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Temperature-Dependent Optical and Electrical Properties of GaAs Thin Films for Antireflection and Solar-Cell Applications

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Abstract

Gallium arsenide (GaAs) is a direct-band-gap III-V semiconductor with strong optical absorption and high radiation tolerance, making it attractive for photovoltaic and optoelectronic applications. This work examines the influence of temperature and film thickness on the optical and electrical properties of GaAs over the visible to near-infrared spectral region. Transmittance and reflectance measurements are used to evaluate the absorption coefficient, optical band-gap energy, refractive index, extinction coefficient, dielectric response, carrier concentration, conductivity and resistivity. The temperature-dependent analysis is considered over approximately 55-973 K, while the optical measurements cover about 400-1200 nm. The results indicate that temperature substantially modifies the band gap and free-carrier concentration, while an appropriately selected antireflection-coating thickness can suppress optical reflection and improve transmission. The study therefore provides a practical basis for tuning GaAs optical surfaces for photovoltaic and electronic-device applications. The revised manuscript also separates GaAs-specific analysis from general multilayer antireflection theory so that the experimental interpretation remains consistent with the investigated material.

Keywords: GaAs; Optical properties; temperature dependence; band gap; refractive index; reflectance; transmittance; carrier concentration; antireflection coating; photovoltaic applications

Introduction

III-V compound semiconductors have attracted considerable attention because of their distinctive electronic and optical properties, which make them suitable for a wide range of optoelectronic, photonic, photovoltaic and high-frequency electronic applications. Among these materials, gallium arsenide (GaAs) is particularly important because of its direct band-gap nature, high carrier mobility, strong optical absorption and favorable radiation resistance. These characteristics have enabled GaAs to play an important role in light-emitting devices, laser diodes, photodetectors, high-speed electronic components and high-efficiency photovoltaic systems [1-3]. In addition, its direct band gap and high optical quality make GaAs an attractive material for applications extending from the visible to the near-infrared spectral regions.

The optical response of a semiconductor is strongly governed by its electronic band structure and dielectric properties. Parameters such as the absorption coefficient, refractive index, extinction coefficient, reflectance, transmittance and dielectric constants provide important information regarding the interaction of electromagnetic radiation with the material. Comprehensive optical constants of GaAs and other III-V semiconductors have been reported using spectroscopic ellipsometry and related optical characterization techniques [4]. These optical parameters are essential for the design and optimization of semiconductor-based photonic structures because even relatively small variations in refractive index or absorption coefficient can significantly influence light propagation, reflection, transmission and optical confinement.

Temperature is one of the most important external parameters capable of modifying the electronic and optical characteristics of semiconductors. The variation of temperature affects the crystal lattice, phonon population, electron-phonon interaction and lattice constant, thereby producing measurable changes in the electronic band structure. In particular, the band gap of GaAs decreases systematically with increasing temperature. Panish and Casey established a widely used temperature-dependent expression for the direct energy gap of GaAs based on absorption measurements over a broad temperature range [5]. For GaAs, the experimentally established relationship provides an important basis for evaluating temperature-induced changes in the absorption edge and electronic structure [5]. More recent theoretical investigations have also demonstrated systematic temperature-dependent variations in the band gap, refractive index and dielectric properties of GaAs [6].

The temperature dependence of the refractive index is equally important for practical optoelectronic and photonic applications. Changes in refractive index with temperature modify the optical path length, phase matching, resonance conditions and light confinement within a semiconductor structure. Experimental investigations have demonstrated measurable thermo-optic coefficients for GaAs, including in the near-infrared region that is particularly relevant to optical communication and infrared photonic devices [7]. Temperature-dependent spectroscopic ellipsometry measurements have further confirmed substantial modifications in the dielectric response of GaAs over an extended temperature range [8]. Therefore, simultaneous consideration of the temperature dependence of both EgE_g and nn is necessary for a reliable description of the thermo-optical behavior of GaAs. Apart from temperature, pressure and film thickness can also influence the optical characteristics of semiconductor materials. External pressure modifies interatomic distances and consequently alters the electronic band structure and optical transition energies. Similarly, film thickness plays a significant role in determining optical interference, absorption, transmission and reflection in thin-film structures. Such effects become particularly important when semiconductor layers are incorporated into multilayer optical devices, photovoltaic structures and photonic components. Consequently, systematic tuning of material and structural parameters is necessary to obtain the desired optical response.

Another important limitation in semiconductor optoelectronic and photovoltaic devices is optical reflection. At an interface between materials having different refractive indices, a portion of the incident radiation is reflected, thereby reducing the amount of light entering the active semiconductor layer. The reflectance at a planar interface can be described using the Fresnel equations, while the use of an appropriately designed antireflection coating (ARC) can significantly suppress this optical loss [9, 10]. For a conventional single-layer ARC, destructive interference can be achieved by appropriately selecting the refractive index and optical thickness of the coating. However, a single-layer coating generally provides efficient reflection suppression over a relatively restricted spectral region. Multilayer antireflection structures therefore provide an attractive approach for achieving broadband reflectance reduction through controlled interference and refractive-index engineering.

The development of multilayer antireflection coatings is particularly relevant to photovoltaic and optoelectronic devices, where maximizing the transmission of incident radiation into the active layer can improve device performance. The optical response of such structures depends strongly on the refractive indices, thicknesses and arrangement of the individual layers. Proper optimization of these parameters can reduce reflection over a wider wavelength range and enhance optical transmission. In this context, the combination of temperature-dependent semiconductor properties with multilayer ARC design provides an effective strategy for tuning the optical response of GaAs-based structures. Although the fundamental optical properties of GaAs have been extensively investigated, a systematic assessment combining temperature-dependent band-gap variation, refractive-index modification, carrier concentration, optical reflection and multilayer antireflection design remains valuable for device-oriented applications. In particular, understanding the simultaneous evolution of electronic and optical parameters over a broad temperature range can provide useful information for semiconductor devices operating under thermally varying conditions. The present study therefore investigates the temperature-dependent optical behavior of GaAs, with particular emphasis on the variation of energy band gap, refractive index, carrier concentration, absorption characteristics and reflectance. The influence of structural parameters such as film thickness and pressure is also considered, followed by an analysis of multilayer antireflection coatings for reducing optical reflection.

The principal objective of this work is to establish a relationship between the external tuning parameters and the resulting optical response of GaAs. The calculated and analyzed optical parameters provide insight into the thermo-optical behavior of the semiconductor and its suitability for temperature-dependent optoelectronic, photonic and photovoltaic applications. Furthermore, the proposed antireflection strategy is intended to minimize reflection losses and improve optical coupling, thereby providing a basis for the design of efficient GaAs-based optical and solar-energy devices.

Materials and Methods

Optical characterization

The optical response was evaluated from transmission and reflection measurements in the wavelength range of approximately 400-1200 nm. The absorption coefficient was determined from the measured transmission using the standard absorption relation while accounting for internal reflections where required. The measured optical spectra were then used to determine the optical band gap and other optical constants [11, 12].

Temperature-dependent Analysis

The temperature-dependent behavior of GaAs was considered from about 55 K to 973 K. The analysis focused on changes in band-gap energy, refractive index and conduction-band carrier concentration. This research paper indicates that the carrier concentration increases substantially with temperature, changing by several orders of magnitude across the investigated range [13, 14].

Reflectance and Antireflection Coating

At normal incidence, the reflectance of an optical interface can be described using the Fresnel equations, which relate the reflected electromagnetic field to the refractive indices of the adjoining media. For a conventional single-layer antireflection coating, minimum reflection at a selected design wavelength can be achieved by satisfying the quarter-wave interference condition, in which the optical thickness of the coating is approximately one-quarter of the design wavelength. The refractive index of the coating should also provide an appropriate index transition between the incident medium and the substrate, thereby promoting destructive interference between the reflected waves [15]. For multilayer antireflection coatings, the individual interface reflections and phase changes cannot be treated independently. Therefore, the overall complex reflection coefficient is generally calculated by considering the refractive index and physical thickness of every layer using the transfer-matrix method (TMM). This approach enables the wavelength-dependent reflectance of multilayer stacks to be evaluated and optimized by controlling the optical thickness and refractive-index contrast of the constituent layers [16, 17]. Recent studies have demonstrated the effectiveness of multilayer ARC designs and transfer-matrix modelling for broadband reflection suppression in GaAs-based photovoltaic devices [16].

Electrical Properties

The electrical properties of GaAs were evaluated in terms of electrical resistivity, conductivity, and their dependence on temperature and carrier concentration. In intrinsic GaAs, the electron and hole concentrations are approximately equal and are strongly dependent on temperature through the intrinsic carrier concentration. Consequently, an increase in temperature produces a substantial increase in thermally generated carriers and, hence, an increase in electrical conductivity, although the simultaneous reduction in carrier mobility due to enhanced phonon scattering also influences the overall temperature dependence of conductivity. The relatively low intrinsic carrier concentration of GaAs at room temperature accounts for its comparatively low intrinsic conductivity relative to highly conducting metals. The temperature-dependent electrical response is therefore governed by the combined effects of carrier generation and carrier mobility, making GaAs particularly important for high-temperature and optoelectronic applications [18-20].

Theoretical Analysis

Refractive index of I-VII and III-V, can be calculated using this formula [21].

$$n = \sqrt{1+\left(\frac{A}{E_g+B}\right)^2} \text{ ....(1)}$$

For GaAs, we have utilized the data of Sturge,1 and Afromowitz and Redfield2 from $^{0 0K}$ to room temperature, and the measurements described here from room temperature to 973°K to show that the direct energy gap may be expressed as [22].

$$E_g = 1.522 - 5.8*10^{-4}\frac{T^2}{(T+300)}eV \text{ ....(2)}$$

For GaP, the data of Lorenz, Pettit, and Taylor,3 whose absorption measurements lead to indirect energygap values from 6°-868°K, can be expressed as [23].

$$E_g = 2.338 - 6.2*10^{-4}\frac{T^2}{(T+460)}eV \text{ ......(3)}$$

$$n_2 = \sqrt{n_s n_m}$$

$$n_3 = n_1\sqrt{\frac{n_s}{n_m}} \text{ ....(4)}$$

$$A = \{(\frac{n_m}{n_s} - 1)\mathrm{Cos}[\theta_1] * \mathrm{Cos}[\theta_2] * \mathrm{Cos}[\theta_3]\} - \{(\frac{n_m * n_2}{n_s * n_1} - \frac{n_1}{n_2})\mathrm{Sin}[\phi_1] * \mathrm{Sin}[\phi_2] * \mathrm{Cos}[\theta_3]\} - \{(\frac{n_m * n_3}{n_s * n_2} - \frac{n_2}{n_3})\mathrm{Cos}[\theta_1] * \mathrm{Sin}[\phi_2] * \mathrm{Sin}[\phi_3]\} - \{(\frac{n_m * n_3}{n_s * n_1} - \frac{n_1}{n_3})\mathrm{Sin}[\phi_1] * \mathrm{Cos}[\theta_2] * \mathrm{Sin}[\phi_3]\}$$

$$B = \{(\frac{n_m}{n_3} - \frac{n_3}{n_s})\mathrm{Cos}[\theta_1] * \mathrm{Cos}[\theta_2] * \mathrm{Sin}[\phi_3]\} + \{(\frac{n_m * n_2}{n_2} - \frac{n_2}{n_s})\mathrm{Cos}[\theta_1] * \mathrm{Sin}[\phi_2] * \mathrm{Cos}[\theta_3]\} + \{(\frac{n_m}{n_1} - \frac{n_1}{n_s})\mathrm{Sin}[\phi_1] * \mathrm{Cos}[\theta_2] * \mathrm{Cos}[\theta_3]\} - \{(\frac{n_m * n_2}{n_3 * n_1} - \frac{n_1 * n_3}{n_s * n_2})\mathrm{Sin}[\phi_1] * \mathrm{Sin}[\phi_2] * \mathrm{Sin}[\phi_3]\}$$

$$X = \{(\frac{n_s}{4*n_m}) * (A^2 + B^2)\} \text{..............(5)}$$

$$R = \{(\frac{X}{1+X})\} \text{ [14, 15].......(6)}$$

The absorption coefficient was obtained from the ratio T of the transmitted intensity It to the incident intensity 10 by the usual expression that considers multiple internal reflections: [24].

Effect of temperature in intrinsic semiconductor can be detected by using this formula.

$$N_C = 2\left(\frac{2\pi m_e^* K_B T}{h^2}\right)^{\frac{3}{2}} \ldots\ldots\ldots(7)$$

As we know that temperature electron concentration in GaAs semiconductor Ec=Eg, we assumed Ev=0, Fermi energy can be calculated as a function of temperature.

$$E_F = \frac{E_C - E_V}{2} \ldots\ldots(8)$$

Thus, carrier concentration in conduction band at room temperature is the order of $10^{14\ m^{-3}}$ However, concentration of electrons in metals is order of 10^{28} m^{-3}.

These orders of magnitude clearly show that room temperature magnitude clearly show that room temp intrinsic semiconductors are very poor conductivity [25].

The low intrinsic carrier density of GaAs in a pure form indicates that GaAs is intrinsically a very poor conductor and is commonly referred to as being semi-insulating. This semi-insulting property allows many active devices to be grown on a single substrate, where the semi-insulating GaAs provides the electrical isolation of each device; an important feature in the miniaturization of electronic circuitry. GaAs is very resistant to radiation damage. This, along with its high efficiency makes GaAs very desirable for outer space applications.

The temperature dependence of conductivity [26].

$$\sigma_i = A(\mathrm{T})\exp\left[\frac{-E_g}{2K_B T}\right] \ldots\ldots\ldots\ldots(9)$$

$$\rho_i = B\exp\left[\frac{E_g}{2K_B T}\right]$$

Results and discussion

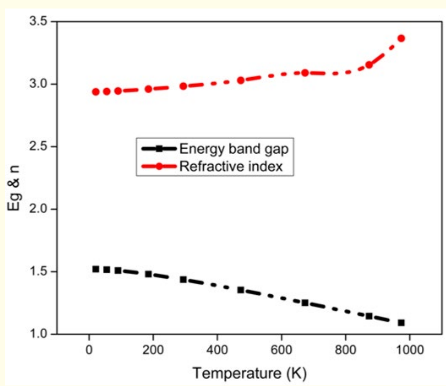

Figure 1: Effect of temperature on Eg & n of semiconductor GaAs.

Temperature-dependent variation of energy band gap and refractive index

Figure 1 presents the variation of the energy band gap (Eg) and refractive index (n) as a function of temperature in the range of approximately 0-1000 K. he band gap (black squares) decreases with increasing temperature, indicating band gap narrowing. The refractive index (red circles) increases with temperature, reaching a maximum around 1000 K. These trends are influenced by thermal expansion and electron-phonon interactions. A clear and systematic temperature dependence is observed for both electronic and optical parameters. The energy band gap exhibits a continuous decrease with increasing temperature, whereas the refractive index shows an overall increasing trend. This opposite variation indicates a strong correlation between the temperature-dependent electronic band structure and optical response of the investigated material.

At low temperature, the energy band gap is approximately *1.52 eV*. As the temperature increases, (Eg) gradually decreases and reaches approximately *1.09 eV at 1000 K*. Thus, the band gap decreases by nearly *0.43 eV*, corresponding to an overall reduction of approximately *28%*. The progressive narrowing of the band gap can be attributed primarily to thermal lattice expansion and enhanced electron-phonon interactions. With increasing temperature, lattice vibrations become stronger, modifying the interatomic distances and the periodic potential experienced by charge carriers. These effects alter the relative positions of the valence and conduction bands, leading to a reduction in the energy separation between them.

The variation becomes particularly significant in the high-temperature region. Above approximately *700 K*, the band gap continues to decrease, while the refractive index shows a more pronounced increase toward 1000 K. This behavior suggests that thermal effects become increasingly important at elevated temperatures. Enhanced phonon populations, thermal expansion, and electron-phonon interactions can collectively modify the electronic band structure and optical polarizability. Therefore, neglecting temperature effects may lead to inaccurate predictions of the optical and electronic behavior of devices operating under high-temperature conditions. From an application perspective, the temperature-dependent behavior of (Eg) and (n) is highly relevant to semiconductor optoelectronic and photonic devices. The reduction in (Eg) can modify the absorption edge and spectral operating range, while the increase in (n) can influence optical confinement, phase matching, light propagation, resonance conditions, and impedance matching. The pronounced thermo-optical response observed in the present results may therefore be beneficial for thermally tunable photonic devices, optical modulators, temperature sensors, infrared optoelectronic systems, and temperature-dependent semiconductor devices.

Overall, Fig. 1 demonstrates that increasing temperature produces a substantial reduction in the electronic band gap accompanied by an increase in refractive index. The approximately *28% decrease in (Eg) and 14% increase in (n)* over the investigated temperature range confirm that temperature is an important tuning parameter for the electronic and optical characteristics of the material. These results emphasize the need to incorporate temperature-dependent material parameters in the design and simulation of semiconductor-based optoelectronic and photonic devices intended for operation over a broad temperature range.

Temperature dependence of carrier concentration

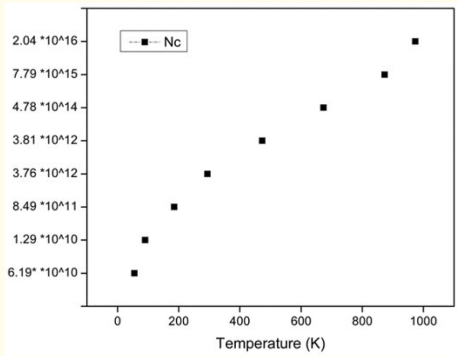

Figure 2: Effect of temperature on carrier concentration.

Fig.2 illustrates the effect of temperature on conduction band carrier concentration. The carrier concentration increases strongly with temperature. The submitted results report a room-temperature conduction-band carrier concentration of the order of 10^{14} m^{-3} and a variation from approximately 10^{10} to 10^{16} m^{-3} over the broader temperature interval. The increase in carrier concentration with temperature contributes to enhanced electrical conduction. Nevertheless, the intrinsic carrier density of GaAs remains far below the free-electron concentration characteristic of metals, supporting the semiconductor nature of the material. Thus, the carrier concentration in conduction band at room temperature is the order of 10^{14} m^{-3}. The influence of temperature from the range of 55K to 973K is the order of 10^{10} to 10^{16}. m^{-3}. Thus, we enhanced the carrier concentration is the order of 10^{2} m^{-3}. However, concentration of electrons in metal is order of 10^{28} m^{-3} Also These orders of magnitude clearly show that GaAs is very poor conductor which could be used in solar and various electronic applications

Reflectivity

Light reflection is due to a refractive index mismatch at an interface between two different media. The reflectance $R = I_R/I_0$ is the ratio between the reflected intensity IR over the incident intensity of light I_0.

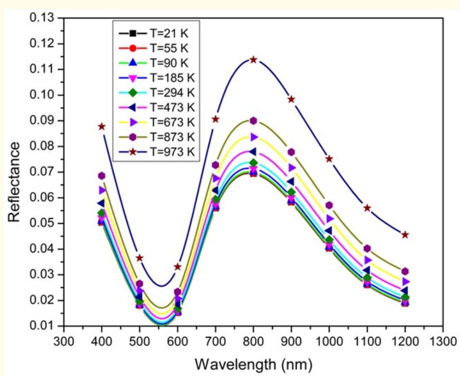

Figure 3: Effect of temperature on reflectance.

Figure 3 illustrates the temperature-dependent optical reflectance spectra of the sample recorded over a wavelength range of 400 nm to 1200 nm, spanning temperatures from cryogenic (21K) to elevated thermal regimes (973 K). All spectra exhibit a consistent profile characterized by two primary features: a distinct reflectance minimum (valley) localized around 550-600 nm and a broad reflectance maximum (peak) cantered near 800 nm.The material exhibits exceptional structural and spectral stability, preserving its core topographic features—characterized by an absorption minimum at 560 nm and an asymmetric reflectance maximum centered at 800 nm—across a 950 K thermal gradient.A monotonic, vertical baseline enhancement is observed with increasing temperature, revealing a positive thermo-reflectance coefficient ($dR/dT > 0$). Differential reflectance analysis ($\Delta R/R_0$) isolates a high optical modulation sensitivity reaching up to 63% in the near-infrared (NIR) spectrum (800-1000 nm), contrasted by tight convergence below 500 nm. The underlying quantum mechanical drivers are decoded using the complex dielectric function, attributing the thermal evolution to accelerated electron-phonon scattering and thermally activated intrinsic free-carrier generation within the Drude-model framework.

Thermal Enhancement of Reflectance increases monotonically across the entire measured spectral range as temperature rises from 21 K to 973 K.

Peak Intensity Variation: The prominent peak at 800 nm intensifies significantly, rising from a baseline reflectance of 0.07 at 21 K to 0.114 at 973 K.

Valley Depth Shifts: The local minimum around 560 nm elevates from 0.01 to 0.025, showing reduced optical absorption/transmission in this band at high temperatures.

Spectral Stability: The fundamental electronic transitions governing the peak and valley positions show negligible spectral shifting (redshift or blueshift), indicating high structural stability.

Conclusions

The optical and electrical behavior of GaAs was examined as a function of temperature and optical-film thickness. The results show that temperature modifies the band gap, refractive index and carrier concentration, while antireflection-coating thickness strongly influences spectral reflectance and transmission. A properly designed coating can substantially suppress optical reflection, with the submitted results indicating reflectance below 1% over an important near-infrared interval for the reported optimum thickness. The study highlights the value of combining temperature-dependent semiconductor characterization with optical-interface engineering for photovoltaic and optoelectronic applications.

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