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The first principle study of the electronic structure of $Si_xGe_{(1-x)}$ alloy films

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ABSTRACT

First principles calculation based on density functional theory (DFT) with the generalized gradient approximation (GGA) are carried out to investigate the electronic band structures of $Si_xGe_{(1-x)}$ alloys nanofilms. The calculation results show that the band gaps of (100), (110) and (111) surfaces $Si_xGe_{(1-x)}$ alloy films with different thickness first increase with the increase of Si content, then flatten out, and finally decrease. At the same time, the transformation of direct band gap and indirect band gap occurs when the thickness of films and Si content of the three surface $Si_xGe_{(1-x)}$ alloy films changes to a certain critical condition. It will be a good way to obtain direct-gap band emission in $Si_xGe_{(1-x)}$ alloys materials.

1. Introduction

In recent decades, SiGe alloys have attracted much attention and been widely used in many fields because of their unique characteristics, which are different from Si or Ge. For example, lattice mismatch caused by difference in lattice constants between silicon and germanium is beneficial to increase carrier mobility in Complementary Metal Oxide Semiconductor (CMOS) process applications [1,2]. By changing the Si and Ge content, the band gap can be well adjusted, which is very favorable for the manufacture of heterojunction bipolar transistors [3]. In addition, due to the smaller bandwidth and higher mobility, the optical absorptivity and photoelectric conversion efficiency are higher, SiGe alloys are also applied in the field of photovoltaic, such as solar cells. Compared with traditional monocrystalline silicon batteries, the SiGe alloy has better effect in short wavelength utilization [4]. In order to improve and expand the application of SiGe alloy, a great deal of research has been carried out in the theory. For example, Zhang, Nambuddee and so on are used to study the band structure, density of States, elastic modulus, elastic modulus, Poisson's ratio constant, heat capacity, Debye temperature, coefficient of thermal expansion and Vivtorinox hardness of SiGe alloy by density functional theory [5–8]. Zhu et al. have studied the band structure of IV family semiconductor alloy by coherent potential approximation, which found that the alloy composition has great influence on the band structure, and plays a decisive role in the transformation of direct band gap and indirect band gap [9]. D'Avezac et al. are used to study the SiGe alloy by genetic algorithm, which found that the Si/Ge(2)/Si(2)/Ge(2)/Si/Ge(n) superlattice grown on the base of $Si_xGe_{(1-x)}$ ($x \leq 0.4$) alloy has a direct band gap [10]. Ali et al. simulated the variation of germanium content in $Si/Si_xGe_{(1-x)}$ film solar cells in the 0.04–0.5 range with the help of PC1D software, who found that the performance of $Si/Si_xGe_{(1-x)}$ film solar cells is better than that of the single crystalline silicon film solar cells in all cases [11].

Due to the quantum confinement effect, the band gap of Si and Ge films broadens relative to the band gap of bulk materials of Si and Ge. Moreover, the band structure of Si and Ge films are greatly influenced by the restricted direction [12,13]. Therefore, the band structure of the SiGe alloy film should also be affected by the restricted direction. In this paper, density functional theory is used to study the band structure of different crystalline $Si_xGe_{(1-x)}$ alloy films, which found that the proportion of silicon and germanium, the orientation of the film surface and the thickness of the film have a great influence on the band structure.

2. Model and calculation method

Electronic structure calculations have been performed for $nSi_xGe_{(1-x)}$ alloy film, in which n indicates the number of single cell layers and x represents the content of Si in the SiGe alloy film.

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Table 1
The lattice constant of three crystal surface films of $1Si_xGe_{(1-x)}$ alloy.

x	Lattice constant /Å								
	111			110			100		
	a	b	c	a	b	c	a	b	c
0	4.06	4.06	23.62	4.04	24.67	5.62	4.30	4.05	26.36
0.2	4.05	4.05	23.74	4.03	24.62	5.60	4.29	4.04	26.22
0.4	4.03	4.03	23.72	4.00	24.55	5.57	4.27	4.01	26.12
0.6	4.00	4.00	23.71	3.98	24.43	5.54	4.25	3.97	25.97
0.8	3.95	3.95	23.68	3.93	24.30	5.50	4.22	3.93	25.78
1	3.90	3.90	23.67	3.88	24.16	5.45	4.17	3.85	25.62

All dangling bonds on the surfaces of $Si_xGe_{(1-x)}$ alloy nanofilms are saturated by hydrogen atoms for obtaining the stable minimum energies. The thickness of film is defined as the distance between the upper surface and the lower surface after hydrogen saturation. The lattice structure and atomic spacing of Si or Ge is taken to be equal to that of bulk Si and Ge material [12], and the Si–H and Ge–H bond length are equal to those determined in SiH_4 and GeH_4 molecules, respectively [13]. In order to avoid interaction between subsequent film structures, a vacuum layer of 2 nm is taken in every model.

The structure optimization and energy band structure calculations of $Si_xGe_{(1-x)}$ alloy nanofilms are performed with first-principles methods based on density functional theory (DFT) using Cambridge Serial Total Energy Package (CASTEP) [14]. The exchange and correlation potential were described with the generalized gradient approximation (Perdew–Burke–Ernzerhof (PBE) functional) [15,16], and the ultrasoft pseudopotential is used.

For the calculation, the plane-wave energy cutoff is set at 380 eV, the SCF convergence tolerance of electronic energy is 1.0×10^{-5} eV/atom, the maximum stress is 0.05 GPa, the maximum ionic displacement is 0.001 Å. The "K point set" selects the "fine" level, and the specific sampling is determined by the size of the cell.

For many alloy materials the calculation results based on the virtual crystal approximation (VCA) method are in good agreement with the experimental results [17–21], so we will also use the VCA method to calculate the band structure of the SiGe alloy film. By changing the Si content, the SiGe alloy electronic structure under different Si content will be obtained.

3. Results and discussions

After geometry optimizations, the lattice constants of the three crystalline surface of $1Si_xGe_{(1-x)}$ alloy films are shown in Table 1. For the (111) surface, when the values of x are 0 and 1, the lattice constants are 4.06 Å and 3.90 Å, which are in accord with the previous results of Wei 4.06 Å and Wang 3.88 Å, respectively [22,23]. At the same time, it can be seen that the three lattice constants of the three crystal surfaces decrease with the increase of Si content, and the law of change can be expressed as the following equation [24]:

$$a_{Si_xGe_{1-x}} = a_{Si}x + a_{Ge}(1-x) - b_{SiGe}x(1-x) \quad (1)$$

where $a_{Si_xGe_{1-x}}$, a_{Si} and a_{Ge} are the lattice constants of $Si_xGe_{(1-x)}$ alloy, Si and Ge, respectively, and b_{SiGe} is the bending coefficient of $Si_xGe_{(1-x)}$ alloy. The fitting curve of lattice constant a of $1Si_xGe_{(1-x)}(111)$ with the variation of x is shown in Fig. 1. It can be seen that the calculation results are in good agreement with the equation (1). The bending coefficient is −0.139. In addition, the lattice constant c indicates the total thickness of the film layer and the vacuum layer.

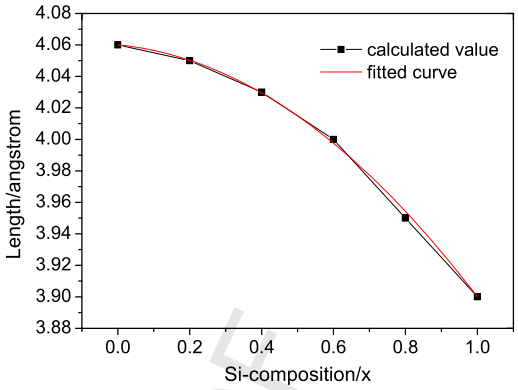

Fig. 1. The curve fitting of lattice constant of $1Si_xGe_{(1-x)}(111)$ with the variation of x.

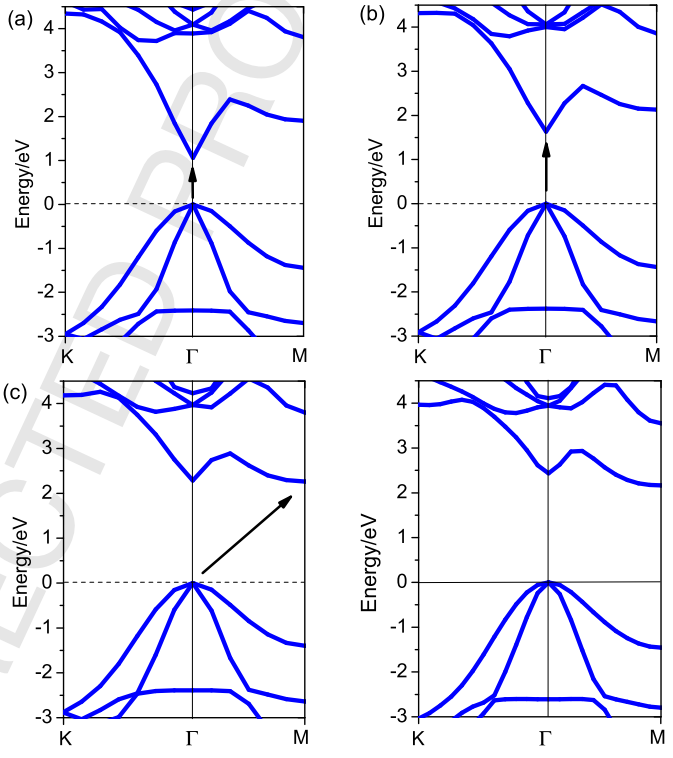

Fig. 2. The band structures of $1Si_xGe_{(1-x)}(111)$ alloy film with x equal to 0 (a), 0.2 (b), 0.8 (c) and 1 (d).

The band structures of $1Si_xGe_{(1-x)}(111)$ alloy film with x equal to 0, 0.2, 0.8 and 1 are shown in Fig. 2. It can be seen that when x is equal to 0 as germanium, it is a direct band gap semiconductor material with a gap of 1.06 eV, and when x is equal to 1 as silicene, it is an indirect band gap semiconductor material with a gap of 2.17 eV, which are consistent with the results of Xia and other previous research [25]. When x value of $1Si_xGe_{(1-x)}$ alloy is gradually increased from 0 to 1, the top of the valence band remained basically unchanged and Γ and M energy levels in the conduction band increase simultaneously. For example, when x is increased from 0 to 0.2, Γ and M energy levels rise from 1.06 and 1.91 eV (Fig. 2(a)) to 1.63 and 2.13 eV (Fig. 2(b)), respectively. When the x is increased to 0.8, the Γ level and M energy level increase to 2.29 and 2.27 eV, respectively, and it turns into indirect band gap.

The change of Γ energy level and M energy level with x in $1Si_xGe_{(1-x)}(111)$ alloy film and $2Si_xGe_{(1-x)}(111)$ alloy film as shown in Fig. 3. We can see that with the increase of x, the Γ