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Elastic, Optical, Transport, and Structural Properties of GaAs

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Abstract

One of the major objectives of physics is to understand the physical properties of compound metals. Based on this very objective, in this chapter, we intend to review the physical as well as chemical properties of Gallium Arsenide material.

Keywords: GaAs, basic principle, physical properties, optical properties, chemical properties, physics

1. Introduction

Each time the creation and refinement of new material growth techniques give rise to the finding of new equipment. The semiconductor which has been found to be most interesting of all (when used), relates to the applications in electronic devices for instance, high speed circuits formed of group III-V compounds along with switches or amplifiers. One of the types of is the Gallium Arsenide (GaAs) [1, 2]. A III-V semiconductor that it is, its composition includes gallium which is an element of the group 3 having orthorhombic trigonal crystal structure coupled with arsenic which belongs to the group 5 and has a trigonal crystal structure. This very combination leads to interesting physical as well as chemical properties in this semiconductor [3, 4]. With different electronic band gaps, these semiconductors can, at ambient temperatures, crystalize into a zinc-blende cubic type crystal structure. Post the discovery of transistor in the year 1947, Gallium arsenide (GaAs) has presented itself as a prominent material for electronic devices. The technological importance and the need of study of Gallium arsenide (GaAs) in the last few years are due to its high melting point at 1238° C along with a density of 5.3176 g/cm³. It is obtained as a by-product from the extraction of ores of zinc and aluminum and is present at 5-15 mg/Kg in Earth's crust [5, 6].

GaAs is the basis of a worldwide industry it has a wide usage area changing from microwave frequency integrated circuits to optical windows. Among III-V semiconductors, GaAs has remained useful as a semiconductor material, widely being used in optoelectronic and microelectronic devices. Given this wide use of GaAs, the idea came to write this chapter focusing on the physical and chemical properties of this important material. While excluding the impurities present and their associated effects, the focus is on the characteristics of GaAs [7, 8].

Included in this chapter, are a few physical as well as chemical properties of gallium arsenide (GaAs) such as the crystal Structure, the direct bandgap of GaAs with its zinc blende type crystal structure, electronic structure, light-emitting

properties, electromagnetic properties, photovoltaic properties, phase transition and mechanical as well as elastic properties. The geometric structures, stabilities, and electronic properties like higher saturated electron velocity and high carrier mobility with a small dielectric constant and high resistivity. This chapter also elaborates on the thermodynamic properties of GaAs such as thermal expansion and thermal conduction.

These great properties led to the production of new and unique devices like high-efficiency light emitters, light sensors, and high-speed switching devices. The GaAs is considered as an outstanding member of the III-V semiconductor family. It has many exceptional features, especially for the recent optoelectronic industry. Hence, special focus has been laid on the examination of physical properties of this material [9–11].

2. GaAs and semiconductors direct bandgap concept

The band structure is the major part of the semiconductors. Briefly explaining it, at absolute zero, a bandgap or an energy gap separates the conduction band (lowest empty band) with the valence band (highest filled band). Therefore, at $T = 0$, electricity is not conducted by the material. The electrons are enabled to be excited into the conduction band through several processes, such as optical absorption or thermal excitation, at finite temperatures and electrical conduction is allowed as there are empty states in the valence band. Energy, in the forms of heat or photons, is released when the electrons return to the valence band [12, 13].

As mentioned in **Figure 1**, two types of bandgaps are there based on different conditions. The first one is if, over the top of the valence band, the bottom of the conduction band does not rest. As a result of this, it is called an indirect gap. Also, photon is necessary in order to provide the momentum required to reach the state in the conduction band, and the electronic transition to happen. However, in case of GaAs and other direct band type semiconductor, the bottom of the conduction band site and the top of the valence band are on top of each other, Therefore even without a change in the wave vector, the electron is able to get excited from the

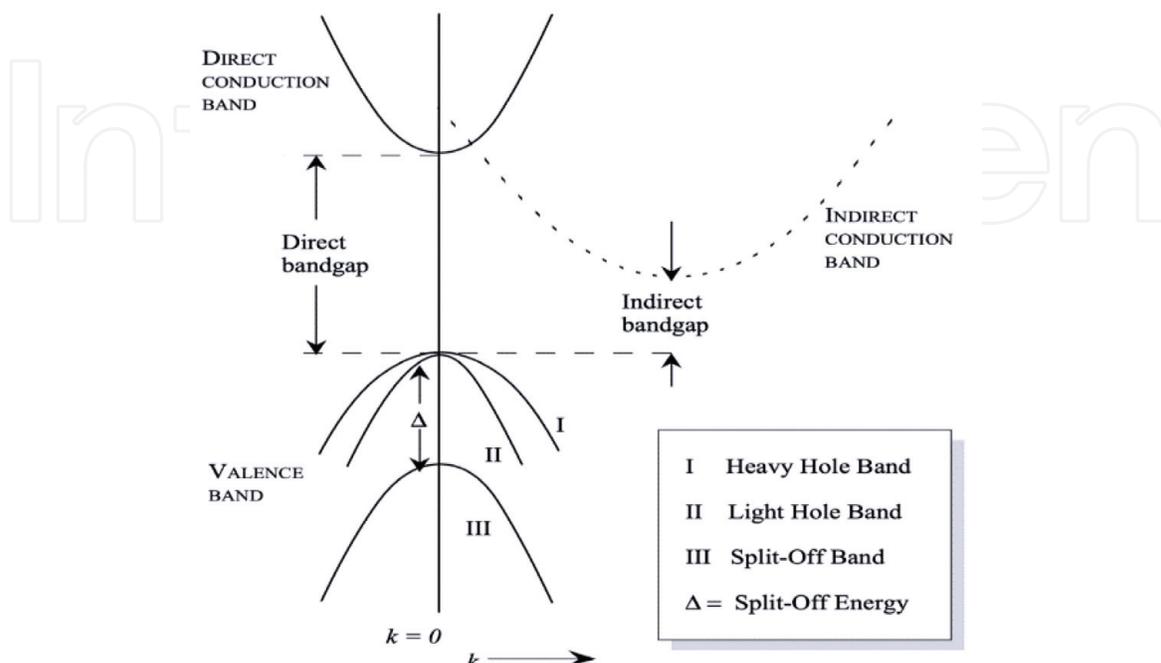


Figure 1. Schematic of the valence band, direct bandgap, and indirect bandgap conduction bands [13].

valence band. A photon on absorbing required energy is sufficient enough for this. Moreover, through the emission of a photon, transition to the valence band from the conduction band can easily be done by the electron. While no interaction of photon is required, emission of light energy of the desired wavelength of 850 nm bandgap occurs and it allows the direct band recombination of holes and electrons. In the absence of defects, the energy released by the dominant mechanism of the indirect bandgap is by photons via electromagnetic radiation. However, photons release energy in the form of heat in the case of indirect bandgap semiconductors [14–16].

Being a good optoelectronic material, direct bandgap in GaAs is considered a useful material in the field of optoelectronics and other electronic fields and is used comprehensively in semiconductor lasers as well as light-emitting diodes. Its use has also been encouraged in the making of high-efficiency solar cells, Gunn diodes, Infrared LEDs, solid-state detectors and radar systems. We have a classification of 1–3 categories depending upon the magnitude of bandgap energy of the materials, namely, narrow, mid and wide-bandgap. Of all the properties of a semiconductor, the presence of energy gap leads all others [16, 17].

Not only band-gap engineering permits the making of band diagrams that have continuous as well as arbitrary band-gap variations, but it is also considered among the strongest tools for the new semiconductor devices and materials. For a specific application, the transport properties of holes, as well as electrons, may be continuous and independent. This approach leads us to a new generation of devices having unique capabilities ranging from resonant tunneling transistors to solid-state photomultipliers. More than for any semiconductor, many band structures for GaAs are precisely known. **Figures 2 and 3** make it clear, showing 1.519 eV as the fundamental energy gap for Gallium Arsenide. Also, the high-temperature performance of GaAs is largely attributed to its wide bandgap [20–22].

Other than this, photoconductivity, a feature semiconductor exhibit under suitable trial conditions is another benefit associated with the bandgap [23]. This occurs when an increase in electrical conductivity happens when an incident light falls on a semiconductor. The suitability of the semiconductor material in optoelectronic devices is also decided by its photoconductive response. Such materials which respond well to the photoconductivity, find themselves useful in the making of infrared sold state detectors. Also, in GaAs, the transport properties of hot electrons

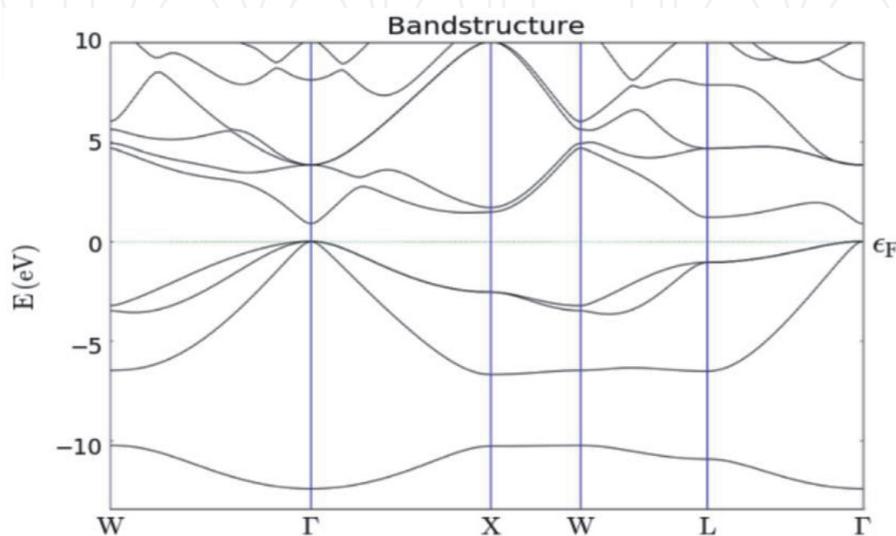


Figure 2.
Structure of GaAs energy band gap [18].

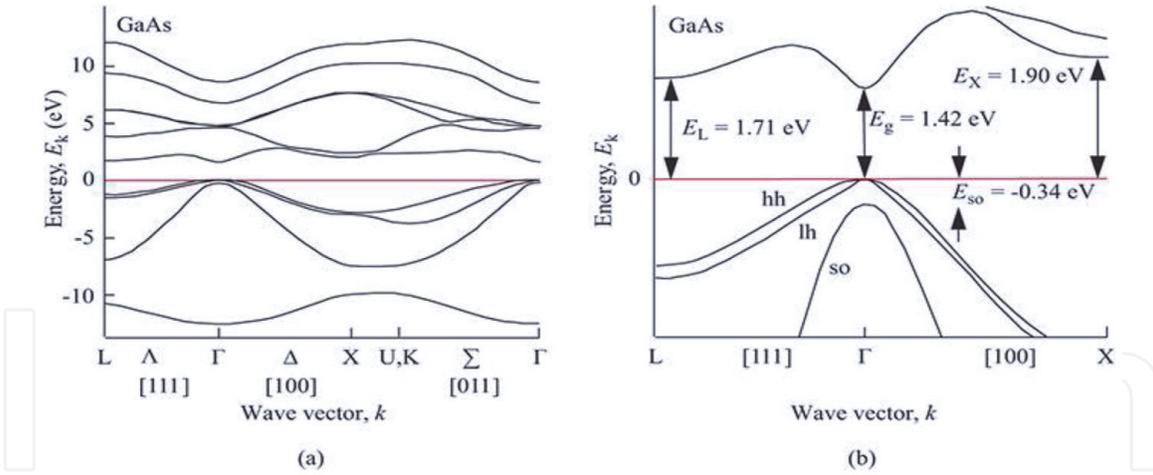


Figure 3.

(a) Calculated band structure of GaAs using the tight binding method. (b) Sketch of GaAs band structure near the Γ -symmetry point showing conduction band, heavy hole band (hh), light hole band (lh), and split-off band (so) in the X [100] and L [111].

are largely affected due to the bandgap. Alloying is another controllable bandgap which useful property of the GaAs [22, 24–26].

The usefulness of GaAs and its alloys in optoelectronics such as solid state lasers and LEDs lies in the bandgap of GaAs which, in the infra-red range results in the emission of photon. The ability of GaAs to retain their semiconductor properties at high temperatures, giving stability to the GaAs comes from the wider bandgap of GaAs [19]. **Figure 3** shows that Calculated band structure of GaAs using the tight binding method with different semiconductor materials.

3. GaAs and semiconductor carrier density

That GaAs is an extremely poor conductor is corroborated by the fact that GaAs has low flow intrinsic carrier density when present in an undoped or pure form. Hence it is mostly considered as semi-insulating. Adding the dopants of either the p- or the n- that is the positive and the negative types respectively, alters this property. Many active devices have been able to be made on a single substrate due to this semi-insulating property, where each device's electrical isolation is provided by the GaAs. For contraction of the electronic circuitry, this characteristic has been found to be quite important [27, 28].

With regards to the transport properties, two important questions that come up where the incorporation of dopants has been done – a) mobility, b) effective carrier concentration [29, 30].

$$n_i = \sqrt{N_C N_V} \exp\left(-\frac{E_g}{K_B T}\right) \quad (1)$$

N_C and N_V , the effective density of states at the band edges, are dependent on temperature and the effective mass of the electron and holes respectively.

$$N_C = 2 \left(\frac{2\pi m_e^* K_B T}{h^2} \right)^{\frac{3}{2}} \quad (2)$$

$$N_V = 2 \left(\frac{2\pi m_h^* K_B T}{h^2} \right)^{\frac{3}{2}} \quad (3)$$

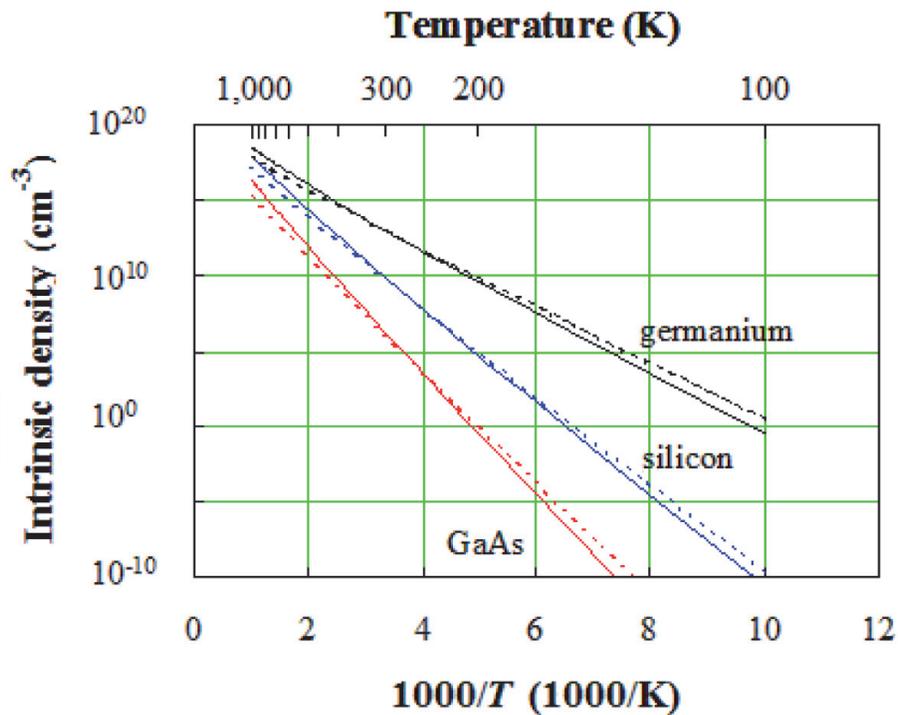


Figure 4. Bandgap energy inverse T for Ge, Si, GaAs in the range 200–1000 K. T [31].

The conductivity is given by

$$\sigma_i = n_i e (\mu_e + \mu_h) \quad (4)$$

Eq. (1) and **Figure 4** can be used to understand the effect of temperature on the concentration of the carrier. It shows the entry of temperature in both exponential as well as pre-exponential terms. There are two effects of increased temperature [31, 32]:

- the effective density of states of the edge of the band is increased (N_V and N_C).
- the exponential portion of Eq. 10 shows a decrease, since its denominator is T .

4. GaAs crystal structure

In solid-state physics, the central theoretical problem happens to be the determination of the energy bands. In other words, in case of solids, the central theoretical problem is the calculation of energy levels of electrons. In order to calculate physical properties such as mechanical properties, magnetic order, optical dielectric or the vibrational spectra, in principle knowledge of the electrons and the energies associated with them is required. In contrast, calculation of lattice constants and other bulk ground state properties such as atomic positions and bulk modulus is considered to be important in physics associated with condensed matter. Such bulk calculations not only help understand as well as characterize the mechanical properties of the matter, but they also help predict their properties in extreme conditions [33–35].

Having a basis and a cubic lattice that is two face centered, the structure of crystal of GaAs is a zincblende structure or cubic sphalerite. In the classic basis, at the origin of the lattice, there is one GaAs molecule. From (0,0,0), the vector of one atom to another at (1/4,1/4,1/4) of the molecule constitutes the basis. Two FCC lattices, one of as while the other being of Ga can also form a crystal as shown in

Figure 5. While arsenic atoms are represented in orange color, the Gallium ones are shown in purple color. As shown, there are 4 arsenic atoms against 14 gallium atoms. This makes a tetrahedral bond, similar to the one in a diamond lattice, but replaced with Ga and as where each Ga is connected to four other atoms. It shows ionic bonding with the presence of two types of atoms [37–39] (**Figure 6**).

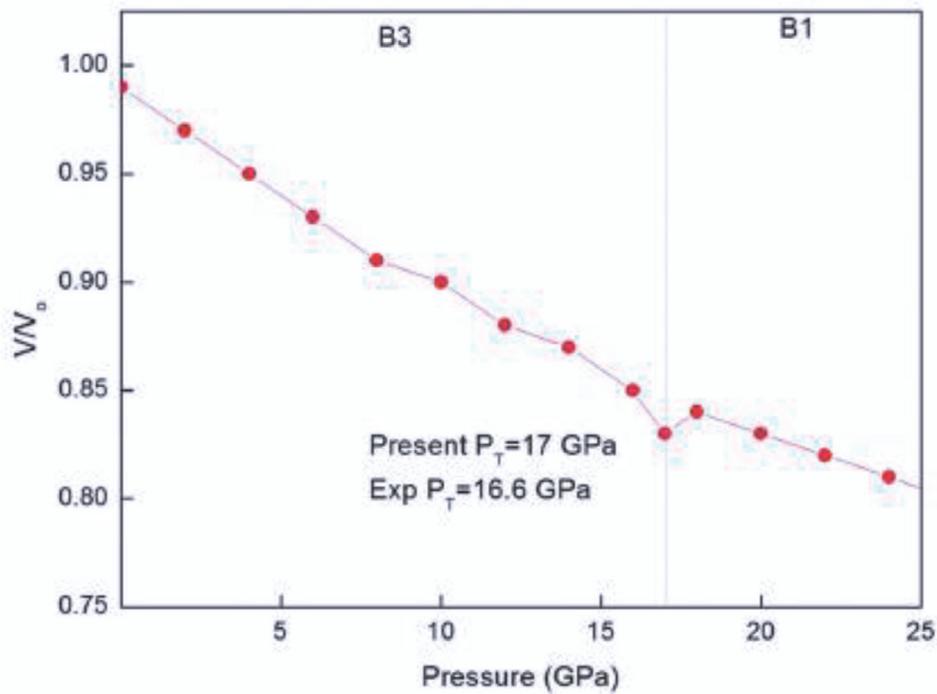


Figure 5.
P-V plot of GaAs up to 25 GPa [36].

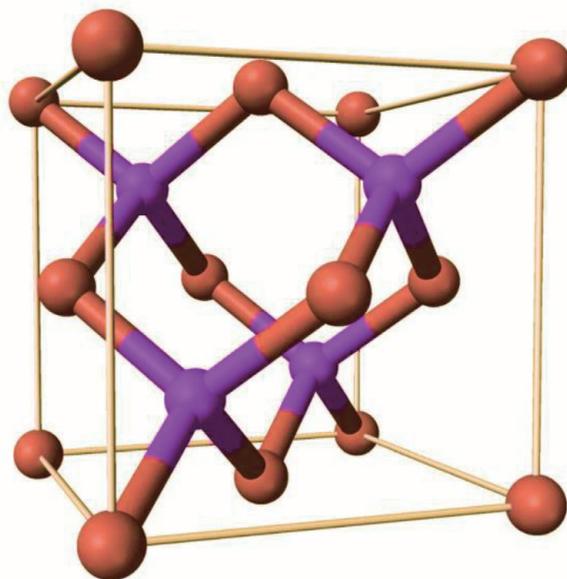


Figure 6.
The crystal structure of GaAs cubic unit cell of GaAs [38].

5. GaAs Fermi level and lattice constant

Figure 7 shows that the drawing of the energy band of the semiconductor, which demonstrates the bandgap along with valence and conduction electrons. An electron leaves a hole in the valence band on moving to the conduction band from

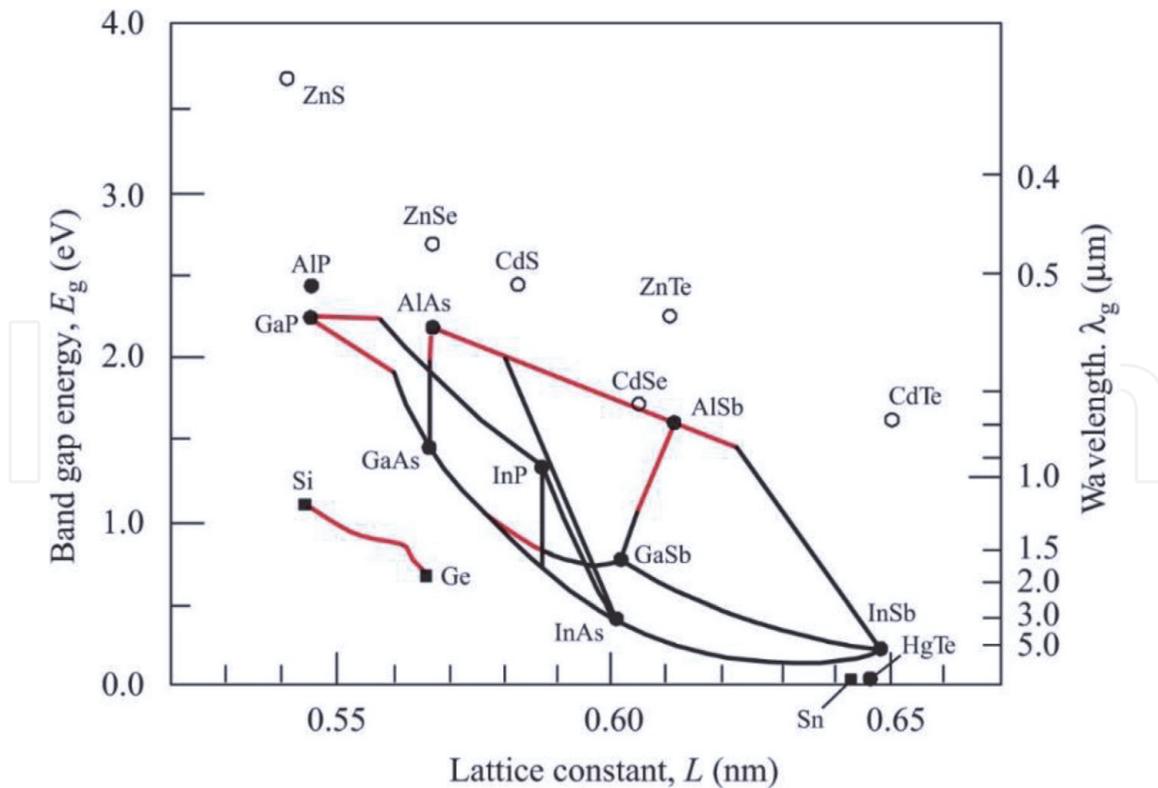


Figure 7. Room-temperature band gap energy, E_g , as a function of lattice constant for several semiconductors. Lines connecting binary compounds such as GaAs and AlAs represent alloy composition with either a direct band gap (thick solid line) or indirect band gap (thin red line). The III-V and II-VI semiconductor compounds in the figure have the zinc blende crystal structure. Si and Ge have the diamond crystal structure [40].

the valence band. For the other electrons in the valence band energy levels, this hole is an empty state and behaves in a manner similar to a $+v_e$ charged particle in the valence band. The number of electrons in the conduction band per unit volume, written as cm^3 , is counted to quantify the electron concentration, and is represented by 'n' [41, 42].

The density of holes in the valence band equals the density of electrons in the conduction band.

$$N_C = \exp\left[\frac{E_F - E_C}{K_B T}\right] = N_V \exp\left[\frac{E_V - E_F}{K_B T}\right] \quad (5)$$

In the above formula,

E_F - Fermi energy.

N_V - effective density of states in the valence band.

E_V - valence band edge.

k_B - Boltzmann's constant.

E_C - conduction band edge.

T - temperature in K.

N_C - effective density of states in the conduction band.

Reordering the above equation, we have

$$\exp\left(\frac{2E_F - E_C - E_V}{K_B T}\right) = \frac{N_V}{N_C} \quad (6)$$

Taking log we have

$$\left(\frac{2E_F - E_C - E_V}{K_B T}\right) = \ln \frac{N_V}{N_C} \quad (7)$$

Solving for E_F

$$E_F = \frac{E_C + E_V}{2} + \frac{K_B T}{2} \ln \left(\frac{N_V}{N_C}\right) \quad (8)$$

It is in the middle of the bandgap that we have the Fermi energy $(E_C + E_V)/2$. Therefore, as shown in 7, the energy bandgap latticed matched for several semiconductors that is related to GaAs and band alignments for sever III-V semiconductor with GaAs (**Figure 8**).

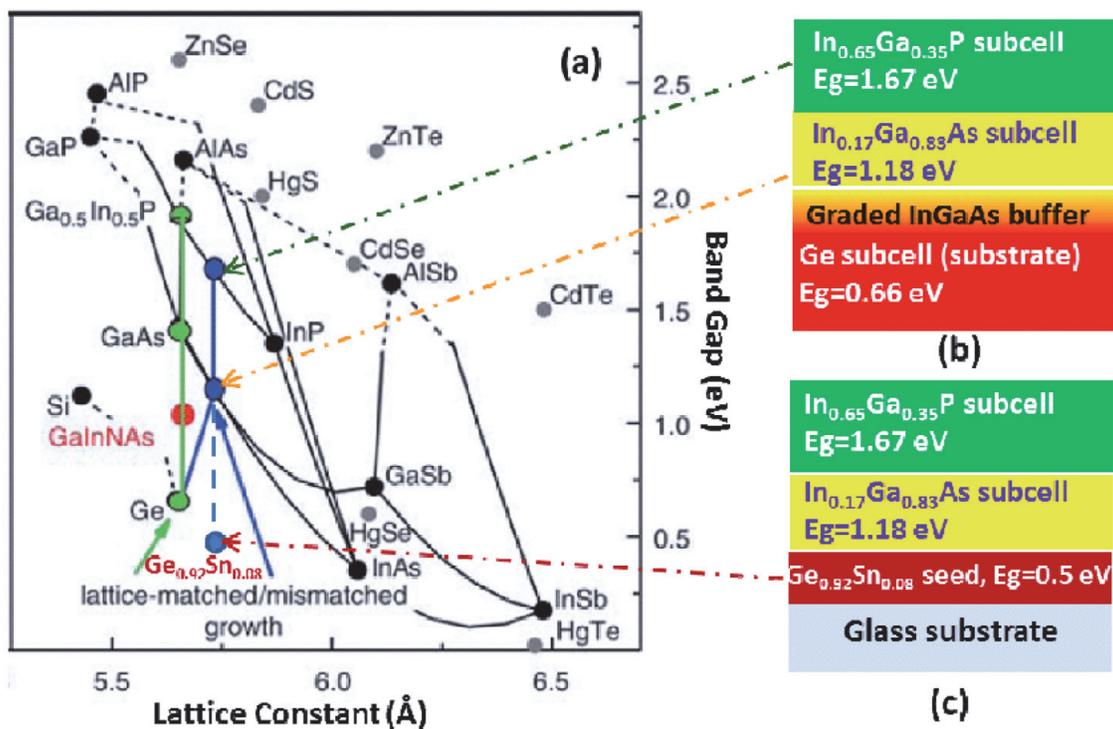


Figure 8.

Band alignments for sever III-V semiconductor with GaAs. (a) Lattice constants and band gaps of different semiconductor materials. The lattice constants of Ge and GaAs are close to a variety of semiconductors with different band gaps, thereby commonly used as substrates for tandem cells. (b) Schematics of a triple-junction tandem cell with optimized compositions of InGaAs and InGaP, which correspond to the blue dots in (a). A buffer layer has to be applied to accommodate the lattice mismatch between the Ge substrate and In 0.17 Ga 0.83 As; (c) Proposed latticematched GeSn/InGaAs/InGaP tandem cell [42].

6. GaAs transport properties

An ionic bond exists between the electrons in the valence band of GaAs atoms. Therefore, in solids, they are not free to transport. However, they can move through a solid if the electron gets excited to the conduction band. Hence, an electron leaves a hole in the valence band on moving to the conduction band from the valence band. An electron jump from one bond to another enables the hole to move in the valence band. Further, these holes and electrons can move upon affected by an electric field [43–45].

The equation that helps derive the acceleration of the electrons (a_e) is-

$$a_e = \frac{eE_x}{m_e} \quad (9)$$

Where m_e is the electron's rest mass and E_x is the electric field. Under an electric field, the interaction of electrons with the solid atoms should also be considered.

In the case of an electron in a solid, under an external field, the interaction with the solid atoms should also be taken into account. Let this interaction of electrons with the atoms of the solid be summed up as $\sum f_{int}$ [46, 47].

$$a_e = \frac{eE_x + \sum f_{int}}{m_e} \quad (10)$$

The conduction electrons are initially in the lowest energy valley, Γ minimum. Here, they are distinguished by a low effective mass and have high mobility. On applying the electric field, these electrons are rapidly accelerated by the field to high velocities: they gain kinetic energy. The electrons' ability gains enough energy to transfer from this valley to the next higher valley, the L minimum. These upper valleys are distinguished by a larger effective mass, and consequently both lower electron mobility and a greater density of available electron positions. The great density of states encourages transfer to these valleys of electrons with suitable energy. There is a fall in the average velocity of all the electrons as the energetic electrons transfer to the upper levels. There is much work available which is focused on the calculation of hot electron transport properties in GaAs. Gallium arsenide exhibits the 'transferred electron' which is commonly known as the TE effect. This transfer of electrons from one region to another energy band structure is an electric-induced field transfer. It has high electron mobility, with a negative resistance being observed and has a small dielectric constant. This is primarily because of extensive utilization of GaAs in ultrahigh frequency, high-temperature resistance and low power circuits and devices [48–53].

$$\text{average velocity } \nu = \frac{n_{\Gamma}\nu_{\Gamma} + n_r\nu_r}{n_{\Gamma} + n_l} \quad (11)$$

7. GaAs optical properties

There are two main categories in which the optoelectronic devices can be categorized. First is the set of those devices in which electrical current get converted into electromagnetic radiation i.e. light. Second is the set of those devices in which light is converted into electric current. An example of the first category of devices is the LEDs. Optoelectronic devices as well as light-emitting devices have GaAs in them. Macroscopic evidence is available for the interaction of matter with light and it is made of four components, namely, incident, reflected, transmitted, and scattered component [52, 54, 55].

Absorption of a photon in a semiconductor can happen in a number of ways. This is commonly known as interband absorption. This happens when in the conduction band an electron is excited up after having absorbed a photon in the valence band. The momentum is unchanged in case of direct gap semiconductor while there is an increase in electron's energy. The momentum is though shifted in case of an indirect gap material. This is made possible by a decrease in bandgap energy with the increase in temperature and a photon being either absorbed or emitted. The two factors responsible for this are lattice vibration (phonons) and thermal expansion. The increase of lattice constant is due to the thermal expansion. This further leads to

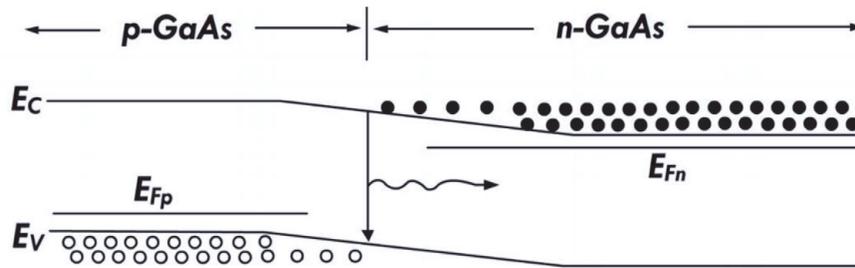


Figure 9. The heterojunction has a higher quantum efficiency since the carriers are localized GaAs [63].

the change in the periodic potential as seen by the electron. The band structure is altered due to these changes [56–59].

Temperature and bandgap shift are related as per the following formula

$$E_g = E_g - \frac{\alpha T^2}{T + \beta} \quad (12)$$

where

E_g - band gap energy

T - temperature

$E_g(0)$ - bandgap at 0 K having units same as that of energy

α has units the same as that of temperature/energy.

Prominently used in optoelectronic as well as microelectronic devices, Gallium arsenide, GaAs is considered a good semiconducting material, having high electron mobility. In the semiconductor material, through the interaction of electron and photons, sunlight is converted into electricity directly by photovoltaic cells [60–62].

Electronic excitation of luminescence is the reason, it is also called as optical radiation. State energy is emitted in the form of EM radiation when the excited electrons move back to the ground. Depending upon the electronic excitation created originally, there are four different types of luminescence, namely,

Photoluminescence – incident light → electronic excitation

Radioluminescence – ionizing radiation (β – rays) → electronic excitation

Cathodoluminescence – electron beam → electronic excitation

Electroluminescence – electrical field → electronic excitation

The functioning of LEDs is by electroluminescence. Using a functional bias, electric current which includes holes and electrons are forwarded to the device. Light is emitted by the recombination of these holes and electrons. In order to increase efficiency, heterostructure LEDs are used. The holes and the electrons, collectively called the carriers are confined in a small spatial region in order to achieve this. Due to the localization of carriers in GaAs, there is higher quantum efficiency at the heterojunction. Hence, it is only in the i-GaAs region, that the recombination takes place. **Figure 9** draws a clear picture of the emitted wavelength in case of both LEDs as shown in **Figure 9** [63–66].

8. GaAs elastic properties

The physical knowledge of the materials namely the phase transitions, interatomic forces and the mechanical features apart from many other features are better understood by examining the elastic properties of the material.

8.1 Density

Being low-density materials, III-V compounds, under pressure, have the ability to show transitions of structural phase to a phase with higher density. **Figure 3** clearly shows that with increase in pressure, the density of GaAs also increases [67].

8.2 Phase transition

Figure 5 shows the P-V graph which helps determine the B3 → B1 phase transition of GaAs. At 17 GPa there is an unexpected decrease in the GaAs's volume. This decrease is attributed to the change in the structural phase related with phase transition of B3 → B1 [23, 36, 68–71].

9. Conclusion

Gallium Arsenide is deemed as an eminent member of the III-V semiconductor group. It has presented itself as a notable material for electronic devices and vastly being used in optoelectronic and microelectronic devices. The precept knowledge of the electrons and the energies related to GaAs is required in order to calculate physical properties. Furthermore, calculation of lattice constants and other bulk ground state properties is considered to be paramount in physics associated with condensed matter.

In this chapter we have reported the basic principle for the GaAs material as well as the physical, optical, and chemical properties. Also, we have reported the crystal growth of the GaAs with another semiconductor material such as In and Al.

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