in Fig.3. The density of states is the sum of those in the three layers below the surface since producing the ideal surface need remove three layers. In Fig.3, we can conclude that the main features of Si(337) are as follows: (1) There are five main surface states in the fundamental gap between the top of valence bands and the bottom of the conduction bands, the states are produced by the dangling bonds of both atoms in the primitive cell, which are all highly localized in the surface layers. These states show both s and p contributions. Along Γ-X line, they show little dispersion and the amplitude of LDOS becomes larger gradually. (2) There is a state in the deeper energy levels from -6.0 to -4.0 eV, it is derived from s orbital of the Si atoms of the surface layers. Along Γ-X line, it has a strong dispersion and the amplitude of LDOS becomes larger rapidly.

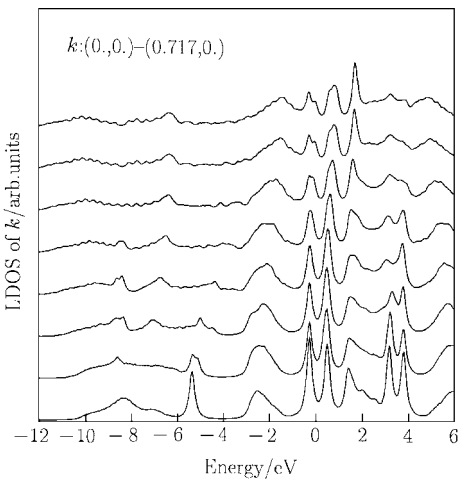


Fig.3. The change of LDOS and dispersion along Γ-X line.

IV. CONCLUSIONS

In conclusion, we have studied the high-index Si(337)1 × 1 surface by using the tight-binding method. The results show that there exist six surface bound states in the range from -12.0 to $+2.0$ eV, the local and the orbital properties of these surface states are discussed. The result is useful for further study of the electronic properties of Si(337) surface in both theoretical and experimental aspects. Further researches, combined with the electronic properties of reconstruction of Si(337)2 × 1 surface, are in progress.

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