Volume 19, Number 2, 2026. pp. 241-248

Jordan Journal of Physics

ARTICLE

Electronic and Elastic Properties of Samarium Monochalcogenides SmX (X = S, Se and Te) at Different Pressure

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DOI: **https://doi.org/10.47011/19.2.10**

Received on: 08/02/2025; *Accepted on: 29/05/2025*

Abstract: In this work, the electronic and elastic properties of samarium monochalcogenides (SmX, where X = S, Se, and Te) are investigated using the plasma oscillation theory of solids. We present a simple relation for the plasmon energy of solids, obtained from the bond length at a given pressure in relation to the homopolar energy gap, heteropolar energy gap, average energy gap, crystal ionicity, electronic polarizability and bulk modulus of Samarium monochalcogenides. The calculated values of the homopolar energy gap, heteropolar energy gap, average energy gap, crystal ionicity, electronic polarizability, and bulk modulus at ambient pressure are found to be 2.458 eV, 5.478 eV, 6.005 eV, 0.8060, 8.93 Å^3 and 58.506 GPa respectively for SmS, 2.218 eV, 5.117 eV, 5.577 eV, 0.8150, 9.731 Å^3 and 52.855 GPa respectively for SmSe, 1.864 eV, 4.576 eV, 4.941 eV, 0.8300, 12.155 Å^3 and 44.765 GPa respectively for SmTe. The calculated results show good agreement with the available experimental and theoretical data.

Keywords: Samarium monochalcogenides, Electronic properties, Bulk modulus, Bond length, Plasmon energy.

1. Introduction

Samarium monochalcogenides (SmX, where X = S, Se, and Te) are divalent compounds and crystallize in the B1-type (NaCl) rock-salt structure below transition pressure [1]. They exhibit metallic behavior when the samarium ion is trivalent and semiconducting behavior when the samarium ion is divalent [2]. The $Sm^{2+}(4f^6)$ ion in SmX possesses a non-magnetic ground state at low temperature obeying Van Vleck paramagnetism and resulting in an insulating state [3]. The plasmon energy of valence electrons in rare-earth chalcogenides is an important parameter for computing mechanical and electronic properties. The average energy gap and bulk modulus of these materials are directly related to the plasmon energy while inversely related with crystal ionicity and polarizability [4]. The motivation for this study arises from the unique semiconducting features and wide range of practical applications of Samarium monochalcogenides in fields like nonlinear optics, electro-optic devices, glass manufacture, abrasive alloys, complex materials, lasers, phosphors, and electronics [5–8]. Spintronics is a branch of electronics that exploits spin-related effects and has gained significant attention due to its capacity for developing advanced devices that mix both transport and magnetic functionalities. As a result, magnetic semiconductors and hybrid structures merging ferromagnets with semiconductors have become major research focuses in the progress of next-generation functional semiconductor devices. These

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materials have been the subject of extensive study for many years. The physical properties of rare-earth chalcogenides are characterized by the 4*f* electrons of rare-earth element. Electronic configuration of rare-earth atom is (Xe) $4f^n5d^16s^2$ or $4f^{n+1}5d^06s^2$. The ionic radius of the rare-earth atom decreases due to the removal of a 4f electron, with values of 1.16 Å and 0.98 Å for Sm^{2+} and Sm^{3+}, respectively. Due to this decrease in ionic radius, divalent rare-earth chalcogenides behave as semiconductors, whereas trivalent compounds exhibit metallic behavior. Localized *f*-electrons determine the valency, whereas band-like *f*-electrons participate in bonding [9]. SmX compounds are ferromagnetic and do not undergo a magnetic-to-nonmagnetic transition while structural phase transition from B_1 to B_2 takes place under pressure due to promotion of electrons from $4f^6,5d^0$ to $4f^5,5d^1$ state [10]. B_1 type (NaCl) i.e., rock-salt structure is most stable and based on band structure computations, these materials show metallic behavior in all states. Spin-polarized calculations revealed that the most stable state in the B1 phase is ferromagnetic [11]. The ionic model defines a process in which electrons move from one atom to another, resulting in the formation of two closed-shell ions that primarily interact through Coulomb forces and short-range repulsion. On the other hand, the covalent model includes the sharing of electrons between atoms rather than actual charge transfer. To measure the ionicity of a crystal, Pauling [12] presented an important approach based on thermo-chemical effects, while Penn [13] later proposed a theory based on a one-electron model. Crystal ionicity is related to bulk modulus, cohesive energy, heat of formation and crystal structure. The heteropolar energy gap, homopolar energy gap, average energy gap and ionicity of binary semiconductor are calculated by using Phillips and Van Vachten (PVV) theory [14]. This theory was modified by Verma and Yadav to calculate ionic energy gap of $R^{+2}X$ and $R^{+3}X$ [15]. Bulk modulus of NaCl type rare-earth divalent and trivalent chalcogenides is calculated by using resultant valence product of anion with cation [16]. Bulk modulus of group IV and II-VI semiconductors having tetrahedral structure is calculated by using relation between plasmon energy and bulk modulus [17]. They extended the relationship between plasmon energy with bond length, homopolar energy gap, heteropolar energy gap, average energy gap, crystal ionicity, bulk modulus and electron polarizability [18]. The aforementioned electronic properties and bulk modulus of rare-earth chalcogenides are calculated only at ambient pressure. In this work, we modify the relationship of plasmon energy with bond length and plasmon energy at different pressures is calculated by using given value of bond length at different pressure. The theoretical concept is explained in Section 2 where an empirical relation of plasmon energy with bond length is developed and methodology for calculation is explained in Section 3. Results and discussion are presented in Section 4. Finally, the conclusions are presented in Section 5.

2. Theory

Theoretically, plasmon energy of compounds is [10]:

$$\hbar\omega_p = 28.8\sqrt{\frac{Z\rho}{W}} \quad (1)$$

where, ρ is the density, Z is the effective number of valence electrons, and W is the molecular weight of the compound. Using the concept that $\rho\left(\frac{W}{d^3}\right)$, the empirical relation between plasmon energy and bond length (d) can be modified as:

$$\hbar\omega_p = \mathrm{K}(d)^{-1.5} \quad (2)$$

where, K = 74.27 such that, if unit of $\boldsymbol{d}$ is in Å then unit of ($\hbar\omega_p$) is in eV. In the case of SmX, the bond length is half of the lattice constant a, and is given by:

$$\boldsymbol{d} = \frac{(\boldsymbol{a})}{\mathbf{2}} \quad (3)$$

According to the modified PVV theory [19], the average energy gap (E_{av}) of a binary crystal is expressed in terms of the heteropolar energy gap (E_{het}) and homopolar energy gap (E_{hom}) as:

$$\mathrm{E}_{\mathrm{av}}^2 = \mathrm{E}_{\mathrm{het}}^2 + \mathrm{E}_{\mathrm{hom}}^2 \quad (4)$$

where,

$$\mathrm{E}_{\mathrm{hom}} = \frac{40.468}{d^{2.5}} \quad (5)$$

and

$$\mathrm{E}_{\mathrm{het}} = \frac{130}{(Z_1Z_2)^{0.7}d^2} \quad (6)$$

where, Z_1 and Z_2 are ionic charges of Sm and X, respectively. Crystal ionicity is given by [4]:

$$\mathrm{f_i} = \frac{\mathrm{E}_{\mathrm{het}}^2}{\mathrm{E}_{\mathrm{av}}^2} \quad (7)$$

Since the homopolar energy gap (E_{hom}), heteropolar energy gap (E_{het}), average energy gap (E_{av}), crystal ionicity (f_i), electronic polarizability (α_e) and bulk modulus (B) of samarium monochalcogenides depend upon the bond length, their empirical relations with plasmon energy can be expressed as:

$$E_{het} = K_1(\hbar\omega_p)^{1.21} \quad (8)$$

$$E_{av} = K_2(\hbar\omega_p)^{1.31} \quad (9)$$

$$f_i = K_3(\hbar\omega_p)^{-0.2} \quad (10)$$

$$\alpha_e = K_4(\hbar\omega_p)^{-2.41} \quad (11)$$

$$B = K_5(\hbar\omega_p)^{1.8} \quad (12)$$

where, $K_1 = 0.2173$, $K_2 = 0.1824$, $K_3 = 1.374$, $K_4 = 5257$ and $K_5 = 0.481$ are adjusting constants.

3. Method of Calculation

The experimentally determined values of the lattice constant ***a*** of SmX at different pressures are given in Table 1 below [1]. As the pressure increases, the bond length ***d*** of SmX decreases. Consequently the plasmon energy increases.

Using relation (2) and the given values of bond length ***d***, i.e., the nearest neighbor distance between Sm and X (S, Se, and Te) at the available pressures (P), the plasmon energy ($\hbar\omega_p$) was first determined ,as presented in Table 1. Using the calculated plasmon energy and Eqs. (2), (4), (8), (9), (10), and (11), the average energy gap (EavE {av}Eav), homopolar energy gap (EhomE_{hom}Ehom), and heteropolar energy gap (EhetE_{het}Ehet) were calculated and are presented in Table 2. Subsequently, the crystal ionicity (fif_ifi), electronic polarizability (αe\alpha_eαe), and bulk modulus (B) of SmX were calculated and are presented in Table 3.

TABLE 1. Calculated values of bond length 'd' and plasmon energy ' $\hbar\omega_p$'

SmX	'P'(GPa)	'a' (Å) [13]	'd' (Å)	'$\hbar\omega_p$' (eV)	
				Theoretical [20]	Calculated
SmS	0.0	5.970	2.985	14.40	14.40
	0.2	5.962	2.981		14.42
	0.4	5.950	2.975		14.47
	0.6	5.944	2.972		14.50
SmSe	0.0	6.200	3.100	13.60	13.61
	0.5	6.173	3.086		13.70
	1.0	6.144	3.072		13.79
	1.5	6.120	3.060		13.87
	2.0	6.108	3.054		13.92
SmTe	0.0	6.594	3.297	12.39	12.41
	0.5	6.570	3.285		12.47
	1.0	6.539	3.269		12.57
	1.5	6.505	3.252		12.66
	2.0	6.482	3.241		12.73
	2.5	6.413	3.206		12.94

TABLE 2. Calculated values of E_{av}, E_{het} and E_{hom}

SmX	'P' GPa	'$\hbar\omega_p$' eV	'E_{het}' eV		'E_{av}' (eV)		'E_{hom}' eV	
			Cal.	Th. [20]	Cal.	Th. [20]	Cal	Th. [20]
SmS	0.0	14.40	5.478	5.470	6.005	6.070	2.458	2.629
	0.2	14.42	5.489		6.017		2.464	
	0.4	14.47	5.513		6.045		2.480	
	0.6	14.50	5.523		6.057		2.487	
SmSe	0.0	13.61	5.117	5.209	5.577	5.724	2.218	2.373
	0.5	13.70	5.157		5.625		2.246	
	1.0	13.79	5.199		5.673		2.270	
	1.5	13.87	5.235		5.717		2.298	
	2.0	13.92	5.258		5.743		2.310	

SmX	'P' GPa	'$\hbar\omega_p$' eV	'E_{het}' eV		'E_{av}' (eV)		'E_{hom}' eV	
			Cal.	Th. [20]	Cal.	Th. [20]	Cal	Th. [20]
SmTe	0.0	12.41	4.576	4.993	4.941	5.396	1.864	2.047
	0.5	12.47	4.603		4.973		1.882	
	1.0	12.57	4.648		5.025		1.910	
	1.5	12.66	4.688		5.072		1.936	
	2.0	12.73	4.720		5.109		1.955	
	2.5	12.94	4.814		5.219		2.016	

TABLE 3. Calculated values of f_i, α_e, and B

SmX	'P'(GPa)	'$\hbar\omega_p$' (eV)	(f_i)		'α_e' (Å^3)		B(GPa)	
			Cal.	Th. [1]	Cal.	Th. [1]	Cal.	Exp. [15]
SmS	0.0	14.40	0.8060	0.8120	8.493	8.165	58.506	60.00
	0.2	14.42	0.8057		8.461		58.673	
	0.4	14.47	0.8051		8.389		59.047	
	0.6	14.50	0.8049		8.359		59.208	
SmSe	0.0	13.61	0.8150	0.8280	9.731	9.598	52.855	52.00
	0.5	13.70	0.8140		9.577		53.486	
	1.0	13.79	0.8130		9.427		54.120	
	1.5	13.87	0.8120		9.297		54.687	
	2.0	13.92	0.8110		9.217		55.042	
SmTe	0.0	12.41	0.8300	0.856	12.155	12.489	44.765	40.00
	0.5	12.47	0.8290		12.014		45.155	
	1.0	12.57	0.8280		11.785		45.809	
	1.5	12.66	0.8270		11.584		46.401	
	2.0	12.73	0.8260		11.431		46.864	
	2.5	12.94	0.8230		10.989		48.264	

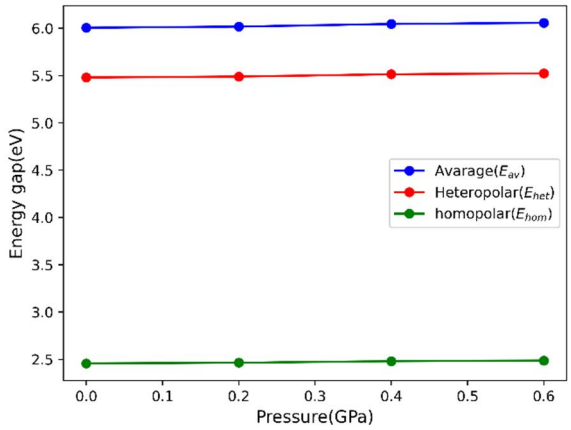
4. Results and Discussion

In this method, the bond length of SmX decreases and the plasmon energy increases with increasing pressure. Using the plasmon energy of the solid and the bond length, five empirical relations were proposed to calculate the electronic and elastic properties of samarium monochalcogenides SmX (X = S, Se, and Te). From the literature, the bond lengths of SmS at pressures of 0, 0.2, 0.4, and 0.6 GPa; SmSe at pressures of 0, 0.5, 1, 1.5, and 2 GPa; and SmTe at pressures of 0, 0.5, 1, 1.5, 2, 2.5 GPa were obtained [1].

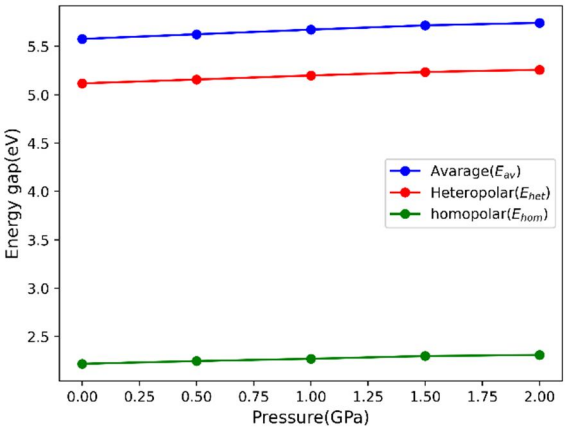
First, using Eq. (2), the plasmon energy ($\hbar\omega_p$) was calculated at the above-mentioned pressures. The electronic and elastic properties of samarium monochalcogenides are functions of plasmon energy. Using this concept, the average energy gap (**E_{av}**), heteropolar energy gap (**E_{het}**), homopolar energy gap (**E_{hom}**), crystal ionicity (**f_i**) electronic polarizability (**α_e**) and bulk modulus (**B**) were calculated. It is found that average energy gap increases slightly from nearly 6.00 eV at 0 GPa to around 6.06 eV at 0.6 GPa for SmS, 5.58 eV at 0 GPa to around 5.73 eV at 2 GPa for SmSe and 4.93 eV at 0 GPa to around 5.25 eV at 2.5 GPa for SmTe. Heteropolar energy gap increases slightly from nearly 5.48 eV at 0 GPa to 5.53 eV at 0.6 GPa for SmS, 5.12 eV at 0 GPa to around 5.26 eV at 2 GPa for SmSe and 4.57 eV at 0 GPa to around 4.80 eV at 2.5 GPa for SmTe. Homopolar energy gap increases very slowly from 2.45 eV at 0 GPa to 2.48 eV at 0.6 GPa for SmS, 2.24 eV at 0 GPa to around 2.31 eV at 2 GPa for SmSe and 1.87 eV at 0 GPa to around 2.03 eV at 2.5 GPa for SmTe. These values are highest for SmS, lower for SmSe, and lowest for SmTe. It is also found that heteropolar energy gap is greater than homopolar energy gap which indicates that samarium monochalcogenides possess a more ionic than covalent character. This trend indicates an increase in atomic size and a decrease in electronegativity from S to Te, resulting in narrower band gaps in the heavier chalcogenides due to weaker Sm–X bonding and more diffuse p orbitals. These findings further show that up to 0.6 GPa, there is no significant change in electronic band structure of SmS, indicating that SmS remains in a stable semiconducting phase. Up to 2 GPa, SmSe exhibits a slight widening of the electronic band gap and also retains its

semiconducting character. However, up to 2.5 GPa, SmTe undergoes an electronic transition, as shown in Fig. 1(a), Fig. 1(b), and Fig. 1(c).

These results are useful for tuning the electronic and optical properties of SmS, SmSe, and SmTe for pressure-dependent applications such as switches, sensors, and thermoelectric devices.



(a) SmS.



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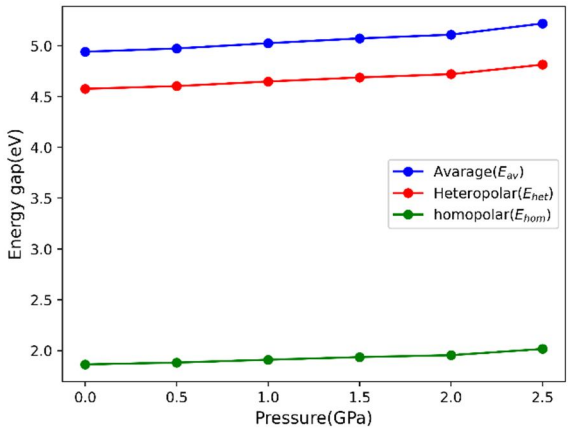


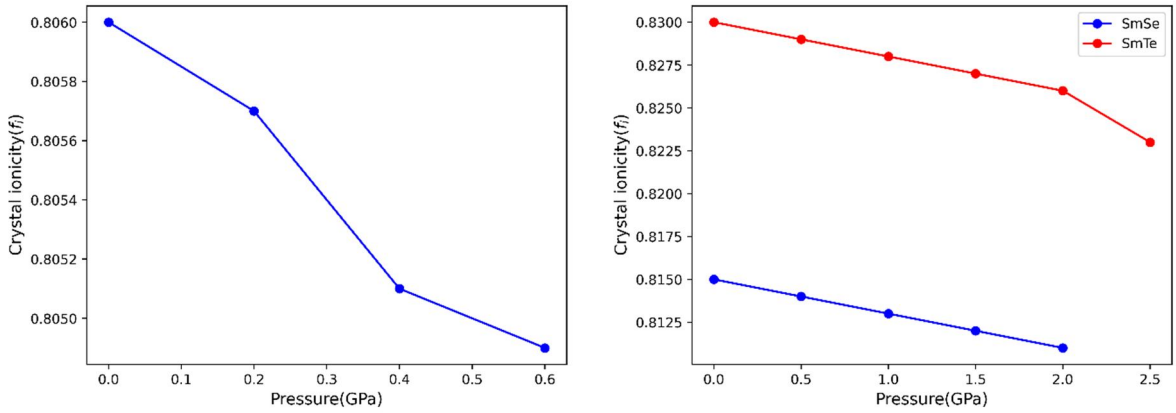
(c) SmTe.

FIG. 1. (a), (b) and (c): Graph of energy gap (average, heteropolar and homopolar) vs. pressure of SmX (X = S, Se, and Te).

Crystal ionicity $\mathbf{f_i}$ is found to decrease gradually with pressure, from 0.8060 at 0 GPa to 0.8049 at 0.6 GPa in case of SmS, as shown in Fig. 2(a). Similarly, it decreases linearly in the case of SmSe, from 0.8150 at ambient pressure to 0.8110 at 2 GPa, and in the case of SmTe, from 0.8300 at 0 GPa to 0.8230 at 2.5 GPa, as shown in Fig. 2(b).

In the case of SmS, which possesses mixed ionic-covalent bonding, external pressure increases the orbital overlap between Sm and S atoms, thereby enhancing the covalent character of the bonding.

The higher value of crystal ionicity for SmTe indicates that Te is less electronegative than Se, resulting in a more pronounced ionic character in Sm–Te bonding at low pressure. However, the linear decrease of ionicity for SmX (X = S, Se, and Te) suggests that covalent interactions become more dominant due to the increased orbital overlap between Sm and X atoms.

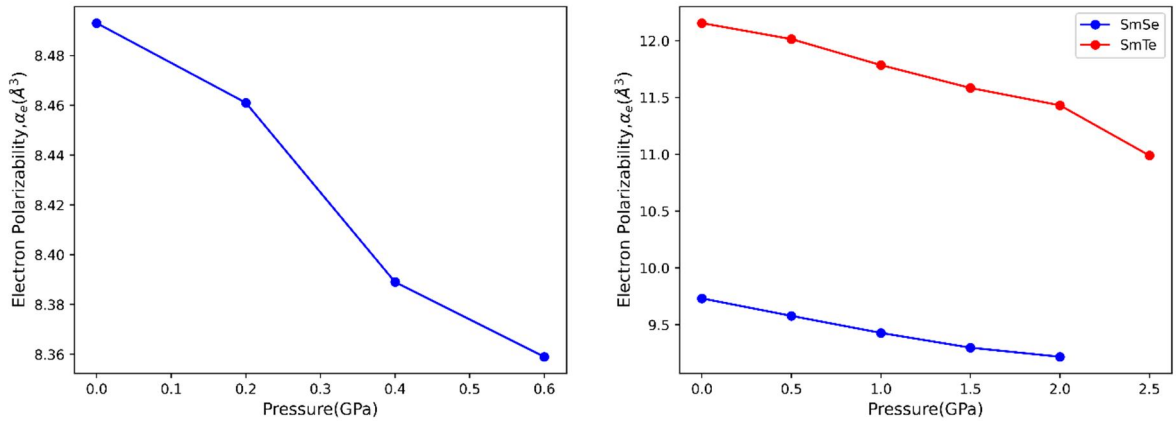


(a) SmS. (b)

FIG. 2. (a) and (b): Graph of crystal ionicity Vs Pressure of SmX (X= S, Se, and Te).

Electronic polarizability was found decrease systematically with increasing pressure, from 8.493 $Å^3$ at 0 GPa to 8.359$Å^3$ at 0.6 GPa for SmS. In the case of SmSe, the electronic polarizability decreased slowly beyond 1.5 GPa, whereas for SmTe, it decreased more rapidly beyond 2 GPa.

The value of electronic polarizability is highest for SmTe and lowest for SmS, as shown in Fig. 3(a) and Fig. 3(b). The decrease in electronic polarizability for SmX (X = S, Se, and Te) with increasing pressure indicates that higher pressure reduces the ease with which the electron cloud can be distorted. The higher electronic polarizability of SmTe indicates a more easily deformable electronic structure. Reduced polarizability results in decreased dielectric screening, which plays an important role in modulating the electronic and optical properties of the material during the semiconducting-to-metallic transition.

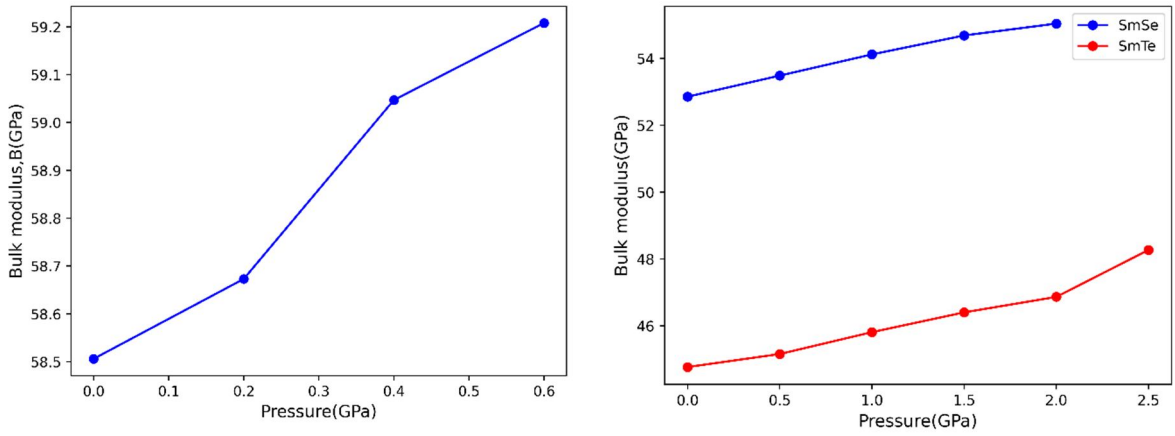


(a) SmS. (b)

FIG. 3. (a) and (b): Graph of electron polarizability vs. pressure of SmX (X = S, Se, and Te).

The bulk modulus was found to increase with pressure. Beyond 1.5 GPa, the bulk modulus increased slowly in the case of SmSe, whereas beyond 2 GPa, it increased more rapidly in the case of SmTe. The values are highest for SmS, lower for SmSe, and lowest for SmTe, as shown in Fig. 4(a) and Fig. 4(b), respectively.

The increase in bulk modulus with pressure suggests greater resistance to compression under elevated pressures. SmS exhibits a higher bulk modulus than SmSe across the entire pressure range, suggesting that SmS has a more rigid crystal structure. This behavior suggests that SmS may be better suited for applications requiring higher mechanical stability under high-pressure conditions.



(a) SmS. (b)

FIG. 4. (a) & (b): Graph of bulk modulus vs. pressure of SmX (X = S, Se, and Te).

5. Conclusion

The calculated values of homopolar energy gap, heteropolar energy gap, average energy gap, crystal ionicity, electronic polarizability and bulk modulus at ambient pressure were 2.458 eV, 5.478 eV, 6.005 eV, 0.8060, 8.93 $Å^3$and 58.506 GPa, respectively, for SmS. For SmSe, the corresponding values were 2.218 eV, 5.117 eV, 5.577 eV, 0.8150, 9.731$Å^{3,}$ and 52.855 GPa, respectively, while for SmTe they were 1.864 eV, 4.576 eV, 4.941 eV, 0.8300, 12.155 $Å^3$ and 44.765 GPa, respectively.

The results are presented in Tables 1, 2, and 3. It was concluded that the nearest-neighbor distance between Sm and X (S, Se, and Te) atoms in samarium monochalcogenides crystals plays a key role in determining the electronic and elastic properties of these compounds. The results further indicate that samarium monochalcogenides exhibit predominantly ionic rather than covalent character. Our study shows that SmS, SmSe, and SmTe possess semiconducting behavior at ambient pressure. With increasing pressure, the energy gap changes significantly, leading to a gradual transition toward metallic behavior. The increase in bulk modulus with pressure indicates that the interatomic distances decrease, resulting in stronger repulsive forces that make further compression more difficult.

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