

Structural, electronic, elastic, optical and thermodynamical properties of zinc-blende SiGe, SiSn and GeSn from first principles

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Abstract

The structural, electronic, elastic, optical and thermodynamical properties of the ordered SiGe, SiSn and GeSn cubic alloy in zinc-blende (B3) structure are investigated using the plane-wave ultrasoft pseudopotential based on the first principles density functional theory (DFT). The ground state properties such as the lattice parameter, bulk modulus, energy derivative, elastic constants C_{ij} , Young's modulus, Poisson's ratio and the Zener anisotropy factor were calculated. The results are in favorable agreement with a previous work. The complex dielectric function, refractive index, extinction coefficient, complex conductivity function, energy loss spectrum, absorption coefficient and optical reflectivity were calculated and the peak position distributions of imaginary parts of the complex dielectric function are explained. The calculated elastic properties are consistent with other calculated results and predicted the Debye temperature, the isochoric heat capacity, the entropy, enthalpy and free energy.

Keywords: density functional theory, elastic properties, optical properties, thermodynamical properties

1. Introduction

In recent years, IV–IV ground compounds such as SiC, SiGe, GeC, SnC and GeSn have attracted both scientific and technological interest. Due to their good chemical stability, wide band gap, high hardness, high stiffness, high melting point and high thermal conductivity, they are considered to be promising materials for electronic and optical devices. It is, therefore, necessary to study their fundamental properties: lattice constants, bulk modulus, energy derivative, structural stability, electronic structure, elastic constants C_{ij} , Young's modulus, Poisson's ratio and Zener anisotropy factor.

Recently, several theoretical studies of SiSn, using the local density approximation within density functional theory and the pseudopotential method have been reported (Amrane *et al.* 1995, Zaouiet *et al.* 1996, Corkill & Cohen 1993, Hatchard & Dahn, 2004, Jensen *et al.* 2011). Other works are also presented on GeC, SnC and GeSn (Benzair *et al.* 2001, Rûcker & Methfessel 1995, Sankey *et al.* 1993, Pandey *et al.* 2000, Pandey *et al.* 1999, Khenata *et al.* 2003, Sahnoun *et al.* 2005, Okoye 2004). Also, experimental works have been devoted to these compounds (Soref 1991, Krishnamurthy 1995, Hôchst *et al.* 1989). However, there have been relatively few theoretical studies of the electronic and structural properties of these materials (Krishnamurthy 1995) compared with SiC and SiGe. All of these studies show that GeC, like SiC, is a wide gap semiconductor with an indirect band gap, but SnC and GeSn are narrow gap semiconductors. The GeC and SnC are also unstable with respect to decomposition into the bulk forms of its separated constituents. The emergence of SiGe, SiSn and GeSn alloys as important materials in the development of strained heterostructure devices has led to an increasing interest in understanding and exploiting their physical properties (Paul 2004, Zhang 2012). It is the development of heterostructures that has enabled band structure and strain engineering to be used in many different ways to improve conventional microelectronic device performance along with allowing new concepts to be explored. These new materials can have a number of remarkable properties and make them particularly worthy of study.

In this paper we investigate theoretically the structural, electronic, optical, elastic and thermodynamical properties of the zinc-blende of SiGe, SiSn, and GeSn compounds. In the frame of the density functional theory (DFT).

This paper is organized as follows. In section 2 the computational approach used in this work is described. Structural parameters, band structure, density of states, elastic, optical and thermodynamical properties results are presented and discussed in section 3. A brief conclusion is present at the end.

2. Method of calculations

The first principle calculations are performed by employing the pseudopotential plane-waves (PP-PW) approach based on density functional theory (Hohenberg & Kohn 1964, Kohn & Sham 1965) and implemented in the most recent version of the CASTEP (Cambridge Serial Total Energy Package) code (Segall et al. 2002) to calculate the total energy, electronic structure, elastic constants, optical spectra and thermodynamical properties. The major advantages of this approach are the ease of computing forces and stresses; the good convergence control with respect to all computational parameters, employed favorable scaling with the number of atoms in the system and the ability to make easier calculations by neglecting core electrons. The exchange-correlation potential was calculated by the local density approximation (LDA) proposed by Ceperley and Alder (Ceperley & Alder 1980) as reformulated by Perdew and Zunger (Perdew & Zunger 1981). In order to reduce the number of plane waves required, chemically inactive core electrons are effectively replaced with the ultrasoft pseudopotential, which in this work were taken from the CASTEP database. The states Si $3s^23p^2$, Ge $4s^24p^2$, and Sn $5s^25p^2$ are treated as valence states. The two parameters that affect the accuracy of calculations are the kinetic energy cutoff, which determines the number of plane waves in the expansion and the number of special k points used for the Brillouin zone integration. A plane wave basis set was used with 300 eV cutoff. The k integrations over the Brillouin zone are performed up to the $5 \times 5 \times 5$ Monkhorst Pack mesh (Monkhorst & Pack 1976). The self consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-6} eV/atom, force 0.03 eV/Å, stress 0.05 GPa and displacement 0.001 Å.

It is well established that the first principle studies based on density functional theory can be used to obtain reliable elastic properties of the ordered SiGe, SiSn and GeSn cubic alloys. Several methods are available for the computation of stiffness coefficients, but currently the stress-strain method seems to be most commonly used and this is the method used in the present work. In this approach, the ground state structure is strained according to symmetry dependent strain patterns with varying amplitudes and to a subsequent computing of the stress tensor after a re-optimization of the internal structure parameters, i.e., after a geometry optimization with fixed cell parameters. The elastic stiffness coefficients are regarded as the proportionality coefficients relating the applied stress to the computed strain (Nye 1985, Karki et al. 1997). In a cubic crystal which has three different symmetry elements (C_{11} , C_{12} , and C_{44}), the one strain pattern, with non-zero first and fourth components, gives stresses related to all three independent elastic coefficients for the cubic system.

The generalized mechanical stability criteria (Sin'ko & Smirnov 2002) are

$$(C_{11} + 2C_{12} + P) > 0, (C_{44} - P) > 0, (C_{11} - C_{12} - 2P) > 0 \quad (1)$$

The adiabatic bulk modulus B and the shear modulus G are given by (Barsoum et al. 2000)

$$B = (C_{11} + 2C_{12})/3 \quad (2)$$

$$G = (G_v + G_r)/2 \quad (3)$$

where $C = (C_{11} - C_{12})/2$, $G_v = (2C + 3C_{44})/5$, $G_r = 15 * (6/C + 9/C_{44})^{-1}$, G_v is the Voigt shear modulus and G_r is the Reuss shear modulus.

The Zener anisotropy factor A is an indicator of the degree of elastic anisotropy possessed by the crystal. For a completely isotropic material, the factor A takes the value of 1. The factor A is calculated in term of the computed data using the following relation (Nye 1985).

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (4)$$

The Young's modulus E and the Poisson's ratio ν are then calculated from these elastic constant using the following relations:

$$E = \frac{9B_s G}{3B_s + G} \quad (5)$$

$$\nu = \frac{3B_s - 2G}{2(3B_s + G)} \quad (6)$$

The optical properties may be acquired from the knowledge of the complex dielectric function $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. The imaginary part $\epsilon_2(\omega)$ was calculated from the momentum matrix elements between the occupied and unoccupied wave functions within the selection rules. The real part $\epsilon_1(\omega)$ of the dielectric function $\epsilon(\omega)$ follows from the Kramer-Kronig relationship. There are two contributions to $\epsilon(\omega)$, namely, intraband and interband transitions. The contribution from the intraband is important only for metals. The interband transitions can further be split into direct and indirect transitions. Here we neglect the indirect transitions which involve

scattering of phonons and are expected to give only a small contribution to $\varepsilon(\omega)$ (Lu et al. 2005). We can calculate important optical functions such as the refractive index $n(\omega)$, optical conductivity function $\sigma(\omega)$, reflectivity $R(\omega)$, electron energy loss spectra, $L(\omega)$ and absorption coefficient $\alpha(\omega)$ using the following expressions (Chang et al. 2008, Elias 2013).

$$n(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2 \right\}^{1/2} + \varepsilon_1(\omega) \right]^{1/2} \quad (7)$$

$$k(\omega) = \frac{1}{\sqrt{2}} \left[\left\{ \varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2 \right\}^{1/2} - \varepsilon_1(\omega) \right]^{1/2} \quad (8)$$

$$R(\omega) = \frac{|\tilde{n} - 1|}{|\tilde{n} + 1|} = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (9)$$

$$\alpha(\omega) = \frac{4\pi k(\omega)}{\lambda} \quad (10)$$

$$L(\omega) = \text{Im}(-1/\varepsilon(\omega)) \quad (11)$$

$$\sigma(\omega) = \frac{2W_{cv}\hbar\omega}{\bar{E}_0^2} \quad (12)$$

where W_{cv} is the transition probability per unit time.

Mechanical properties can be related to thermodynamical parameters such as the Debye temperature, specific heat, thermal expansion and melting point, as they play an important role in understanding the thermal response of the solids. According to the standard thermodynamics, if the system is held at a fixed temperature T and pressure P then the Gibb's free energy (G) of the system is expressed as (Blanco et al. 2004):

$$G(V, P, T) = E(V) + PV - TS \quad (13)$$

where $E(V)$ is the total energy, V is the volume and S is the entropy of the system. Since the electronic structure calculations are performed in the static approximation, i.e., at $T=0$ K and neglecting zero-point vibrational effects, the corresponding Gibb's free energy in this case becomes $G(V, P) = E(V) + PV$. So we have chosen the quasi-harmonic Debye model (Chang et al. 2008) and according to this model the non-equilibrium Gibb's free energy function is given by

$$G^s(V, P, T) = E(V) + PV + A_{vib}(\Theta(V), T) \quad (14)$$

where $\Theta(V)$ is the Debye temperature, PV corresponds to the constant hydrostatic pressure condition and A_{vib} is the vibrational Helmholtz free energy.

The thermodynamic properties such as heat capacity (C_v), entropy and the vibrational internal energy can be calculated using the following relations (Blanco et al. 2004):

$$C_v = 3nk \left[4D\left(\frac{\Theta}{T}\right) - \frac{3\frac{\Theta}{T}}{e^{\Theta/T} - 1} \right] \quad (15)$$

$$C_v = nk \left[4D\left(\frac{\Theta}{T}\right) - 3\ln(1 - e^{-\Theta/T}) \right] \quad (16)$$

$$C_v = nkT \left[\frac{9\Theta}{8T} + 3D\left(\frac{\Theta}{T}\right) \right] \quad (17)$$

where n is the number of atoms per formula unit, $D(\Theta/T)$ represents the Debye integral.

3. Results and discussion

3.1. Structural, electronic, and elastic properties

The equilibrium volume of the ground state of the zinc-blende phase of SiGe, SiSn and GeSn cubic alloys is determined by calculating the total energy per primitive unit cell as a function of the volume (V). The calculated results are shown in figure 1. The Murnaghan's equation of state (Elias&Saadi 2013, Murnaghan 1944) is then used to fit the calculated energy-volume data. The obtained structural parameters such as a , B , and B' are evaluated and compared in table 1 along with the theoretical results. Here, it is difficult to compare with experiments because there is not experimental data available. The computed lattice parameters were utilized to observe the success and consistency of the present model in predicting the other physical properties. The calculated values of lattice parameters for SiGe, SiSn and GeSn are 5.4519, 5.904 and 6.2261 Å, respectively.

These values agree quite well with the theoretical results obtained by using the Abinit Code (Zhang et al. 2012) which gives 5.46, 5.81 and 6.11Å, respectively. These calculated lattice parameters, bulk module and their pressure derivatives are given in table 1 and are in good agreement with the theoretical values (Zhang et al. 2012). Table 1: The lattice constants a (Å), bulk modulus B (GPa), their energy derivative B' , elastic constants C_{ij} , Young's modulus E , Poisson's ratio ν and Zener anisotropy factor A of SiGe, SiSn and GeSn in the ZB structure at zero pressures within the LDA compared to available other theoretical work.

		a	B	B'	C_{11}	C_{12}	C_{44}	E	ν	A
SiGe	Present	5.4519	87.619	4.518	150.6733	57.8432	74.9668	118.58152	0.2774	1.61514
	Previous [*]	5.46	88.6	4.34	150.2	57.8	75	150.3	0.216	1.62
SiSn	Present	5.904	68.554	4.446	110.7954	48.02636	52.85843	81.74990	0.3024	1.68422
	Previous [*]	5.81	72.47	4.40	118.5	49.5	51.2	107.5	0.252	1.48
GeSn	Present	6.2261	43.178	5.127	96.40062	42.70148	46.64714	70.18367	0.3070	1.737351
	Previous [*]	6.11	53.8	5.126	90.4	35.5	37.3	82.2	0.245	1.36

* Ref.(Zhang et al. 2012)

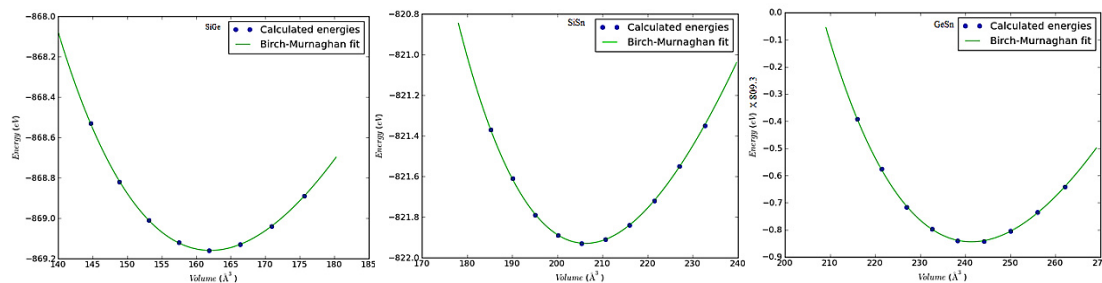


Figure 1. The variation of the total energy with volume in the zinc-blende structure for SiGe, SiSn and GeSn

The elastic constants provide a link between the mechanical and dynamical behavior of the crystals. For a cubic lattice, there are three independent components, C_{11} , C_{12} and C_{44} . They can be determined by the analysis of changes in calculated stress values resulting from changes in the strain.

The traditional mechanical stability conditions of the elastic constants in a cubic crystal are known to be $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$. For three compounds, the present elastic constants in Table 1 satisfy these stability conditions in the zinc-blende structure, indicating that it is a mechanically stable state at ambient pressure. The calculated results of the Zener anisotropy factor A are presented in Table 1. From Table 1, we can see that the A values are larger than 1.0 and we cannot regard SiGe, SiSn, and GeSn as elastically isotropic. The Poisson's ratio ν and Young's modulus E , which are the most interesting elastic properties for applications, are often measured for polycrystalline materials when investigating their hardness. The Poisson's ratio ν provides more information about the characteristics of the bonding forces than any of the other elastic constants, which usually range from 0.25 to 0.5. The calculated Poisson ratios are very close to 0.25, which means that the three materials have predominantly central inter-atomic forces (Nye 1985). The bigger the Poisson ratio is, the better the plasticity is. Thus, GeSn is the one which shows the best plasticity. While for SiGe, the Poisson ratio is the smallest corresponding to the poorest plasticity.

For the zinc-blende of SiGe, SiSn, and GeSn, the calculated electronic band structure (left panel) and the total density of state (TDOS) (right panel) along the various symmetry lines at 0 GPa are illustrated in Figure 2. It can be seen that the top of the valence band (VB) is at the G -symmetry point and the bottom of the conduction band (CB) is at the X -symmetry point, which suggests that the zinc-blende SiGe, SiSn, and GeSn has an indirect gap occurring between the G and X points. Figure 2 shows that at 0 GPa, the indirect band gap ($E_V - E_C$) occurs at 0.521 eV for SiGe, 0.539 for SiSn and 0.490 for GeSn respectively.

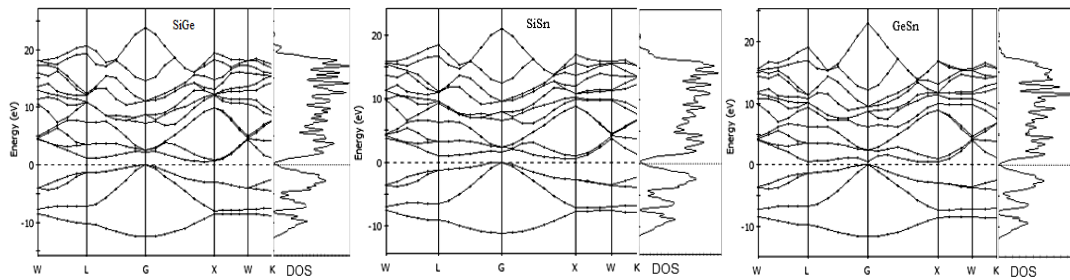


Figure 2. Electronic band structures for SiGe, SiSn and GeSn compounds in the ZB structure from LDA.

3.2 Optical properties

The electronic structure of solids allows various interband and intraband optical transitions, while the tensor components of the complex dielectric function, i.e., $\epsilon(\omega)=\epsilon_1(\omega)+i\epsilon_2(\omega)$, can be helpful for the identification of these transitions.

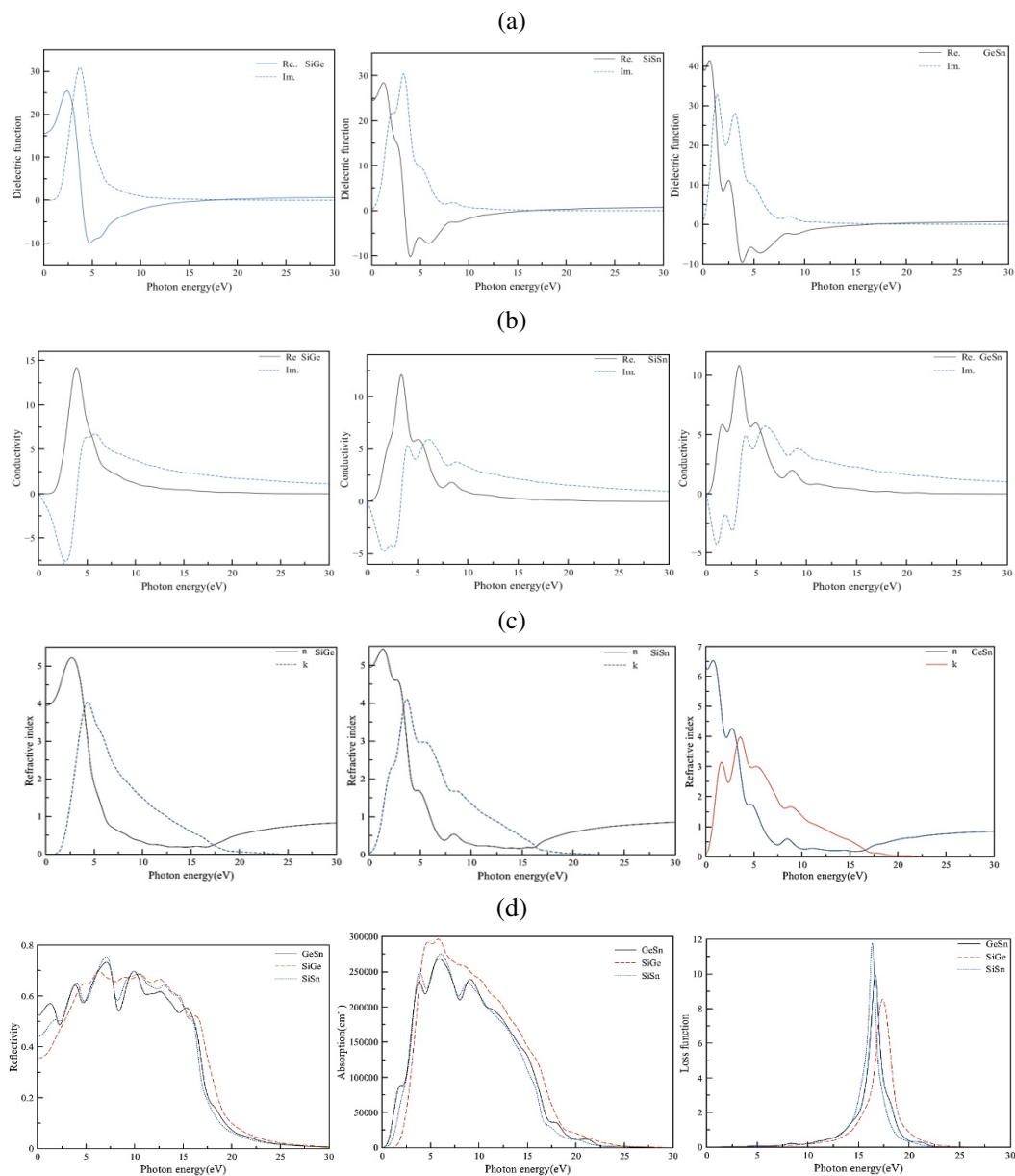


Figure 3. Dielectric function (a) conductivity (b) refractive index (c) reflectivity, absorption coefficient and loss function (d) for SiGe, SiSn and GeSn compounds in the ZB structure from LDA.

The complex dielectric function describes the complete response of a material to the disturbances caused by the electromagnetic radiations. The calculated real part $\epsilon_1(\omega)$ and imaginary part $\epsilon_2(\omega)$ of the dielectric function for SiGe, SiSn and GeSn, in the energy range 0-30 eV are shown in figure 3a. The present analysis of the $\epsilon_2(\omega)$ curves shows that the first critical points of the dielectric function occurs at 1.94eV, 0.75eV, and 0.12eV for SiGe, SiSn, and GeSn, respectively. These points are GV–GC splitting, which gives the threshold for direct optical transitions between the valence band maximum (VBM) and the conduction-band minimum (CBM). This is known as the fundamental absorption edge. The main contribution to the optical spectra originates from the transition from the top three valence bands to the lower three conduction bands. The present results of calculated $\epsilon_1(\omega)$ are shown in figure. 3a. An important quantity of $\epsilon_1(\omega)$ is the zero frequency limit $\epsilon_1(0)$, which represents the dielectric response to the static electric field. Note that we do not include phonon contributions to the dielectric screening, and that $\epsilon_1(0)$ corresponds to the static optical dielectric constant ϵ_1 . The present calculated optical dielectric constants $\epsilon_1(\omega)$ are 15.78 , 24.62 and 38.87 for SiGe, SiSn, and GeSn, respectively. The frequency dependent optical conductivity is also calculated and is shown in figure 3b. Optical conduction starts responding to the applied energy field from 1.11eV, 0.12eV and 0.07eV for SiGe, SiSn and GeSn, respectively. Maximum optical conductivity of SiGe, SiSn and GeSn occur at 3.80 eV, 3.34 eV and 3.18 eV, and have magnitudes 14.26 1/fs, , 12.04 1/fs and 10.90 1/fs, respectively.

The knowledge of the refractive index of an optical material is important for its use in optical devices such as photonic crystals, wave guides, etc. The calculated refractive indices $n(\omega)$ are shown in figure 3c. All the peaks that appeared in the spectrum of the refractive index are related to the peaks that appeared in the imaginary part of the dielectric function. We note that at low energy, the refractive index for the compounds studied in this work varied between 4.0 to around 6.0. At high energies, a rapid decreasing occurs in the refractive indices of all compounds.

The absorption coefficient $\alpha(\omega)$ for the zinc-blende structure of SiGe, SiSn and GeSn, is shown in figure 3d. It is clear from the figure that the three peaks at (4.63, 5.77, 8.52) eV are for SiGe, (3.70, 5.98, 8.83) eV are for SiSn and (3.8, 5.82, 9.03) eV are for GeSn. There is almost no absorption at the lower energy region from about 0 to 1.5 eV for SiGe, 0 to 0.75eV for SiSn and 0 to 0.23 eV for GeSn. This means that the material is transparent from the partially ultra-violet to the visible light area because photon energy at such range is just within the forbidden band.

The calculated reflectivity spectrum $R(\omega)$, is shown in figure 3d. According to the graph one can say that these compounds show small reflectivity at low energies.

A rapid increase in the reflectivity occurs at intermediate and high energies. The reflectivity maximum arise from the inter-band transitions. They occur between the energy range 5.98-6.75eV for SiGe, 6.52-7.32eV for SiSn, and 6.18-7.48eV for GeSn which is in the ultraviolet region. SiGe, SiSn and GeSn can therefore serve as a possible shield for ultraviolet radiation. The electron energy loss function $L(\omega)$ is an important factor describing the energy loss of a fast electron traversing a material. Prominent peaks in $L(\omega)$ spectra represent the characteristics associated with the plasma oscillations and the corresponding frequencies are the so-called screened plasma frequencies. One may note from figure 3d that the main peaks of $L(\omega)$ are located at about 17.53 eV, 16.60 eV, and 16.18 eV for SiGe, SiSn, and GeSn respectively, which correspond to the abrupt reduction of $R(\omega)$, and to the zero crossing of $\epsilon_1(\omega)$.

3.3. Phonon dispersion curves and density of states

Figure 4 shows the calculated phonon dispersion curves of SiGe, SiSn and GeSn, along several symmetry lines together with the corresponding total densities of states (DOS). The acoustic phonon branches have positive frequency values, indicating the stability of these compounds in the zinc-blende structure at zero pressure. From the plotted total densities of states, the lower frequency modes are due to the motion of the heavier atom, while the higher frequency modes are associated with the lighter ones.

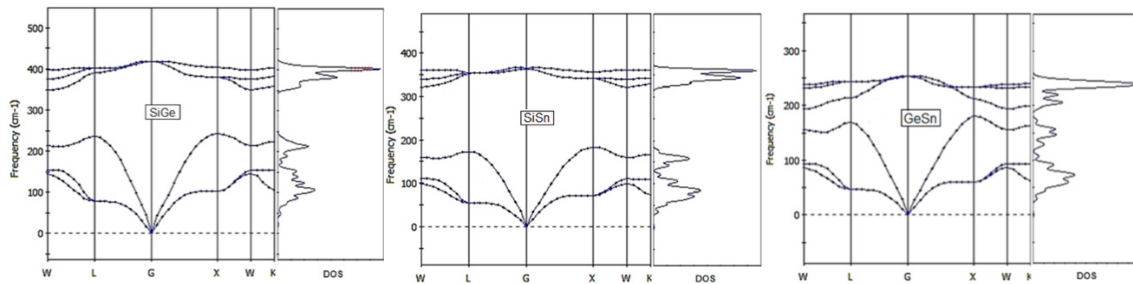


Figure 4. Calculated phonon dispersions and density of states (DOS) for SiGe, SiSn and GeSn, at zero pressures.

Some numerical values of the mode frequencies at the high symmetry points G, X and L are also listed in Table 2 for the binaries and the elemental components, together with the available theoretical data.

Table 2. Phonon frequencies (in cm^{-1}) calculated at the high-symmetry points G, X and L, for SiGe, SiSn and GeSn compared to available other theoretical work.

		G_{TO}	G_{LO}	X_{TO}	X_{LO}	L_{TO}	L_{LO}
SiGe	Present	418	418	402	382	400	385
	Previous *	416.72	416.72	398.89	384.81	398.80	376.98.
SiSn	Present	362	362	360	340	350	350
	Previous *	358.02	351.64	337.20	332.83	336.62	322.59
GeSn	Present	255	250	225	210	230	210
	Previous *	209.03	209.03	191.67	170.04	172.44	173.56

*Ref.(Zhang et al. 2012)

The obtained LO and TO frequencies at the zone center (G) agree well with the results of Zhang et al. They correspond to 418 (362)250 and 418 (362)255 for LO(G) and TO(G) modes, respectively for SiGe (SiSn) GeSn. These results are also in agreement with previous theoretical results of Zhang et al. (Zhang et al. 2012).

After obtaining the phonon spectrum over the entire BZ, we calculated the Helmholtz free energy F , enthalpy H , entropy S , and constant-volume specific heat C_v at zero pressure of three compounds by using the phonon density of states and quasi-harmonic approximation.

The contribution to the free energy, enthalpy, the entropy, and heat capacity from 0 K to 1000 K are shown in figure 5. It is noted that the enthalpy and entropy change increase rapidly when the temperature increases at low temperature. It is obvious that the free energy decreases, when the temperature increases. The change of the heat capacity C_v at constant volume versus temperature is also shown in figure 5. For the heat capacity at constant volume C_v , with increasing temperature, C_v values increase sharply at a lower temperature, then increase slowly at a higher temperature and then approach the Dulong Petit limit. At high temperature, C_v approaches approximately 11.5 cal/cell K for SiGe and SiSn crystal. As an important physical quantity, the Debye temperature is a suitable parameter to describe phenomena of solid-state physics which are associated with lattice vibration, elastic constants, specific heat and melting point. The Debye temperature is not a strictly determined parameter, and various estimates may be obtained through well-established empirical or semiempirical formulas.

These results are of significant importance for a better understanding of the thermodynamic properties of zincblende SiGe, SiSn and GeSn, crystal. These predicted high-temperature behaviors could give some information when SiGe, SiSn and GeSn, anneal at different temperature to improve their performance. It is difficult to evaluate the magnitude of errors between calculations and experiments. The results calculated in this work can be seen as a prediction for future investigations.

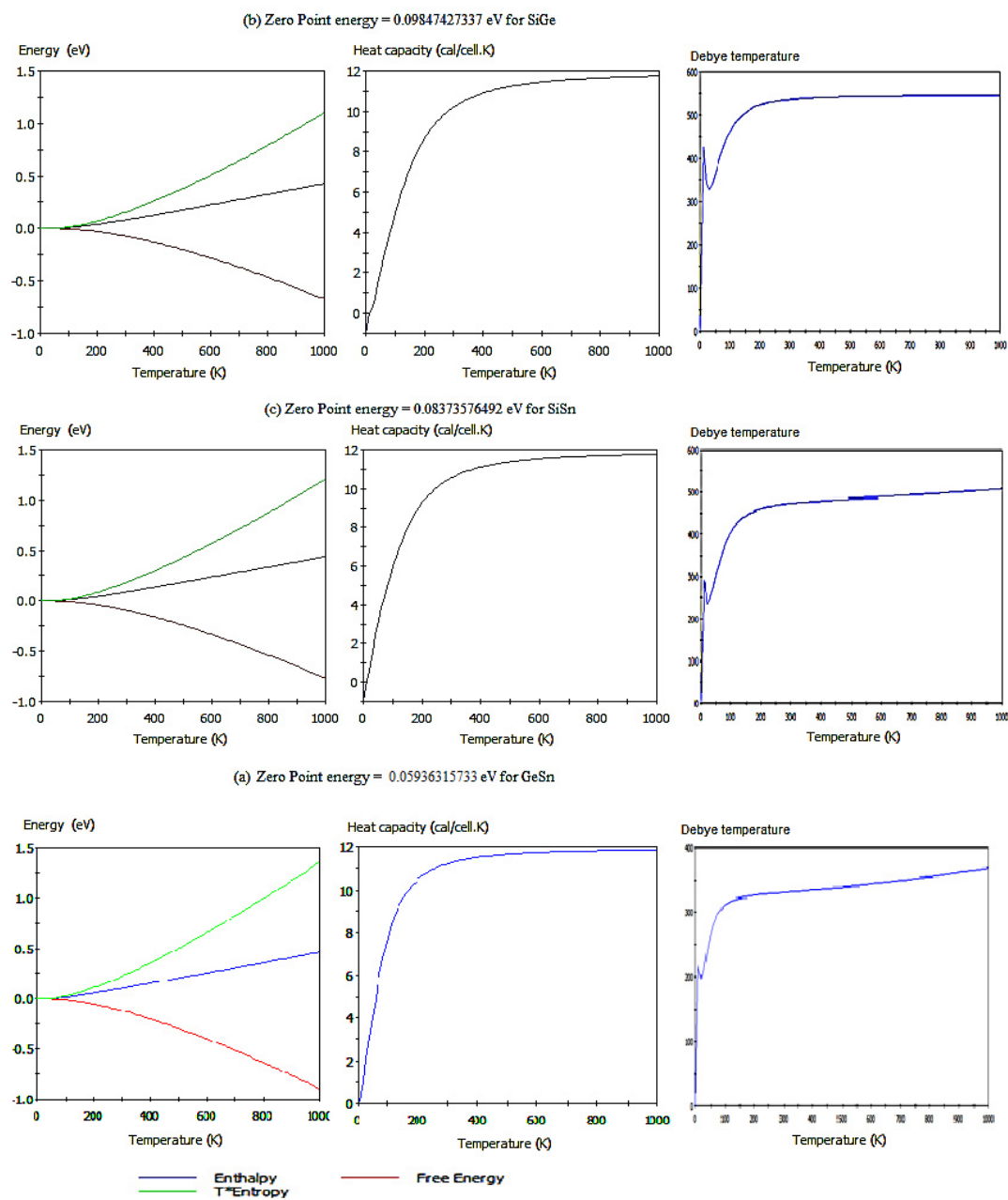


Figure 5. The temperature dependence of the vibrational contribution to the free energy, enthalpy, entropy, and heat capacity for the zinc-blende SiGe, SiSn and GeSn.

4. Conclusions

The structural, electronic, optical elastic and thermodynamic properties of zinc-blende SiGe, SiSn and GeSn have been studied by means of density functional theory within the local density approximation (LDA). The most relevant conclusions are summarized as follows:

1. The calculated ground state properties of these compounds at zero pressure are in agreement with the available theoretical data.
2. The calculations of the electronic structure showed that SiGe, SiSn and GeSn are semiconductors. The dielectric function, refractive index and electron energy loss were calculated in the energy range of 0-30 eV.
3. The elastic constants, shear modulus, Young's modulus and Poisson's ratio were calculated. The elastic constants obey stability conditions for SiGe, SiSn and GeSn compounds.
4. Finally, by phonon calculations some thermodynamic properties such as the vibrational contribution to the Helmholtz free energy, enthalpy, entropy, and the heat capacity were also successfully obtained. These results can give much help in the annealing process used to improve the properties of these semiconducting materials.

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