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Study of the elastic, opto-electronic and thermoelectric properties of ternary chalcogenides X$_2$Sb$_2$Se$_5$ (X=Ge, Sn)

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Abstract

There search on phase change materials in the last decades has extensively been outlined. Fascinating and promising as these materials and their applications are a profound understanding of the material physics is desire. The chalcogenide material Ge$_2$Sb$_2$Te$_5$ *is the prototype phase-change material. The effect of replacing Ge by Sn et Te by Se was studied for a systematic understanding and prediction of new potential candidates for PCRAM applications.*

The structural, elastic,opto-electronic and thermoelectric properties of Ge$_2$Sb$_2$Se$_5$ *and* Sn$_2$Sb$_2$Se$_5$ *ternary alloys have been investigated using the full-potential (linearized) augmented plane wave method. To make the results comparably the opto-electronic calculations, were performed using two methods, namely generalized gradient approximation developed by Perdew-Burke-Emzerhof (PBE-GGA), and recently developed modified Becke–Johnson (mBJ) potential. This is found to be a semiconductor with energy band gap equal to 0.64 eV and 0.57 eV for* Ge$_2$Sb$_2$Se$_5$ *and* Sn$_2$Sb$_2$Se$_5$ *respectively . All the elastic constants obey the Born–Huang criteria, suggesting that they are mechanically stable This material is being reported as thermoelectric material. The Seebeck coefficient increases with temperature and attains the maximum value 650 µV/K and 580 µV/K at T=300 K for* Ge$_2$Sb$_2$Se$_5$ *and* Sn$_2$Sb$_2$Se$_5$ *respectively. The material has achieved the maximum value of ZT is 0.92 for* Ge$_2$Sb$_2$Se$_5$ *and 0.97 for* Sn$_2$Sb$_2$Se$_5$ *at 300 K.*

Keywords: Phase change memory; FP-LAPW; DFT; GGA, mBJ; band gap; optical properties; thermoelectric properties

1. Introduction

The developments in multi-media applications as well as the nature of the internet lead to larger and more efficient data storage needs. One of the methods currently used is optical storage based on the phase change of chalcogenide materials [1-7]. This idea had been suggested for the first time by S.Ovestein [8] and it is the origin of the realization of "Digital Versatile Disk" (DVD). PCM materials exhibit a significant variation in certain physical properties when passing from the amorphous to the crystalline state whose storage principle is based on the electrical conductivity between the two phases of the materials. In fact, the transition from the crystalline state to the amorphous state takes place very quickly in a reversible manner under the application of an electric pulse [9-12]. GST alloys used in PCM can be presented in numerous arrangements around three elements Ge, Te and Sb which are chalcogenides glasses. The Ge$_2$Sb$_2$Te$_5$ alloy has received considerable attention due to its properties such as long life, high electrical contrast and fast crystallization speed. The Sb-Se chalcogenide system is also important because of its continuous variation of the band gap energy and the network constant, as well as the electrical properties [13, 14]. The addition of a third element such as Ge, Sn, to the Sb-Se system has also produced a significant effect on the structural, physical, optical, electronic and thermal properties [15-20]. Telluride materials are not the only chalcogenide materials to be used for memory development. Thus a new generation of memories using glasses of selenide chalcogenides. The effect of replacing Ge by Sn et Te by Se was studied for a systematic understanding and prediction of new potential candidates for phase change random access memory (PCRAM) applications. A deep understanding of electronic and optical properties of materials like Ge$_2$Sb$_2$Se$_5$ and Sn$_2$Sb$_2$Se$_5$ is quintessential for turning their properties with an outlook towards both optical as well as electronic future applications.

2. Details of calculations

The first principles calculations based on the density functional (DFT) to compare the previously proposed models have been reported by Sun .[21] and Sosso. [22]. The authors have concluded that the most stable configuration of GST is one proposed by Kooi and Dee Hosson [23]. We proposed the same staking configuration of Ge$_2$Sb$_2$Se$_5$ and Sn$_2$Sb$_2$Se$_5$.

In our work, we studied the physical properties of ternary alloys Ge$_2$Sb$_2$Se$_5$ and Sn$_2$Sb$_2$Se$_5$ using the augmented and linearized plane wave method (FP-LAPW). This first principle method based on the functional theory of density (DFT) is implemented in the Wien2k code [24,25]. The exchange-correlation potential is calculated within the generalized gradient approximation (GGA) by

Perdew_Burke Ernzerhof (PBE) [26]. We have also used the modified version of the original Becke-Johnson exchange potential [27] , known mBJ (modified Becke-Johnson) potential [28] which is considered to be quite precise in elaborating electronic and optical properties of insulators and semiconductors.

In the FP-LAPW method, the unit cell is divided into two regions, a region composed of spheres which do not overlap and which are centered on each atom (Muffin-tin spheres) of radius RMT, and an interstitial region between the Muffin-Tins, in which the basis set consists of plane waves region. The value of the Muffin-tin radius RMT has been set at 2.5, for all atoms, The cut-off energy which defines the separation between the core and valence states is set at -6.0 Ry. The basic functions, the electronic densities, and the potentials are extended in combination of spherical harmonics inside the Muffin-tin spheres and in Fourier series in the interstitial region with a cutoff (cut-off radius) $R_{MT}K_{max}=7$ (where R_{MT} is the smallest radius of the MT sphere, Kmax is the standard of the largest wave vector used for the development of eigen functions in plane waves). We use 1000 k-points in the Brillouin zone, which corresponds to meshes 16x16x3. Self-consistent calculations are considered to be converged when the total energy of the system is stable within 0.0001 Ry.

3. Results

3.1. Structural and elastic properties

The crystal structure of $X_2Sb_2Se_5$ (X=Ge, Sn) has been proposed the layer sequence of Se-X-Se-Sb-Se-Se-Sb-Se-X [29]. Firstly, we have optimized the internal structure of hexagonal phase at the experimental lattice parameters of GST [30] $a_0 = b_0 = 4{,}2217\,\AA$ and $c_0 = 17{,}2391\,\AA$. The volume versus energy is fitted by the Birch-Murnaghan equation of state [31]. From this fit, we can get the equilibrium lattice constant$(a, b\ c)$, bulk modulus (B) and pressure derivative of the bulk modulus (B') . These values are shown in table 1.

Table1: Atomic positions, calculated lattice parameters, bulk modulus B0, pressure and derivative (B') of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

	Lattice parameters ($\AA$)	B(GPa)	B'
$Ge_2Sb_2Se_5$	$a = b = 4.0145$ $c = 16.8856$	57.16	4.18
$Sn_2Sb_2Se_5$	$a = b = 4.1426$ $c = 17.4246$	52.33	4.20

Our calculated equilibrium lattice parameter (a, b, c) is in reasonable agreement with the experimental of GST.

Elastic properties of a solid are important because they relate to various fundamental solid-state properties such as interatomic potentials, equation of state, and phonon spectra. The values of elastic constants provide valuable information on the structural stability of materials.

The calculated values of five independent elastic constants for hexagonal crystals (C_{11}, C_{12}, C_{13}, C_{33} and C_{44}), bulk (B) and shear modulus (G) in Voigt, Reuss and Voigt-Reuss-Hill [32,33] approximations of the two materials in the hexagonal structure are given in table 2.

Table2: Elastic constants of the Hexagonal phase of $Ge_2Sb_2Se_5$ an $Sn_2Sb_2Se_5$

	C_{11}(GPa)	C_{12}(GPa)	C_{13}(GPa)	C_{33}(GPa)	C_{44}(GPa)	C_{66}(GPa)	B(GPa)	G(GPa)
$Ge_2Sb_2Se_5$	178.31	62.66	83.17	77.67	25.85	120.86	74.97	54.93
$Sn_2Sb_2Se_5$	111.42	10.68	73.76	72.91	51.22	61.05	68.11	56.45

First of all, Cij constants for the two systems are satisfy the Born–Huang criteria [34] for mechanically stable crystals: $C_{44} > 0$, $C_{11} > |C_{12}| > 0$ and $C_{11}+C_{33} + 2C_{13} > 0$.

we notice that the bulks obtained by the optimization are closer than those calculated by the elastic constants Cij for the two materials. According to the empirical formula of Pugh [35], the critical value of the B/G which separates between the ductile and brittle behavior of materials is around 1.75. If B/G > 1.75 the material behaves as ductile and if B/G <1.75 the material is fragile. The values of B/G for $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ are respectively 1.36, 1.21 which shows that the two materials have a fragile behavior.

3-2. Electronic properties

We have studied in this part the electronic properties of ternary compounds. In solid state physics, the energy bands give the possible energies of an electron in function of the k wave vector. From the dispersion equation E (k) which represents a very important property in the case of semiconductors, these electronic properties include band structures, gap energies (Eg), state densities. The band structures obtained for each compound by the use of two approximations have almost the same appearance, this is why only the curves obtained using the (GGA-mBJ) are illustrated in figure1.

From these curves, we can notice that for $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ compounds, the maximum of the valence band is located at the point of symmetry Γ and the minimum of the conduction band is at the point of symmetry Γ. Consequently, the two compounds have a direct gap under the direction (Γ→Γ). The results of the direct energy gaps obtained by the two approximations GGA-PBE and GGA- mBJ are given in the table3.

Table 3: Energy gap at high symmetry points for $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

Method	$Ge_2Sb_2Se_5$	$Sn_2Sb_2Se_5$	$Ge_2Sb_2Te_5$
GGA-PBE	0.38 eV	0.32 eV	0.20 eV[[27]
GGA-mBJ	0.64 ev	0.57 eV	0.40 eV[36]]

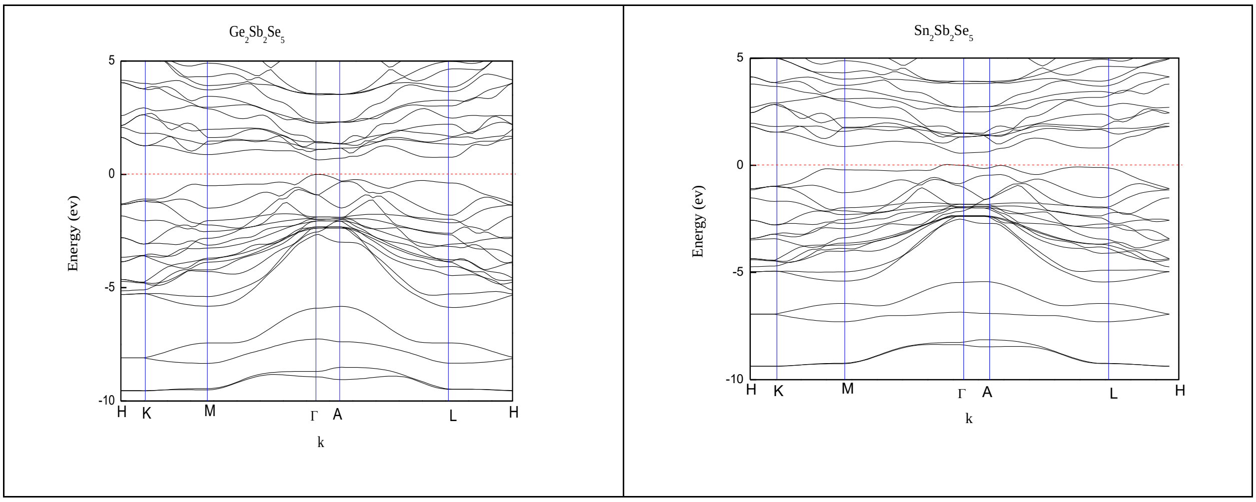

Figure1. Band structure along the high symmetry point using the GGA-mBJ methods of *$Ge_2Sb_2Se_5$* and of *$Sn_2Sb_2Se_5$*

It is a well known fact that GGA-PBE exchange-correlation potentials underestimate the band gap of semiconductors. The calculated GGA-mBJ band gap values for $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ are in excellent agreement with those obtained of GST. Hence we conclude that GGA-mBJ method is more suitable for the study of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ compounds. This method provides the band gaps almost equal to the experimental values of GST $E_g^{exp} = 0.5$ eV [37].

The calculated electronic density of state of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ at theoretical equilibrium volume is reported in Figure2.

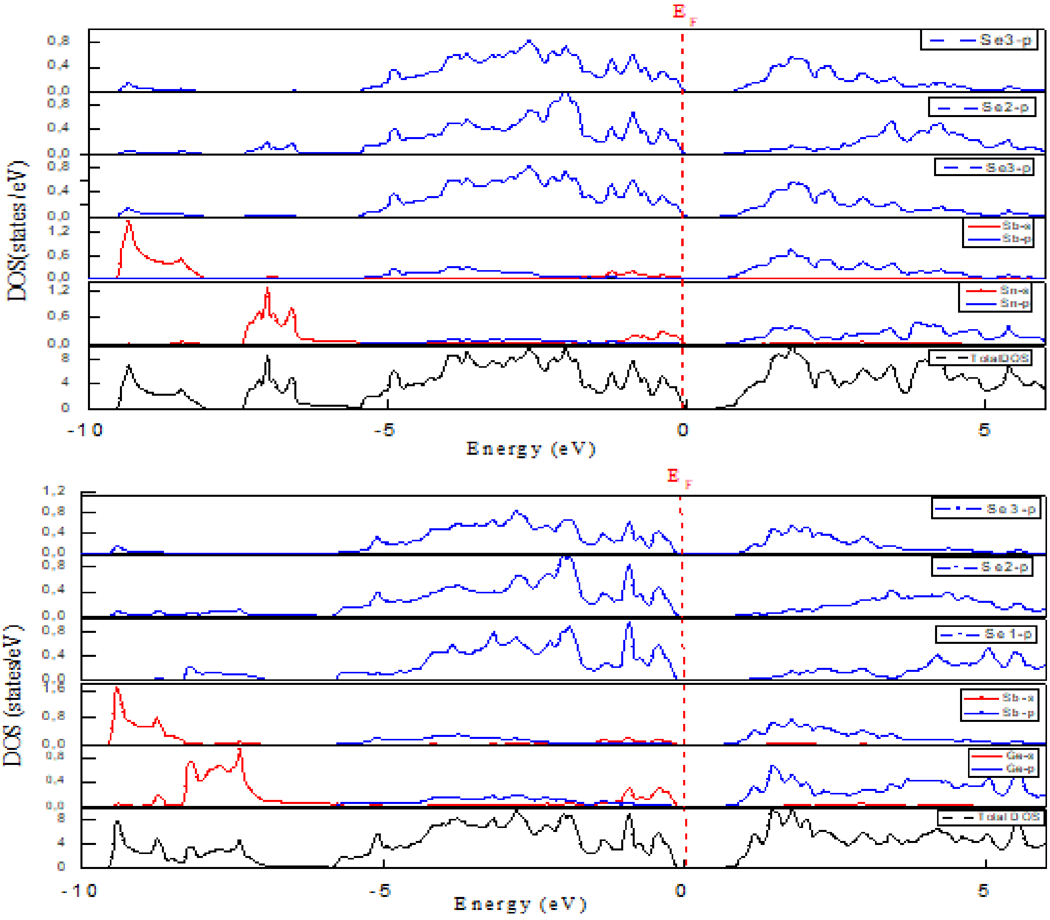

Figure 2. Total and partial density of states of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

The total and partial state densities, calculated by the GGA-mBJ for the compounds $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ are illustrated in the figure2. In case of $Ge_2Sb_2Se_5$, the valence bands in the energy range -10 eV to -5 eV are dominated by majority contribution the s states of Ge and Sb atoms and minority contribution of p states of Se atom. In the energy range -5 eV to 0 eV are mainly contributed by p states of Ge, Sb and Se atoms. The region above the Fermi level is the conduction band, in energy bands range 0-5eV majority contribution is from p state of Se. Along with this majority contribution, the minority contributions from p states of Ge, Sb atoms is observed. A similar of behavior, is also viewed in case of $Sn_2Sb_2Se_5$, with a variation in the energy values.

3-2. Optical properties

Optical properties in solid state physics describe the interaction of electromagnetic radiation with a material and they induce polarization effects as well as the displacement of the conduction electrons. These processes are the answer optics of the material and can be characterized by the dielectric function $\varepsilon(\omega)$ which plays a important role in the study of optical properties. We have studied and determined in this section the optical properties of the two compounds. The formula of dielectric function is defined by: $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$

The real part $\varepsilon_1(\omega)$ is related to the polarization, and the imaginary part $\varepsilon_2(\omega)$ depends on the electronic transition at the origin of absorption which defines the optical gap. Among the optical properties which describe the interaction of light with the medium, finds the refractive index complex. At low frequency ($\omega = 0$), we have $n(0) = \varepsilon_1^{1/2}(0)$.

The calculation results of the imaginary part $\varepsilon_2(\omega)$ of the dielectric function in the energy range from 0 to 10 eV for these ternary compounds are illustrated in the figure 3.

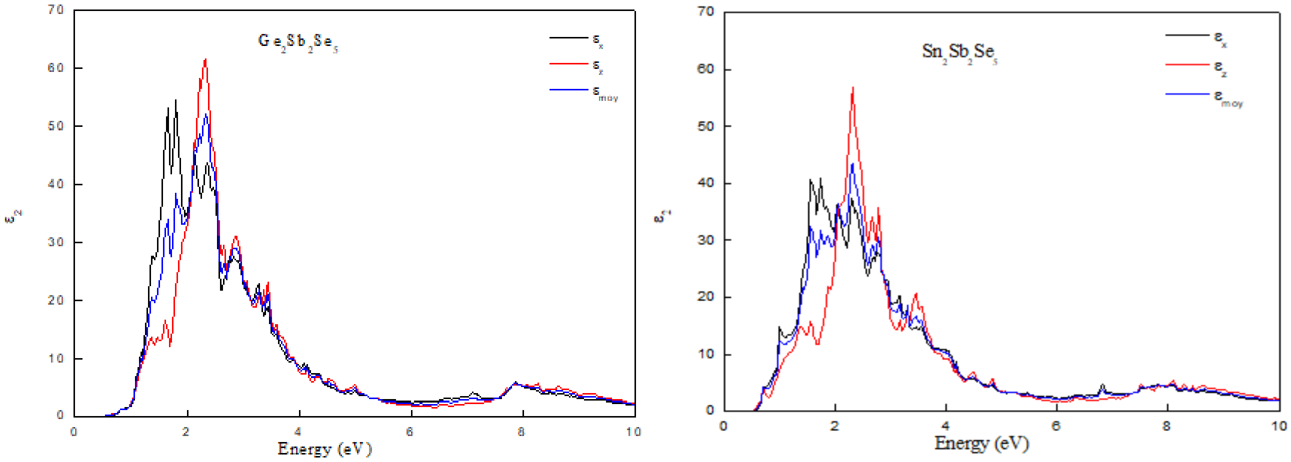

Figure 3. Imaginary part ε_2 of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

Analysis of these spectra shows that the behavior of ε_2 is almost similar for the two compounds, and the first critical points of the dielectric function which corresponds to the fundamental absorption thresholds start at around 0.6 eV, and 0.5 eV of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ respectively. The origin of these points is due to the optical transition between the highest valence band and the lowest conduction band, these values define the optical gap which are close to the values of the electronic gap. Then the values of the critical points correspond to the transition ($\Gamma_v \rightarrow \Gamma_c$) for $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$. So, we notice next to the fundamental peak the main peaks which reflect the maximum absorption, are located 2.3 eV. These peaks characterize the transitions ($L_v \rightarrow L_c$).

Figure4 shows the calculated results of the real (dispersive) part $\varepsilon_1(\omega)$ of the dielectric function of the compounds $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$. The zero crossing of the spectra means there is no scattering. We noticed that the function $\varepsilon1(0)$ is canceled at the following energy values: 25.44 eV of $Ge_2Sb_2Se_2$ and 24.46 eV of $Sn_2Sb_2Se_5$, where the dispersion is zero and therefore the absorption is maximum.

We have determined the static dielectric constant $\varepsilon1(0)$ which is a larger quantity and given by the lower limit of the energy of $\varepsilon(\omega)$. The static refractive index n(0) obtained of $Ge_2Sb_2Se_2$ and $Sn_2Sb_2Se_5$ are 5.04 and 4.94 respectively.

The imaginary part and the extinction coefficients of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ as well as the experimental results of the GST are shown in the figure5. We see that the GST curves are similar to those of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

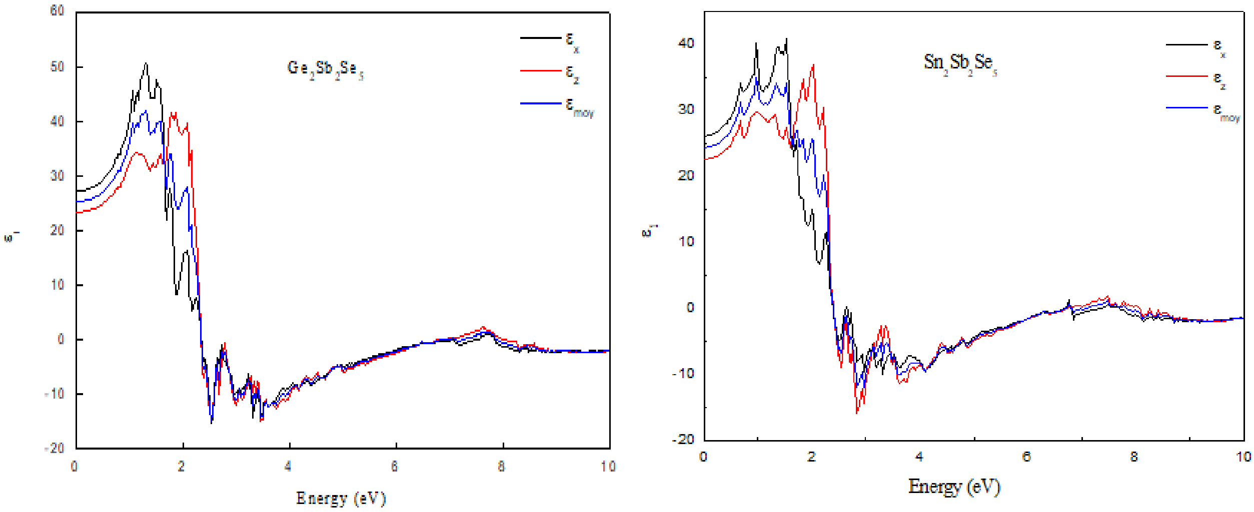

Figure 4. Imaginary part ε_1 of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

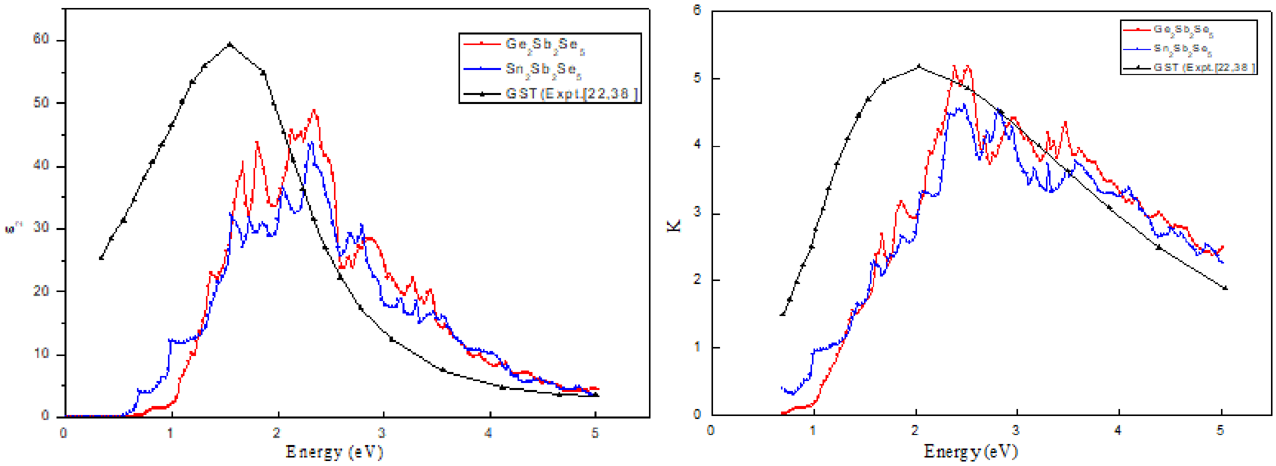

Figure 5. The imaginary part and the extinction coefficients of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ and the experimental results of the GST

3-3 Thermoelectric properties

Another approach consists in recovering the wasted electricity by reconverting the heat produced into electricity, this is achievable by the thermoelectric phenomenon. The thermal properties of materials are the basis of solid state physics and technological applications. It becomes necessary to study the thermal properties of materials in order to expand our knowledge of their specific behavior when they undergo strong pressure or temperature constraints. In our study, we have examined the effect of temperature on the thermal properties of materials semiconductors. DFT has been used to obtain the minimum energy structure and, the ground state energy for each band with index n and a wave vector k (E_0(n; k)). Boltzmann transport theory, as implemented in the BOLTZTRAP code [39], uses E0(n; k) to determine thermoelectric properties of the compounds. The thermoelectric phenomenon was first observed by Thomas Johann Seebeck. He showed that a voltage could be generated by heating a junction of two different metals (thermocouple). By heating the junction, electrons and holes travel in opposite directions creating a voltage difference. The generated voltage is proportional to the temperature difference ($V = S\Delta T$), where the proportionality constant is known as the Seebeck coefficient (S). The performance of a thermoelectric material is measured by figure of merit ZT which is defined as: $\mathrm{ZT} = \frac{\mathrm{S}^2\sigma}{\mathrm{k}}\mathrm{T}$,where σ is electrical conductivity and k is thermal conductivity. In the calculations of the thermoelectric properties of the compounds $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$ by the approximation (PBE-GGA), we used the equilibrium mesh parameter and a number of 50000 points k in the Brillouin zone, because the calculation of these properties requires a large number of eigen values corresponding to eigen vectors.

The variations of the seebeck coefficient (S), electrical conductivity (σ/τ), thermal conductivity (k/τ)and the power factor (PF) with the chemical potential at 300, 600 and 800 °K of the two compounds are shown in Figure 6.

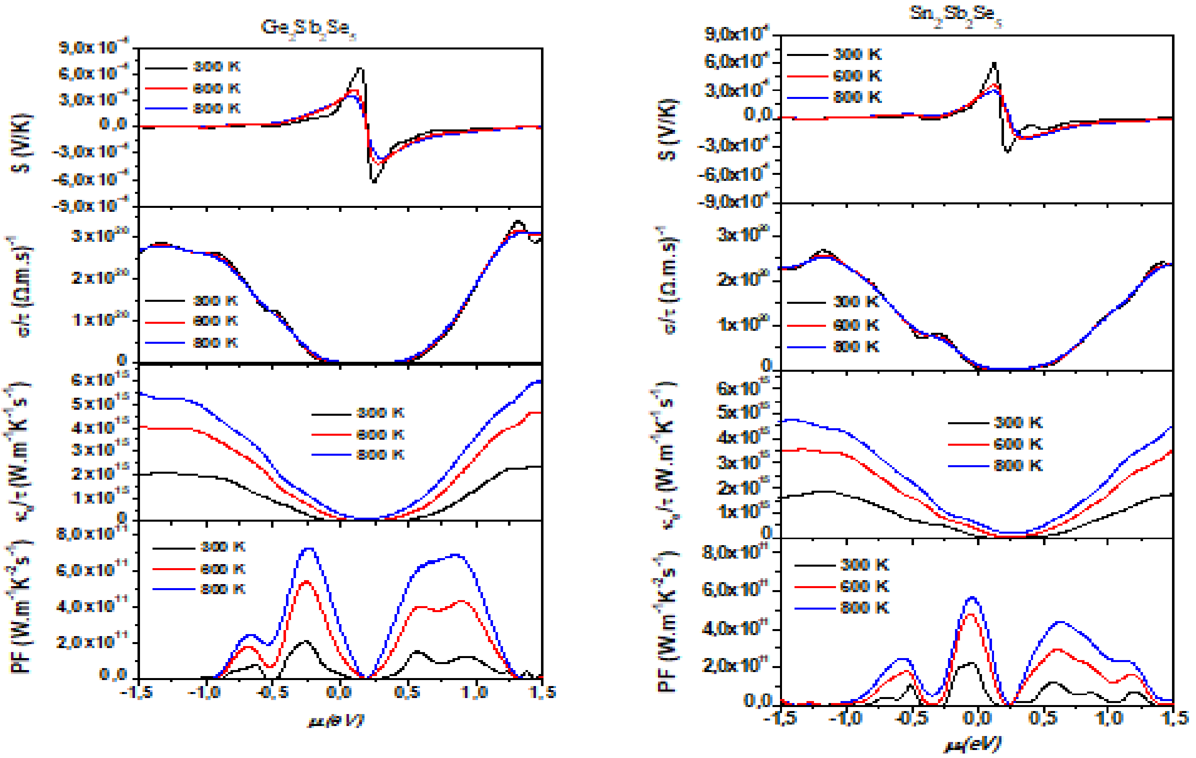

Figure 6. Seebeck coefficient, electrical conductivity, thermal conductivity and the power factor of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$

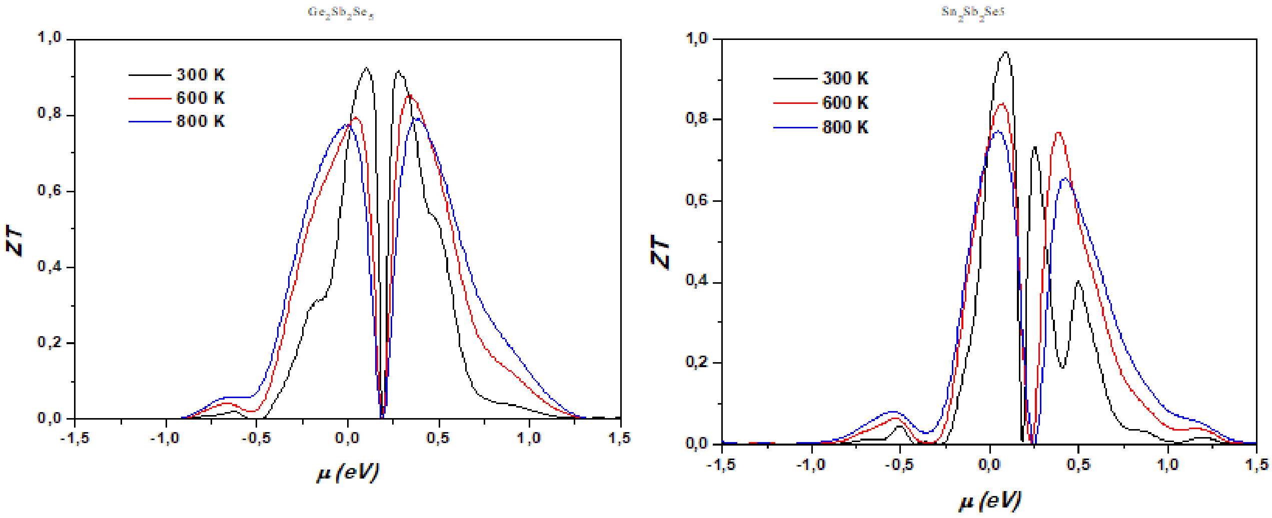

Figure 7. Merit factor of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$.

We notice that the two materials have the same appearance for the different properties. we can see on figure 6, that the Seebeck coefficient reaches high values between 0 and 0.25 eV of chemical potential, while outside this region the Seebeck coefficient decreases. At room temperature, it reaches the maximum with a value of $650\,\mu V/K$ for Ge_2Sb_2Se and $580\,\mu V/K$ for $Sn_2Sb_2Se_5$. The figure shows that the thermal and electrical conductivity is negligible at zero chemical potential and increases as the chemical potential increases. Electrical and thermal conductivity is minimum between $\mu = 0$ and $\mu = 0.5eV$ for different temperatures. Also, we notice that the electrical conductivity curves coincide for all temperatures. We observe that the power factor increases as a function of chemical potential and reaches the first maximum at $\mu = -0.27\,eV$ for $Ge_2Sb_2Se_5$ and $\mu = -0.05\,eV$ for $Sn_2Sb_2Se_5$. The power factor decreases and is canceled at $\mu = 0.2\ eV$ then it reaches the second maximum at $\mu = 0.6\ eV$. This maximum values increase with temperature.

Figure 7 shows the variation of merit factor ZT as a function of the chemical potential at 300, 600 and 800 °K. The ZT reaches its maximum for the temperature 300 °K with a value of 0.92 at $\mu = 0.1\ eV$ and $\mu = 0.3\ eV$ for $Ge_2Sb_2Se_5$ and 0.97 at $\mu = 0.1\ eV$ for $Sn_2Sb_2Se_5$. These values are close to unity which shows that the two materials are good candidates for thermoelectric devices[40].

4. Conclusion

In summary, using the FP-LAPW method, we have investigated the structural, elastic, opto-electronic and thermoelectric properties of $Ge_2Sb_2Se_5$ and $Sn_2Sb_2Se_5$. Our main results are as follows:

(a) The calculated lattice constants and bulk modulus for the ternary compounds are in reasonable agreement with the experimental data and previous theoretical results of GST.

(b) The elastic constants have been predicted and satisfy the generalized criteria for mechanically stable crystals.

(c) The study of electronic structures allowed us to conclude that the two materials have a semiconductor behavior with a direct gap indicating that the fundamental band gap is direct (Γ - Γ)

(d) The calculated of the optical properties indicates that the two compounds have an optical gap (absorption threshold) close to the value of the electronic gap.

(f) Moreover, thermoelectric transport coefficient analysis shows that the ZT reaches its maximum for the temperature 300 °K with a value of 0.92 and for $Ge_2Sb_2Se_5$ and 0.97 for $Sn_2Sb_2Se_5$. These values are close to unity which shows that the two materials are good candidates for thermoelectric devices.

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