Available online at www.sciencedirect.com

ScienceDirect

Physics Procedia 11 (2011) 134–137

Physics Procedia

www.elsevier.com/locate/procedia

Proceedings of APAC-SILICIDE 2010

First-principles Calculations on the Electronic Structure and Optical Properties of Mg_2Si Epitaxial on Si (111)

Qian Chen[a,b], Quan Xie[a,b,*]

[a]*College of Science, Guizhou University, Guiyang, 550025, P.R.China*
[b]*Institute of New type Optoelectronic Materials and Technology, Guizhou University, Guiyang, 550025, P.R.China*

Abstract

The electronic structure and optical properties of Mg_2Si for the epitaxial relationship Mg_2Si (111)//Si (111) are calculated by using the first-principles pseudopotential method based on the density functional theory. The results show that Mg_2Si is the most steady state when the lattice parameter a of the primitive cell is 0.4522 nm; Mg2Si is an indirect semiconductor with the band gap

Keywords: Mg_2Si; epitaxial; first-principles; electronic structure; optical properties;

1. Introduction

There has been increasing attention to the semiconducting silicides which are composed of non- or less toxic and abundantly natural elements in the earth's crust for the applications to photoelectronic and thermoelectric devices. These silicides belong to the most promising materials for the modern solid-state electronics because of their technological compatibility with silicon, high thermal stability, resistance to oxidizing and aggressive media, and chemical inertness. These silicides are called ecologically friendly semiconductor materials [1]. Mg_2Si belongs to one of the most promising ecologically friendly semiconductor materials.

The first calculations of the band structures of Mg_2Si were made in the early 1960s. P. M. Lee [2] calculated the electronic energy-band spectra of magnesium silicide and magnesium germanide in 1964. N. O. Folland [3] applied the self-consistent method to calculate the energy band structure of Mg_2Si in 1967. In 1969, M. Y. Au-Yang [4] used the empirical pseudopotential method to calculate the band structures and dielectric function of Mg_2Si and predicted the indirect band gap to be 0.53 eV. The early empirical pseudopotential calculation of F. Aymerich [5]

* Corresponding author. Tel. and fax: +86-851-3623248.
E-mail address: qxie@gzu.edu.cn.

1875-3892
doi:10.1016/j.phpro.2011.01.022

was 0.49 eV in 1970. D. M. Wood [6] calculated the band structures, equilibrium lattice constants, and electronic charge densities of Mg_2Si using self-consistent pseudopotential band theory within the local-density formalism in 1986. J. L. Corkill [7] applied the ab initio pseudopotential method to Mg_2Si in 1993 and predicted the indirect band gap to be 0.118 eV. P. Baranek [8] calculated the electronic structure, lattice parameters, phonon frequencies at the Brillouin zone center, and first-order elastic constants at the ab initio Hartree−Fock level using either all-atomic-electron basis sets or basis sets associated with core pseudopotentials. B. Arnaud [9] used GW approximation (GWA) based on an all-electron full-potential projector-augmented-wave method to calculate the electronic properties of semiconductors. Y. Imai [10] used the first-principles pseudopotential method to calculate the electronic structure and densities of states of Mg_2Si in 2002 and predicted the indirect band gap to be 0.28 eV. Q. Chen [11] used the first-principles pseudopotential method to calculate the electronic structure, densities of states and optical properties of Mg_2Si in 2008.

However, no studies have been done for Mg_2Si//Si (111) system to our knowledge. In the present paper, we give the results of the calculation of the electronic structure and optical properties of Mg_2Si//Si (111).

2. Computational details

The calculations have been done by using CASTEP (Cambridge Serial Total Energy Package) developed by Payne et al. [12], which is the first-principles pseudopotential method based on the density-functional theory (DFT) [13] to describe the electron-electron interaction, a pseudopotential description of the electron-core interaction, and a plane-wave expansion of the wave-functions. As for the method of approximation to the exchange-correlation term of the DFT, the gradient corrected exchange-correlation functional was used. We expanded the valence electronic wave functions with the plane-wave basis set and set the cutoff energy E_{cut}=380 eV for the plane wave, which converges the total energy of unit cell to better than 1 meV/atom. The electron-ion interaction is described by Vanderbilt's ultrasoft pseudopotentials [14].

The intermetallic silicide Mg_2Si is the only stoichiometric silicide in Mg-Si system. Mg_2Si has an anti-CaF_2 type structure (Fm3m, No.225) with the lattice constant of 0.635 nm [15]. The Si atoms occupy fcc sites and the eight Mg atoms are at the points ± (1/4, 1/4, 1/4)a in the unit cell, where a is the lattic constant. The crystal structure of Mg_2Si is shown in Figure 1.

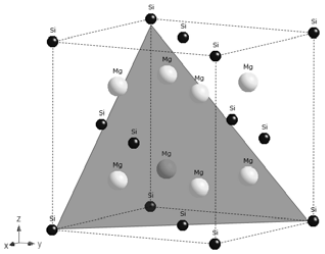


Figure 1 Crystal structure of Mg_2Si

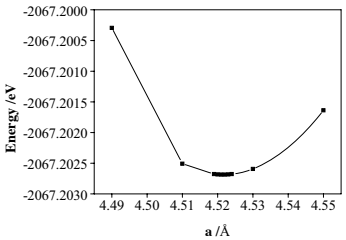


Figure 2 Relation curve of the lattice parameter a and the total energy of Mg_2Si primitive cell

3. Results and discussion

3.1 System optimization

Structural matching is one of the main factors to determine the quality of an epitaxial growth. The geometrical concept of the lattice match for any pair of crystal lattices in any given crystal direction has been proposed by Zur et al. [16,17]. A small lattice mismatch is a favorable prerequisite for epitaxial layer growth. For good quality epitaxial layers, the lattice mismatch between the silicide and the silicon substrate is typically less than 3% [18].

Mg_2Si has a cubic structure which is similar to silicon but with a larger lattice parameter. For a=0.635 nm a side of the unit cell on the Mg_2Si (111)1×1 surface is 0.449 nm, that is about 1.3% longer than 0.4434 nm, which is

$2/3\sqrt{3}$ times the surface lattice parameter of the ideal Si (111)1×1 surface (0.384 nm). Due to the small lattice mismatch high quality epitaxial growth of Mg_2Si onto monocrystalline silicon appears to be possible.

In order to gain the stable structure we let b=c=0.4434 nm and calculate the total energy of the primitive cell near a=0.449 nm. Figure 2 shows the relation curve of the lattice parameter a and the total energy of Mg_2Si primitive cell. As shown in Figure 2, the most steady state is a=0.4522 nm.

3.2 The band structure

According to the optimization results, the calculated band structure is plotted in Figure 3, where the dotted line represents the Fermi level. As shown in Figure 3, Mg_2Si is an indirect-gap semiconductor with E_g= 0.2261 eV and the direct-gap is 1.8831 eV. The valence band maximum is located at the Γ_{15} point, whereas the conduction band minimum is located at the X_1 point.

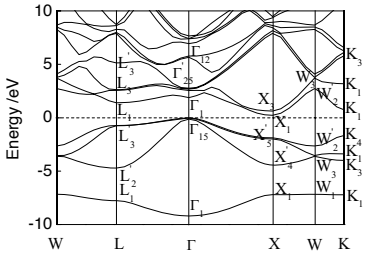


Figure 3 The calculated band structure of Mg_2Si

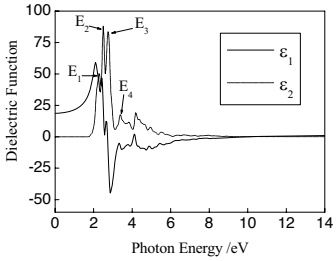
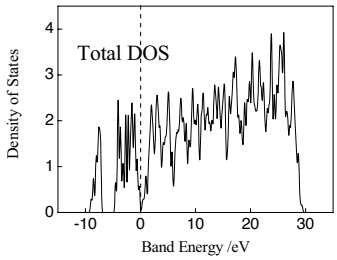
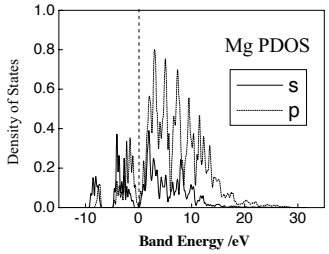


Figure 5 The dielectric function of Mg_2Si

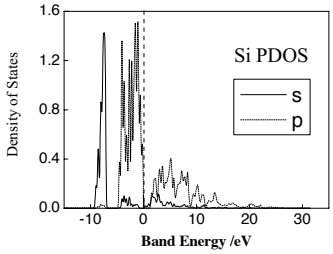
3.3 The density of states



(a)



(b)



(c)

Figure 4 The total densities of states of Mg_2Si (a) and the partial densities of states of Mg (b) and Si (c)

The calculated partial densities of states for Mg_2Si is shown in Figure 4. According to the calculations, the s states of Si have a pronounced effect only on the first valence band, whereas their effect near the Fermi level is minor; therefore their spectra are excluded from consideration. The dominant contribution to the valence band is made by the s and p states of Mg hybridized with p states of Si. The lower conduction band is characterized by the hybridization of all states of Si and Mg, the total contribution of Mg states being greater than the total contribution of Si. Therefore, the valence bands of Mg_2Si near the Fermi surface are composed of Si 3p, Mg 3s, 3p and the conduction bands are mainly composed of Mg 3s, 3p as well as Si 3p.

3.4 The optical properties

The dielectric function is an important parameter for the material, because it is the fundamental feature of the linear response to an electromagnetic wave and uniquely determines the propagation behavior within the radiation. Figure 5 shows the calculated real part $\varepsilon_1(\omega)$ and the imaginary part $\varepsilon_2(\omega)$ of dielectric function for Mg_2Si. The calculated static dielectric function $\varepsilon_1(0)$ is 18.7369. In Figure 5, there are four obvious peaks in the ε_2 curve at the energy range of 0~4 eV. Peaks E_1 (2.2762 eV), E_2 (2.4955 eV), E_3 (2.7514 eV) and E_4 (3.3728 eV) correspond with $X'_5 \rightarrow X_1$ and $L'_3 \rightarrow L_1$, $X'_5 \rightarrow X_3$, $\Gamma_{15} \rightarrow \Gamma'_{25}$, $L'_3 \rightarrow L_3$ transitions in Figure 3 respectively.

4. Conclusions

The electronic structure and optical properties of Mg_2Si for the epitaxial relationship Mg_2Si (111)//Si (111) are calculated. The results show that Mg_2Si is the most steady state when the lattice parameter a of the primitive cell is 0.4522 nm; Mg_2Si is an indirect semiconductor with the band gap of 0.2261 eV; the direct transition is 1.8831 eV; the valence bands of Mg_2Si near the Fermi surface are composed of Si 3p, Mg 3s, 3p and the conduction bands are mainly composed of Mg 3s, 3p as well as Si 3p; the static dielectric function is 18.7369.

Acknowledgements

This study was supported by the National Natural Science Foundation of China (Grant No. 60566002), the Top Talent's Scientific Research Project of Organization Department of Guizhou Province (Grant No. Z053123), the Nomarch's Foundation for Outstanding Science and Education Scholars of Guizhou Province (Grant No.Z053114), the undergraduate carve out project of department of Guiyang science and technology (Grant No. 6-5).

References

[1] Yunosuke Makita, Proceeding of Japan-UK joint Workshop on Kankyo-Semiconductors (2000) 29.
[2] P. M. Lee, Phys. Rev. **135** (1964) A1110.
[3] N. O. Folland, Phys. Rev. **158** (1967) 764.
[4] M. Y. Au-Yang and M. L. Cohen, Phys. Rev. **178** (1969) 1358.
[5] F. Aymerich and G. Mula, Physica Status Solidi. **42** (1970) 697.
[6] D. M. Wood and Alex Zunger, Phys. Rev. B **34** (1986) 4105.
[7] J. L. Corkill and M. L. Cohen, Phys. Rev. B **48** (1993) 17138.
[8] P. Baranek and J. Schamps, J. Phys. Chem. B **101** (1997) 9147.
[9] B. Arnaud and M. Alouani, Phys. Rev. B **62** (2000) 4464.
[10] Y. Imai, A. Watanabe, M. Mukaida, Journal of Alloys and Compounds **358** (2003) 257.
[11] Q. Chen, Q. Xie, W. J. Yan et al., Science in China Series G: Physics, Mechanics & Astronomy **38** (2008) 825.
[12] M. C. Payne, M. P. Teter, D. C. Allan, et al., Reviews of Modern Physics **64** (1992) 1045.
[13] W. Kohn and L. J. Sham, Phys. Rev. **140** (1965) A1133.
[14] D. Vanderbilt, Phys. Rev. B **41** (1990) 7892.
[15] P. Villars and L. D. Calvert, Pearson's Handbook of Crystallographic Data for Intermetallic Phases (Second Edition) (1991)
[16] A. Zur, T. C. McGill, Journal of Applied Physics **55** (1984) 378.
[17] A. Zur, T. C. McGill, M. A. Nicolet, Journal of Applied Physics **57** (1985) 600.
[18] L. A. Clevenger and R. W. Mann, Formation of epitaxial TM silicides, in: Properties of Metal Silicides (1995)