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Electronic Properties of Rare Earth Intermetallic Chalcogenides under Effect of Pressure

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Abstract. In this present paper, we have investigated and evaluated the electronic and structural properties of mixed rare earth chalcogenides ($SmSe_xTe_{1-x}$) and rare earth intermetallic chalcogenides ($Sm_xYb_{1-x}Te$) using Vegard's law under the effect of pressure (0.0 to 2.0 GPa). We have presented the expressions relating the lattice constant and activation energy with carrier effective mass and dielectric constant of given compound for different concentration (x). The lattice constant decreases or increases with increasing Se or Sm concentration. The activation energy of ($SmSe_xTe_{1-x}$) increases while that of ($Sm_xYb_{1-x}Te$) decreases on increasing Se and Sm concentration respectively. At ambient pressure carrier effective mass exhibit linearly increases with Se concentration except pressure 0.5–2.0 GPa. The carrier effective mass of ($Sm_xYb_{1-x}Te$) predicted that the linearly decreases with Sm concentration at lower pressure while increases as same trend at higher pressure. Finally, change in dielectric constant with concentration have shown decreases at lower pressure and increases at higher pressure for ($SmSe_xTe_{1-x}$) while only increases for ($Sm_xYb_{1-x}Te$) at all pressure. We have implemented modified relation on carrier effective mass and activation energy to obtain their respective result.

KEY WORDS: Vegard's law, intermetallic chalcogenides, carrier effective mass, activation energy, dielectric constant.

1 Introduction

Rear earth chalcogenides crystalized in B_1-type crystal structure at zero pressure. They show metallic behavour when rare earth ions are trivalent state while semiconducting at divalent state of rare earth ion [1]. Outermost electronic configuration of samarium is $4f^6 5s^2 5p^6 5d^0 6s^2$. Under the hydrostatic pressure semiconductor-metal transition taken place in samarium chalcogenides due to delocalization of 4f electron i.e., $4f^6 5d^0$ to $4f^5 5d^1$ and change in valence from $2+$ to $3+$ [2]. Ritu Dubey et al. [3] found the phase transition pressure of SmS and their alloys ($SmS_{1-x}Se_x$) forming by the substitution of Se. The result have shown the discontinuous to continuous transition on decreasing the concentration of Se with the value of x [4].

In $Sm_{1-x}Y_xS$, a discontinuous transition is taken place at $x = 0.15$ while replacement of Yb^{2+} for Sm^{2+} does not show any valence mixing and substitution of (La^{3+} for Sm^{2+} or Sb^3 for S^2) gives a weak, regular transition to mixed valence [5]. $Sm_{1-x}Y_xS_{0.78}Se_{0.22}$ compounds was obtained using ball-milling and hot pressing. $Sm_{1-x}Y_xS_{0.78}Se_{0.22}$ exhibited a reduced minimum thermal conductivity of 1.26 W/(m K) in comparision to original SmS. Yttrium doping was then introduced to $Sm_{1-x}Y_xS_{0.78}Se_{0.22}$ to modify the carrier concentration. The carrier concentration and electrical conductivity increased with higher Y content [6]. Pseudobinary alloy system $TmSe_{1-x}Te_x$ shows the semiconductor-metal transition under pressure due to change in valency of Tm atom as a result single-crystal $TmSe_{1-x}Te_x$ at low temperature was investigated [7]. Energy gap of TmTe is about 300 meV where localized Tm^{2+} i.e., $4f^{13}$ level is lies between p band as filled anion and $5d6s$ band as empty cation. This energy gap goes on decreasing due to substitution of Se and becomes 40 meV for $TmSe_{0.60}Te_{0.40}$. $TmSe_{1-x}Te_x$ is ferromagnetic in the range ($0.1 \leq x \leq 0.18$) having critical temperature 1.8–3.7 K while antiferromagnetic in the range ($0.4 \leq x \leq 1$) having critical temperature 0.2–0.3 K [8].

Semiconducting to metallic transition is taken place in the range ($0.2 < x < 0.5$) for $TmSe_{1-x}Te_x$ similar to first order semiconductor-metal transition in SmS having energy gap 0.15 eV and lattice constant 5.9–6.0 [9]. Realistic Interaction Potential (RIP) model helps to find the elastic constants and phase transition from B_1 to B_2 under normal temperature and high pressure. In this research work we have used a theoretical model in order to determine the electrical transport properties of rare earth mixed crystal system ($SmSe_xTe_{1-x}$) and rare earth intermetallic chalcogenides ($Sm_xYb_{1-x}Te$) known as alloys of Samarium chalcogenides. This model is belonging to only two parameters namely lattice constant and activation energy for the calculation of carrier effective mass and dielectric constant.

2 Theoretical Methodology

Vegard's law [10,11] explains that, the lattice parameter of a solid solution which obtained by the substitution of new atom is always varies linearly with the concentration of substituent atoms at constant temperature such that nature of bonding is not altered i.e., similar to the constituent phase. The Substituting atoms are statistically arranged and the lattice parameter is influenced by the size of atom.

In the case of mixed crystal system ($SmSe_xTe_{1-x}$, and $Sm_xYb_{1-x}Te$), i.e., ($Sm_xYb_{1-x}Te$) is also known as rare earth intermetallic chalcogenides, virtual crystal approximation (VCA) [12] can be applied. According to this approximation: masses, force constants effective charge, activation energy and lattice constant of average ions varies linearly with concentration (x) and hence they follow the Vegard's law as,

Lattice constant (a) of mixed crystal (mixed rare earth chalcogenides) is given by

$$a = (1-x)a_1 + xa_2\,, \tag{1}$$

where a_1 is the lattice constant of pure crystal (SmTe and YbTe) and a_2 is the lattice constant of pure crystal (SmSe and SmTe), respectively.

Similarly, activation energy (ΔE) of mixed rare earth chalcogenides is given by

$$\Delta E = (1-x)\Delta E_1 + x\Delta E_2\,, \tag{2}$$

where ΔE_1 is activation energy of pure crystal (SmTe andYbTe) and ΔE_2 is activation energy of pure crystal (SmSe and SmTe), respectively.

The carrier effective mass of given mixed crystal is predicted by relation [13]

$$\frac{m_0}{m^*} = 1 + \frac{2\hbar^2}{m_0 a^2 \Delta E}\,, \tag{3}$$

where m_0 is the rest mass of electron, $\hbar = h/2\pi$ and h is Plank's constant. Equation 3 can be modified as

$$m^* = 9.1\times 10^{-31}\Big(1 + \frac{15.26}{a^2\Delta E}\Big)^{-1}. \tag{4}$$

Here a is in Å and ΔE is in eV so that m^* is in kg.

Pure rare earth chalcogenides are ionic semiconductor when rare earth atom is divalent [14]. Due to thermal motion and diffusion a vacant site is created to one of lattice ions creating coulomb field. This Coulomb field is determined by dielectric constant of lattice given by [15]

$$\varepsilon = \Big(\frac{13.53 m^*}{\Delta E\, m}\Big)^{1/2}. \tag{5}$$

Numerical value of dielectric constant is given by

$$\varepsilon = \left(\frac{1.4868m^*}{\Delta E}\right)^{1/2}. \tag{6}$$

2.1 Method of calculation

Experimentally determine value of latttice constant of pure rare earth chalcogenides SmTe and YbTe at various pressure represents a_1 in equation (1) is given in Table 1 when $x = 0$. Similarly, experimentally determine value of latttice constant of pure rare earth chalcogenides SmSe and SmTe at various pressure represents a_2 in equation (1) is given in Table 1 when $x = 1$.

Experimentally determine value of activation energy of pure rare earth chalcogenides SmTe and YbTe at various pressure represents ΔE_1 in equation (2) is given in Table 2 when $x = 0$. Similarly, experimentally determine value of activation energy of pure rare earth chalcogenides SmSe and SmTe at various pressure represents ΔE_2 in equation (2) is given in Table 2 when $x = 1$ [16].

Putting the value of a_1 and a_2 in equation (1), lattice constant of $SmSe_xTe_{1-x}$, and $Sm_xYb_{1-x}Te$ for $0 < x < 1$ is determined and presented in Table 1. Similarly, putting the value of ΔE_1 and ΔE_2 in equation (2), activation energy of $SmSe_xTe_{1-x}$, and $Sm_xYb_{1-x}Te$ for $0 < x < 1$ is determined and presented in Table 2. Finally, with the help of lattice constant and activation energy along with theoretical model given in equation (4) and equation (6), carrier effective mass (m^*) and dielectric constant (ε) of $SmSe_xTe_{1-x}$, and $Sm_xYb_{1-x}Te$ for $0 \leq x \leq 1$ is determined and presented in Tables 3 and 4, respectively.

Table 1. Lattice constant of mixed rare earth chalcogenides at different pressure

Mixed RE Chalcogenide	Pressure, P (Gpa)	Lattice constant a (Å)					
		$x = 0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1$
$SmSe_xTe_{1-x}$	0.0	6.5940	6.5152	6.4364	6.3576	6.2788	6.2000
	0.5	6.5700	6.4906	6.4112	6.3318	6.2524	6.1730
	1.0	6.5390	6.4600	6.3810	6.3020	6.2230	6.1440
	1.5	6.5050	6.4280	6.3510	6.2740	6.1970	6.1200
	2.0	6.4820	6.4072	6.3324	6.2576	6.1828	6.1080
$Sm_xYb_{1-x}Te$	0.0	6.3600	6.4068	6.4536	6.5004	6.5472	6.5940
	0.5	6.2740	6.3332	6.3924	6.4516	6.5108	6.5700
	1.0	6.1890	6.2590	6.3290	6.3990	6.4690	6.5390
	1.5	6.1470	6.2186	6.2902	6.3618	6.4334	6.5050

Table 2. Activation energy of mixed rare earth chalcogenides at different pressure

Mixed RE Chalcogenide	Pressure, P (Gpa)	Activation energy ΔE (eV)					
		$x = 0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1$
$SmSe_xTe_{1-x}$	0.0	0.3600	0.3760	0.3920	0.4080	0.4240	0.4400
	0.5	0.3500	0.3532	0.3564	0.3596	0.3628	0.3660
	1.0	0.3340	0.3256	0.3172	0.3088	0.3004	0.2920
	1.5	0.3210	0.3008	0.2806	0.2604	0.2402	0.2200
	2.0	0.1220	0.1256	0.1292	0.1328	0.1364	0.1400
$Sm_xYb_{1-x}Te$	0.0	0.4600	0.4400	0.4200	0.4000	0.3800	0.3600
	0.5	0.4050	0.3940	0.3830	0.3720	0.3610	0.3500
	1.0	0.3500	0.3468	0.3436	0.3404	0.3372	0.3340
	1.5	0.3000	0.3042	0.3084	0.3126	0.3168	0.3210

Table 3. Carrier effective mass of mixed rare earth chalcogenides at different pressure

Mixed RE Chalcogenide	Pressure, P (Gpa)	Effective mass m^* ($\times 10^{-31}$ kg)					
		$x = 0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1$
$SmSe_xTe_{1-x}$	0.0	4.6079	4.6521	4.6915	4.7264	4.7571	4.7839
	0.5	4.5272	4.4926	4.4571	4.4207	4.3835	4.3454
	1.0	4.3993	4.2863	4.1714	4.0547	3.9364	3.8164
	1.5	4.2855	4.0848	3.8752	3.6564	3.4284	3.1908
	2.0	2.2893	2.2982	2.3064	2.3128	2.3175	2.3205
$Sm_xYb_{1-x}Te$	0.0	5.0011	4.9324	4.8601	4.7823	4.6984	4.6079
	0.5	4.6509	4.6296	4.6075	4.5831	4.5564	4.5272
	1.0	4.2573	4.2859	4.3154	4.3441	4.3720	4.3993
	1.5	3.8801	3.9613	4.0434	4.1248	4.2055	4.2855

Table 4. Dielectric constant of mixed rare earth chalcogenides at different pressure

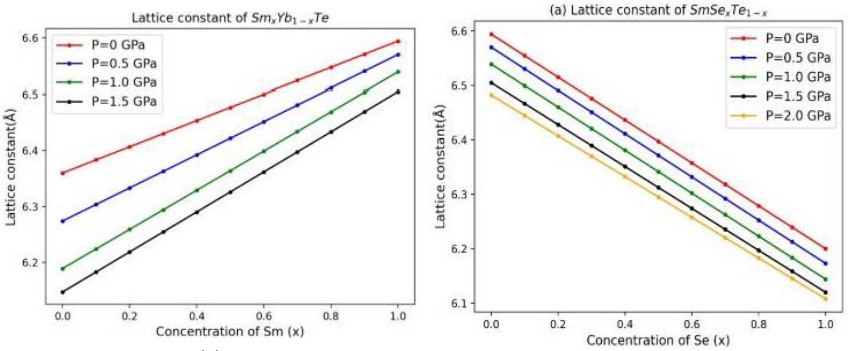
Mixed RE Chalcogenide	Pressure, P (Gpa)	Dielectric constant ε					
		$x = 0$	$x = 0.2$	$x = 0.4$	$x = 0.6$	$x = 0.8$	$x = 1$
$SmSe_xTe_{1-x}$	0.0	4.3624	4.2890	4.2183	4.1501	4.0843	4.0206
	0.5	4.3854	4.3487	4.3120	4.2753	4.2384	4.2015
	1.0	4.4253	4.4241	4.4218	4.4184	4.4139	4.4082
	1.5	4.4553	4.4934	4.5313	4.5691	4.6066	4.6437
	2.0	5.2820	5.2159	5.1519	5.0886	5.0261	4.9642
$Sm_xYb_{1-x}Te$	0.0	4.0205	4.0825	4.1479	4.2161	4.2876	4.3624
	0.5	4.1321	4.1797	4.2292	4.2799	4.3320	4.3854
	1.0	4.2526	4.2866	4.3212	4.3559	4.3906	4.4253
	1.5	4.3852	4.4001	4.4151	4.4293	4.4427	4.4553

3 Results and Discussion

The study finds the physical, electronic, and dielectric properties of mixed crystal system and rare earth intermetallic chalcogenides ($SmSe_xTe_{1-x}$ and $Sm_xYb_{1-x}Te$), under the variation of pressure. The lattice constant, activation energy, carrier effective mass and dielectric constant were methodically analyzed for pressures 0.0, 0.5, 1.0, 1.5 and 2 GPa and different compositions (x).

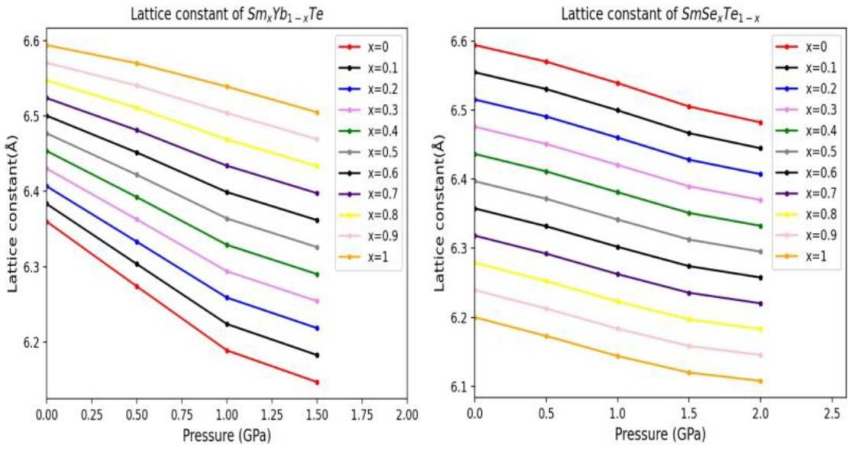
The variation of the lattice constant a with Selenium (Se) concentration x in $SmSe_xTe_{1-x}$ at different pressures 0.0 to 2.0 GPa is shown in Figures 1(a) and 2(a). The lattice constant shows a flat decrease as the concentration of Se (x) increases from 0 (pure SmTe) to 1 (pure SmSe) for all pressure. This indicate that, the substitution of larger Se^{2+} ions in SmTe by smaller Te^{2+} ions lead to a reduction of lattice constant. The lattice constant decreases steadily when pressure increases from 0.0 to 2.0 GPa for constant concentration of Se resulting compression of $SmSe_xTe_{1-x}$. The regularity of compression at different pressures shows that the arrangement keeps its structural same without phase transitions within the considered pressure range. The variation of the lattice constant a with Samarium (Sm) concentration x in $Sm_xYb_{1-x}Te$ at different pressures 0.0 to 1.5 GPa is shown in Figures 1(b) and 2(b). The lattice constant increases as the concentration of Sm (x) increases from 0 (pure YbTe) to 1 (pure SmTe) for all pressure. This indicate that, the substitution of larger Sm^{2+} ions in YbTe by smaller Yb^{2+} ions lead to the increase of lattice constant. The lattice constant decreases with increasing pressure for constant Sm concentration x resulting the reduction of inter atomic distance. The linearly variation of lattice constant shows a stable mixed phase transition with out structural change.

The variation of activation energy (ΔE) of $SmSe_xTe_{1-x}$ with concentration of Se (x) at different pressures 0.0 to 2.0 GPa as shown in Figures 3(a) and 4(a). The activation energy increases consistently with concentration of Se (x) at am-



(a) (b)

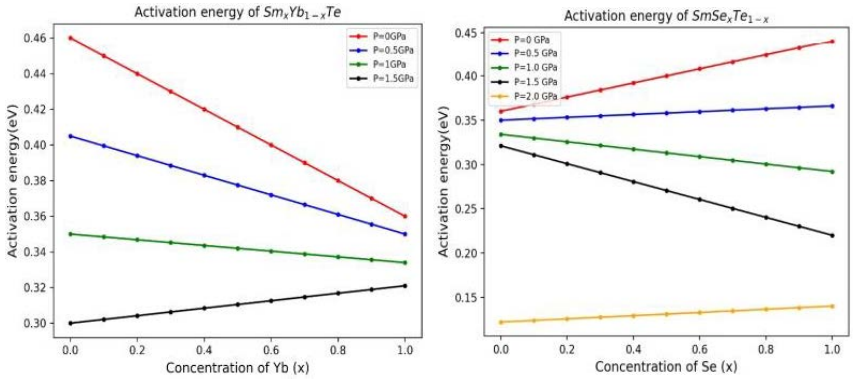
Figure 1. Variation of lattice constant with concentration (x) at given different pressure.



(a) (b)

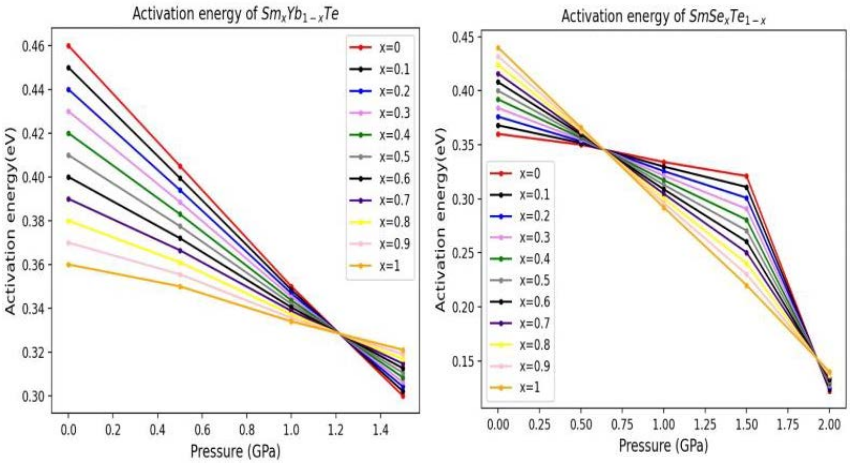
Figure 2. Variation of lattice constant with pressure at given different concentration (x).

bient pressure indicating that, substitution of Se ions for Te ions increases the energy gap, i.e., bandgap of SmSe is wider than that of SmTe. At $P = 0.5$ GPa, ΔE almost remain constant. But the activation energy decreases with increasing Se concentration, representing a probable structural or electronic change at higher pressures (2.0 GPa $> P \geq$ 1.0 GPa). This shows that pressure makes band gap contraction, reducing the excitation energy. At 2.0 GPa, ΔE again increases which advises a probable pressure-induced insulator-metal phase transition due to delocalization of carrier in the material. Increase in pressure often causes to increased hybridization of electronic state, resulting a decrease in the semiconducting gap and which makes electronic transitions easier. The varia-



(a) (b)

Figure 3. Variation of activation energy with concentration (x) at given different pressure.

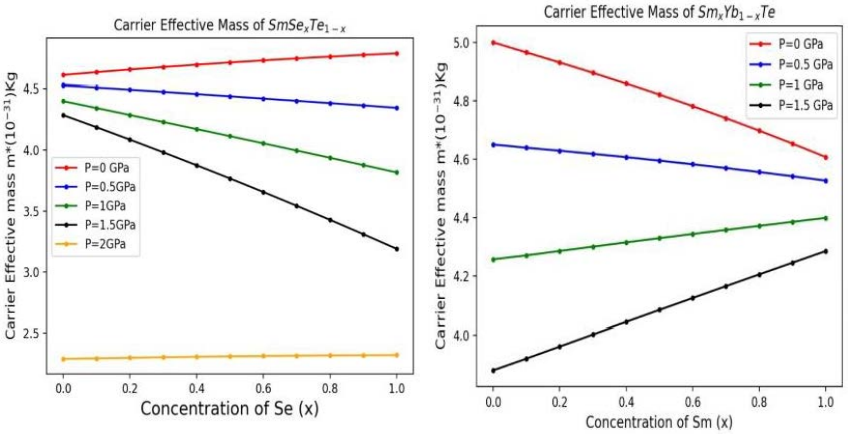


(a) (b)

Figure 4. Variation of activation energy with pressure at given different concentration (x).

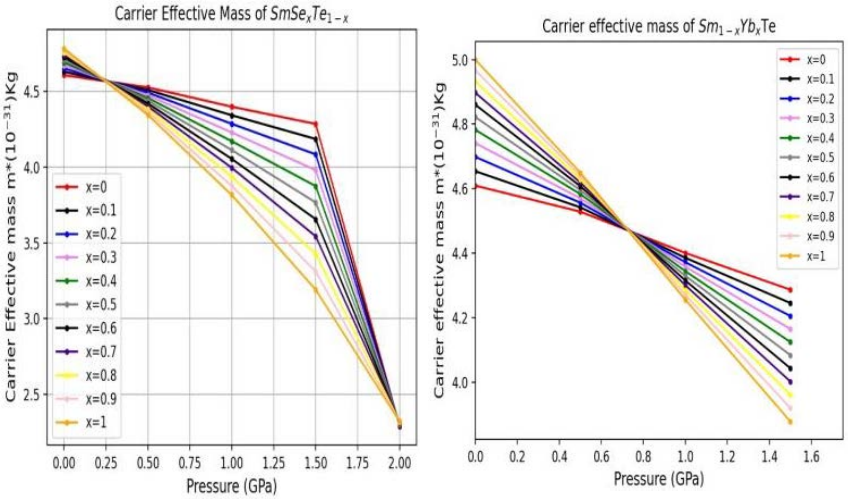
tion of activation energy (ΔE) of $Sm_xYb_{1-x}Te$ with concentration of Sm (x) at different pressures 0.0 to 1.5 GPa as shown in Figures 3(b) and 4(b). The activation energy decreases linearly and fast with concentration of Sm (x) at ambient pressure indicating that, substitution of Sm ions for Yb ions decreases the energy gap, i.e., bandgap of SmTe is wider than that of SmTe. At $P = 0.5$ GPa, ΔE decreases linearly and slow. The activation energy again decreases with increasing Se concentration, representing a probable structural or electronic change at higher pressures (1.0 GPa). This shows that pressure makes band gap contraction, reducing the excitation energy. At 1.5 GPa, ΔE again increases which advises a probable pressure-induced insulator-metal phase transition due to delocalization of carrier in the material. Increase in pressure often causes to increased hybridization of electronic state, resulting a decrease in the semiconducting gap and which makes electronic transitions easier.

The variation of carrier effective mass m^* with Selenium (Se) concentration x in $SmSe_xTe_{1-x}$ at different pressures 0.0 to 2.0 GPa as shown in Figures 5(a) and 6(a). m^* increases consistently with concentration of Se (x) at ambient pressure indicating that Se combination increases the density of states, may be due to an improved band structure. After pressure 0.5 GPa, m^* decreases upto 1.5 GPa such that decreasing rate is higher for higher pressure. This indicates pressure-induced band expansion and a reduction in the carrier's localized character. The carrier effective mass is almost constant which shows that a transition to a more delocalized electronic state at $P \geq 2.0$ GPa. The variation of carrier effective mass m^* with Samarium (Sm) concentration x in $Sm_xYb_{1-x}Te_{\ x}$ at different pressures 0.0 to 1.5 GPa as shown in Figures 5(b) and 6(b). On increasing Sm



(a) (b)

Figure 5. Variation of carrier effective mass with pressure at given different concentration (x).



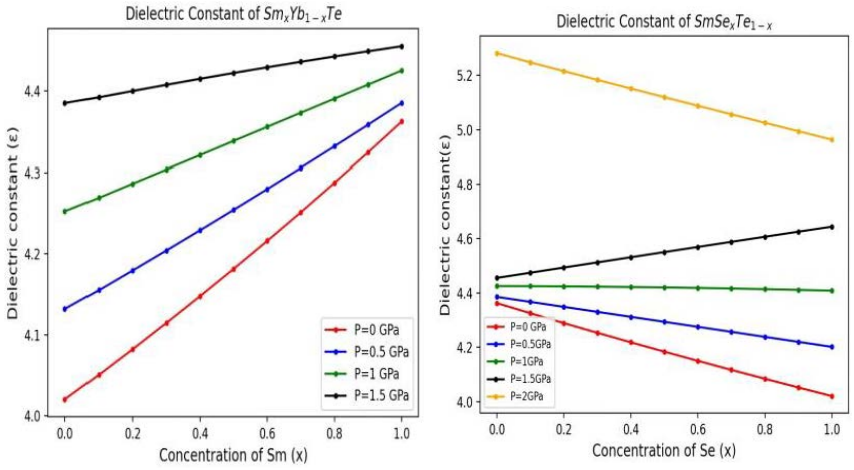
(a) (b)

Figure 6. Variation of carrier effective mass with concentration (x) at given different pressure.

concentration, increases band distribution resulting decreases in carrier effective mass up to pressure 0.5 GPa. At pressure 1.0 GPa, equilibrium state is obtained and the carrier effective mass decreases with slow rate. At high pressure, increasing Sm concentration, the band distribution increases resulting increases in carrier effective mass which advises that pressure alters the electronic states, per-

haps making localization effects. The results indicate a transition in electronic structure under pressure were adding the concentration of Sm reduces carrier effective mass at low pressures where as increases at high pressures by reason of stronger electronic correlations.

The variation of dielectric constant ε with Selenium (Se) concentration x in $SmSe_xTe_{1-x}$ at different pressures 0 to 2.0 GPa as shown in Figures 7(a) and 8(a). At pressure 0.0 to 0.5 GPa, ε decreases due to increasing ionicity and decreasing polarizability on increasing Se concentration. At pressure 1.0 GPa, ε steadies, i.e., does not depend on concentration Se ions. At $P = 2.0$ GPa, ε increases with concentration of Se ions due to greater electronic polarizability and structural phase transitions. Te is more metallic than Se and has lesser electronegativity that changes dielectric properties. At lower pressures, on increasing concentration of Se, the material become more ionic resulting decrease of dielectric constant. At higher pressures, on increasing concentration of Se, the electronic structure and bonding features change resulting an increase in the dielectric constant. The variation of Dielectric constant ε with Selenium (Se) concentration x in $Sm_xYb_{1-x}Te_{\ x}$ at different pressures 0 to 1.5 GPa as shown in Figures 7(b) and 8(b). ε increases linearly with concentration of Se for all pressure range and increasing rate is icreases on increasing pressure. Here, the dielectric constant is depended up on polarizability. Yb has a more localized $4f$-state, while Sm has a more delocalized $4f$-orbital resulting greater electronic polarization. Hence Sm concentration increases the polarizability of $Sm_xYb_{1-x}Te_{\ x}$ leading to an increase in the dielectric constant.



(a) (b)

Figure 7. Variation of dielectric constant with concentration (x) at given different pressure.

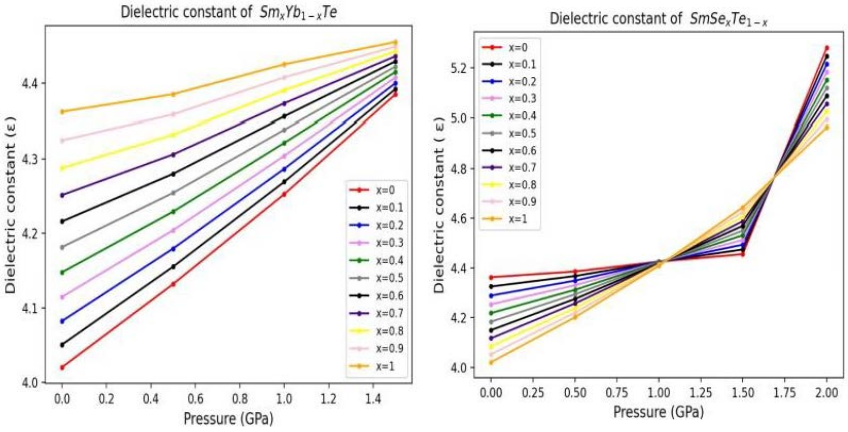


Figure 8. Variation of dielectric constant with pressure at given different concentration (x).

4 Conclusion

The result of this study concludes that the lattice constant decreases for $SmSe_xTe_{1-x}$ while increases for $Sm_xYb_{1-x}Te_x$ with increasing Se or Sm concentration, signifying stability of material without change in phase under the given pressure range. On increasing Se concentration in $SmSe_xTe_{1-x}$, the activation energy increases significant with broadening bandgap, but it decreases in $Sm_xYb_{1-x}Te_x$, suggesting bandgap narrowing. Narrowing of bandgap under pressure and electronic hybridization properties results possible insulator-metal transitions. On increasing Se concentration in $SmSe_xTe_{1-x}$, the carrier effective mass increases at ambient pressure while decreases beyond 0.5 GPa due to delocalization properties and expansion of band. On increasing Sm concentration in $Sm_xYb_{1-x}Te_x$, the carrier effective mass is initially decreases at lower pressure but at higher pressures increases due to localization effects. On increasing Se concentration in $SmSe_xTe_{1-x}$ the dielectric constant is initially decreases at lower pressures while increases at higher pressures. But in $Sm_xYb_{1-x}Te_x$, it increases constantly with Sm concentration due to greater electronic polarizability. These findings make available understandings into the pressure induced electronic and structural properties of Sm-based chalcogenides, applicable for semiconductor, optoelectronics and thermoelectric devices.

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