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Temperature dependence of the optical and lattice vibration properties in gallium arsenide

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ABSTRACT

The temperature dependence of the band gaps, refractive index, high-frequency and static dielectric constants and optical phonon frequencies in GaAs has been computed by using a pseudopotential approach. Our findings for all features of interest at given temperatures yielded values that agree with those previously reported. The variation of the features being studied here versus temperature showed a monotonic behavior. The transverse optical (TO) and longitudinal optical (LO) phonon frequencies are shifted towards low frequencies when the temperature is raised from 0 to 600 K. The change in the LO-TO splittings by raising temperature reflects the change in the ionicity character of the material under investigation.

1. Introduction

III-V family of compound semiconductors provide the materials basis for new cutting-edge classes of electronic and optoelectronic devices and have found a good deal of applications [1,2]. Particularly important member of this family is gallium arsenide (GaAs) which is a well-known material with great potential for use in different applications such as semiconductor devices, multilayer structures and so on [3]. The material of interest is a direct band-gap semiconductor with a zinc-blende crystal structure. It is used in the manufacture of devices such as microwave frequency integrated circuits, infrared light-emitting diodes, optical windows and solar cells [4–7]. Besides, it can be used as a substrate material for the epitaxial growth of other III–V semiconductors. Very recently, Yaremchuk et al. [8] have optimized and fabricated a gold-coated GaAs diffraction gratings and reported that the investigated structure can be applied to the optical refractive index sensor systems.

Like other III-V semiconductors [9,10] the physical properties of GaAs are sensitive to external influences such as pressure, temperature, external magnetic fields and strain [11–17]. These features make GaAs a strong candidate for sensors of several kinds. As a matter of fact, for semiconductors the physical properties and their temperature dependence are essential material parameters in the design and fabrication of devices. They are also important in the determination of epitaxial growth conditions [18–20]. Varying the temperature makes it possible for tuning the physical properties and in turn the frequency for generation and detection of radiations.

Previous experimental and theoretical attempts have been made to investigate the temperature dependence of some fundamental properties of semiconductor materials [9,15,21–24]. However, most of them still not well established. This has motivated us to take such a study for GaAs. In the present contribution a pseudopotential approach has been employed in order to investigate the

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Table 1
Experimental band-gap energies [29] for GaAs fixed in the fits at room temperature.

$E_{\Gamma\text{-}\Gamma}$ (eV)	$E_{\Gamma\text{-}X}$ (eV)	$E_{\Gamma\text{-}L}$ (eV)
1.42	1.81	1.72

temperature dependence of the optical properties and optical phonon frequencies in GaAs. A highly adjusted form factors in conjunction with a non-linear least-squares method are used so as to construct the potential at various temperatures ranging from 0 to 600 K. Our results are compared when possible with experiment and previous theoretical data.

2. Computational details

The present calculations are mainly based on the empirical pseudopotential method (EPM) [25]. The pseudopotential form factors (PFFs) are adjusted so as to reproduce the experimental energy band gaps of GaAs at some selected high-symmetry points in the Brillouin zone at different temperatures ranging from 0 to 600 K. The optimization of the empirical pseudopotential parameters has been made using the non-linear least-squares method as described in Refs. [26–28]. The dimension of the eigenvalue matrix is taken to be 136 × 136. The energy band gaps of GaAs at Γ, X and L high-symmetry points in the Brillouin zone fixed in the fits at room temperature are given in Table 1. Table 2 lists the final adjusted PFFs for GaAs at various temperatures in the range 0–600 K.

The refractive index (n) has been calculated using the Reddy and Anjaneyulu model [30]. The model has been preferred to other models quoted in the literature [31] because it has been reported to provide better results compared to experiment as regards n for III-V semiconductors [32,33]. The optical high-frequency and static dielectric constants, the longitudinal optical (LO) and transverse optical (TO) phonon frequencies of the material of interest are determined using the same methodology as that used by Bouarissa et al. [34].

All calculated optical parameters of interest depend on the fundamental energy band gap (E_g) which in turn depends on temperature. Thus, the knowledge of the temperature dependence of E_g allowed the determination of the optical parameters such as the refractive index, high-frequency dielectric constant, static dielectric constant, LO and TO phonon frequencies as a function of temperature.

3. Results and discussion

The variation of the direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) band gap energies as a function of temperature for GaAs is plotted in Fig. 1. Note that by raising temperature from 0 up to 600 K, all band gap energies of interest decrease monotonically and non-linearly. Generally, two mechanisms are thought to be responsible for the temperature dependence of energy band gaps. These mechanisms are the thermal expansion and the electron-phonon interaction [35–37]. The first mechanism results from the dependence of the band gap energy on the lattice parameter. The second mechanism that is due to the electron-phonon interaction has the major contribution. The behavior of the energy band gaps (Γ-Γ) and (Γ-L) of GaAs versus temperature appears to be opposite to that versus pressure [16], whereas that of the indirect band gap (Γ-X) follows the same trend as that versus pressure. Generally, this is the behavior commonly reported for direct and indirect band gap energies of binary tetrahedral semiconductors versus pressure and temperature [2,23,38,39]. At zero temperature, our results yielded a value of 1.519 eV for the fundamental direct band-gap (Γ-Γ). This value is in good accord with that of 1.517 eV reported by Lautenschlager et al. [40] who examined a large number of samples by ellipsometry.

The optical characteristics of a material medium can be described by the knowledge of the refractive index of the material in question. Thus, an accurate determination of n is very useful in the design of optical devices [31,41,42]. Furthermore, the temperature dependence of n is of fundamental interest in many optical and optoelectronic applications. For that purpose, n has been calculated using the model of Reddy and Anjaneyulu [30] as stated in Section 2. Our results regarding the variation of n as a function of temperature are displayed in Fig. 2. We observe that when the temperature is increased from 0 to 600 K, n increases from 3.17 to 3.35. The increase is monotonic. It should be noted that at a temperature of 300 K, our findings yielded a value of n = 3.24 for GaAs semiconductor material. This value deviates by less than 4% from the known value of 3.35 quoted in Ref. [43] for GaAs.

Table 2
Symmetric V_S and antisymmetric V_A pseudopotential form factors (in Ryd) for GaAs at various temperatures ranging from 0 to 600 K.

Temperature (K)	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$
0	−0.240579	0.0126	0.060453	0.067159	0.05	0.01
100	−0.239480	0.0126	0.059782	0.068588	0.05	0.01
200	−0.237322	0.0126	0.058461	0.071332	0.05	0.01
300	−0.239833	0.0126	0.059625	0.060536	0.05	0.01
400	−0.231666	0.0126	0.055067	0.078560	0.05	0.01
500	−0.228390	0.0126	0.053144	0.082742	0.05	0.01
600	−0.225005	0.0126	0.051189	0.086920	0.05	0.01

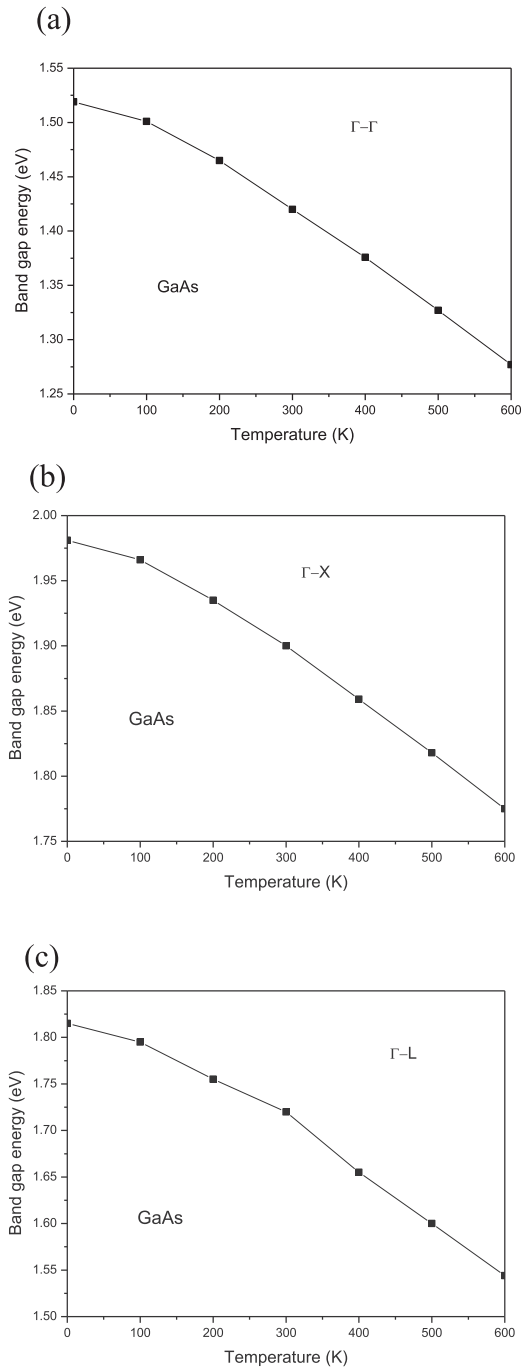

Fig. 1. (a) Direct band-gap energy (Γ-Γ) in GaAs versus temperature (b) Indirect band-gap energy (Γ-X) in GaAs versus temperature (c) Indirect band-gap energy (Γ-L) in GaAs versus temperature.

Our calculations of the optical properties have been extended to include both the high-frequency dielectric constant (ε_∞) and the static dielectric constant (ε_0). As a matter of fact, the knowledge of ε_∞ and ε_0 is needed to properly design and apply instruments. In the present contribution ε_∞ for GaAs is determined to be 10.51 at a temperature of 300 K. This value agrees to within 4% with that of 10.89 reported in Ref. [43]. The variation in ε_∞ as a function of temperature is illustrated in Fig. 3. Note that by raising the temperature on going from 0 to 600 K, ε_∞ increases from 10.07 to 11.20. The behavior is monotonic as expected from that of n versus temperature.

As far as ε_0 is concerned, our results yielded a value of about 12 for GaAs at a temperature of 300 K. This value agrees reasonably well with that of 12.9 reported in Ref. [43]. The variation in ε_0 as a function of temperature in the range 0–600 K is shown in Fig. 4. By

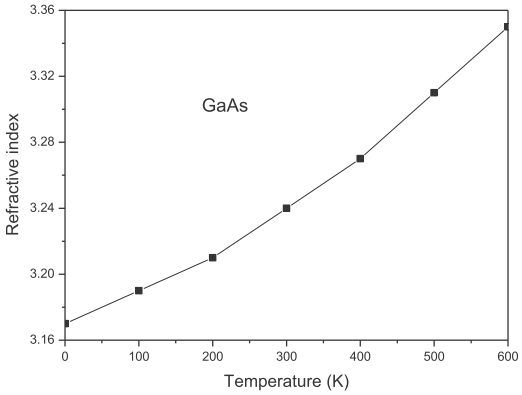

Fig. 2. Refractive index in GaAs versus temperature.

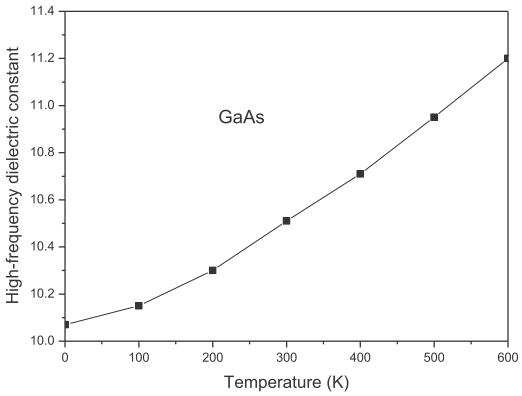

Fig. 3. High-frequency dielectric constant in GaAs versus temperature.

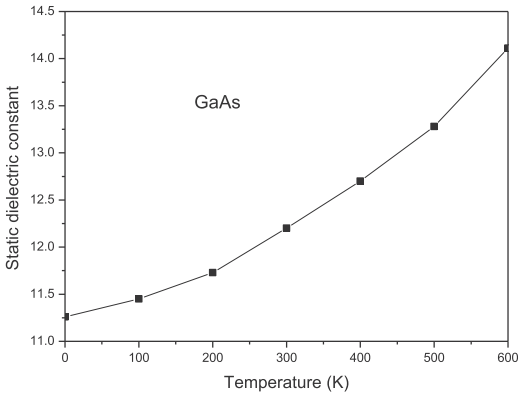

Fig. 4. Static dielectric constant in GaAs versus temperature.

observing Fig. 4 one can note that ε_0 increases from 11.26 (at 0 K) to 14.11 (at 600 K). The increase is monotonic and qualitatively similar to that of ε_∞. Accordingly, one can conclude that the increase of temperature leads to the increase of both ε_∞ and ε_0 suggesting thus that the effect of GaAs semiconductor material on a capacitor becomes higher when increasing the temperature. This effect seems to be opposite to that of pressure which has been reported for ε_∞ and ε_0 in the case of InAs semiconductor material [44].

One of the important part of condensed matter physics is the study of vibrational properties. In fact, phonons play a major role in several of the fundamental properties of condensed matter. Hence, an accurate knowledge of the lattice vibration properties leads to a better understanding of band parameters which are responsible for the optical devices efficiency [10,45–47]. In the present work, we are dealing with GAs in the zinc-blende structure. Hence, we have only two modes to be considered: the longitudinal optical (LO) and the transverse optical (TO) phonon frequencies. These frequencies are referred to in the text as ω_{LO} and ω_{TO}, respectively and are taken at the high-symmetry point Γ in the Brillouin zone. At a temperature of 300 K, our findings yielded values of $\omega_{LO} = 6.60 \times 10^{13}$ s^{-1} and $\omega_{TO} = 6.13 \times 10^{13}$ s^{-1} for GaAs semiconductor material. These values are in reasonable agreement with those of $\omega_{LO} = 5.5 \times$

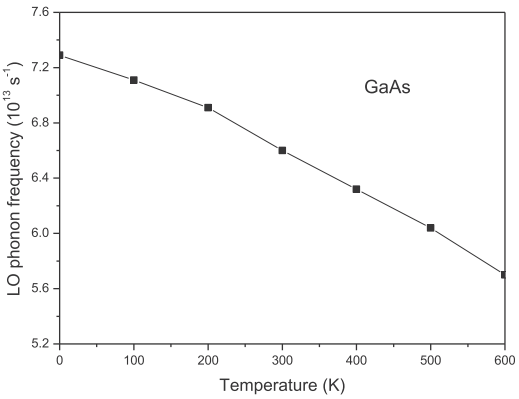

Fig. 5. LO phonon frequency in GaAs versus temperature.

10^{13} s^{-1} and $\omega_{TO} = 5.1 \times 10^{13}$ s^{-1} quoted in Ref. [48].

The temperature dependence of ω_{LO} and ω_{TO} for GaAs in the zinc-blende structure is shown in Figs. 5 and 6, respectively. By observing Fig. 5, we note that as the temperature raises from 0 up to 600 K, ω_{LO} decreases from 7.29×10^{13} s^{-1} to 5.70×10^{13} s^{-1} showing a monotonic behavior. The same qualitative behavior can be observed for ω_{TO} as seen in Fig. 6 where ω_{TO} decreases from a value of 6.90×10^{13} s^{-1} to a value of 5.08×10^{13} s^{-1} when the temperature changes from 0 to 600 K. However, it should be noted that the rate of shift of ω_{LO} towards lower frequencies (lower energies) when raising temperature is different from that of ω_{TO}. This is an indication of the variation of the LO-TO splittings when the temperature is raised which reflects the change in the ionicity of the material of interest when the temperature is changed.

4. Conclusion

In summary, the temperature dependence of direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) band-gap energies, refractive index, high-frequency and static dielectric constants, and LO and TO phonon frequencies of GaAs in the zinc-blende structure was investigated. The considered temperature range was taken from 0 up to 600 K. The calculations were performed using a pseudopotential approach. Our results were found to be in good accord with those reported in the literature for given temperatures. All features of interest were found to vary monotonically with raising temperature. The behavior of both LO and TO phonon frequencies versus temperature showed a shift of both parameters at the Γ point in the Brillouin zone towards low frequencies (low energies) with raising temperature. The LO-TO splitting was found to change with changing the temperature indicating thus the variation of the crystal ionicity character with raising temperature. The present work showed that a pseudopotential approach with highly adjusted form factors can yield good results regarding the temperature dependence of the optical properties of GaAs.

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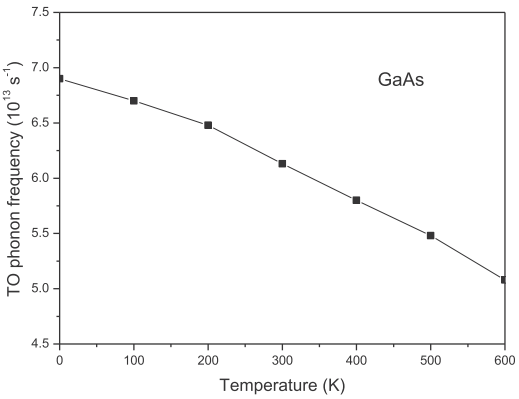

Fig. 6. TO phonon frequency in GaAs versus temperature.

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