Lattice vibration, optical, and mechanical properties of aluminum phosphide (AlP) compound under the influence of temperature

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(Received 11 January 2023; Revised 24 March 2023)

We have studied the lattice vibrations, optical and mechanical characteristics of the zinc-blende aluminum phosphide (AlP) compound. Investigations have been done into the effect of temperature on refractive index, optical dielectric constant, static dielectric constant, longitudinal and transversal sound velocities, reflectivity, susceptibility, phonon frequencies, micro-hardness, ionicity, and transverse effective charge. AlP is a wide-indirect band gap semiconductor and has a wide range of uses in high-performance optoelectronic devices, such as the manufacturing of infrared photo-detectors and light-emitting diodes. It's important to know the physical properties of semiconductor materials, like the AlP compound, to develop new technologies and devices. The calculations were carried out using the empirical pseudo-potential method (EPM). Comparative analysis with the existing experiment and other theoretical calculations reveals a satisfactory level of agreement.

Document code: A **Article ID:** 1673-1905(2023)08-0472-4

DOI https://doi.org/10.1007/s11801-023-3004-2

III-V semiconductors have a wide range of uses in high-performance optoelectronic devices[1], because of its superior electrical properties, which include high electron mobility, a straight band gap, and a low excitons binding energy[2]. The aluminum phosphide (AlP) is a III-V semiconductor with an indirect band gap[3]. Alloying this material with other binary compound semiconductors is possible. This might be beneficial for things like light-emitting diodes[4,5]. To create new technologies and devices, it is essential to comprehend the physical properties of semiconductor materials[6]. AlP is a wide-indirect band gap semiconductor[2]. Under normal conditions, AlP crystallizes in the zinc-blende structure. The material of study has a variety of uses, particularly in the manufacturing of infrared photo-detectors and light-emitting diodes[7]. To investigate the pressure-induced phonon stiffening and softening in III-V phosphide, SHINDE et al[8] used the rigid ion and deformation bond approximation models. Using the ab initio method, KHANIN et al[3] investigated the high-temperature and high-pressure thermo-physical characteristics of AlP semiconducting material. The influences of pressure and temperature give the semiconducting materials new essential features. The electronic, structural, thermoelectric, and dielectric properties of AlP with the presence of sulfur impurities with various concentrations were studied using the first-principles density functional theory (DFT) by AHMOUM et al[9]. It is essential to investigate how temperature and pressure affect the physical characteristics of semiconducting materials[10-13].

The effect of temperature on the electronic, optical, mechanical characteristics, phonon frequencies, and sound velocities of GaP was investigated by AL MAAITAH et al[14]. In this work, the temperature influence on the mechanical, optical, and lattice vibration properties of the AlP compound has been studied. The two papers studied the physical properties of the AlP and GaP by the pseudopotential method. Each application has its requirements, so we must study the properties of all materials to distinguish and classify between these materials. It is necessary to understand the material's properties can help to better predict the manufacturing outcome. The materials' properties will determine the processing conditions, storage conditions, final application, performance, and useful lifetime that the material could perform. Additionally, the material's inherent qualities might not provide the desired use, but mixing between these materials might produce beneficial properties that can be applied to a variety of significant applications. For some combinations of GaP and AlP layers, it is possible to create short-period superlattices (SLs) that have a quasi-direct band gap. These SLs are a novel family of materials with the potential for use in optical systems operating in the visible (green) wavelength range.

The empirical pseudo-potential method (EPM) has been used to calculate the electronic properties of the AlP binary compound[15]. The AlP compound is considered to be a zinc-blende structure. Only six pseudo-potential form factors are taken into consideration for the zinc blend structure[16]. To reach convergence, 65 plane waves are

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considered. Correlating the energy band gap and semiconductors' refractive indices have been the subject of numerous investigations. Herve and Vandamme's relation was used to calculate the refractive index in this paper[17].

$$n=\sqrt{1+\left[\frac{13.6}{3.4+E_{\mathrm{g}}}\right]^2}. \tag{1}$$

We could determine the sound velocity using the elastic constants and the crystal density (g), as shown in Ref.[18]

$$v(T)=\sqrt{\frac{c_{ij}(T)}{g}}. \tag{2}$$

By employing the Lyddane-Sachs-Teller relation, it can determine the optical phonon frequencies ω_{LO} and ω_{TO}[18] as follows

$$\frac{\omega_{\mathrm{TO}}^2}{\omega_{\mathrm{LO}}^2}=\frac{\varepsilon_\infty}{\varepsilon_{\mathrm{S}}}, \tag{3}$$

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

where M is the reduced mass multiplied by two and Ω_{O} is the volume that one atom takes up. The temperature-dependent transverse effective charge $e_{\mathrm{T}}^{*}(T)$ is determined from the following relation[19]

$$2e_{\mathrm{T}}^{*}(T)=-\Delta Z+\frac{8\alpha_{\mathrm{P}}(T)}{1+\alpha_{\mathrm{P}}^2(T)}, \tag{5}$$

$$\Delta Z=Z_{\mathrm{Al}}-Z_{\mathrm{P}}, \tag{6}$$

where Z_{Al} and Z_{P} are the valences of aluminum and phosphide compounds, respectively.

The longitudinal and transversal optical phonon frequencies are among the vibrational properties that are the current focus of our discussion. Fig.1 depicts how temperature affects the longitudinal and transversal phonon frequencies (ω_{LO} and ω_{TO}) of AlP material. As temperature rises from 0 to 300 K, the longitudinal and transverse phonon frequencies decrease and after 300 K they raises. A thorough description of fundamental vibrational events is required for the exploration of transport and optical characteristics in polar semiconductors. Our results and the available data agree to a reasonable degree[20]. Our findings for ω_{LO} and ω_{TO} are predictions. The following equations describe a fit of these two almost nonlinear curves in Fig.1.

$$\omega_{\mathrm{LO}}=10.844-0.000\,3T+2\times10^{-6}T^2, \tag{7}$$

$$\omega_{\mathrm{TO}}=12.228-0.000\,3T+1\times10^{-6}T^2. \tag{8}$$

The mode of acoustic waves in the [111] direction is thought to be crucial in applications of piezoelectric devices with a zinc blende structure in AlP due to the significant interaction between the piezoelectric field and the propagation of ultrasonic waves along the direction. Fig.2 shows how temperature affects the longitudinal and transverse sound velocities of an AlP semiconductor. Raising the temperature causes the components of sound velocity to slightly rise. Our findings and those in Ref.[18] demonstrate a very high level of agreement. The measurement of the longitudinal sound velocity in the [111] direction is one of the most important elastic properties. The components of the sound velocity can be used to calculate the elastic constants of the subject material at various temperatures.

The compressional wave speed and the shear wave speed can be calculated from the elastic constants of the single crystals by calculating the isotropic shear, Young's, and bulk moduli. Fig.3 shows the shear, compressibility, and average velocities of the AlP compound as a function of temperature. For the next experimental work, the sound velocity values at high temperatures could serve as a reference. The temperature dependence of the shear and average velocities demonstrates an increase in these parameters with increasing temperature and a decrease in the compressional wave speed according to the following relationships

$$Sh=4.409\,2-3\times10^{-5}T+3\times10^{-7}T^2, \tag{9}$$

$$Co=7.791\,3-5\times10^{-5}T+5\times10^{-7}T^2, \tag{10}$$

$$Av=4.903\,4-3\times10^{-5}T+3\times10^{-7}T^2. \tag{11}$$

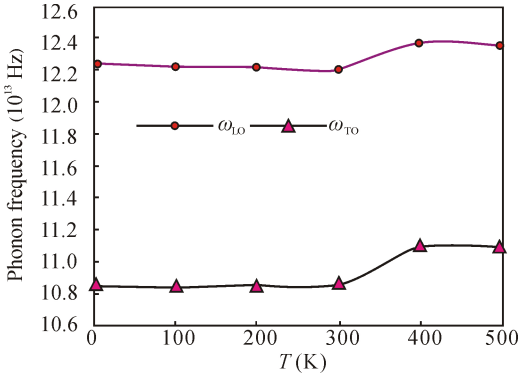


Fig.1 Longitudinal and transversal phonon frequencies of the AlP compound as a function of temperature

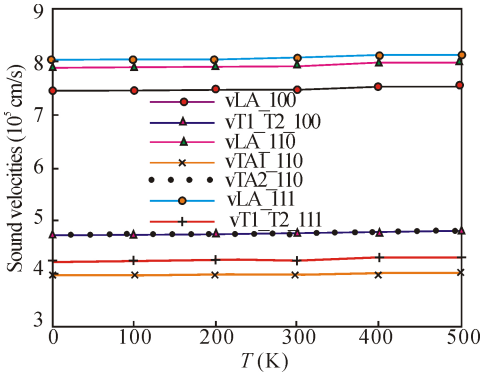


Fig.2 Temperature-dependent longitudinal and transversal sound velocities of AlP material

A significant factor determining semiconductors' optical and electrical behavior is their refractive index. Fig.4 demonstrates the refractive index, optical dielectric constant, and static dielectric constant of the AlP compound as a function of temperature. Since the energy gap is known to diminish with the refractive index of a material, it is considered that there is some connection between these two essential characteristics. It should be observed that as the temperature rises, the refractive index somewhat increases. One of the most important characteristics of semiconductors is the dielectric constant, which controls their electrical behavior. The optical dielectric constants behave similarly to the refractive index, which is

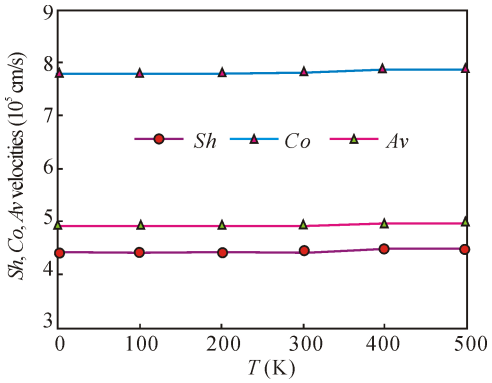


Fig.3 Variations of shear, compressibility, and average velocities of the AlP compound as a function of temperature

marginally increased by increasing temperature. Our results of the refractive index, optical dielectric constant, and static dielectric constant are in good agreement with the values that have already been published at 300 K. The behavior of the refractive index, optical dielectric constant, and static dielectric constant can be modeled by the following polynomials

$$n=2.335\ 3+3\times10^{-5}T+4\times10^{-8}T^2, \quad (12)$$

$$\varepsilon_\infty=5.453\ 6+0.000\ 1T+2\times10^{-7}T^2, \quad (13)$$

$$\varepsilon_0=6.933\ 1+0.000\ 2T-4\times10^{-7}T^2. \quad (14)$$

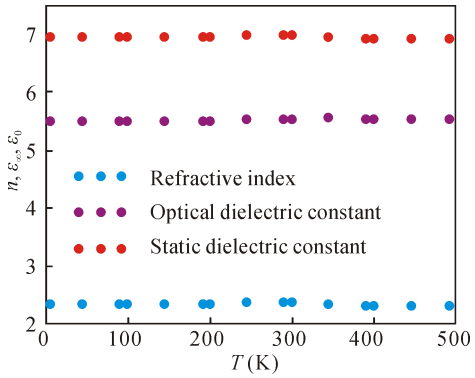


Fig.4 Temperature-dependent refractive index, optical dielectric constant, and static dielectric constant of the AlP compound

By adding an absorbing substance, reflectivity refers to the reduction in reflected power. Fig.5 illustrates how the reflectivity (R) and susceptibility (S) of AlP change with temperature. By raising the temperature, the reflectivity is increased. Modern optical communication systems highly depend on susceptibility. Increased temperature results in increasing in susceptibility. The analytical formulas are produced from the estimated reflectivity and susceptibility data as follows

$$R=0.160\ 3+4\times10^{-6}T+7\times10^{-9}T^2, \quad (15)$$

$$S=4.451\ 8+0.000\ 2T+2\times10^{-7}T^2. \quad (16)$$

The effective charge, Cauchy ratio, Born ratio, and ionicity of AlP as a function of temperature are displayed in Fig.6. The ionicity regulates the relative charge on the cation and anion sites in the lattice. The ionicity of the semiconductor and the anti-symmetric gap are related to each other. It can be seen that raising the temperature causes the ionicity to decrease. The Cauchy ratio restriction problem can be solved by incorporating many-body interaction into the pair potential. It is observed that rising temperature causes the Cauchy ratio to slightly rise. As the temperature rises, it can be seen that the Born ratio minimizes. The charge transferred from the two types of atoms to the bond is described by effective charge. It is clear that raising the temperature causes the effective charge to reduce.

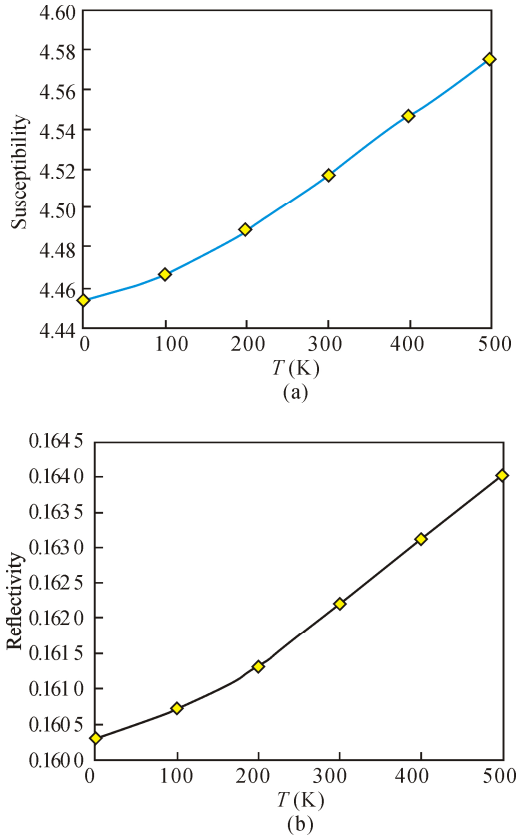
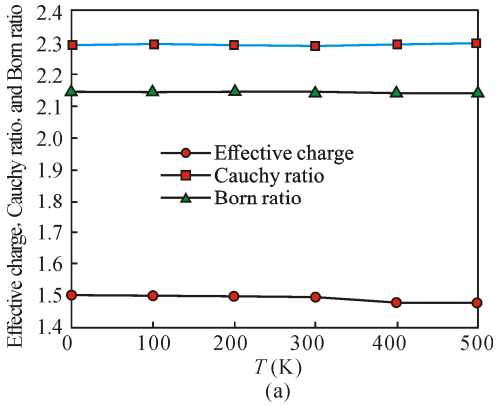


Fig.5 Temperature-dependent (a) reflectivity and (b) susceptibility of the AlP compound



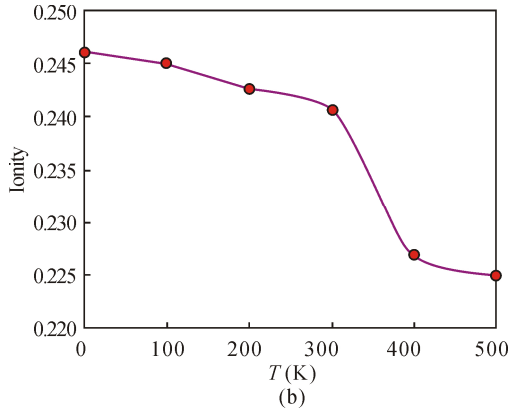


Fig.6 (a) Effective charge, Cauchy ratio, and Born ratio and (b) ionicity for the AlP compound as a function of temperature

We studied the lattice vibration properties of the zinc-blende AlP material. The mechanical properties of the AlP semiconductor were investigated. The optical characteristics of the AlP compound were determined. The impact of temperature on the studied properties has been investigated. The EPM was used to analyze these properties. The results demonstrated that the sound velocities and phonon frequencies are optimized with good agreement with the existing data within a 0.5% error. Our findings are well in accordance with other theoretical research and the available experimental data.

Ethics declarations

Conflicts of interest

The authors declare no conflict of interest.

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