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Optoelectronic, Elastic and Thermal Properties of Cubic Perovskite-Type SrThO₃

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The electronic structure, elastic, thermal and optical properties of the cubic strontium thorate $SrThO_3$ are calculated using the full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory with generalized gradient approximations GGA and local density approximation LDA. The modified Becke-Johnson potential (mBJ) is applied in electronic structure for calculating the energy gap. The obtained results are the Young modulus, shear modulus, the Poisson ratio, isotropic shear modulus, longitudinal, transverse and average sound velocities, the Zener anisotropy factor, the Kleinman parameter and the Debye temperature of the systems. All results are discussed and compared with the available experimental data.

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1. Introduction

Broadly speaking, perovskites are important materials for optoelectronics field, where many studies of their physical properties are part of scientific research today. They reveal much more important properties from theoretical and experimental point of view, such as ferroelectricity, superconductivity, optical and magnetic properties [1, 2].

The first synthesis of SrThO₃ by conventional solid route was reported in 1947 by Marie-Szabo [3]. Recently, Subasri et al. [4] have noted the limited thorium oxide solubility in SrO and that the formation of the pure ternary phase is not achieved. On the other hand, the samples of SrThO₃ are prepared correctly by a sol-gel technique followed by the combustion of gel [5, 6].

The properties of perovskites, such as strontium thorate SrThO₃, have attracted a lot of interest over the last decade [4–7]. The values of the Gibbs energy of SrThO₃ show that this compound is meta-stable with respect to its constituent oxides (SrO and thorium), and therefore it is difficult to eliminate the synthesis of strontium thorate. $SrThO_3$ is reported to be prepared by a conventional solid state route [8, 9], Purohit et al. [7] have studied the synthesis of nano-crystalline powders of $SrThO_3$ by a gel combustion route. To date we have the structural data [3-7]. The coefficients of linear thermal expansion [7] were also reported. Shein et al. have calculated the electronic and elastic properties of SrThO₃ in the cubic phase [10], using the FPLAPW method within GGA approximation. Though there is some experimental and theoretical work on the compound, however any detailed data concerning the optical properties of SrThO₃ is probably not available in literature.

In this work, we will contribute to the study of the structural, elastic, thermal, electronic and optical properties of $SrThO_3$ using the full potential linearized augmented plane wave (FP-LAPW) method in the density-functional theory (DFT) framework within GGA, LDA and mBJ approximation using the WIEN2K code.

2. Computational method

The first-principles calculations are performed using the full-potential augmented plane wave (FP-LAPW) method as implemented in WIEN2K code [11]. The exchange-correlation potential was calculated within the local density approximation (LDA), developed by Ceperley and Alder and parameterized by Perdew and Zunger [12, 13], as well as the generalized gradient approximation (GGA) of Perdew, Burke and Ernzerhof [14]. We have used the Tran and Blaha modified Becke-Johnson potential [15, 16] (mBJ) for calculating the electronic properties of the material. The mBJ functional cannot be used for total energy calculations but yields improved band gaps in a wide variety of materials [15–17]. In this work, we have introduced 2300 plane waves in the structure of the the cubic perovskite $SrThO_3$. A satisfactory degree of convergence is achieved by considering a number of basic functions FP-LAPW $R_{\rm MT}K_{\rm max} = 7$, where $R_{\rm MT}$ is the average radius of the Muffin-Tin spheres and K_{max} is the maximum value of the wave vector K = k + G.

The elastic coefficients were determined from firstprinciples calculations by applying a set of given homogeneous deformations with a finite value and calculating the resulting stress with respect to optimizing the internal atomic degrees of freedom [18]. A cubic crystal has three independent elastic constants, namely C_{11} , C_{12} , and C_{44} . One strain pattern, with non-zero first and fourth components, gives stresses related to all three independent elastic coefficients for the cubic system. Three positive

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and three negative amplitudes were used for each strain component with the maximum value of 0.5%, and then the elastic stiffness coefficients were determined from a linear fit of the calculated stress as a function of strain.

The study of thermal effects was done within the quasiharmonic Debye model implemented in the Gibbs program [19]. For a solid described by an energy-volume (E - V) relationship in the static approximations, the Gibbs program allows us to evaluate the Debye temperature, to obtain the Gibbs free energy G(V; P, T) and to minimize G for deriving the thermal equation of state V(P,T). Other macroscopic properties related to P and T can be also derived by using standard thermodynamic relations [19, 20].

3. Results and discussion

3.1. Structural properties

The calculated structural properties of $SrThO_3$, using the FP-LAPW method within both the LDA and the GGA approximations, are quoted in Table I along with the available experimental and theoretical data. It is evident from the table that our calculated lattice parameter is in good agreement to the experimental [21] and other theoretical results [22].The calculated lattice parameters (a, b and c) using the LDA and GGA approximations are 4.49 Å and 4.52 Å respectively, which show a good agreement with experimental values. Consequently, the GGA approximation was found to be very successful when applied to systems of perovskite $SrThO_3$ (see Fig. 1).



Fig. 1. The variation of the total energy as a function of the volume of $\rm SrThO_3$.

The lattice constants of the perovskites are also calculated by the ionic radius method, using the following relation [23]:

 $\begin{array}{l} a_0 = \alpha + \beta \left(r_{\rm Sr} + r_{\rm O} \right) + \gamma \left(r_{\rm Th} + r_{\rm O} \right), \qquad (1) \\ \text{where } \alpha = 0.06714, \ \beta = 0.4905, \ \gamma = 1.2991 \ [24], \ r_{\rm Sr} \text{ is} \\ \text{the ionic radius of Sr (1.44 Å) and } r_{\rm Th} \text{ is the ionic radius} \\ \text{of Th (0.94 Å), while } r_{\rm O} \text{ is the ionic radius of O (1.35 Å)}. \end{array}$

It is clear from the table that our lattice constants calculated by ionic radius method are 4.49 Å for SrThO₃, is in close agreement (less than 1%) with the experimental results [20–21]. Critical radius plays an important role in the activation energy of oxygen migration, ion conductivity and it also provides a guideline for doping selection. The critical radii for the compound are calculated by using the following mathematical formula [25, 26]:

$$r_{\rm c} = \frac{-r_{\rm A}^2 + \frac{3}{4}a^2 - \sqrt{2}ar_{\rm B} + r_{\rm B}^2}{2r_{\rm A} + \sqrt{2}a - 2r_{\rm B}},\tag{2}$$

$$a = 2(r_{\rm B} + r_{\rm O})t < 1, (3)$$

$$t = \frac{r_{\rm A} + r_{\rm O}}{\sqrt{2}(r_{\rm A} + r_{\rm B})}.\tag{4}$$

The values of the bulk modulus are 120.17 GPa (127.59 GPa), using GGA (LDA) approach and with a pressure derivative which is equal to 4.062.

TABLE I

Calculated, analytic and experimental values of lattice constants, volume, bulk modulus, pressure derivative of bulk modulus, band gap $E_{g,\Gamma-\Gamma}$, E_g (mBj) and critical radii r_c , tolerance factors, elastic constants, Zener anisotropy factor A, Poisson's ratio v, Kleinman parameter ζ , Young's modulus E, and shear modulus C' of SrThO₃.

Damama	Experim.	LDA	Present	Other	Analytical			
Faram.		GGA	work	work	work			
a [Å]	4.5426^{a} 4.42^{b}	4.49	4.53	4.43^{c}	4.316^{d}			
vol. $[Å^3]$		611.8017	627.1834					
B [Gpa]		127.5928	120.1704					
B'		4.1011	4.0620					
$E_{g,\Gamma-\Gamma}$		1.912	2.058	3.00^{a} 2.25^{a}				
$E_g(mBj)$		4.202	4.230					
r_c					0.653			
t				$0.780\ ^a$	0.8614			
C_{11}		141.98	209.64	197.3^{a}				
C_{12}		95.72	72.33	67.10^{a}				
C_{44}		32.59	32.18	31.90^{a}				
A		1.40	0.47	0.49^{a}				
v		0.551	0.476	0.467^{a}				
$\zeta [{ m kg/m^3}]$		0.12	0.13	0.229^{a}				
E [GPa]		78.54	116.98	113.31^{a}				
$C'[{\rm GPa}]$		23.13	68.65	65.10^{a}				

a:[21]; b:[20]; c:[3]; d:[25].

3.2. Elastic properties

For cubic system, there are three independent elastic constants (C₁₁, C₁₂ and C₄₄). Each of them represents the directional mechanical responses of the crystal for different directions of applied forces [27]. In this work, we have used the IRelast method developed by J.Morteza and implemented in the WIEN2K package [11]. The elastic constants (C_{ij}) for cubic SrThO₃ calculated using the FP-LAPW method within both LDA and GGA approximations, are summarized in Table I. Under pressure P, the calculated elastic constants are positive and satisfy the generalized elastic stability criteria [28, 29]:

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

$$\frac{1}{3} (C_{11} + C_{12} + P) > 0,$$

 $(C_{44} - P) > 0$, see Table I. (3) The bulk modulus *B* should also satisfy the criterion: $C_{12} < B < C_{11}$.

The bulk modulus B, calculated by the formula

$$B = \frac{1}{3} \left(C_{11} + 2C_{12} \right), \tag{4}$$

is similar to those obtained by LDA and GGA approximation.

The most interesting elastic constants (listed in Table II), the anisotropy factor A, Poisson's ratio v, Young's modulus E, isotropic shear modulus G, Kleinman parameter ζ and shear modulus C' can be calculated using the following relations [30]:

$$A = \frac{2C_{44}}{C_{11} - C_{12}}, \quad v = \frac{3B - 2G}{2(2B + G)},$$
$$E = \frac{9GB}{G + 3B} \quad \text{and} \quad G = \frac{G_V + G_R}{2}.$$
(5)

Here G_V is Voigt's shear modulus, corresponding to the upper bound of G values and G_R is Reuss's shear modulus, corresponding to the lower bound of G values. They can be expressed as:

$$G_{\rm V} = \frac{{\rm C}_{11} - {\rm C}_{12} + 3{\rm C}_{44}}{5},$$

$$\frac{5}{G_{\rm R}} = \frac{4}{({\rm C}_{11} - {\rm C}_{12})} + \frac{3}{{\rm C}_{44}},$$
(6)

$$\zeta = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}.$$
(7)

And shear modulus [31] is given by:

$$C' = \frac{C_{11} - C_{12}}{2}.$$
(8)

The Kleinman parameter ζ describes the relative positions of cation and anion sub lattices under volume conserving strain distortions for which positions are not fixed by symmetry.

The anisotropy factor A is equal to one for an isotropic material, while any value smaller or larger than one indicates anisotropy. We obtain that the value of the anisotropy factor A is 0.85 in the LDA (0.47 in the GGA). This indicates that our compound is anisotropic. Young's modulus E is a good indicator about the stiffness of the material. When it is higher for a given material, the material is stiffer. Poisson's ratio v provides more information for dealing with the characteristic of the bonding forces than does any of the other elastic properties. The value of the Poisson ratio v for covalent materials is small (v < 0.1), whereas for ionic materials a typical value of v is 0.25 [32]. In our calculations v is 0.551 for LDA and 0.476 for GGA. Hence, a higher ionic contribution in an inter-atomic bonding for this compound should be assumed. The shear modulus G represents the resistance to plastic deformation, while the bulk modulus Brepresents the resistance to fracture. We know that there is a criterion for B/G ratio which separates the ductility and brittleness of materials. According to Pugh's criteria [33], the critical value is 1.75, if B/G > 1.75 the material is ductile, otherwise it is brittle. For the $SrThO_3$, the B/G ratio within LDA is 3.91 and 2.69 within the GGA. Thus according to Pugh's criteria, our material is ductile. Besides, for covalent and ionic materials, the typical relations between bulk and shear modulus are: G = 1.1Band G = 0.6B, respectively. For SrThO₃ the calculated values of G/B are 0.31 within LDA and 0.37 within the GGA, indicating that the ionic bonding is suitable, which is upper than 1.75. Thus $SrThO_3$ is naturally ductile. The Kleinman parameter ζ quantifies internal strain and thus indicates the relative ease of bond bending against bond stretching. It also implies resistance against bond bending or bond angle distortion. In a system, minimizing of bond bending leads to $\zeta = 0$ and minimizing of bond stretching leads to $\zeta = 1$. In the present study, the parameter ζ is found to be 0.12 within LDA and 0.13 within GGA. It is clear that SrThO₃ shows more resistance to bond bending and bond angle distortion among the materials. The Debye temperature is a fundamental physical parameter which is closely related to many physical properties, such as specific heat and melting temperature. At low temperatures, the vibrational excitations arise solely from acoustic vibrations. Hence, at low temperatures the Debye temperature calculated from elastic constants is the same as that determined from specific heat measurements. The Debye temperature $\theta_{\rm D}$ is calculated from the elastic constants data using the average sound velocity $\vartheta_{\rm m}$, by the following common relation [34]:

$$\theta_{\rm D} = \frac{h}{k} \left[\frac{3n}{4\pi} \left(\frac{N_{\rm A} \rho}{M} \right) \right]^{\frac{1}{3}} \vartheta_{\rm m},\tag{9}$$

where h is Planck's constant, k is Boltzmann's constant, N_A is Avogadro's number, n is the number of atoms per formula unit, M the molecular mass per formula unit, $\rho = M/V$ is the density, and ϑ_m is given [35] as:

$$\vartheta_m = \left[\frac{1}{3}\left(\frac{2}{\vartheta_t^3} + \frac{1}{\vartheta_1^2}\right)\right]^{\frac{1}{3}}.$$
(10)

Here ϑ_1 and ϑ_t are the longitudinal and transverse elastic wave velocities, respectively, which are obtained from Napier's equations [36]:

$$\vartheta_1 = \left(\frac{3B+4G}{3\rho}\right)^{\frac{1}{2}}, \quad \vartheta_t = \left(\frac{G}{\rho}\right)^{\frac{1}{2}}.$$
 (11)

The calculated Debye temperature and sound velocities, as well as the density of the SrThO₃ compound are given in Table II. Our calculated ϑ_1 , ϑ_t and θ_D values are 4761.8 m/s, 2079.2 m/s and 263.9 K, respectively, within LDA, are to be compared with the values of $\vartheta_1 = 5148.1$ m/s, $\vartheta_t = 2564.8$ m/s and $\theta_D = 324.9$ K within GGA.

TABLE II

Calculated values of the isotropic shear modulus G, longitudinal sound velocity ϑ_1 , transverse sound velocity ϑ_t , average sound velocity ϑ_m and Debye temperature θ_D .

	C.TLO	ρ	ϑ_1	ϑ_{t}	ϑ_{m}	θ_{D}	
	$SrinO_3$	$[kg/m^3]$	[m/s]	[m/s]	[m/s]	[K]	
Our	^a LDA	6571.8	4761.9	2079.2	2347.9	263.93	
work	^a GGA	6660.5	5148.1	2564.8	2877.9	324.95	

^a:IRelast method

3.3. Thermodynamic properties

The thermal properties of SrThO₃ are determined in the temperature range from 0 to 1200 K, where we have applied the quasi-harmonic Debye approximation. The pressure effect is studied in the range from 0 to 15 GPa. In order to determine the structural parameters at P = 0 and T = 0, we have fitted with a numerical EOS the total energy versus primitive cell volume, and then derive the macroscopic properties as function of Pand T from standard thermodynamic relations.

In Fig. 2, we have plotted the temperature effects on the lattice parameters of $SrThO_3$ at several pressures. The lattice constant increases with increasing temperature at a given pressure. The effect of increasing temperature on the lattice parameter is just the same as that of the decreasing pressure.



Fig. 2. Variation of the lattice constant as a function of temperature at pressure of 0, 5, 10 and 15 GPa for $SrThO_3$.

On the other hand, it is noted from Fig. 3 that the bulk modulus is nearly constant from 0 to 100 K and decreases linearly with increasing temperature from T > 200 K. The effect of increasing pressure on the material is the same as the that of the decreasing temperature.

We present in Fig. 4 the variation of the thermal expansion coefficient α as function of temperature and pressure. It is shown that, at a given pressure, α increases with the



Fig. 3. Variation of the bulk modulus as a function of temperature for $SrThO_3$ at pressure of 0, 5, 10 and 15 GPa for $SrThO_3$.

increase of temperature up to 200 K. When T > 200 K, α gradually approaches a linear increase, which means that the temperature dependence of α is very small at high temperature. At 400 K and zero pressure, α is equal to 3.490×10^{-5} K⁻¹.



Fig. 4. Variation with temperature of the thermal expansion coefficient, at pressure of 0, 5, 10 and 15 GPa for $SrThO_3$.

The investigation of the heat capacity of crystals is an old topic of condensed matter physics with which illustrious names are associated [37]. We show in Fig. 5 variation of the heat capacities C_V versus temperature at 0 to 15 GPa. It is shown that when T < 600 K, the heat capacity C_V is depending on both the temperature and the pressure. When the temperature is constant, C_V decreases with the applied pressure. At high temperature (T > 600 K) C_V tends to the Dulong-Petit limit [38], which is common to all solids at high temperature. At high temperature C_V tends to approach 121.86 J mol⁻¹K⁻¹. At zero pressure and 300 K, C_V is equal to 113.41 J mol⁻¹K⁻¹.



Fig. 5. Variation with temperature of the specific heat at constant volume, C_V , at pressure of 0, 5, 10 and 15 GPa for SrThO₃.



Fig. 6. Variation with temperature of the Debye temperature, $\theta_{\rm D}$ at pressure of 0, 5, 10 and 15 GPa for SrThO₃.

Finally, in Fig. 6, we present the dependence of the Debye temperature $\theta_{\rm D}$ on temperature and pressure. It can be seen that $\theta_{\rm D}$ is nearly constant from 0 to 100 K and increases linearly with increasing temperature from T > 200 K. It is also shown that when the temperature is constant, the Debye temperature increases almost linearly with applied pressure. Our calculated $\theta_{\rm D}$ at zero pressure and zero temperature is equal to 422.58 K, which is in agreement with the value of 324 K computed accurately in terms of the elastic constants (Table II). This might be an indication that the quasi-harmonic Debye model is a very reasonable alternative to account for the thermal effects, with no expensive task in terms of computational time.

3.4. Electronic properties

The band structure, charge density and the electronic density of states are calculated with the well converged self-consistent solution of FP-LAPW, shown in Fig. 3. The band structure is calculated along the high symmetry directions of the 1st Brillouin zone, using two approximations, LDA and GGA. The zero of energy is chosen to coincide with the Fermi energy level. It is clear from Fig. 7 that, SrThO₃ is a direct band gap compound at the high point of symmetry Γ with a band gap of 4.23 eV, calculated with mBj method. In this compound, the upper valence band maximum and the lower conduction band minimum occur at Γ points of the Brillouin zone (the optical transitions are direct). The important features of the band structure for this compound are given in Table I along with the results of previous works.



Fig. 7. Energy band structure and partial density of states (PDOS) of SrThO₃ (a) LDA approximation and (b) GGA approximation .



Fig. 8. Total and partial density of states for $SrThO_3$ within LDA, GGA and mBJ approximations.

The calculated total (TDOS) and partial density of states for $SrThO_3$ is shown in Fig. 8. The overall TDOS profiles are in good agreement with previous theoretical results [10]. It is clear from the figures that the density of states can be mainly divided into four parts. The first and second part are located between -18.30 and -16 eV and between -14.80 and -11.30 eV, respectively. The first and the second region are dominated with O-2s, Sr-4p and Th-6p respectively; the third part from -3.90 to 0 eV in the valence band is mainly made from of O-2p orbitals; the forth part extending from 2.25 to 8 eV in

the conduction band. The conduction band for $SrThO_3$ consists of the Th-5f with Th-6d character. It is clear for $SrThO_3$, that the covalent bonds in the crystal are due to the mixing of oxygen 2p orbital with thorium 6d and 5f orbitals, whereas in this energy region the occupied Sr states are practically absent at the Fermi level energy.



Fig. 9. Total electron density for $SrThO_3$ in the (110) plane, calculated with GGA and LDA approximation.

Charge density maps serve as a complementary tool for achieving a proper understanding of the electronic structure of the system being studied. We have calculated the charge density of $SrThO_3$ in the (110) plane. It can be seen from Fig. 9 that most of the charge density is located in the Th-O bond direction and there is a large transfer of charge among Sr and O atoms with a very small contour among the ions, hence Sr–O bond is strongly ionic with very weak covalent nature. We also show that electrons are strongly shared and distributed along the Th–O bond. Hence, this bond is strongly covalent with the bond length of 2.31 Å.

3.5. Optical properties

In this theoretical method, the dielectric function and other optical properties can be calculated by using the momentum matrix elements. The optical properties of the cubic perovskite SrThO₃ can be calculated using complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, where $\varepsilon_1(\omega)$ is the real part and $\varepsilon_2(\omega)$ is the imaginary part of the dielectric function. It is directly related to the electronic band structure of the material and describes the absorptive behaviour.

In this section, we present in Figs. 10 and 11 the optical properties, as well as, the dielectric function, the refractive index, the absorption coefficient, and the optical conductivity of $SrThO_3$.



Fig. 10. Real and imaginary part of dielectric function of SrThO₃.

The imaginary part of dielectric function is depicted in Fig. 10. The optical band gap obtained from this function is 4.39 eV, which is close to the values obtained from the band structure. The gap was shifted closer to the experimental data due to mBJ results.

The maxima in the imaginary part of $\varepsilon_2(\omega)$ are four peaks A, B, C and D at 7.4, 5.7, 5.2 and 3.6, corresponding to the energies of 8, 9, 12 and 24 eV respectively, in the GGA approximation. The origin of these peaks lies in the inter band transitions which can be related to the density of states of the compound shown in Fig. 8. The peaks are due to the transition of electrons from 2p-O to 4d-Sr and 5f-Th states, and from 6d-Th, 4d-Sr to 5d-Th states in the conduction band. It is clear from these values that the band gap of SrThO₃ is larger than 3.1 eV. Thus it should work well in the ultraviolet (UV) region of the spectrum [39, 40]. This direct and wide band gap material could be suitable for the high frequency UV device applications.

Similarly, using mBJ-LDA and mBJ-GGA we have found three high peaks 5.2, 4.4 and 2 eV, corresponding to the energies of 6.8, 7.5, 8.5 and 12 eV. The peaks are from the interband transitions between the O-2p to Th-5d.

The high peaks in the vacuum ultraviolet energy regions indicate the strong optical activity of this material, which can be used for optoelectronic devices.

The real part of dielectric function $\varepsilon_1(\omega)$ is displayed in Fig. 10. The calculated static dielectric constant $\varepsilon_1(0)$



Fig. 11. Optical parameters of SrThO₃.

is at about 3.52 eV within GGA and 2.86 eV within LDA approximation. The static dielectric constant is very important in GGA compared to LDA. The main peak is at about 7.10 within LDA and 7.55 within GGA at 7.63 eV and 7.88 eV, respectively. Above the maximum the curve decreases and becomes flattened with small variations. It is further noted that the real part of dielectric function become negative in the energy ranges of 10.40–11.19 eV, 11.74–12.06 eV and 24.25–32.20 eV. In these ranges the photon beam is completely absorbed in the optical medium and the material shows metallic nature.

Figure 11 shows a strong absorption nature in the different parts of spectra, ranges 3.30–30 eV. Thus this material can be also used as a filter for various energies in the UV spectrum.

The knowledge of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ allows using equations

$$\alpha\left(\omega\right) = \frac{2\pi}{\lambda} K\left(\omega\right),\tag{12}$$

$$\alpha\left(\omega\right) = \frac{2\pi\omega}{c}\sqrt{\frac{-Re\left(\varepsilon\left(\omega\right)|\varepsilon\left(\omega\right)|\right)}{2}},\tag{13}$$

$$n(\omega) = \frac{1}{2} \left[\varepsilon_1(\omega)^2 + \left(\varepsilon_2(\omega)^2 \right)^{\frac{1}{2}} + \varepsilon_1(\omega) \right]^{\frac{1}{2}}, \qquad (14)$$

$$R = \left| \frac{N-1}{N+1} \right| = \frac{(n-1)^2 + K}{(n+1)^2 + K},$$
(15)

$$\sigma(\omega) = -\frac{i\omega}{4\pi}\varepsilon(\omega). \tag{16}$$

The critical point of the absorption coefficient $\alpha(\omega)$ (Fig. 11) is at 6.21 eV. The compound has strong response to the incident photons in the range 6.25–32 eV. The highest peak value, which corresponds to the maximum absorption of $\alpha(\omega)$, is at 23 eV.

The refractive index $n(\omega)$ is displayed in Fig. 11 along XX-direction. The static refractive index $n_0(\omega)$ is found to be 1.68 within LDA and 1.88 within GGA approximation. The refractive index reaches a maximum value of 2.80 within LDA and 2.92 within GGA at 7.90 eV and 7.76 eV, respectively.

The reflection coefficient is a very important parameter which characterizes the part of reflected energy at the interface of the solid. From Fig. 11, the zero frequency limit of reflectivity of SrThO₃ is found to be 0.065 within LDA and 0.093 within GGA approximation. There are high reflection peaks at energies 8.5, 10.5, 13.5 and 29 eV corresponding to the negative value of $\varepsilon_1(\omega)$.

The optical conductivity is a complex quantity. This complex quantity was also calculated and is shown in Fig. 11. From the figure it is noted that the optical conductance starts responding to the applied energy field from 5.79 eV. The good response is found in the range 5.8–32 eV. The maximum optical conductivity of the compounds is at about 23.74 eV.

4. Conclusions

We presented our results of the optoelectronic, structural, thermal and elastic properties of $SrThO_3$ in the cubic phase, calculated using the FP-LAPW method with the LDA, GGA approximations and mBJ. By comparison with other reports we confirm that theoretically predicted lattice constant and bulk modulus of this compound are in a good agreement with the available data. The independent elastic constants and their pressure derivatives are evaluated and linear pressure dependences of the bulk modulus and elastic constants are found. Through the quasi-harmonic Debye model, the dependences of the lattice constant, bulk modulus, thermal expansion parameter, heat capacity and Debye temperature on temperature and pressure have been obtained and compared successfully. Moreover, we have noticed that there is a small difference between the LDA and GGA approximation results in the most parts of the properties study. This difference is remarkable in the density of state. Consequently, we have introduced the mBj approximation that gives a correct band gap, allowing to define the correct transition in the imaginary part of dielectric function. The direct and wide band gap with the spectra of the imaginary part of the dielectric function confirm that this material is useful for optoelectronic device applications in the UV region of spectrum.

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