Effect of temperature on the electronic, optical, mechanical characteristics, phonon frequencies, and sound velocities of GaP

Ibtisam F Al Maaitah*

Applied Physics Department, Faculty of Science, Tafila Technical University, P. O. Box 179, Tafila, Jordan

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We report a theoretical analysis of the electronic, optical, and mechanical properties of zinc-blende GaP semiconductor material. High-temperature impact on the interesting features has been reported. The temperature dependence of sound velocity and phonon frequencies of GaP has been determined. The pseudopotential technique has been used in our study. The current study can help in our comprehension of how temperature affects the electronic characteristics of GaP material. Our findings show generally a good accordance with the experiment. The prediction properties could be used in optoelectronic applications in the high-temperature range.

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Optoelectronics is a technologically interesting area for III-V semiconductors. Among III-V semiconductors, GaP has attracted much attention because it is one of the most promising materials for the development of optoelectronics[1]. At normal temperature, GaP, a broad band-gap compound semiconductor material, has a zinc-blende structure with an indirect band-gap[2]. Applications for electroluminescent devices are made by the material of interest. It is one of the most crucial III-V semiconductors from a commercial viewpoint[2]. For a wide range of scientific and technical applications, it is interesting to have an understanding of the material physical properties under extreme conditions[3]. Because of the significance of III-V semiconductors for technology, both their electronic and optical properties have attracted significant study in both theory and experiment[1,4-6]. The relationship between temperature and pressure and the electronic, optical, and mechanical properties of semiconductors has been studied[7-10]. For device analysis and design, a thorough understanding of the electrical, optical, and mechanical properties of III-V semiconductors is required. The examination of materials' electrical and optical properties also requires the use of excitons and lattice vibrations.

In the present study, the effect of temperature has been investigated on the band parameters, mechanical, and optical characteristics in zinc blende GaP. The high-temperature dependence of zinc-blende GaP has attracted much attention. The computations are mainly based on a pseudopotential approach. In this work, the empirical pseudopotential method (EPM) is used for the calculations[11-13].

The wave equation with crystal pseudopotential is solved in the pseudopotential-energy-band calculation. In the EPM, one has to fit the atomic form factors to experiment. The experimental value of the fundamental energy band gap E^{Γ} and polarity at normal temperature is the guidance to obtain the temperature reliance of the energy gaps. The pseudopotential form factors employed to achieve this agreement will reveal some information about the actual potential. The computations of E^{Γ} will be adapted to agree with the experimental value of E^{Γ}. The energy gap at each temperature from 0 to 500 K will then be determined using the suggested temperature dependency of the pseudopotential form factors. Moreover, the polarity is calculated by the symmetric and anti symmetric form factors (W^{s3}, and W^{a3}). After that, the mechanical parameters could be determined. Adittionally, the sound velocity could be calculated. The transverse effective charge (*TEC*) e_{T}^{*} is obtained using the relation[14]

$$e_{\mathrm{T}}^{*}=\frac{1}{2}\left[-\Delta z+\frac{8\alpha_{\mathrm{p}}}{1+\alpha_{\mathrm{p}}^{2}}\right], \tag{1}$$

where Δz is the valence difference and is given by $\Delta z=z_3-z_5$, and z is the valence of the semiconductor material. The optical phonon frequencies ω_{LO} and ω_{TO} are calculated using the Lyddane-Sachs-Teller relation[15] as

$$\frac{\omega_{\mathrm{TO}}^{2}}{\omega_{\mathrm{LO}}^{2}}=\frac{\varepsilon_{\infty}}{\varepsilon_{0}}, \tag{2}$$

* E-mail: ibtrand1@yahoo.com

with the relation[16] of

$$\omega_{\mathrm{LO}}^2-\omega_{\mathrm{TO}}^2=\frac{4\pi e_{\mathrm{T}}^{*2}e^2}{M\Omega_0\varepsilon_\infty}, \tag{3}$$

where M is twice the reduced mass and Ω_0 is the volume occupied by one atom. According to Anderson, the elastic constants of the single crystals are used to calculate the isotropic shear, Young's and bulk moduli, which are then used to derive the compressional, shear and average wave speeds[17]. Using the elastic constants and crystal density (g), as demonstrated inRef.[16], we can calculate the sound velocity as

$$v(T)=\sqrt{\frac{C_{ij}(T)}{g}}. \tag{4}$$

The micro-hardness, ionicity, *TEC*, reflectivity, and susceptibility of the GaP semiconductor compound at different values of temperature are listed in Tab.1. At normal temperature, there is a good accordance between our results and the experimental and published values[16,18]. The calculated values of micro-hardness, ionicity, *TEC*, reflectivity, and susceptibility of GaP material at high temperatures are new results and may serve as a reference for the experimental work.

Tab.1 Micro-hardness, ionicity, *TEC*, reflectivity, and susceptibility of GaP semiconductor at different temperatures

T (K)	Micro-hardness (GPa)	Ionicity	*TEC*	Reflectivity	Susceptibility
0	7.02	0.197 1	2.299 2	0.166 3	4.650 8
100	7.01	0.196 3	2.297 0	0.169 3	4.751 0
200	7.00	0.195 0	2.295 5	0.173 5	4.893 2
300	6.99 9.45[16]	0.195 4	2.294 7 2.040 0[19] 2.800 0[18]	0.181 7	5.178 2
400	6.98	0.194 6	2.292 5	0.186 8	5.361 4
500	6.96	0.194 3	2.291 7	0.202 0	5.929 4

Fig.1 shows the micro-hardness of the GaP semiconductor as a function of temperature. It is seen that the micro-hardness is decreased by increasing temperature from 0 to 500 K. There are several indications that the dislocations produced during these devices' fabrication have a significant impact on their operating performance and deterioration behavior[16]. The hardness test has been used for a very long time as a simple way to describe the mechanical behavior of solids. The interest in semiconductor hardness is mostly due to the use of semiconductors in several device applications[16]. The compressional wave speed and the shear wave speed might be calculated from the elastic constants of the single crystals by calculating the isotropic shear, Young's and bulk moduli.

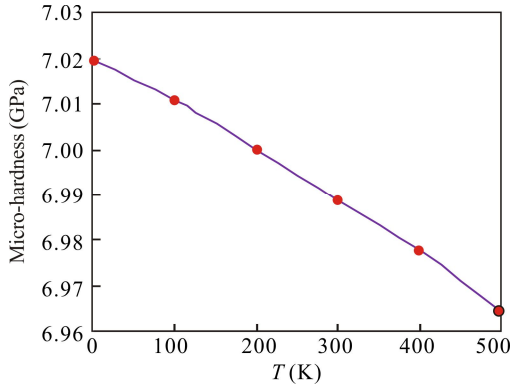

Fig.1 The micro-hardness of GaP semiconductor as a function of temperature

The compressional wave speed (C_0), shear wave speed (Sh), and average wave speed (Av) of GaP material are displayed in Fig.2. It has been found that rising temperature reduces the GaP material's compressional wave speed, shear wave speed, and average wave speed. One of the most crucial elastic parameters to be determined is the longitudinal sound velocity along the [111] direction. One can derive sound velocities from the elastic constants of the majority of binary materials. The mode of acoustic waves propagating along the [111] direction is expected to play a significant role in the applications of piezoelectric devices[20] owing to the strong coupling between the piezoelectric field and the ultrasonic wave propagation along that direction that can be estimated with a zinc blende structure of GaP.

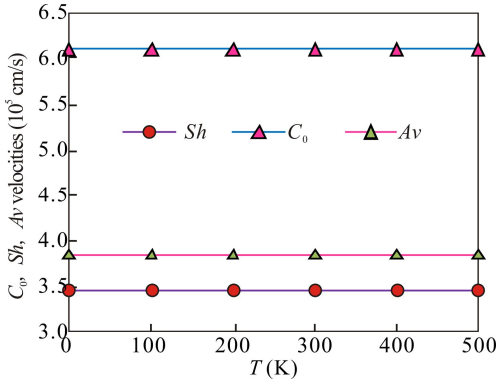

Fig.2 The compressional wave speed, shear wave speed, and average wave speed of GaP material as a function of temperature

The values of the longitudinal and transverse sound velocities propagating along the three principal directions [100] (v_{LA} and $v_{\mathrm{TA1,\,TA2}}$), [110] (v_{LA}, v_{TA1}, and v_{TA2}), and [111] (v_{LA} and $v_{\mathrm{TA1,\,TA2}}$) of GaP for various temperatures in the range of 0—500 K are provided in Tab.2 and shown in Fig.3. It is seen that the longitudinal and transverse sound velocities are slightly varied by increasing

temperature. The longitudinal and transverse sound velocity components are considered constant with the variation of temperature. This is due to the longitudinal and transverse sound velocity components depending on the elastic constants, whereas the elastic constants are slightly affected by temperature. Our calculated values of sound velocities at room temperature are in good agreement with the experimental data[16].

Tab.2 The longitudinal and transverse sound velocities (10^5 cm/s) of GaP semiconductor propagating along the three principal directions [100], [110], and [111] for various temperatures

T (K)	v_{LA_100}	$v_{T1\_T2\_100}$	v_{LA_110}	v_{TA1_110}	v_{TA2_110}	v_{LA_111}	$v_{T1\_T2\_111}$
0	5.858 0	3.718 6	6.200 0	3.115 1	3.718 6	6.309 9	3.328 4
100	5.858 4	3.718 9	6.200 4	3.115 4	3.718 9	6.310 3	3.328 7
200	5.857 8	3.718 6	6.199 8	3.115 1	3.718 6	6.309 7	3.328 4
300	5.856 6 5.830 0[16]	3.717 8 4.130 0[16]	6.198 5 6.450 0[16]	3.114 5 3.080 0[16]	3.717 8 4.130 0[16]	6.308 4 6.640 0[16]	3.327 8 3.470 0[16]
400	5.856 5	3.717 9	6.198 5	3.114 6	3.717 9	6.308 3	3.327 8
500	5.855 0	3.716 9	6.196 8	3.113 7	3.716 9	6.306 6	3.327 0

The susceptibility of GaP material as a function of temperature is shown in Fig.4. It is noticed that the susceptibility of GaP material is nonlinearly increased by increasing temperature. According to the definition of the reflection coefficient, which exposes the optical response of a material's surface, the reflection coefficient is defined as the ratio of the reflected power to the incident power. The reflection coefficient can be calculated from the refractive index of a substance. Fig.5 shows the variation of the reflection coefficient of the GaP semiconductor with temperature. It is observed that the reflection coefficient is nonlinearly increased by enhancing temperature. This is due to the ratio of the reflected power to the incident power raises with raising the temperature.

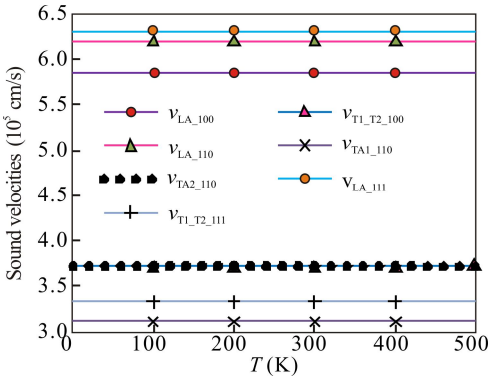

Fig.3 The longitudinal and transverse sound velocities of GaP semiconductor propagating along the three principal directions [100], [110], and [111] as a function of temperature

The ionicity of the semiconductor is linked with the anti-symmetric gap. Ionicity and polarity act as indicators of the relative charge that the cation and anion sites in the lattice are holding. Fig.6 displays the ionicity of the GaP semiconductor as a function of temperature. The ionicity is found to decrease when temperature increases from 0 to 500 K. This is because ionicity is related to the energy difference between the first and second valence bands at the X-point.

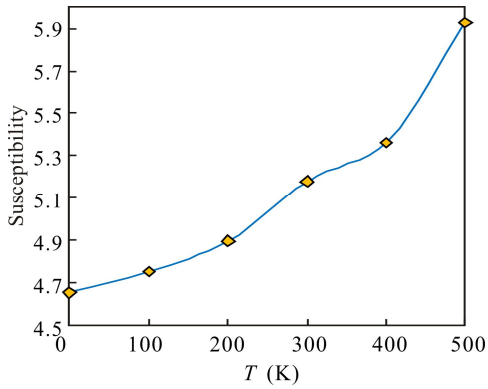

Fig.4 The susceptibility of GaP material as a function of temperature

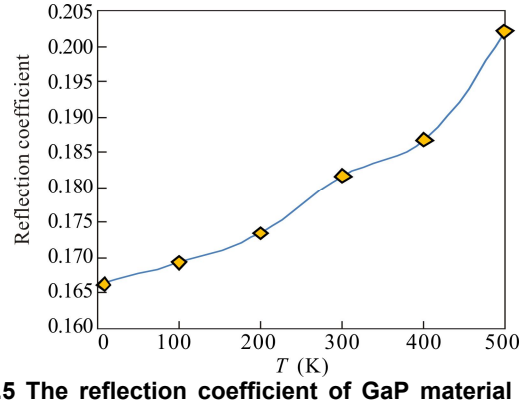

Fig.5 The reflection coefficient of GaP material as a function of temperature

An accurate description of basic vibrational properties is extremely important in the study of transport and optical properties in polar semiconductors. The longitudinal and transversal optical phonon frequencies are some examples

of the vibrational properties that are currently the focus of our discussion. The computed LO (Γ) and TO (Γ) phonon frequencies for the GaP semiconductor, as well as its temperature dependence, are displayed in Fig.7. It is observed that the longitudinal and transversal optical phonon frequencies (ω_{LO}, ω_{TO}) are decreased by increasing temperature from 0 to 500 K. This is because the optical high-frequency dielectric constant varies with different temperatures. These quantities have a relationship with the optical high-frequency dielectric constant which has a relationship with the refractive index.

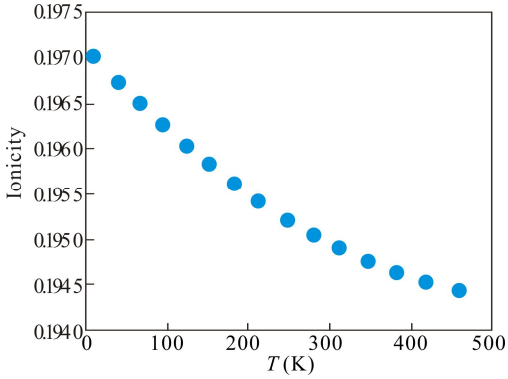

Fig.6 The ionicity of GaP semiconductor as a function of temperature

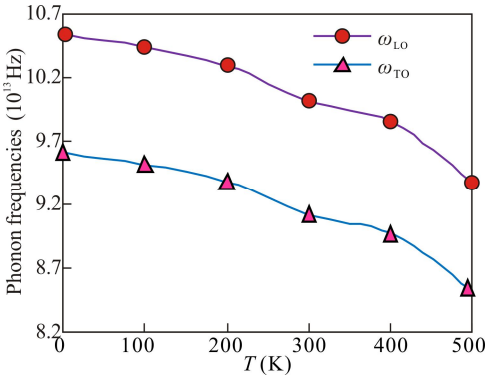

Fig.7 The longitudinal and transversal optical phonon frequencies (ω_{LO}, ω_{TO}) of GaP semiconductor as a function of temperature

The *TEC* calculation is extremely fascinating because it sheds light on the phonon activity in the infrared spectrum of materials. The *TEC* is a crucial quantity that describes the leading coupling between lattice displacement and the electrostatic field. Infrared lattice-reflection spectra can be used to deduce a theoretically prescribed *TEC*, even though it cannot be experimentally measured. Fig.8 shows the *TEC* of GaP material as a function of temperature. It is seen that the *TEC* is decreased by enhancing temperature. This may indicate that the material has more covalent bonds due to the drop in *TEC*.

The electronic, optical, mechanical characteristics, phonon frequencies, and sound velocities of the semiconductor material made of zinc-blende GaP have been

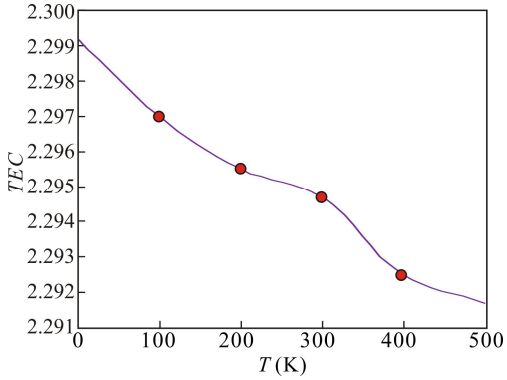

Fig.8 The *TEC* of GaP material as a function of temperature

investigated. The variation of temperature on the considered properties was taken into account. It has been stated that high temperatures have an impact on fascinating features. In our investigation, the pseudopotential method was employed. Our results demonstrated good agreement with the experimental data. The calculated results at high temperatures were new values and considered as a reference for future experimental data. The optoelectronic applications in the high-temperature region could make use of the predictive properties.

Statements and Declarations

The authors declare that there are no conflicts of interest related to this article.

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