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Structural investigation of Si$_{0.5}$Ge$_{0.5}$ alloy for optoelectronic applications: Ab initio study

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**ABSTRACT**

The structural, electronic and optical properties of the binary silicon–germanium alloy have been investigated using the projector augmented-wave (PAW) calculations with a powerful VASP package (Vienna ab initio simulation package). The structural properties of Si$_{0.5}$Ge$_{0.5}$ alloy have been calculated using total energy calculations and compared with our empirical model of bulk modulus. The electronic band structure and density of state of Si$_{0.5}$Ge$_{0.5}$ alloy show that the conduction band minimum (CBM) is located at the $X$ point and the valence band maximum (VBM) is located at the $\Gamma$ point, resulting in indirect ($\Gamma$–$X$) energy band gap of 0.48 eV. The results of the refractive index and optical dielectric constant of Si$_{0.5}$Ge$_{0.5}$ alloy are also obtained. The PAW’s results are in good agreement with experimental, theoretical and our model results.

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1. Introduction

The optoelectronic properties of SiGe alloys are realized for applications in quantum-well intersubband technology [1,2]. Many interesting possibilities of these alloys are suggested [3]. Fundamental measurements of parameters that influence device performance of SiGe-based devices are preceded [4]. The change in the electronic structure of semiconductors is caused by the formation of the semiconductor alloys. A strong revival is in the electronic properties of Si$_{1-x}$Ge$_x$ alloys within the context of superlattice physics [5]. A considerable interest has focused on the electronic band structure of Si$_{1-x}$Ge$_x$ alloys. The available calculations are: virtual-crystal approximation (VCA) applied with empirical pseudopotential [6], tight-binding model [7] and with self-consistent pseudopotential; other calculations were carried out with coherent potential approximation (CPA) [8,9].

Different theoretical calculation methods of band gaps are available. Empirical pseudopotential [10,11] calculations require a large number of fitting parameters to obtain acceptable agreement with the experimental results [12]. The first-principle calculations are technically involved and computationally time consuming. To calculate the electronic band structure of semiconductors and insulators, there is a known problem [13], the energy gap is underestimated by as much as 50–100%.

Shen et al. [14] have illustrated the lattice constant of Si$_{1-x}$Ge$_x$ alloys and the bond length to be simply predicted. Eq. (1) in Ref. [14] has used to calculate the average bond length for Si$_{1-x}$Ge$_x$ alloys. On the basis of Vegard’s picture [15], the lattice constant is given simply by $4d/\sqrt{3}$. Si$_{1-x}$Ge$_x$ alloy is elaborated by X-ray diffraction and extends X-ray absorption fine-structure (EXAFS) experiments [14]. Theoretical studies of pressure-induced phase transition in SiGe alloy are presented using fully ab initio approach based on DFT-LDA [16] and first-principle pseudopotential approaches [17]. These results are noticed in comparison with the experimental value of transition pressure.

Finally, Adolph et al. [18] have demonstrated the accuracy of projector augmented-wave (PAW) approach for the calculation of optical spectra. Explicitly, they have selected a set of elemental and binary semiconductors with different bonding properties. Their PAW results are compared with those obtained employing a full All-Electron (AE) method or norm-conserving pseudopotentials (PP) approach.

The aim of this paper is to present a self-consistent electronic structure study for Si$_{0.5}$Ge$_{0.5}$ alloy. Projector augmented-wave (PAW) calculations with a powerful package VASP (Vienna ab initio simulation package) have been used to calculate the structural and electronic properties, to investigate optical properties of refractive index and to confirm our bulk modulus model of Si$_{0.5}$Ge$_{0.5}$ alloy.

2. Computational method

The density-functional theory within local-density approximation (LDA) [19] is applied on the plane wave basis. We have used the

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Table 1

<table>
<thead>
<tr>
<th>Compound</th>
<th>(a) (Å)</th>
<th>(B) (GPa)</th>
<th>(B')</th>
<th>(B'') (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GeSi0.5Ge0.5</td>
<td>Present</td>
<td>5.51</td>
<td>84.74</td>
<td>4.56</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.535 (^{a})</td>
<td>87.4 (^{a})</td>
<td>4.48 (^{a})</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.519 (^{b})</td>
<td>85 (^{b})</td>
<td>4.0 (^{b})</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.538 (^{c})</td>
<td>89.4 (^{c})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.48 (^{d})</td>
<td>88 (^{d})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.454 (^{e})</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ge</td>
<td>Present</td>
<td>5.64</td>
<td>72.52</td>
<td>4.85</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.65 (^{f})</td>
<td>73 (^{f})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.60 (^{g})</td>
<td>72 (^{g})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.74 (^{h})</td>
<td>71 (^{h})</td>
<td>5.1 (^{h})</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.63 (^{i})</td>
<td>75.3 (^{i})</td>
<td></td>
</tr>
<tr>
<td>Si</td>
<td>Present</td>
<td>5.40</td>
<td>99.13</td>
<td>2.94</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.43 (^{j})</td>
<td>96 (^{j})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.43 (^{k})</td>
<td>98.9 (^{k})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.45 (^{l})</td>
<td>96 (^{l})</td>
<td>4.1 (^{l})</td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>5.39 (^{m})</td>
<td>100.2 (^{m})</td>
<td></td>
</tr>
</tbody>
</table>

\(^{a}\) Ref. [6], \(^{b}\) Ref. [24], \(^{c}\) Ref. [25], \(^{d}\) Ref. [16], \(^{e}\) Ref. [17], \(^{f}\) Ref. [26], \(^{g}\) Ref. [27], \(^{h}\) Ref. [28], \(^{i}\) Ref. [29], \(^{j}\) Ref. [30].

The PS wave functions \(\psi_n\) are the variational quantities. The index \(i\) is a shorthand for the atomic site \(R_i\), the angular momentum numbers \(l = l_i, m_i\), and an additional index \(k\) is referring to the reference energy \(E_{idl}\). A detailed description of the PAW method for calculating the occupancies of each augmentation channel \((i, j)\), \(\rho_{ij}\), from the pseudo-wave-functions applying to the projector functions, \(\beta_i\), and the pseudized core density \(\beta_{ik}\), are available in Ref. [32].

### 3. Results and discussion

#### 3.1. Structural properties

In order to calculate the ground state properties for zinc-blende structure of SiGe0.5 alloy, the total energy is calculated and fitted to Murnaghan’s equation of state [23] as given by

\[
V = V_0 \left[ 1 + \frac{B_0}{B_0'} \left( \frac{P}{B_0} \right)^{1/\gamma_0} \right]^{-\gamma_0}
\]

where \(B_0\) and \(B_0'\) are the bulk modulus and its derivative at the equilibrium volume \(V_0\).

The calculated equilibrium lattice constants, bulk moduli and first derivative of bulk moduli of Ge, Si are given in Table 1 together with the available experimental and theoretical data. The computed lattice constant \(a\) using LDA deviates from the measured ones within 0.1 and 0.5% [26, 29] for Ge and Si, respectively. The slight deviation of the lattice parameters in comparison with the experimental results is mainly due to the use of local density approximation (LDA). To establish the reliability of our computational scheme for Ge and Si, we next turn to SiGe0.5 alloy. The PAW’s calculated results give good agreement with the experimental ones and better than ultra-soft pseudopotential (US-PP) results [30]. We have adopted a zinc-blende (ZB) structure for the calculation of SiGe0.5 alloy. The ZB structure of SiGe0.5 alloy has two sites occupied by Si and Ge, respectively. The atoms are arranged without taking into consideration the disorder effect coming with the random occupation of all sites with either Si or Ge. Fitting the variation of total energy versus volume (Fig. 1) of SiGe0.5 alloy, gave us the ground state properties (Table 1). Our results are in good agreement with the available data [6, 24].

In order to confirm our empirical model of bulk modulus [31], we have carried out this calculation of SiGe0.5 alloy using the equilibrium lattice parameter. The computation of \(B''\) is trivial and
the accuracy of the results reaches that of ab initio calculations. We used the following expression [31]

\[ B^* = [3000 - \lambda 1000]^{\alpha - 3.5/2} \]  

where \( \alpha \) is the lattice constant in (Å) and \( \lambda \) is an empirical parameter which accounts for the effect of \( B^*; \lambda = 0 \) for group-IV, 2 is in (Å) and the first term in (GPa). The calculated bulk moduli \( B^* \) values compared with experimental [16,27] and theoretical [6,17,24–26,28–30] ones are given in Table 1. We may conclude that the present \( B^* \) calculated in a different way than the definition of others are in good accord with the experimental values and exhibit the same chemical trends as those found in the values derived from the experimental and theoretical approaches values as seen in Table 1. The results of empirical model of bulk moduli are in agreement with others.

3.2. Electronic properties

The band structure of Si0.5Ge0.5 alloy for zinc-blende structure is calculated by means of VASP method. The details of the VASP calculations for different types of materials are given elsewhere [33–35]. The frozen-core PAW method turns out to be as powerful as US-PP method since it is also restricted to a variational treatment of the valence states only. The basic variational quantities are again non-norm-conserving pseudo wave functions. The major difference between the PAW and US-PP methods concerns only the augmentation of the charges or wave functions inside the core region. Fig. 2 shows the electronic band structure of the relaxed Si0.5Ge0.5 alloy (corresponding to the zinc-blende structure SiGe, with the average of bulk values of Si and Ge).

It is clearly seen that this alloy is an indirect band gap (\( \Gamma-X \)). Our results agree well with the self-consistent full potential LMTO calculations of Schmid et al. [36], especially for the minimum gap (near X point) and for the band ordering (\( E_{\Gamma-X} > E_{\Gamma-\Gamma} > E_{\Gamma-X} \)). The very important notice is the band gap derived from LDA eigenvalues which is too small; LDA underestimates the band gaps as mentioned previously in introduction. Thus, although the minimum gaps are brought close to experiments, the dispersion of the present band structure may not predict future experiments very well. In this LDA, the electronic properties are determined as a function of the electronic density by applying local relations appropriate for a homogeneous electronic system. It should be noticed, however, that the experimental data of the energy gaps of Si0.5Ge0.5 alloy are not sufficiently available to allow an accurate determination of the potential parameters. The calculated principal band gaps for zinc-blende structure of Si0.5Ge0.5 alloy are summarized in Table 2; the accordance with others including US-PP [30] is shown and the differences are mentioned due to different methods used in calculations. Using PAW with VASP, the density of state is computed. Fig. 3 displays the computed density of state for zinc-blende structure of Si0.5Ge0.5 alloy. The lower part of the valence band (VB) is dominated by Si 3s state while 4s state of Ge is contributed to both parts of VB. The large component of s state of Ge is in the upper VB while its absence in the bottom of the conduction band (CB) suggests Ge resembles an anion. This indicates that p electrons of Ge significantly affect the electronic properties.

It is clear that Si0.5Ge0.5 alloy is a semiconductor, to understand the chemical bonds of the alloy, the electronic band structure (Fig. 2) and the density of state (Fig. 3) of Si0.5Ge0.5 alloy have been calculated.

3.3. The refractive index

The refractive index \( n' \) is a very important physical parameter related to the microscopic atomic interactions. From theoretical viewpoint, there are basically two different approaches: the refractive index will be related to the density and the local polarizability of these entities [38].

On the other hand, considering the crystalline structure represented by a delocalized picture; \( n' \) will be closely related to the energy band structure of the material, complicated quantum mechanical analysis requirements and the very particular obtained results. Consequently, many attempts have been made in order to relate the refractive index and the energy gap \( E_g \) through simple relationships [39–44]. Currently, we are using the PAW’s calculated energy gap to those relationships.

However, these relations of \( n' \) are independent of temperature and incident photon energy. The various relations between \( n' \) and \( E_g \) will be reviewed. Ravindra et al. [44] had been suggested different relationships between the band gap and the high frequency refractive index and presented a linear form of \( n' \) as a function of \( E_g \):

\[ n' = \alpha + \beta E_g \]

(5)

<table>
<thead>
<tr>
<th>Compound</th>
<th>( E_{\Gamma-X} ) (eV)</th>
<th>( E_{\Gamma-\Gamma} ) (eV)</th>
<th>( E_{\Gamma-X} ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si0.5Ge0.5 alloy</td>
<td>Present</td>
<td>1.70</td>
<td>0.48</td>
</tr>
<tr>
<td></td>
<td>2.33(^d), 1.239(^c), 1.36(^c)</td>
<td>1.06(^a)</td>
<td>1.43(^a)</td>
</tr>
</tbody>
</table>

\( ^a \) Ref. [6].  
\( ^b \) Ref. [30].  
\( ^c \) Ref. [10].  
\( ^d \) Ref. [20].

Fig. 2. Band structure of Si0.5Ge0.5 alloy in the zinc-blende structure with the average of bulk values of Si and Ge.

Table 2. Calculated principal direct and indirect energy gaps for Si0.5Ge0.5 alloy in its zinc-blende structure at the equilibrium volume compared to theoretical values.

Fig. 3. Total density of state (DOS) of Si0.5Ge0.5 alloy in the zinc-blende structure at the equilibrium volume.
where $\alpha = 4.048$ and $\beta = -0.62 \text{ eV}^{-1}$. To be inspired by simple physics of light refraction and dispersion, Herve and Vandamme [45] proposed an empirical relation as follows:

$$n^2 \approx 1 + \frac{A}{(E_g + B)^2},$$

(6)

where $A = 13.6 \text{ eV}$ and $B = 3.4 \text{ eV}$. Ghosh et al. [46] have taken a different approach to the problem by considering the band structure and quantum-dielectric formulations of Penn [47] and Van Vechten [48], respectively.

Introducing $A$ as the contribution from the valence electrons and $B$ as a constant additive to the lowest band gap $E_g$, the expression for the high-frequency refractive index is written as:

$$n^2 - 1 = \frac{A}{(E_g + B)^2},$$

(7)

where $A = 2SE_g + 212$, $B = 0.21E^2 + 4.25$ and $(E_g + B)$ refers to an appropriate average energy gap of the material. Thus, these three models of variation $n^2$ with energy gap have been calculated. The results for Si$_0.5$Ge$_0.5$ alloy displayed in Table 3. This is verified by the calculation of the optical dielectric constant $\varepsilon_{\infty}$, which depends on the refractive index. Note that $\varepsilon_{\infty} = n^2$ [49]. In Table 3, the investigation of the calculated values of $\varepsilon_{\infty}$ using three models are given. A linear dependence of these properties on the energy gap is observed and the refractive index for high $E_g$ tends to shift towards the blue-green.

### 4. Conclusion

In this paper, we have studied the structural, electronic and optical properties following the projector augmented-wave (PAW) method within the local density approximation. It is found that Si$_0.5$Ge$_0.5$ alloy is a semiconductor with a small indirect band gap. Our bulk modulus model results are in good agreement with experimental and other data. The results of refractive index and optical dielectric constant of Si$_0.5$Ge$_0.5$ alloy using phenomenological models are investigated. Good agreement with experimental, in accordance with theoretical results and better than ultra-slow pseudopotential (US-PP) data are shown.

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### References

[12] For example, the empirical pseudopotential band structure calculations, which generally need fewer fitting parameters than the empirical tight-binding parameters, require six fitting parameters to calculate energy bands at zero pressure. See e.g. M. Rahab, Y. Al-Douri, M. Sehil, D. Rashid, Pressure effect on electronic band structure of III–V compounds, Mater. Chem. Phys. 80 (2003) 34–38.
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