



# Analysis of Band-gap and Lattice Vibration Properties Based Temperature on GaAs - Based LED

Win Tun Oo<sup>1</sup>, Tin Tin Hla<sup>2</sup> & Maung Maung Latt<sup>3</sup>

<sup>1</sup>Win Tun Oo, <sup>2</sup>Tin Tin Hla, PhD. & <sup>3</sup>Maung Maung Latt, PhD

<sup>1,2</sup> Department of Electronic Engineering, Mandalay Technological University, Myanmar

<sup>3</sup> Faculty Department of Electronic Engineering, Technological University (Taungoo), Myanmar  
Republic of the Union of Myanmar

**Abstract:** Gallium arsenide (GaAs) is a III-V direct band gap semiconductor with its zinc blende type crystal structure at ambient conditions. The phonons of GaAs material is an important to determine the important characteristics of the applications they are thermal transport, carrier mobility, and breakdown voltage. This paper describes calculation of phonon dispersion, including the effects of LO vs frequency and TO vs frequency for the infrared of the material. when the temperature is raised from 0 to 600 K, the transverse optical (TO) vs frequency and longitudinal optical (LO) vs frequency are varied according to the frequency ranges. The change in energy band gap and the LO-TO splitting by raising temperature reflects the change in the ionicity character of the material under investigation. LO VS frequency and TO vs frequency are simulated by using MATLAB software. This paper will help the researchers who analyze the LEDs.

**Keywords:** GaAs, temperature, energy band gap, transverse optical, longitudinal optical, MATLAB

## 1. INTRODUCTION

Every solid has its own characteristic energy-band structure. This variation in band structure is responsible for the wide range of electrical characteristics observed in various materials. In semiconductors and insulators, electrons are confined to a number of bands of energy, and forbidden from other regions.

The energy band gap is the energy difference between the top of the valence band and the bottom of the conduction band. electrons are able to jump from valence band to conduction band and vice versa. an electron jumps from a valence band to a conduction band, the electron acquires a minimum amount of energy for the transition. The required energy depends on the different types of the materials. Electrons can get enough energy to jump from valence band to the conduction band either by electrical excitation or photon excitation.

The electromagnetic boundary conditions which apply at semiconductor surfaces are the source of many interesting physical effects, such as surface and guided wave phonon polarizations. In these phenomena the normal modes of bulk excitations are significantly altered by the presence of a dielectric interface. III-V family of compound semiconductors provide the materials basis for new cutting-edge classes of optoelectronic devices and have found a good deal of applications [1,2]. Thermal properties and vibrational properties are determined such as by their band gap, thermal conductivity, carrier concentration, Fermi energy and phonon frequency.

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[3]. The slab modes bear the surprising property that a transverse vibration occurs at the bulk longitudinal optic (LO) frequency, while the longitudinal mode occurs at the bulk transverse optic (TO) frequency. Vibrations with this behavior were detected in the infrared absorption of thin (4000 Å) alkali-halide films. The present study represents the first identification of light scattering by such vibrational modes in a semiconductor super lattice.

One of the important parts of condensed matter physics is the study of vibrational properties. In fact, phonons is an important 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. In the present work, this paper dealing with GaAs in the zinc-blende structure. So, this work only two modes to be considered: the longitudinal optical (LO) vs frequency and the transverse optical (TO) vs phonon frequencies. These frequencies are referred to in the text as  $\omega_{LO}$  and  $\omega_{TO}$ , respectively and are taken at the high-symmetry point  $\Gamma$  in the Brillouin zone.

## 2. COMPUTATIONAL METHODS

### 2.1 Band Structure of GaAs

The energy bandgap of semiconductors decrease according to the temperature is increased. this effect is based on the linear expansion by temperature coefficient of a material. an increased lattice spacing decreases the average potential of the electrons in the material, which cause to reduce the size of the energy bandgap. this result cause the interatomic spacing increases when the amplitude of the atomic vibrations increases due to the increased thermal energy.

$$E_g = E_g(0) - \frac{\alpha T^2}{T + \beta} \tag{1}$$

Where,

$E_g$  = Band-gap energy

$T$  = Temperature (K)

$\alpha$  and  $\beta$  = Fitting Parameters (frequently called the Varshni parameters)

The change in band-gap energy vs temperature is shown with the associated result Figure 1. The eleven materials are tested for the band-gap vs temperature, among them three are illustrated in Figure 1. Based on fitting parameters, the energy gap values are shown in Table 1.

Table 1. Energy gap values based on fitting parameters

Materials	Ge	Si	GaAs
$E_g(0)$ (eV)	0.7437	1.166	1.519
$\alpha$ (meV/K)	0.477	0.473	0.541
$\beta$ (K)	235	636	204

### 2.2 Lattices vibrational phonon energies

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, the longitudinal optical (LO) and transverse optical phonon frequencies as a function of temperature.

The effects of temperature on the phonon energies measured by RS are due primarily to the thermal expansion coefficient of the crystal lattice. The dependence of phonon energy with temperature T will be

$$\omega(q, t) = \omega_0(q) \left( 1 - \frac{\alpha_L^2 a_0}{k_L k_B} T \right) \quad (2)$$

Where,

- $\omega_0(q)$  = Phonon dispersion of the harmonic linear chain,
- $a_0$  = Lattice constant
- $\alpha_L$  = Coefficient of linear expansion
- $k_L$  = Compressibility of the linear chain
- $k_B$  = Boltzmann's constant,
- $q$  = phonon wave vector.

### 3. RESULTS AND DISCUSSIONS

In Figure 1, the band-gap energy is the main factor for the temperature dependence. The inspection of the figure reveals that the temperature increases, the energy gap of the semiconductors decreases. Therefore, the energy gap is temperature dependent for the materials of the device. As the temperature increases, the energy band-gap of GaAs, Si and Ge also decreases. Among the materials, Si and Ge has the lowest energy band-gap.

The change in band-gap energy as a function of temperature is shown with the associated result Figure 1. Some materials are tested for the band-gap as a function of temperature. The band-gap energy is the main factor for the temperature dependence. When the temperature is increased, the energy gap of the semiconductor decreases. Therefore, the energy gap is temperature dependent for the materials of the device. As the temperature increases, the energy band-gap of GaAs, Si and Ge also decreases. Among the materials, Ge has the lowest energy band-gap. The energy band gap of semiconductors tends to decrease as the temperature is increased. The variation of the energy gap with temperature is the fundamental problems in semiconductor physics. It is also major problem in light sources where in devices are exposed to temperature varying conditions.

The energy band gap of semiconductors tends to decrease as the temperature is increased. This means that the interatomic spacing increases when the amplitude of the atomic vibrations increases due to the increased thermal energy. This effect is quantified by the linear expansion coefficient.

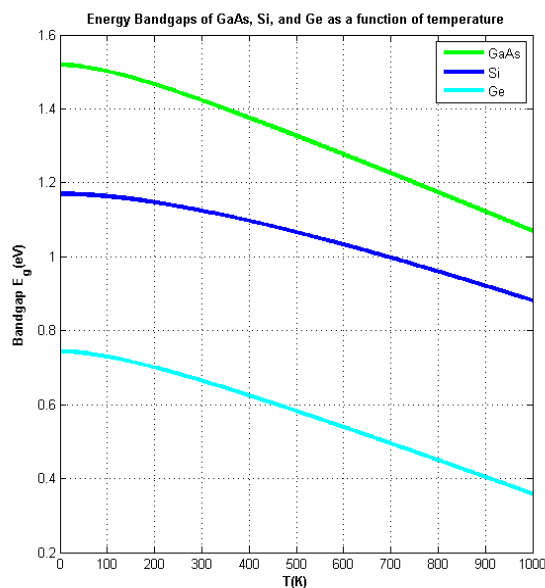


Figure 1. Energy Bandgap of GaAs, Si and Ge vs Temperature

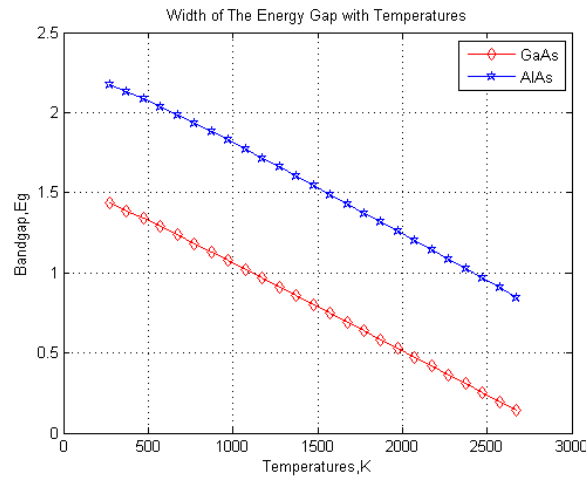


Figure 2. The Energy Gap of GaAs and AlAs as the Function of Temperature

The heterojunction structure was constructed for light sources. The material systems are designed based on bandgap simulation. Figure 2 shows the bandgap variation as the function of temperature from 0K to 300K. The band gap energy is important for material selection for solar cell design. The band gap energies of GaAs and AlAs are showed. The energy of GaAs is 1.424 eV at 300 K, after that the curve dramatically decreases to 0 eV for the increasing the temperature of 3000 K. AlAs band energy is 2.163 eV at 300 K and the energy gap decreases to 0.5 eV at 3000K. The energy of AlGaAs depends on these materials' energy variation.

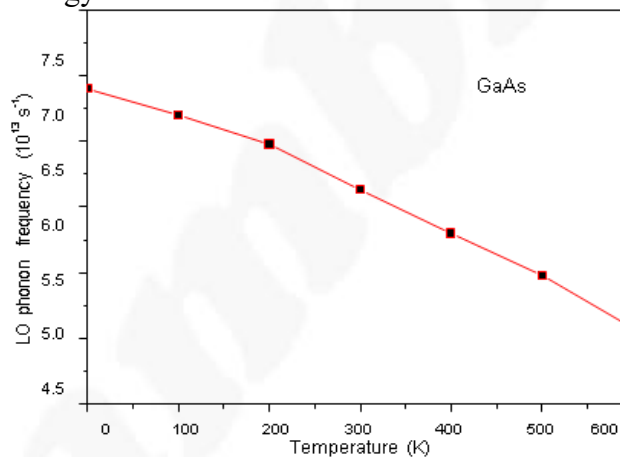


Figure 3. LO phonon frequency in GaAs versus Temperature

This expression predicts a linear decrease in phonon energy with an increase of Temperature. The temperature dependence of  $\omega_{LO}$  and  $\omega_{TO}$  for GaAs in the zinc-blende structure is shown in Figure 3 and 2 respectively. Figure 1 note that as the temperature raises from 0 up to 600 K,  $\omega_{LO}$  decreases from  $7.29 \times 10^{13} \text{ s}^{-1}$  to  $5.70 \times 10^{13} \text{ s}^{-1}$  showing a monotonic behavior. The same qualitative behavior can be observed for  $\omega_{TO}$  as seen in Figure 4 where  $\omega_{TO}$  decreases from a value of  $6.90 \times 10^{13} \text{ s}^{-1}$  to a value of  $5.08 \times 10^{13} \text{ s}^{-1}$  when the temperature changes from 0 to 600 K. However, it should be noted that the rate of shift of  $\omega_{LO}$  towards lower frequencies (lower energies) when raising temperature is different from that of  $\omega_{TO}$ . This is an indication of the variation of the LO-TO splitting when the temperature is raised which reflects the change in the ionicity of the material of interest when the temperature is changed.

The behavior of both LO and TO phonon frequencies versus temperature showed a shift of both parameters at the  $\Gamma$  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.

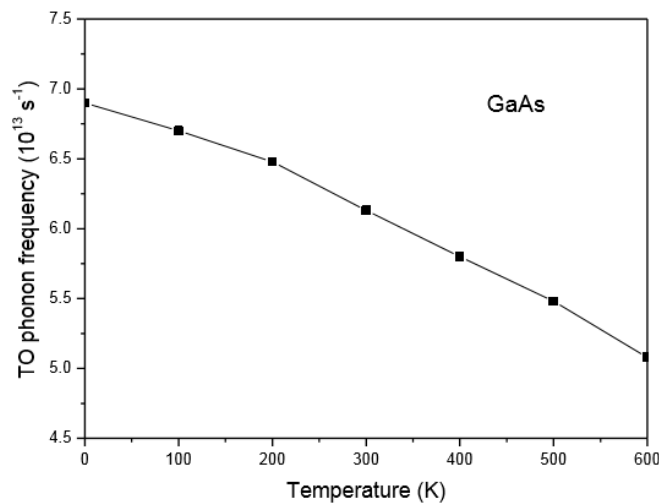


Figure 4. TO phonon frequency in GaAs versus Temperature

#### 4. CONCLUSION

In summary, the implementations for band diagram design based on the physical parameters of semiconductor materials other thermal properties and vibrational properties have been discussed. The numerical analyses are also evaluated with the help of MATLAB. Finally, these novel results in detail may be helpful to the future theoretical works of GaAs.

#### 5. ACKNOWLEDGMENT

The author would like to thank colleagues from the Department of Electronic Engineering of Mandalay Technological University (MTU).

#### 6. REFERENCES

1. L. Zhaojun, H. Tongde, L. Qiang, L. Xing, Z. Xinbo, Compound Semiconductor Materials and Devices, Morgan & Claypool Publishers, (2016).
2. Vurgaftman, J. R. Meyer, L. R. Ram-Mohan, Band parameters for III-V compound semiconductors and their alloys, J. Appl. Phys. 89 (2001) 5815-5875
3. N. G. Einspruch, W. R. Wisseman, GaAs Microelectronics, VLSI Electronics Microstructure Science, Academic Press (2014)
4. P. B. Allen, V. Heine, Theory of the temperature dependence of electronic band structures, J. Phys. C 9 (1976) 2305-2312

Zambrut Journal, Link Access;

<https://zambrut.com>

<https://zambrut.com/vibration-temperature/>

© Copyright International Journal of Zambrut | Zambrut, Inc.