Investigation of recombination lifetime of gallium antimonide through different recombination processes in particular of Auger recombination process

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Contents

Acronym

[acronym]glossaries GaSbGaSbGallium Antimonide SRHSRHShockley-Read-Hall Recombination RRRRRadiative Recombination ARARAuger Recombination PLPLPhotoluminescence IVIVCurrent-Voltage CVCVCapacitance-Voltage SRVSRVSurface Recombination Velocity XRDXRDX-ray Diffraction LEDLEDLight emitting diode JDOSJDOSJoint density of states VRSVRSVan Roosbroeck Shockley [type=, title=List of Acronyms]

Abstract

Recombination of electrons and holes may take place in the host crystal or at impurity Centre's, the energy being removed by radiation of a light quantum, by multi phonon emission, or by an Auger process. The investigation of recombination lifetime of gallium antimonide (GaSb) using the Van Roosbroeck-Shockley method is crucial for understanding the materials performance in optoelectronic devices such as photo detectors, infrared LEDs, and lasers. GaSb is a narrow band gap semiconductor with unique electronic and optical properties. It is highly effective in mid infrared applications due to its small band gap. The recombination lifetime in GaSb significantly influences its device efficiency by determining the carrier dynamics. The van Roosbroeck –Shockley method provides a framework to calculate recombination rate and recombination lifetime of GaSb based on radiative recombination process. The band gap energy variation of GaSb as a function of wave vector k were calculated. The result shows that the band gap energy of GaSb increases with increasing of wave vector k and also decrease with increasing of temperature. Absorption and emission rate are both calculated since emission rate is decreased with increasing photon energy that emitted the absorption rate is increased with increasing photon energy. The recombination rate was calculated by pointing different dependencies. At the last the recombination lifetime of GaSb were calculated by using different recombination mechanisms. The radiative recombination lifetime is longer than the Auger recombination lifetime. Keywords: Gallium Antimonide (GaSb), Van Roosbroeck-Shockley method, recombination rate, emission rate, absorption rate, recombination, recombination process.

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Chapter 1

INTRODUCTION

1.1 Background of the study

Semiconductors are a group of materials having electrical conductivities between conductors and insulators [1]. GaSb and related semiconductors refers to the groups III–V semiconductors that contain the Sb element among these materials, GaSb has a prominent position among the III–V compound semiconductors. GaSb has a lattice constant of 6.0959 Å that mediates between ternary and quaternary III–V compound semiconducting materials, which enables perfect lattice matching of GaSb to be achieved with many III–V phosphonium-type materials, which is then favorable for high-quality antimony material growth. GaSb can be readily obtained in bulk form through the Czochralski (Cz) growthtechnique [2]. The minority carrier's recombination lifetime is one of the most important parameters as it both characterizes the semiconductor materials and it strongly influences devices properties [3]. The generation of excess carriers in a semiconductor may be accomplished by either electrical or optical means. The conduction and valence band in semiconductors are separated by an energy gap. The electron in the conduction band is in a meta-stable state with higher energy compared to the valence band energy level. It can become stable in the valence band, as there is less energy there. When the electron in the conduction band surpasses the energy gap and reaches the valence band, it becomes stable and occupies the position of a hole in the valence band. With this action, the electron and hole disappear. This is called electron-hole pair recombination or simple recombination in semiconductors. Recombination in semiconductorseliminates the free electrons and holes, thus creating equilibrium in steady state [4]. There are different types of recombination mechanisms in a semiconductor. According to the application of semiconductors and the conditions prevailing, one of the recombination mechanisms becomes active and more efficient than other types. Recombination in semiconductors can be categorized into two groups: radiative and non-radiative recombination. Radiative recombination occurs when an electron from the conduction band recombines with a hole in the valence band. As a result of electron-hole recombination, a photon is emitted. Radiative recombination is the radiative

transition of the electron from the conduction band to the valence band, which involves optical processes: spontaneous emission, absorption or gain, and stimulated emission. This kind of recombination is prominent in direct-band gap semiconductor laser.In non-radiative recombination, electron-hole recombination takes placenon-radiatively. Non-radiative recombination mechanisms in semiconductors are:1. Auger recombination: In Auger recombination, the energy released during electron-hole recombination is transferred to excite another electron in the same band to higher energy levels. The excited electron achieves thermal equilibrium by dissipating the energy to lattice vibrations or phonon. Auger recombination is predominant non-radiative recombination in long-wavelength semiconductor lasers. As the doping density of the semiconductor increases, the Auger recombination lifetime decreases [4]. 2. Recombination through defects: Recombination through defects is a two-step process where electrons recombine with holes through defect energy levels in the band gap. Defects are introduced in the crystal lattice intentionally or unintentionally. The defects in the semiconductor crystal lattice establish a forbidden region and an electron gets trapped by the energy state in that region. If a hole acquires the same energy state before the electron gets re-emitted into the conduction band, electron-hole recombination takes place. This type of recombination is also called Shockley-Read-Hall (SRH) recombination.This type of recombination is utilized in injection lasers [4]. 3.Surface recombination: A strong perturbation of crystal lattice can be called a surface. The surfaces in semiconductor crystal lattices create dangling bonds that are exposed to the ambient. Such exposed surfaces absorb impurities from the ambient and become localized centers of defects. The high concentration of defects in surfaces increases the probability of non-radiative recombination. Cleaved facets in injection lasers are introduced for enhancing recombination in semiconductors through surface recombination [4]. The term “lifetime” is used in physics in a totally intuitive manner to indicate the temporal interval between the generation and the death of a particle. Nevertheless, often the “death” is only a change of the particle state, like in the case of the recombination process in the semiconductors theory. In fact, the recombination lifetime refers to the time in which the electron returns from an excited state to the equilibrium state. The excitation can be obtained, for example, by a photon absorption or an electrical injection process in the forward-biased p-n junction. The electron comes back in the equilibrium state, occupying the vacancy left by the excitation. The lifetime of an excess electron-hole pair associated with radiative recombination is called the radiative carrier lifetime and that associated with non-radiative recombination is called the non-radiative carrier lifetime [3, 5]. If both electrons and holes are present, the carrier lifetime is limited by recombination [6]. The total recombination rate is a superposition of several recombination mechanisms [7]. The focus of this thesis is investigating the recombination lifetimes of gallium antimonide (GaSb) through different recombination processes. hypertargetresearch-questions

1.2 Research questions

The present study seeks answer to the following research questions

- How the band-gap energy is affected by wave vector k of intrinsic GaSb?
- What is the impact of carrier concentration,temperature and photon energy on both absorption and emission rate and also recombination rate of Gallium antimonide?
- How does the recombination mechanisms affect the recombination lifetime of Gallium antimonide (GaSb)?
- How does the recombination mechanisms affect the recombination lifetime of Gallium antimonide (GaSb)?

1.3 Objectives

1.3.1 General Objective

The general objectives of this study are to investigate the recombination lifetime for different recombination processes in gallium antimonide (GaSb).

1.3.2 Specific Objectives

The specific objectives of this study is;

- To calculate the energy versus wave vector for gallium antimonide (GaSb).
- To calculate the recombination rate of gallium antimonide(GaSb) in all recombination mechanisms.
- To calculate absorption and emission rate of gallium antimonide (GaSb).
- To calculate the carriers lifetime of gallium antimonide (GaSb) in different recombination processes.

1.4 Statement of the problem

The minority carriers' recombination lifetime is one of the most important parameters as it both characterizes the semiconductor materials and it strongly influences devices properties. As more than 95% of all the produced electronic devices are fabricated through CMOS process, nowadays the majority of the studies on recombination lifetime concerns power electronics, diodes, IGBTs—where lifetime killing methodologies are mostly employed or solar cells,

where recombination parameters are directly related to the conversion capability of these devices [8]. The semiconductor material, Gallium antimonide (GaSb) plays significant role in the production of light emitting diodes (LEDs) and other optoelectronic devices. So, it is aimed to investigate the recombination lifetime for different recombination processes in gallium antimonide (GaSb).

1.5 Significance of the Study

Understanding the recombination lifetime of many different semiconductor (in particular GaSb) helps to develop the knowledge of the nature of semiconductors in detail. Moreover it helps to develop computational skills of others.

1.6 Scope of the Study

The scope of this study will be limited to the calculation of the energy versus wave vector for gallium antimonide(GaSb), calculation of absorption and emission rate of gallium antimonide(GaSb), calculation of the recombination rate of gallium antimonide(GaSb) in all recombination mechanisms and finally calculating the carriers lifetime of gallium antimonide(GaSb) in different recombination processes.

Chapter 2

LITERATURE REVIEW

2.1 Introduction

This chapter focuses on the basic Quantum mechanical description of many- body system up to the theoretical background of the recombination processes and recombination lifetime calculations methodologies. For approximately solving many electrons and holes lifetimes problems, radiative recombination lifetimes, non radiative recombination lifetimes and finally to perform calculations of a system, recombination rate and factors affecting recombination lifetimes can be reviewed.

2.2 General Properties of Gallium antimonide (GaSb)

GaSb is an exciting semiconductor material with several attractive properties such as high charge carrier mobility and small (direct) band gap of 0.727 eV at room temperature [7]. It is mechanically stable narrow band gap with melting point of 712oc, average molar mass of 191.483g/mol and density of 5.614g/cm3. The shift in the fiber loss minima towards higher wavelengths from 0.8 mm over the past two decades has shifted the material of interest from time to time [10]. Gallium antimonide (GaSb) have promising potential to resolve the future challenges of IR optoelectronic devices such as the need for extending the wavelength for optical communication beyond 1.55m to minimize absorption losses in optical fibers [9]. GaSb can be readily obtained in bulk form through the Czochralski (Cz) growth technique [2].

2.2.1 Chemical properties of gallium antimonide (GaSb)

The surface instability mechanism in GaSb has beendiscussed by Schirm et.al, low temperature process can produce on GaSb a non-equilibrium$Ga_2O_3 - Sb_2O_3$surface layer as follows

$$2GaSb + 3O_3 \rightarrow Ga_2O_3 + Sb_2O_3$$

The only stable phases that can exist in thermodynamic equilibrium with GaSb are Ga_2O_3 and elemental antimony. Any Sb_2O_3 should react with GaSb to give rise to Ga_2O_3 plus free Sb as

$$2GaSb + Sb_2O_3 \rightarrow Ga_2O_3 + 4Sb$$

This reaction spontaneously occurs (G = -12Kcal/mol) even at room temperature. Thus a GaSb surface exposed to air will form a native oxide layer consisting of Sb_2O_3, Ga_2O_3 and a fraction of a monolayer frees Sb. This fractional Sb monolayer is quite sufficient to drastically increase recombination velocity and surface leakage [27].

2.2.2 Mechanical and thermal properties of GaSb

GaSb has molecular weight of 191.483g/mol. Gallium Antimonide (GaSb) is a crystalline semiconductor compound of gallium and antimony of the III-V family [10]. The crystal structure of Gallium Antimonide (GaSb) is Zinc blende.the basic properties of gallium antimonide is given below

Table 2.1: Physical properties of GaSb

Properties	**Zinc Blende GaSb**
Thermal expansion coefficient ($^{\circ}C^{-1}$)	7.75×10^{-6}
Thermal diffusivity (cm^2s^{-1})	0.23
Thermal conductivity ($W.cm^{-1}.^{\circ}C^{-1}$)	0.32
Index of refraction (n)	3.8
Band gap energy (eV) at 300K	0.726
Lattice constant (Å)	6.09593

2.3 Crystal structures of GaSb

GaSb crystallizes in zinc-blende structure, which belongs to the space group $F^{-}43m$ in the Hermann–Mauguin notation, or T2d in the Schoenflies notation [11]. The zinc blende structure is identical to that of the diamond lattice except that each Ga atom has four tetrahedral arranged Sb neighbors and vice versa. However, unlike the diamond structure, the zinc-blende structure does not possess a center of inversion, and opposite directions in the crystal are not necessarily equivalent. The zinc-blende structure has the distinct property that it is a very open lattice, leaving space for relatively large interstitial species. In GaSb, where the covalent radii of Ga and Sb are 1.26 and 1.38 Å respectively, 66% of the lattice volume is empty. A crystal will always have a finite concentration of defects at a finite temperature. While it is true that adding defects to a perfect crystal increases its internal energy, the total free energy (G) of a crystal at a temperature T is made up of the sum of the internal energy (H) and the entropy (S), which becomes more negative by the addition of defects [12].

2.4 Application of gallium antimonide GaSb

GaSb is the most important one, as it provides a wide range of electronic energy gaps .

- It has high potential in the extending the wavelength for optical communication beyond 1.55m to minimize absorption losses in optical fibers optoelectronic devices.
- It has high potential for fabricating high frequency optoelectronic devices operating with low power consumption.
- It has a huge application in the production infrared LEDs.
- Gas purity monitoring and trace moisture detection in corrosive gases like HCl in semiconductor processing.
- Detecting micro leaks of toxic gases such as PH3.
- monitoring of plasma etching
- Detecting hazardous gases like HF and H2S in chemical plants.
- Monitoring greenhouse gas fluxes.
- It also used in laser and thermos voltaic system.

2.5 Energy bandgap

Materials can be classified into three categories, namely insulators, metals and semiconductors. These materials can be distinguished by their energy gap. The lowest energy levels of any system, which are filled with electrons, are called valence band, and the upper available states are called conduction band. The maxima of the valence band and the minima of the conduction band are separated. by an energy gap (E_g). For insulators E_g is very high, for metals $E_g \sim 0\ eV$ and for semiconductorsE_g is between $0.17ev$ and $6ev$. The maxima of valence and minima of conduction at k = 0 is approximately parabolic and their energy is given by The conduction band energy E_c and valence band energy E_v are given by:

$$E_c = E_g + \frac{\hbar^2 k^2}{2m_e} \tag{2.1}$$

$$E_v = -\frac{\hbar^2 k^2}{2m_h} \tag{2.2}$$

where h represents Plank's constant, m_e and m_h are the mass of electron and hole, respectively. At 0K electrons in the valence band do not have enough energy to be excited to the conduction band, and therefore a semiconductor behaves as an insulator at 0K. In this case all the electrons occupy the valence band (Mohsen Aziz, et.al(2014)). The band gap is the difference in energy between the lowest point of the conduction band and the highest point of the valence band [11]. If the conduction band minimum and the valence band maximum are located at the same k-value in the first Brillion zone, such as the-point at the zone center, then the semiconductor is called the direct band gap semiconductor [13]. Therefore GaSb is the one from the direct band gap semiconductor.

2.6 Recombination

Recombination refers to the inverse processes by which the electron-hole pairs are lost due to the spontaneous transition of an excited electron from conduction band to an unoccupied state in valence band. The excess energy and the change in the momentum released are either as photons or phonons or transferred to other carriers, which ensure energy and momentum conservation for the individual processes of electron hole recombination [14]. In thermal equilibrium the relationship $pn = n^2$ is valid. If excess carriers are introduced to a semiconductor so that $pn > n^2$, we have a nonequilibrium situation. The process of introducing excess carriers is called carrier injection. Most semiconductor devices operate by the creation of charge carriers in excess of the thermal equilibrium values.We can introduce excess carriers by optical excitation or forward-biasing a p–n junction. Whenever the thermal-equilibrium condition is disturbed (i.e., $\neq n^2$), processes exist to restore the system to equilibrium (i.e., $pn = n^2$). In the case of injection of excess carriers, the mechanism that restores equilibrium is recombination of the injected minority carriers with the majority carriers. Depending on the nature of the recombination process, the energy released from the recombination process can be emitted as a photon or dissipated as heat to the lattice. When a photon is emitted, the process is called radiative recombination; otherwise, it is called non radiative recombination [15].

2.6.1 Radiative Recombination

Radiative recombination is the inverse process of direct band-to-band photon absorption and, therefore, has the same dependence on band structure. Hence, the probability for this event to occur under thermal equilibrium conditions can be derived from the sum of the probabilities of photon absorption for all electron-hole pairs having an energy separation equal to the photon energy. The processes associated with the radiative recombination of electron-hole pairs in semiconductors are spontaneous emission, optical absorption or gain, and stimulated emission [4]. However, a much simpler approach proposed by vanRoosbroeck and Shockley is to start with the measured optical absorption constant. The approach requires the knowledge of only a

few basic parameters, namely the bandgap energy, the absorption coefficient, and the refractive index [16]. In a direct band gap semiconductor, the fundamental absorption process is usually dominated by the vertical transition. The energy dependence of the fundamental optical absorption coefficient for a direct band gap semiconductor can be expressed by

$$\alpha_i = \left(\frac{2^{\frac{2}{3}}q^2}{3nm_0ch^2}\right)\left(m_r^{\frac{3}{2}} + m_0 m_r^{\frac{1}{2}}\right)(h\nu - E_g)^{\frac{1}{2}} \tag{2.3}$$

where n is the index of refraction, is E

m_r^{-1} is the reduced electron and hole effective mass, andm_0 is the freeelectron mass, Equation (2.3) shows that for $h\nu \geq E_g$, the optical absorption coefficient for a direct bandgap semiconductor is proportional to the square root of the photon energy. In order to correlate the rate of capture probability coefficient Br to the optical absorption coefficient d, one can treat the semiconductor as a blackbody radiation source and use the principle of detailed balance under thermal equilibrium conditions. B_rMay be determined by setting the rate of radiative recombination equal to the rate of total blackbody radiation absorbed by the semiconductor due to band-to-band radiative recombination, which can be expressed by

$$B_r n_i^2 = \int \frac{n^2 \alpha E^2 dE}{\pi} \tag{2.4}$$

Where $E = h\nu$ is the photon energy,

$$B_r n_i^2 = \int \frac{n^2 \alpha E^2 dE}{\pi} \tag{2.5}$$

$$m_r^{-1} = \frac{m_e + m_h}{m_e m_h} \tag{2.6}$$

the right-hand side of (2.4) is obtained from the Planck blackbody radiation formula. Solving (2.3) and (2.4), one obtains the rate of capture probability Br for the direct transition, which reads

$$B_r = \left(\frac{E_g}{n_i}\right)^2 (2\pi)^{\frac{2}{3}} \tag{2.7}$$

It is important to note from (2.5) that B_r is inversely proportional to the square of the intrinsic carrier density, which shows an exponential dependence of B_r on temperature. This implies that the band-to-band radiative recombination lifetime is a strong function of temperature [13]. Combining the corrected absorption constant,α, with the Plank distribution for photon density at thermal equilibrium givesthe radiative generation rate,G_r which is the same as the spontaneous radiative recombination rate r_{sp}in thermal equilibrium as

$$G_r = r_{sp} = \frac{8\pi n_R^2}{h^3 c^2} \int_0^\infty e^{-\frac{\hbar\omega}{K_B T}} d(\hbar\omega) \tag{2.8}$$

where n is the index of refraction and c is the speed of light. Radiative recombination can be decomposed into spontaneous and stimulated emission components, "i.e.,$B_r = r_{sp} + r_{st}$ general and $B_r = R_{sp} + R_{st} \ = G_r$, in thermal equilibrium. Spontaneous emission occurs as a result of the "lifetime" of a metastable excited state, whereas stimulated emission is the result of the interaction between the electric and magnetic fields of a photon and the wave function of an excited electron. In thermal equilibrium the ratio of spontaneous to stimulated rates at a given photon energy is$e^{\frac{\hbar\omega}{K_B T}} - 1$. When thermal equilibrium is disturbed, the radiative recombination components are modified with the factor $\frac{np}{n_i^2}$for non-degenerate cases, neglecting the effect of photon recycling. The total recombination rate is

$$B_r = r_{sp} + r_{st} = (R_{sp} + R_{st}) \frac{n_p}{n_i^2} = G_r \frac{n_p}{n_i^2} \tag{2.9}$$

Therefore, assuming no spatial dependence, the continuity equation gives

$$\frac{dn}{dt} = g_r - r_r = -G_r \frac{(np - n_i^2) + n'p'}{n_i^2} \tag{2.10}$$

$$= -G_r \frac{n'(n_0 + p_0 + n')}{n_i^2} \tag{2.11}$$

where the simplification that $n^{'} = p^{'}$ has been employed in the last step. Thus, the radiative recombination lifetime can be written as

$$\tau_R = \frac{n_i^2}{G_r (n_0 + p_0 + n')} \tag{2.12}$$

which exhibits an inverse dependence on earner concentration in high-level injection becoming constant in low-level injection. When the temperature of the semiconductor is increased, the number of equilibrium photons increases at all frequencies. This causes a change in G_r which depends on the distribution of photons with energy above the bandgap. It gives an approximate temperature dependence proportional to $e^{-(\frac{E_g+\delta}{K_B T})}$ where δ is a small value compared to the band gap. Hence an increase in G_r, is expected with temperature resulting in a radiative lifetime proportional to $T^3 e^{\frac{\delta}{K_B T}}$ which has an inverse temperature dependence at low temperatures and a direct dependence at room temperature [17].

2.6.2 Auger recombination

Auger recombination occurs as the energy and momentum of two carriers, an electron in the conduction band and a hole in the valence band, are transferred to a third carrier, another electron or hole. This process is the inverse of the impact ionization process, which can be split into two types: electron-electron collisions and hole-hole collisions [2]. Such an event must occur in a manner which conserves both energy and momentum, and the probability for such processes is enhanced if the ratio $(\frac{m_c}{m_v})$ is considerably smaller than or larger than unity [18]. Auger recombination in n-type semiconductors involves two electrons and one hole, while p-type semiconductors involve two holes and one electron. In order to evaluate the equilibrium recombination rate, the nature and occupancy of the valence and conduction bands must be known. Typically, Bloch functions are assumed for the wave functions in the valence and conduction bands and their occupancy is described by the Fermi-Dirac distribution function. The interaction between the recombining particles is Columbic in nature. In degenerate semiconductors, however, when the doping level approaches or exceeds the density of states the Coulomb potential is screened due to the effect of the high concentration of majority carriers. The transition probability is described in terms of matrix elements of the interaction Hamiltonian in perturbation theory. The sum of the matrix elements is taken over all permissible initial and final states, weighted by the respective occupancy probabilities [19]. For the thermal equilibrium condition the resulting Auger recombination rate is given by

$$R_a = G_0 = C_n n_0^2 p_0 + C_p p_0^2 n_0 \tag{2.13}$$

Under non equilibrium conditions, the Auger recombination rate is given by

$$r_A = C_n n^2 p + C_p p^2 n \tag{2.14}$$

Therefore, the net Auger recombination rate under steady-state conditions can be obtained from

(2.12) and (2.13), which yields

$$U_A = r_A - G_0 = C_n\left(n^2 p - p_0 n_0^2\right) + C_p\left(p^2 n - p_0^2 n_0\right) \tag{2.15}$$

Where C_n and C_p are the capture probability coefficients when the third carrier is either an electron or a hole. Both C_n and C_p can be calculated from their inverse process, namely, impact ionization. In thermal equilibrium, the rate at which carriers are annihilated via Auger recombination is equal to the generation rate averaged over the Boltzmann distribution function in which the electron–hole pairs are generated by impact ionization. Thus, oneobtains

$$C_n n_0^2 p_0 = \int_0^\infty P(E)\left(\frac{dn}{dE}\right) dE \tag{2.16}$$

Where $P(E)$ is the probability per unit time that an electron with energy E makes an ionizing collision. It can be described by

$$P(E) = \left(\frac{mq^4}{2h^3}\right) G\left(\frac{E}{E_t} - 1\right)^s \tag{2.17}$$

Where G $<$ 1 is a parameter that is a complicated function of the band structure of the semiconductor. The exponent s is an integer that is determined by the symmetry of the crystal in momentum space at threshold energyE_t. The value of E_t for impact ionization is roughly equal to $1.5E_g$, where E_g is the energy band gap of the semiconductor. By substituting (2.16) into (2.15), one obtains

$$n_i^2 C_n = \left(\frac{s}{\sqrt{\pi}}\right)\left(\frac{mq^4}{h^3}\right) G\left(\frac{K_B T}{E_t}\right)^{s-\frac{1}{2}} e^{-\frac{E_t}{K_B T}} \tag{2.18}$$

Equation (2.17) shows that the Auger capture coefficient C_n for electrons depends exponentially on both the temperature and energy band gap of the semiconductor.The Auger lifetime may be derived from (2.14), with the result

$$\tau_A = \frac{\Delta n}{U_A} = \frac{1}{n^2 C_n + 2n_i^2\left(C_n + C_p\right) + p^2 C_p} \tag{2.19}$$

For an extrinsic semiconductor, τ_A is inversely proportional to the square of the majority carrier density. For the intrinsic case, the Auger lifetime can be obtained from (43) and (44) with s = 2 and$C_n \neq C_p$, which yields

$$\tau_{Ai} = \frac{1}{3n_i^2(C_n + C_p)} = 3.6 \times 10^{-17} \left(\frac{E_t}{K_B T} \right)^{\frac{3}{2}} e^{\frac{E_t}{K_B T}} \tag{2.20}$$

Which shows that the intrinsic Auger lifetime is an exponential function of temperature and energy band gap. The Auger recombination has been found to be the dominant recombination process for degenerate semiconductors and small-band-gap semiconductors. For small-band-gap semiconductors, one expects the Auger recombination to be the predominant recombination process even at smaller injection level [20].

2.6.3 Shockley-Read-Hall Recombination

An allowed energy state, also called a trap, within the forbidden band gap may act as a recombination center, capturing both electrons and holes with almost equal probability. This equal probability of capture means that the capture cross sections for electrons and holes are approximately equal. The SRH theory of recombination assumes that a single recombination center, or trap, exists at an energyE_t within the band gap [1]. The emission and capture rates of charge carriers determine the occupancy of a center at equilibrium. The Fermi function at the trap energy is given by

$$f_F(E_t) = \frac{1}{1 + e^{\left(\frac{E_t - E_F}{K_B T} \right)}} \tag{2.21}$$

After some lengthy analysis of the dynamics involved in this process, we see that that the recombination rate R_T involved with traps is dependent on the volume density of trapping defects and the energy of the trapping level:

$$R_T = \frac{np - n_i^2}{\tau_{ho}(n + n_1) + \tau_{eo}(p + p_1)} \tag{2.22}$$

Where ‘n’ and ‘p’ are the concentrations of electrons and holes respectively, n is the “intrinsic carrier concentration”, and τ_{ho} and $\tau_{eo}$are lifetime parameters (for holes and electrons respectively) whose values depend on the type of trap and the volume density of trapping defects. The quantities $n_1$and $p_1$are parameters that introduce the dependency of the recombination rate on the trapping energy level E_t as follows

$$n_1 = N_c e^{\left(\frac{E_t - E_c}{K_B T}\right)} \tag{2.23}$$

$$p_1 = N_v e^{\left(\frac{E_v - E_t}{K_B T}\right)} \tag{2.24}$$

$$n_1 p_1 = n_i^2 \tag{2.25}$$

It is simply noted that when the flaw density is small enough to keep n_e and p_e essentially the same, then the hole lifetime τ_{ho} equals the electron lifetime τ_{eo} This lifetime has the form

$$\tau_{ho} = \tau_{eo} = \frac{\tau_0 (n_0 + p_0) + \tau_\infty (n_e)}{n_0 + p_e + n_e} \tag{2.26}$$

Where τ_0 andτ_∞, are the limiting values of lifetime for very small and very large disturbances of equilibrium and are each inversely proportional to the density of recombination centers [21].

2.7 Band structure

A commonly used approximation of the exact band structure in a direct-gap semiconductor is the parabolic band model. In this model the energy-versus-wave vector (E versus k) relation is assumed to parabolic, that is,

$$E_C = \frac{h^2 k^2}{2m_e} \qquad \text{for electrons} \tag{2.27}$$

$$E_h = \frac{h^2 k^2}{2m_h} \qquad \text{for holes} \tag{2.28}$$

Where m_e and m_h are the effective masses of electrons and holes, respectively, and k is the magnitude of the wave vector k. In a direct-gap semiconductor, the minimum in the conduction band curve and the maximum in the valence band curve occur at the same value of the wave vector k (k value zero). Since a photon carries negligible momentum compared with the carrier

momentum *hk*,adiative transitions occur between free electrons and free holes of essentially identical wave vectors. At a given temperature T, the available number of electrons and holes are distributed over a range of energies.

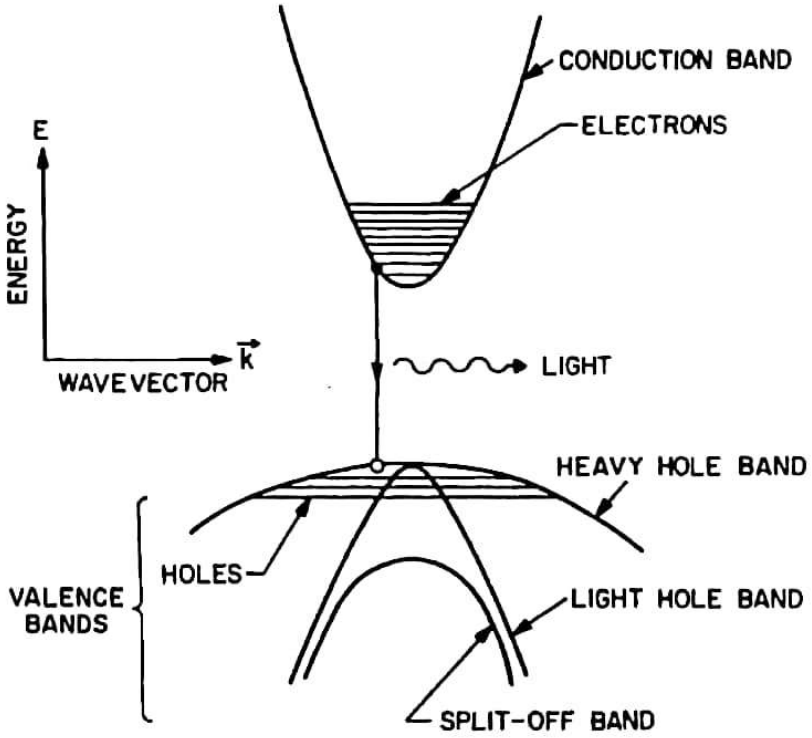

Figure 2.1: Energy versus wave-vector diagram of a direct-band-gap semiconductor

The occupation probability f_c of an electron with energy E_e is given by the Fermi-Dirac statistics, and is

$$f_c(E_c) = \frac{1}{\exp\left(\frac{E_c - E_{fc}}{K_B T}\right) + 1} \tag{2.29}$$

Where E_{fc} is the quasi-Fermi level for the conduction band,similarly, for the valence-band holes, the occupation probability of ahole with energy $E_h$is

$$f_h(E_v) = \frac{1}{\exp\left(\frac{E_h - E_{fv}}{K_B T}\right) + 1} \tag{2.30}$$

Where E_{fv} is the quasi-Fermi level for the valence band. The notations used here assume that E_c and E_{fc} are measured from the conduction-band edge and are positive into the conduc-

tion band.On the other hand, E_v and E_{fv} are measured from the valence-band edge and are positive into the valence band. Note that $f_v represents the occupation probability of the hole and not of the electron. Co$ the band gap. The photon can be absorbed creating an electron of energy Ee and a hole of energy Ev. The absorption rate is given by

$$R_a = B\,(1-f_c)\,(1-f_v)\,\rho(E) \tag{2.31}$$

Where B is the transition probability, p(E) is the density of photons of energy E, and the factors

$$1-f_c$$

and

$$1-f_v$$

represent the probabilities that the electron and hole states of energy E_c and E_v are not occupied. The stimulated-emission rate of photons is given by

$$R_e = B f_c f_v \rho(E) \tag{2.32}$$

Where the Fermi factors f_c and f_v are the occupation probabilities of the electron and hole states of energy E_c and E_v respectively. The stimulated emission process is accompanied by the recombination of an electron-hole pair. The condition for net stimulated emission or optical gain is

$$R_e > R_a \tag{2.33}$$

Using Eqs. (2.29) and (2.30), this condition becomes

$$f_c + f_v > 1 \tag{2.34}$$

With the use of f_c and f_v given by Eqs. (2.27) and (2.28), this becomes

$$E_{fc} + E_{fv} > E_c + E_v \tag{2.35}$$

By adding E_g to both sides and noting that E_c + E_v+ E_g =hv, it follows that the separation of the quasi-Fermi levels must exceed the photon energy in order for the stimulated-emission rate to exceed the absorption rate. This is the necessary condition for net stimulated emission or optical gain.[22]

2.8 Theory of radiative recombination

The theory of radiative recombination is first discussed in terms of a rigorous quantum mechanical model. Subsequently recombination is discussed in terms of a semi classical model based on equilibrium generation and recombination. This model was developed by van Roosbroeck and Shockley (1954). Finally, the Einstein model of spontaneous and stimulated transitions in a two-level atom is discussed.

2.8.1 Quantum mechanical model

The quantum mechanical calculation for the spontaneous emission rate is based on the induced emission rate given by Fermi's Golden Rule which gives the transition probability per unit time (called transition rate) from a quantum mechanical state j to a state m.

$$W_{j\to m} = \frac{d}{d(t)}\left|a_m^{'}(t)\right|^2 = \frac{2\pi}{\hbar}\left|H_{mj}^{'}\right|^2 \rho\left(E = E_j + \hbar\omega_0\right) \tag{2.36}$$

Where$H_{mj}^{'}$ is the transition matrix element [16]. The spontaneous-emission rate and the absorption rate for photons in a semiconductor can be calculated using time-dependent perturbation theory and summing over the available electron and hole states. We first consider the case of two discrete energy levels of energy E_i and E_i The electron makes a transition from an initial state of energy E_i to a final state of energy E_f and in the process a photon of energy E = E_i - E_f is emitted. The transition probability or the emission rate W of such a process is given by Fermi's golden rule

$$W = \frac{2\pi}{h}\left|H_{if}^{'}\right|^2 \rho\left(E_f\right)\delta W\left(E - E_i + E_f\right) \tag{2.37}$$

where $H_{if}^{'}$ is the matrix element $< i|H^{'}|f >$ of the time-independent part of the perturbation Hamiltonian H_I between the initial state $|i>$ and final state $|f>$. and $\rho(E_f)$ is the density of the final states. For optical transitions between the conduction and valence band, the electron momentum must be conserved because the photon momentum ($p = k$) is negligibly small. The conservation of momentum condition is known as the k-selection rule. In obtaining Eq. (46), the perturbation Hamiltonian is assumed to be of the form

$$H_I = 2H^{'} \sin \omega t \tag{2.38}$$

The time-dependent sinusoidal part gives rise to the delta function of Eq. (2.35) arising from the energy conservation during the emission process. For photons interacting with free electrons of massm_0, the perturbation Hamiltonian is given by

$$H_I = -\frac{q}{m_0} A \cdot P \tag{2.39}$$

Where **A** is the vector potential of the electromagnetic field and **p** is the electron-momentum vector. The vector potential is related to the electric field ε by the equation

$$\varepsilon = -\frac{\partial A}{\partial t} \tag{2.40}$$

For a traveling plane wave with the angular frequency (ω), the electric field is written as

$$\varepsilon = E_0 \overrightarrow{\in} \cos\left(\widehat{\omega t - \overrightarrow{k}} \cdot \overrightarrow{r}\right) \tag{2.41}$$

where $\overrightarrow{\in}$ is a unit vector determining the polarization of the field, E_0 is its amplitude, and $\overrightarrow{k}$ denotes the propagation vector such that $\overrightarrow{\in} x \overrightarrow{k} = 0$. The magnitude of the electric field E_0 associated with one photon can be obtained asfollows. The magnitude of the Poynting vector that represents the energy flux is given by

$$\overrightarrow{S} = \left| \langle \overrightarrow{\varepsilon} \times \overrightarrow{B} \rangle \right| \tag{2.42}$$

where angular brackets denote time averaging and $\overrightarrow{B}$ is the magnetic field, which can be obtained using Maxwell's equations Using them, we obtain

$$\overrightarrow{S} = \frac{1}{2} E_0^2 \overline{\mu} \varepsilon_0 c \tag{2.43}$$

where $k = \frac{\overline{\mu}\omega}{c}$ and $\overline{\mu}$ is the refractive index of the medium. The factor 1/2 arises from time averaging over one optical cycle. The energy flux per photon is also given by the product of the photon energy $\hbar\omega$ and the group velocity $\frac{c}{\overline{\mu}}$ Hence it follows that

$$\overrightarrow{S} = \frac{\hbar\omega c}{\overline{\mu}} \tag{2.44}$$

the vector potential A is given by

$$A = - \in \left(\frac{2\hbar}{\in_0 \overline{\mu}^2 \omega}\right)^{\frac{1}{2}} \sin(\omega t - \overrightarrow{k} \cdot \overrightarrow{r}) \tag{2.45}$$

the perturbation Hamiltonian becomes

$$H_I = \frac{q}{m_0}\left(\frac{2\hbar}{\varepsilon_0 \overline{\mu}^2 \omega}\right)^{\frac{1}{2}} (\widehat{\varepsilon} \cdot \mathbf{p}) \sin(\omega t - \mathbf{k} \cdot \mathbf{r}) \tag{2.46}$$

The square of the transition matrix element H'_{if} is now given by

$$|H'_{if}|^2 = \frac{q^2}{m_0^2} \frac{2\hbar}{\varepsilon_0 \overline{\mu}^2 \omega} \frac{1}{4} |\langle i|\varepsilon \cdot \mathbf{p}|f\rangle|^2 \tag{2.47}$$

Where we have made the usual assumption that the electron wave functions spread over a linear dimension shorter than the wavelength $(r \ll \lambda)$ so that $k.r \ll 1$. For stimulated emission or absorption, $\rho(E_f) = 1$, and the absorption or emission rate at a photon energy $E = \hbar\omega$ for transitions between two discrete levels obtained is given by

$$W = \frac{\pi q^2}{m_0^2 \varepsilon_0 \overline{\mu}^2 \omega} \left|M_{if}\right|^2 \delta\left(E_i - E_f - \hbar\omega\right) \tag{2.48}$$

Where $M_{if}$is the momentum matrix element between the initial and final electron states. In the case of absorption, the number of photons absorbed per second is W. Since a photon travels a distance $\frac{c}{\overline{\mu}}$ in 1sec, the number of photons absorbed per unit distance or the absorption coefficient $\alpha = \frac{\overline{\mu}W}{c}$. the absorption coefficient for photons of energy E equal to $\hbar\omega$ becomes

$$\alpha(E) = \frac{q^2 h}{2\varepsilon_0 m_0^2 c \overline{\mu} E} \left|M_{if}\right|^2 \delta\left(E_i - E_f - \hbar\omega\right) \tag{2.49}$$

For spontaneous emission, the quantity $\rho(E_f)$ in Eq. (2.28) equals the number of states for photons of energy E per unit volume perunit energy. It is given by

$$\rho\left(E_f\right) = \frac{\overline{\mu}^3 \omega^2}{\pi^2 c^3 \hbar} \tag{2.50}$$

the spontaneous emission rate per unit volume at the photon energy E isgiven by

$$r_{sp}(E) = \frac{4\pi q^2 \overline{\mu} E}{\varepsilon_0 m_0^2 c^3 h^2} \left|M_{if}\right|^2 \delta\left(E_i - E_f - E\right) \tag{2.51}$$

We now calculate the spontaneous-emission rate and the absorption coefficient for direct-gap semiconductors. These quantities are obtained by integrating Eqs. (2.46) and (2.49) over the occupied electrons and holes states in a semiconductor [23]. A realistic band model for a $-V$ direct-gap semiconductor is the four-band model [24] In this model the valence band is represented by three sub bands: the heavy-hole band, the light-hole band, and the spin-split-off-hole band. The Light- and heavy-hole bands are degenerate at $k = 0$. Usually the split-off energy A is large compared with the thermal energy $K_B T$; hence the split-off band is full of electrons, that is, no holes are present. The quasi-Fermi levels for the conduction and valence bands can be obtained from the known effective masses and the density of states in each band. For the conduction band, E_{fc} is obtained using

$$n = \int \frac{\rho_c(E) dE}{1 + \exp\left(\frac{E - E_{fc}}{K_B T}\right)} \tag{2.52}$$

Where $\rho_c(E)$ is the conduction-band density of states and n is the number of electrons in the conduction band. The density of states for electrons of energy E can be obtained by

$$\rho_c(E) = 2\frac{4\pi K^2}{(2\pi)^3}\frac{dK}{dE} = 4\pi\left(\frac{2m_c}{h^2}\right)^{\frac{3}{2}} \tag{2.53}$$

Where $E = \frac{h^2 K^2}{2m_c}$, and m_c is the conduction-band effective mass. The factor 2 in Eq. (2.51) arises from the two electronic spin states. Equation (2.50) can be rewritten as

$$n = N_c \frac{2}{\pi^{\frac{1}{2}}} \int \frac{\varepsilon^{\frac{1}{2}} dE}{1 + \exp\left(\varepsilon - \varepsilon_{fc}\right)} \tag{2.54}$$

Where

$$N_c = 2\left(\frac{2\pi m_c K_B T}{h^2}\right)^{\frac{3}{2}}$$

and $\varepsilon_{fc} isequalto \frac{E_{fc}}{K_B T}$. Equation (2.52) can be used to calculate ε_{fc} for a given electron concentration. A useful approximation for ε_{fc} is given by [25], they show that $epsilon_{fc}$ can be represented by a convergent series of the form

$$\varepsilon_{fc} = \ln\left(\frac{n}{N_c}\right) + \sum_{i=1}^{\infty} A_i \left(\frac{n}{N_c}\right)^i \tag{2.55}$$

For a non-degenerate electron gas ($n \ll N_c$), all terms except the first in Eq. (2.53) can be neglected and the Fermi energy is given by

$$E_{fc} = K_B T \ln\left(\frac{n}{N_c}\right) \tag{2.56}$$

the occupation probability becomes is

$$E_{fc} = K_B T \ln\left(\frac{n}{N_c}\right) \tag{2.57}$$

The occupation probability becomes:

$$f_c(E) \approx \frac{n}{N_c} \exp\left(\frac{-E}{K_B T}\right) \tag{2.58}$$

This is often referred to as the Boltzmann approximation. The use of Eq. (2.55) simplifies considerably the calculation of recombination rates in semiconductors.

The quasi-Fermi level for the holes in the valence band can be similarly calculated. The hole density is given by:

$$p = \sum_{i=l,h} \int \frac{\rho_{vi}(E) dE}{1 + \exp\left(\frac{E - E_{fv}}{K_B T}\right)} \tag{2.59}$$

where $\rho_{vi}(E)$ is the density of states for holes, and the summation is over the light-hole and heavy-hole bands.

The density of states is given by:

$$\rho(E) = N_v \frac{2}{\pi^{\frac{1}{2}}} \int \frac{\varepsilon^{\frac{1}{2}} d\varepsilon}{1+\exp(\varepsilon - \varepsilon_{fv})} \tag{2.60}$$

where

$$N_v = 2\left(\frac{2\pi K_B T}{h^2}\right)^{\frac{3}{2}} \left(m_{lh}^{\frac{3}{2}} + m_{hh}^{\frac{3}{2}}\right) \tag{2.61}$$

Here, m_{lh} and m_{hh} are the effective masses of light and heavy holes, respectively.

For the non-degenerate case where p N_v, Eq. (2.61) can be simplified to obtain the following expressions for the quasi-Fermi energy and the hole occupation probability.

The quasi-Fermi level for holes in the valence band is given by:

$$E_{fv} = K_B T \ln\left(\frac{p}{N_v}\right) \tag{2.62}$$

The hole occupation probability is:

$$f_v(E) = \frac{p}{N_v} \exp\left(\frac{-E}{K_B T}\right) \tag{2.63}$$

For non-degenerate semiconductors, the quasi-Fermi levels for electrons and holes, E_{fc} and E_{fv}, can be used to determine carrier concentrations and recombination rates. These equations are essential in semiconductor physics, particularly in analyzing carrier dynamics under thermal equilibrium and external perturbations.

The spontaneous-emission rate at the photon energy E is given by

$$r_{sp}(E) = \frac{2q^2 \overline{\mu} E \left|M_b\right|^2}{\pi \varepsilon_0 m_0^2 c^3 h^2} \left(\frac{2m_r}{\hbar^2}\right)^{\frac{3}{2}} (E - E_g)^{\frac{1}{2}} f_c(E_c) f_v(E_v) \tag{2.64}$$

Thus the total spontaneous-emission rate per unit volume due to electron-heavy-hole transitions is given by

$$R = \int_{E_g}^{\infty} r_{sp}(E) dE \tag{2.65}$$

2.8.2 The van Roosbroeck–Shockley model

The VRS model allows one to calculate the spontaneous radiative recombination rate under equilibrium and non-equilibrium conditions. To calculate the recombination rate, the model requires the knowledge of only a few basic parameters, namely the band gap energy, the absorption coefficient, and the refractive index. All of these parameters can be determined by simple, well-known experimental methods. Consider a semiconductor with an absorption coefficient () given in units of cm^{-1}. A photon is generated in the semiconductor by electron–hole recombination and is subsequently absorbed, The mean distance a photon of frequency travels before being absorbed is simply $\alpha(v)^{-1}$. The time it takes for a photon to be absorbed is given by

$$\tau(v) = \frac{1}{\alpha(v)V_{gr}} \tag{2.66}$$

Where V_{gr} is the group velocity of photons propagating in the semiconductor, The group velocity of photons is given by

$$V_{gr} = \frac{d\omega}{dk} = \frac{dv}{d(\frac{1}{\lambda})} = c\frac{dv}{d(\overline{n}v)} \tag{2.67}$$

Where $\overline{n}$ is the refractive index, Inserting the group velocity into Eq. (2.63) yields

$$\frac{1}{\tau(v)} = \alpha(v)V_{gr} = \alpha(v)c\frac{dv}{d(\overline{n}v)} \tag{2.68}$$

This equation gives the inverse photon lifetime or photon absorption probability per unit time. The product of the absorption probability and the photon density yields the photon absorption rate per unit time per unit volume. Under equilibrium conditions, the density of photons per unit volume in a medium with refractive index n is given by Planck's black-body radiation formula.

$$N(\lambda)d\lambda = \frac{8\pi}{\lambda^4}\frac{1}{e^{\frac{hv}{K_BT}} - 1} \tag{2.69}$$

From which we can readily obtain $N(v)dv$, the number of photons having frequencies in the interval v and $vplusdv$ We have

$$\lambda = \frac{c}{(\overline{n}v)} \tag{2.70}$$

so that $d\lambda$ is equal to $-\frac{c}{(\overline{n}v)^2}\frac{d(\overline{n}v)}{dv}dv$ Inserting eq(2.66) this value in Eq. (2.65) yields Planck's black-body photon distribution as a function of frequency

$$N(v)dv = \frac{8\pi v^2\overline{n}^2}{c^3}\frac{d\,(\overline{n}v)}{dv}\frac{1}{e^{\frac{hv}{K_BT}}-1}dv \tag{2.71}$$

The absorption rate per unit volume in the frequency interval and +d is given by the photon density divided by the mean lifetime of photons.

$$R_0(v) = \frac{N(v)}{\tau(v)} = \frac{8\pi v^2\overline{n}^2}{c^3}\frac{d\,(\overline{n}v)}{dv}\frac{1}{e^{\frac{hv}{K_BT}}-1}\alpha(v)c\frac{dv}{d\,(\overline{n}v)} \tag{2.72}$$

Integration over all frequencies yields the absorption rate per unit volume

$$R_0 = \int_0^\infty R_0(v)dv = \int_0^\infty \frac{8\pi v^2\overline{n}^2}{c^2}\frac{\alpha(v)}{e^{\frac{hv}{K_BT}}-1}dv \tag{2.73}$$

Which is the celebrated van Roosbroeck–Shockley equation. The vanRoosbroeck–Shockley equation can be simplified by writing the absorption coefficient as

$$\alpha = \alpha_0\sqrt{\frac{(E\ -\ E_g\ )}{E_g}} \tag{2.74}$$

The square-root dependence of the absorption coefficient is motivated by the proportionality of the absorption coefficient and the density of states, which in turn follows a square-root dependence on energy. Note that 0 is the absorption coefficient at

$$h\nu\ =\ 2Eg$$

. The vanRoosbroeck–Shockley equation can be simplified further by neglecting the frequency dependence of the refractive index and using the refractive index value at the band edge. One obtains

$$R_0 == 8\pi c\bar{n}^2\alpha_0\sqrt{\frac{K_BT}{E_g}}\left(\frac{K_BT}{ch}\right)^3\int_{x_g}^{\infty}\frac{x^2\sqrt{x-x_g}}{e^x-1}dx \tag{2.75}$$

where

$$x = h\nu\ /(kT)\ = E\ /(k_BT) \tag{2.76}$$

and

$$x_g = E_g\ /(k_BT) \tag{2.77}$$

Owing to the strong increase of the exponential function with x, only a small range of energies close to the bandgap contributes to the integral. Under equilibrium conditions, the carrier generation rate (photon absorption rate) is equal to the carrier recombination rate (photon emission rate). Thus the van Roosbroeck Shockley model provides the equilibrium recombination rate [16]. The recombination rate is now given by

$$R = Bn_i^2 \tag{2.78}$$

2.8.3 The Einstein model

The first theory of optical transitions was developed by Albert Einstein. The Einstein model includes spontaneous and stimulated or induced transitions. Spontaneous transitions occur spontaneously, that is, without an external stimulus. In contrast, stimulated transitions are induced by an external stimulus, namely a photon. Thus, the induced transition rates are proportional to the photon density or radiation density [16].

2.9 Continuity Equations and Carrier Lifetimes

Suppose that conduction band electrons are created at a rate g_E as a result of some external influence. In addition to this, there are natural rates of generation, g, and recombination, r, resulting from a variety of energy transformation mechanisms. Then if we concentrate on the free electron population and its dependence on time, we must be able to express an electron continuity equation in the form

$$\frac{\partial n}{\partial t} = (g - r) + g_E + e^{-\nabla}.I_n \tag{2.79}$$

Here the last term represents the tendency of excess electrons to move elsewhere if their distribution is not uniform. Now it is plausible to assume that $(r - - - g)$ will be crudely proportional to the excess electron density n_e equal to (n — n_0) when this excess density is not unduly large. It is convenient to define the electron lifetime τ_n by

$$\tau_{n_e} = \frac{n_e}{r - g} \tag{2.80}$$

Recognizing that a lifetime so defined will probably not be entirely independent of n_e. Thus in a semiconductor situation for which spatial dependences can be ignored, the electron continuity equation reduces to

$$\frac{dn_e}{dt} = \frac{dn}{dt} = g_E - \frac{n_e}{\tau_n} \tag{2.81}$$

A continuity equation for holes can be formulated in the same manner,thus

$$\frac{dp_e}{dt} = \frac{dp}{dt} = g_E^{'} - \frac{P_e}{\tau_P} \tag{2.82}$$

Holes and electrons have equal lifetimes if generation and recombination are both exclusively band to band processes [26].

Chapter 3

Materials and Methodology

3.1 Materials

The study was involved both theoretical and computational methods. The books, articles, journals, published thesis and dissertations carried out based on the thesis title are to be sources of information in theoretical analysis. Computer and software are essential instruments to help us in computational part of my study, All of them are used to accomplish the study.

3.2 Methodology

The calculation of recombination lifetime of GaSb is performed by different radiative recombination models, those models are quantum mechanical model, van Roosbroeck and Shockley model and Einstein model. The simplest approach to calculate the recombination lifetime GaSb is the Van Roosbroeck and Shockley model. It is semi classical method of calculating the recombination life time of the non-degenerate bimolecular semiconductors like GaSb. There our further analysis for my thesis is more focus on this method.

Chapter 4

Results and Discussions

4.1 Introduction

In this chapter, the recombination lifetime of gallium antimonide is calculated within the framework van Roosbroeck- Shockley method. The important aspects in studied recombination lifetime of Gallium antimonide (GaSb) are energy versus wave vector, absorption and emission rate, recombination rate and the carriers lifetime of gallium antimonide(GaSb) in different recombination processes. Results are mainly presented in figures. The first result are the energy versus wave vector for gallium antimonide(GaSb) and second result is absorption and emission rate of GaSb then comes the result of recombination rate and carriers recombination lifetimes of GaSb. Graphs were plotted to obtain the optimized parameters for GaSb recombination lifetime, within joint density of states (JDOS) correlation functional.

4.2 The energy versus wave vector for gallium antimonide (GaSb)

The energy band gap of GaSb with respect to the wave vector K was investigated. by keeping all energy band gap dependency of GaSb constant except the wave vector k. The band gap energy of GaSb is around 0.726ev at a temperature of 300K, this is because the minimum conduction band and maximum valence band are both located at the same K-space, K=0 (the Gamma point in Brillouin zone). The calculated result was shown on Figure 2. The curve shows that the band gap energy is maximum at both maximum and minimum K-value of the wave vector. It means that at both K=±10^9 m^{-1} K-value the graph shows maximum band gap energy of around 1.79*ev.* the graph shows the parabolic shape and this curve shows how the band gap energy of GaSb is increased with increasing the K-values of wave vector and it justifies identity points of symmetry in the band structure. And the following equation yields

$$E_g(k) = E_g + \frac{h^2k^2}{4m_em_h}[m_e + m_h] \tag{4.1}$$

Table 4.1: The results of energy band gap of GaSb with respect to wave vector

Wave vector (m^{-1})	Energy band-gap (eV)
0	0.726
2×10^8	0.7684633
4×10^8	0.895853202
6×10^8	1.108169704
8×10^8	1.405412807
1×10^9	1.787582511

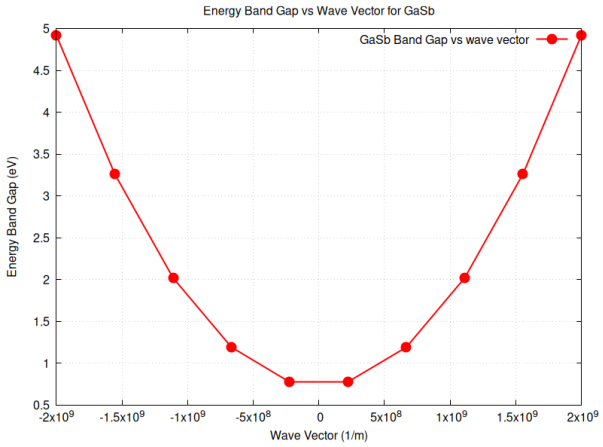

Figure 4.1: Band gap energy versus wave vector graph

4.3 Emission rate and Absorption rate of Gallium Antimonide (GaSb)

4.3.1 Emission rate of Gallium Antimonide (GaSb)

The spontaneous emission rate (emission of photon due to electron-hole recombination) was calculated based on JDOS. The JDOS describes the number of electron-hole pairs at each energy level that can participate in photon emission. For GaSb the JDOS will be significant near the band gap and will gradually increase with photon energy. On the graph below we had observed peak, this peak indicates that the photon energy ranges where radiative recombination and photon emission is most likely to occur. GaSb is a direct band gap semiconductor with band gap energy of around 0.726ev. Photon emission cannot occur below this energy, as there is not

enough energy to transition across the band gap. At peak point as shown in Figure 3 below, the radiative recombination is most efficient. Beyond the peak the emission rate may start to decline or saturate even as photon energy increases. This is because at higher photon energies, the JDOS may not continue increasing significantly, and fewer electron hole pairs exist at this higher energy level. Generally the emission rate at high photon energies may diminish due to a lack of available states or reduced recombination probability. Table 3 shows the grids between photon energy and spontaneous emission. The following equation yield's

The emission rate of photons in GaSb is derived from the principle of **detailed balance**, which states that in thermal equilibrium, the **emission rate** must be equal to the **absorption rate** when no external excitation is applied.

Spontaneous Emission Rate

The spontaneous emission rate per unit volume per unit energy is given by:

$$R_{\text{em}}(E) = A_{cv}(\omega)\rho_{\text{ph}}(E)\left[f_c(E) - f_v(E)\right] \tag{4.2}$$

where:

- $R_{\text{em}}(E)$ is the photon emission rate per unit volume per unit energy.
- $A_{cv}(\omega)$ is the spontaneous emission coefficient.
- $\rho_{\text{ph}}(E)$ is the **photon density of states**, given by:

$$\rho_{\text{ph}}(E) = \frac{8\pi n^3 E^2}{(hc)^3} \tag{4.3}$$

- $f_c(E)$ and $f_v(E)$ are the Fermi-Dirac distributions for electrons in the conduction and valence bands, respectively.

Total Emission Rate

The total spontaneous emission rate per unit volume is obtained by integrating over all photon energies:

$$R_{\text{em}} = \int_{E_g}^{\infty} R_{\text{em}}(E)dE. \tag{4.4}$$

Expanding the emission rate using the **Einstein relations**, we express it in terms of the absorption coefficient:

$$R_{\text{em}}(E) = \alpha(E)\frac{B_{cv}}{A_{cv}}\rho_{\text{ph}}(E). \tag{4.5}$$

where B_{cv} and A_{cv} are the Einstein coefficients for absorption and spontaneous emission.

Emission and Blackbody Radiation

In thermal equilibrium, the **photon emission rate** is also related to the **blackbody radiation distribution**:

$$R_{\text{em}}(E) = \alpha(E)\frac{I_{\text{bb}}(E)}{E} \tag{4.6}$$

where:

$$I_{\text{bb}}(E) = \frac{2E^3}{(hc)^2}\frac{1}{e^{E/k_BT}-1} \tag{4.7}$$

is the **blackbody radiation intensity** at temperature T.

Detailed Balance Condition

From detailed balance, in thermal equilibrium, the absorption and emission rates satisfy:

$$R_{\text{abs}}(E) = R_{\text{em}}(E). \tag{4.8}$$

This implies:

$$\alpha(E)\frac{I(E)}{E} = \alpha(E)\frac{I_{\text{bb}}(E)}{E}, \tag{4.9}$$

which leads to the equilibrium photon flux being given by Planck's law.

In Considerations for GaSb

- GaSb has a direct bandgap of approximately $E_g \approx 0.726$ eV at room temperature.
- The spontaneous emission coefficient $A_{cv}(\omega)$ depends on the electronic band structure.
- The photon density of states $\rho_{\text{ph}}(E)$ influences the rate of emission.
- The refractive index n of GaSb varies with wavelength (typically $n \approx 3.8$ in the infrared range).

For precise calculations, numerical simulations such as **Density Functional Theory (DFT)** or **empirical fitting models** are recommended.

Table 4.2: Emission rate of GaSb as a function of energy band gap

Photon energy (eV)	Spontaneous emission rate ($\text{cm}^{-3}s^{-1}$)
0.72600001096725464	0.0000000000000000
0.75002403499127868	$2.7241423576949791 \times 10^{-2}$
1.0002742852415289	$1.2927834129908399 \times 10^{-5}$
1.1944684794357232	$1.0092618455108621 \times 10^{-8}$
1.2004744854417291	$8.0716582360128329 \times 10^{-9}$
1.2260000109672546	$3.1196090615391520 \times 10^{-9}$

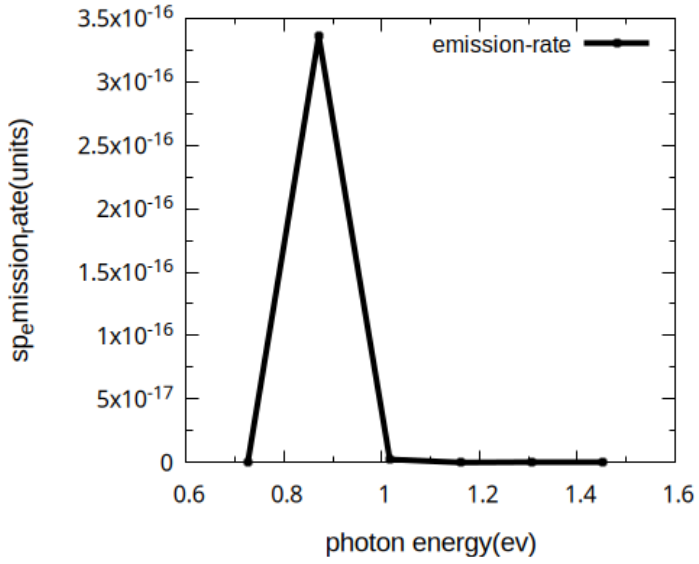

Figure 4.2: Emission rate of GaSb as a function of energy band gap

4.3.2 Absorption Rate of GaSb with respect to the photon energy

The absorption rate was calculated using VRS which related the optical absorption coefficient to the rate of spontaneous emission. The VRS expression for absorption involves calculating the transition rate based on DOS (Density of state) and occupation probabilities in the conduction and valence bands. In this part of my analysis I have to describe the spontaneous absorption rate as the rate at which photons are absorbed by semiconductor without external stimulation. By using mathimatica codes I have generated the data to plot the graph of spontaneous absorption rate against the photon energy that absorbed intrinsic GaSb. We analyze the absorption rate of GaSb by comparing the photon energy when it is adjusted below the band gap energy of GaSb and above the band gap energy of GaSb as shown in Figure 4 below. In region below the band gap energy (Ephoton¡Eg) GaSb shows minimal absorption rates as photon do not have energy to excite electrons across the band. This theoretical data was collected at a temperature T=300K, we made the temperature constant to avoid the variation of band gap energy. The grids are shown in the Table 4.

The absorption coefficient $\alpha(E)$ in the van Roosbroeck–Shockley formalism is given by:

$$\alpha(E) = \frac{c^2}{n^2 \hbar \omega} A_{cv}(\omega) \left[f_c(E) - f_v(E) \right] \tag{4.10}$$

where:

- c is the speed of light in vacuum.
- n is the refractive index of GaSb.
- $\hbar$ is the reduced Planck's constant.

- ω is the angular frequency of the photon, $\omega = E/\hbar$.
- $A_{cv}(\omega)$ is the spontaneous emission coefficient.
- $f_c(E)$ and $f_v(E)$ are the Fermi-Dirac distributions for the conduction and valence bands, respectively.

The absorption rate per unit volume is given by:

$$R_{\text{abs}} = \int_{E_g}^{\infty} \alpha(E) \frac{I(E)}{E} dE \tag{4.11}$$

where:

- R_{abs} is the absorption rate (number of absorbed photons per unit volume per second).
- $I(E)$ is the spectral photon flux (number of incident photons per unit area per second per energy range).
- E_g is the bandgap energy of GaSb ($E_g \approx 0.726$ eV at room temperature).

In Considerations for GaSb

- GaSb has a direct bandgap of approximately $E_g \approx 0.726$ eV at room temperature.
- The joint density of states (JDOS) and transition matrix elements influence $A_{cv}(\omega)$.
- The refractive index n of GaSb depends on wavelength (typically $n \approx 3.8$ in the infrared range).

For precise calculations, the absorption coefficient $\alpha(E)$ can be derived using numerical methods such as density functional theory (DFT) or empirical models.

Table 4.3: Variations of absorption rate of GaSb as a function of photon energy

Photon energy (eV)	Absorption Rate ($\text{cm}^{-3}s^{-1}$)
0.726	0
1.011714286	7.64×10^{26}
1.297428571	1.08×10^{27}
1.583142857	1.32×10^{27}
1.868857143	1.53×10^{27}

In region where the photon energy is above the band gap energy (Ephoton¿Eg) absorption rate increase as photon energy surpasses the band gap energy. The curve steepness shows the involvement of electron transition. From the above Figure 4 we understand that the rate of absorption is spontaneously increased with increasing the photon energy just above the threshold energy of GaSb.

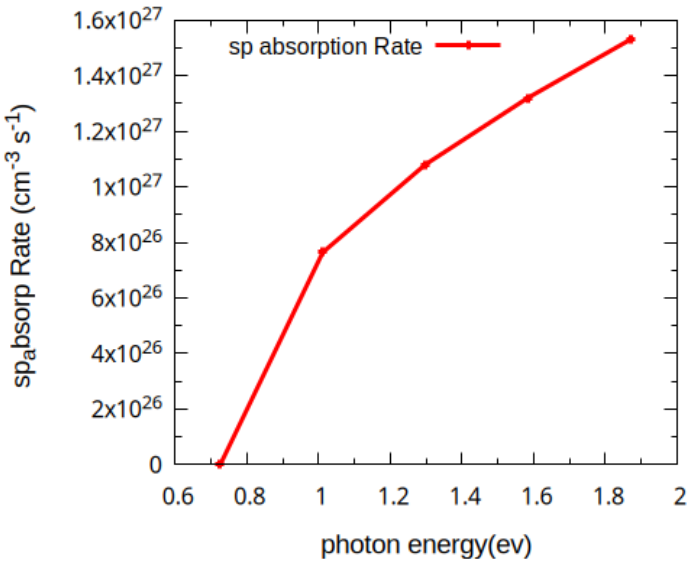

Figure 4.3: Absorption rate of GaSb as a function of photon energy

4.4 Recombination rate of GaSb

Under equilibrium conditions, the carrier generation rate (photon absorption rate) is equal to the carrier recombination rate (photon emission rate) thus the VRS provides the equilibrium recombination rate.

4.4.1 Radiative Recombination Rate of GaSb

Energy band gap dependency of Radiative recombination rate of GaSb

In this part of my analysis we will see all dependency of radiative recombination rate. The band gap energy E_g impacts the recombination rate because it determines the energy difference between conduction band and valence bands. Figure 5 show that the radiative recombination rate is expected to decrease with increasing the band gap energy. This decrease in radiative recombination rate is due to for a given carrier density higher energy gaps make radiative transitions less. The result is more illustrated on the Table 5 below. The result below is obtained from the equation below; The radiative recombination rate in a direct bandgap semiconductor like GaSb is given by the van Roosbroeck–Shockley relation, which describes the balance between spontaneous emission and absorption.

General Expression for Radiative Recombination

The **radiative recombination rate** per unit volume is given by:

$$R_{\text{rad}} = Bnp, \tag{4.12}$$

where:

- R_{rad} is the radiative recombination rate (carrier recombinations per unit volume per second).
- B is the **radiative recombination coefficient**.
- n is the **electron concentration** in the conduction band.
- p is the **hole concentration** in the valence band.

The radiative recombination coefficient B depends on the bandgap energy E_g through the spontaneous emission process, which can be derived from the van Roosbroeck–Shockley formalism:

$$B(E_g, T) = \frac{e^2}{\varepsilon_0 m_0 c n^2} \int_{E_g}^{\infty} \frac{g_c(E) g_v(E) |\mathbf{M}_{cv}|^2}{E^2} f_c(E) f_v(E) dE. \tag{4.13}$$

Here:

- e is the elementary charge.
- ε_0 is the permittivity of free space.
- m_0 is the free electron mass.
- c is the speed of light.
- n is the refractive index of GaSb.
- $g_c(E)$ and $g_v(E)$ are the conduction and valence band density of states.
- $|\mathbf{M}_{cv}|^2$ is the transition matrix element squared.
- $f_c(E)$ and $f_v(E)$ are the Fermi-Dirac distributions.

Approximating $B(E_g, T)$
For a direct bandgap semiconductor like GaSb, B is often approximated as:

$$B(E_g, T) \approx B_0 \left(\frac{E_g}{k_B T} \right)^{3/2} e^{-E_g / k_B T}. \tag{4.14}$$

where:

- B_0 is a material-dependent constant.
- k_B is Boltzmann's constant.
- T is the temperature in Kelvin.

Total Radiative Recombination Rate

Integrating over all energies, the total radiative recombination rate becomes:

$$R_{\text{rad}} = \int_{E_g}^{\infty} \alpha(E) I_{\text{bb}}(E) dE. \tag{4.15}$$

in Considerations for GaSb

- GaSb has a direct bandgap of approximately $E_g \approx 0.726$ eV at room temperature.
- The radiative recombination rate is crucial for optoelectronic devices such as LEDs and infrared detectors.
- The band structure and temperature dependence affect the efficiency of recombination processes.

For precise calculations, numerical simulations such as **Density Functional Theory (DFT)** or **empirical fitting models** are recommended.

Where is the bandgap at 0K around 0.812ev , and are constant specific for GaSb.

Table 4.4: Energy band gap dependency of radiative recombination

Energy Band Gap (eV)	Radiative Recombination Rate ($cm^{-3}s^{-1}$)
0.5	7.69×10^{-10}
0.7	5.45×10^{-13}
0.9	3.43×10^{-16}
1.1	2.01×10^{-19}
1.3	1.12×10^{-22}
1.5	6.04×10^{-26}

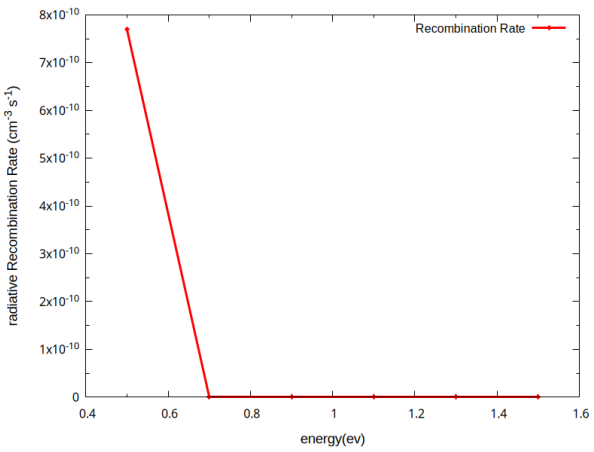

Figure 4.4: Variation of radiative recombination rate of GaSb with the function of energy band gap

Radiative Recombination Rate and Carrier Density of GaSb

The expected result for low carrier density regime indicates that the radiative recombination rate might increase near linearly with carrier density. A sharp increase at lower densities may indicate higher radiative efficiency, while saturation is observed at higher densities. At extremely high carrier densities we might eventually observe a plateau, or saturation due to effects band filling or Auger recombination. This plot is valuable in understanding the operating ranges for GaSb based devices.

The radiative recombination rate in a direct bandgap semiconductor like GaSb follows the van Roosbroeck–Shockley model, where the recombination process is governed by the electron-hole interaction.

General Expression for Radiative Recombination

The radiative recombination rate per unit volume is given by:

$$R_{\text{rad}} = Bnp, \tag{4.16}$$

where:

- R_{rad} is the radiative recombination rate (number of recombination events per unit volume per second).
- B is the **radiative recombination coefficient**.
- n is the **electron density** in the conduction band.
- p is the **hole density** in the valence band.

Carrier Density Dependence in Equilibrium

In **intrinsic semiconductors**, the carrier densities satisfy:

$$np = n_i^2, \tag{4.17}$$

where n_i is the intrinsic carrier concentration, given by:

$$n_i = \sqrt{N_c N_v} e^{-E_g/2k_B T}. \tag{4.18}$$

Here,

- N_c and N_v are the effective density of states in the conduction and valence bands.
- E_g is the bandgap energy.
- k_B is Boltzmann's constant.
- T is the absolute temperature.

Thus, for an intrinsic semiconductor:

$$R_{\text{rad}} = Bn_i^2. \tag{4.19}$$

Radiative Recombination in Doped Semiconductors

For an **n-type semiconductor**, where the electron density is approximately equal to the doping concentration ($n \approx N_d$) and assuming low-level injection ($p \ll n$):

$$R_{\text{rad}} = BN_d p. \tag{4.20}$$

For a **p-type semiconductor**, where the hole density is approximately equal to the doping concentration ($p \approx N_a$):

$$R_{\text{rad}} = BnN_a. \tag{4.21}$$

High-Carrier Injection Case

Under **high-injection conditions**, where excess carriers ($\Delta n = \Delta p$) are generated (e.g., under intense illumination or electrical injection):

$$R_{\text{rad}} = B(\Delta n + n_0)(\Delta p + p_0). \tag{4.22}$$

Approximating for large carrier injection ($\Delta n \gg n_0, p_0$):

$$R_{\text{rad}} \approx B\Delta n^2. \tag{4.23}$$

Total Radiative Recombination Rate

To obtain the total recombination rate, we integrate over all energy states:

$$R_{\text{rad,total}} = \int_{E_g}^{\infty} B(E)n(E)p(E)dE. \tag{4.24}$$

in Considerations for GaSb

- GaSb has a direct bandgap of approximately $E_g \approx 0.726$ eV at room temperature.
- The radiative recombination coefficient B is temperature-dependent and varies with doping levels.
- At high carrier injection, recombination scales as $B\Delta n^2$, which is important for LED and laser applications.

For precise modeling, numerical simulations such as **Density Functional Theory (DFT)** or **empirical fitting models** are recommended.

Table 4.5: Results for radiative recombination rate with respect to carrier density

Carrier Density (cm^{-3})	Radiative Recombination Rate ($cm^{-3}\ s^{-1}$)
$1.00 \times 10^{+13}$	$1.00 \times 10^{+16}$
$1.00 \times 10^{+14}$	$1.00 \times 10^{+18}$
$1.00 \times 10^{+15}$	$1.00 \times 10^{+20}$
$1.00 \times 10^{+16}$	$1.00 \times 10^{+22}$
$1.00 \times 10^{+17}$	$1.00 \times 10^{+24}$
$1.00 \times 10^{+18}$	$1.00 \times 10^{+26}$
$1.00 \times 10^{+19}$	$1.00 \times 10^{+28}$

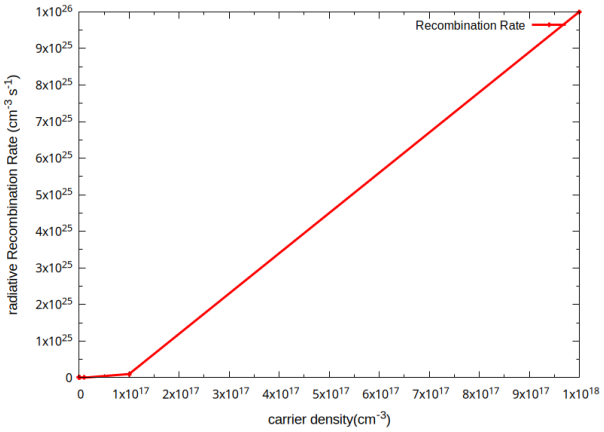

Figure 4.5: Radiative recombination rate of GaSb versus its carrier density

Radiative Recombination Rate and Temperature Dependency of GaSb

Radiative recombination as a function of temperature was studied. In this investigation, we analyzed that as temperature increases, the radiative recombination rate rises sharply. This is due to the increase in the intrinsic carrier concentration $n_i, which has an exponential dependency on temperature.$

The radiative recombination rate in GaSb increases sharply with temperature due to the exponential increase in intrinsic carrier concentration. The band gap of GaSb narrows with increasing temperature. As $E_g decreases, the exponential term in n_i is less suppressed, further accelerating the increa$

The radiative recombination rate per unit volume is:

$$R_{\text{rad}} = B(T)np, \tag{4.25}$$

where:

- R_{rad} is the radiative recombination rate (number of recombination events per unit volume per second).
- $B(T)$ is the **radiative recombination coefficient**, which varies with temperature.

- n and p are the electron and hole concentrations.

Carrier Density Dependence on Temperature

The intrinsic carrier concentration n_i depends on temperature as:

$$n_i = \sqrt{N_c N_v} e^{-E_g/2k_B T}. \tag{4.26}$$

where:

- N_c and N_v are the effective density of states in the conduction and valence bands, given by:

$$N_c = 2\left(\frac{2\pi m_c^* k_B T}{h^2}\right)^{3/2}, \tag{4.27}$$

$$N_v = 2\left(\frac{2\pi m_v^* k_B T}{h^2}\right)^{3/2}. \tag{4.28}$$

- m_c^* and m_v^* are the effective masses of electrons and holes in GaSb.
- k_B is Boltzmann's constant.
- T is the absolute temperature.
- E_g is the bandgap energy of GaSb.

Thus, the intrinsic carrier concentration varies as:

$$n_i \propto T^{3/2} e^{-E_g/2k_B T}. \tag{4.29}$$

Temperature Dependence of the Radiative Recombination Coefficient

The radiative recombination coefficient $B(T)$ is related to the transition probabilities and the joint density of states, leading to an approximate dependence:

$$B(T) \propto T^{-3/2}. \tag{4.30}$$

Thus, the radiative recombination rate in intrinsic GaSb varies with temperature as:

$$R_{\text{rad}}(T) \propto T^{-3} e^{-E_g/k_B T}. \tag{4.31}$$

Total Radiative Recombination Rate

Integrating over all energy states, the total recombination rate is:

$$R_{\text{rad,total}} = \int_{E_g}^{\infty} B(T) n(E,T) p(E,T) dE. \tag{4.32}$$

in Considerations for GaSb

- GaSb has a direct bandgap of approximately $E_g \approx 0.726$ eV at room temperature.
- As temperature increases, n_i increases exponentially, leading to higher recombination rates.
- The recombination coefficient $B(T)$ decreases with temperature due to the broadening of the density of states.
- At high temperatures, non-radiative recombination (e.g., Auger recombination) becomes dominant over radiative recombination.

For precise modeling, numerical simulations using **Density Functional Theory (DFT)** or empirical fitting models are recommended.

Table 4.6: Results of radiative recombination rate as a function of temperature

Temperature (K)	Radiative Recombination Rate ($cm^{-3}s^{-1}$)
300	4.97×10^{-19}
350	6.65×10^{-17}
400	2.72×10^{-15}
450	5.01×10^{-14}
500	5.28×10^{-13}
550	3.68×10^{-12}
600	1.89×10^{-11}

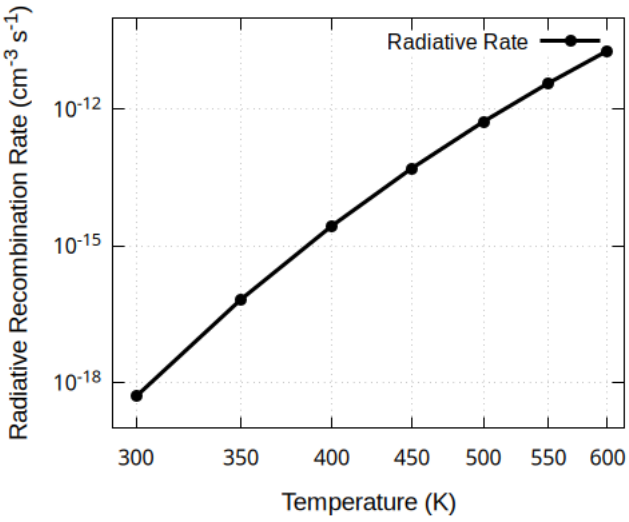

Figure 4.6: Radiative recombination rate of GaSb versus temperature variation

4.4.2 Auger Recombination Rate of GaSb

We investigated the Auger recombination rate of GaSb as a function of different parameters, including temperature, carrier density, injection level, and band gap energy. Like the radiative recombination rate, the Auger recombination rate increases with increasing carrier density and temperature. In this section, we focus on carrier injection and band gap energy.

Auger Recombination Rate Dependency on Band Gap Energy

The Auger recombination rate of GaSb was analyzed against the band gap energy and plotted. The band gap energy of GaSb was varied from 0.5 eV to 1.2 eV in steps of 0.1 eV. The Auger recombination rate decreases as the band gap energy increases.

Auger recombination is a non-radiative recombination process where the energy released by electron-hole recombination is transferred to another charge carrier rather than being emitted as a photon. This process becomes significant at high carrier concentrations and affects the performance of GaSb-based optoelectronic devices.

General Auger Recombination Expression

The Auger recombination rate is generally expressed as:

$$R_{\text{Auger}} = C_n n^2 p + C_p n p^2, \tag{4.33}$$

where:

- R_{Auger} is the Auger recombination rate (number of recombinations per unit volume per second).
- C_n and C_p are the Auger recombination coefficients for conduction band and valence band processes, respectively.
- n is the electron density in the conduction band.
- p is the hole density in the valence band.

Dependency on bandgap energy

The Auger recombination coefficient depends on the bandgap energy E_g, as it is related to the density of states and transition probabilities. The general empirical dependence is given by:

$$C_n, C_p \propto E_g^{-3} e^{-E_g/k_B T}. \tag{4.34}$$

Thus, the Auger recombination rate scales with bandgap energy as:

$$R_{\text{Auger}} \propto E_g^{-3} e^{-E_g/k_B T} (n^2 p + n p^2). \tag{4.35}$$

Total Auger Recombination Rate

Integrating over all energy states, the total Auger recombination rate is:

$$R_{\text{Auger,total}} = \int_{E_g}^{\infty} C(E)n(E)p(E)(n(E)+p(E))dE. \tag{4.36}$$

in Considerations for GaSb

- GaSb has a relatively small direct bandgap ($E_g \approx 0.726$ eV at room temperature), making Auger recombination significant at high carrier concentrations.
- The Auger coefficient follows an inverse cubic dependence on E_g, meaning materials with smaller bandgaps experience stronger Auger recombination.
- In highly doped or high-injection conditions, Auger recombination dominates over radiative recombination, reducing efficiency in LEDs and laser diodes.
- Suppression of Auger recombination is critical for achieving high efficiency in GaSb-based optoelectronic devices.

For precise calculations, numerical simulations using **Density Functional Theory (DFT)** or empirical fitting models are recommended.

Table 4.7: Auger recombination rate with respect to band gap energy

Band Gap Energy (eV)	Auger Recombination Rate ($cm^{-3}s^{-1}$)
0.5	2.48×10^{11}
0.6	7.49×10^{8}
0.7	2.26×10^{6}
0.8	6834.30
0.9	20.64
1.0	0.06236
1.1	0.000188
1.2	5.69×10^{-7}

Auger Recombination Rate vs. Injection Level

The Auger recombination rate was also analyzed as a function of the carrier injection level. Injection level is defined as the excess concentration of charge carriers introduced into the material compared to its thermal equilibrium state. The results indicate that the Auger recombination rate increases significantly with increasing injection levels. Auger recombination is a non-radiative process in which the energy released from electron-hole recombination is transferred to another free carrier. This process plays a significant role at high carrier injection levels in GaSb-based optoelectronic devices.

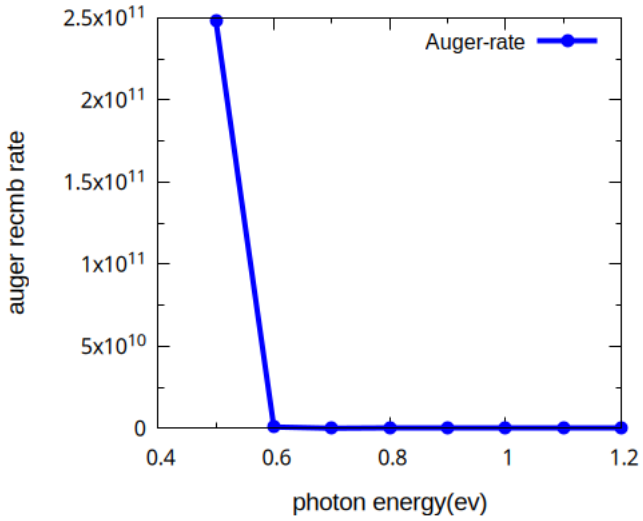

Figure 4.7: Relation between band gap energy and Auger recombination rates

General Auger Recombination Expression

The Auger recombination rate is given by:

$$R_{\text{Auger}} = C_n n^2 p + C_p n p^2, \tag{4.37}$$

where:

- R_{Auger} is the Auger recombination rate (recombinations per unit volume per second).
- C_n and C_p are the Auger recombination coefficients.
- n is the electron concentration.
- p is the hole concentration.

Injection-Level Dependence

The carrier densities depend on the injection level Δn:

- **Low-level injection** ($\Delta n \ll n_0, p_0$): The excess carrier concentration is small compared to the doping levels. - **High-level injection** ($\Delta n \gg n_0, p_0$): The excess carrier concentration dominates over the equilibrium carrier densities.

(a) Low-Injection Case ($\Delta n \ll n_0, p_0$)

For an **n-type** semiconductor where $n \approx N_d$ and $p = n_i^2/N_d$:

$$R_{\text{Auger}} \approx C_n N_d^2 \Delta n. \tag{4.38}$$

For a **p-type** semiconductor where $p \approx N_a$ and $n = n_i^2/N_a$:

$$R_{\text{Auger}} \approx C_p N_a^2 \Delta n. \tag{4.39}$$

Thus, at **low injection levels**, the Auger recombination rate increases **linearly** with excess carrier density.

(b) High-Injection Case ($\Delta n \gg n_0, p_0$)

At high injection levels, where $n \approx p \approx \Delta n$:

$$R_{\text{Auger}} \approx (C_n + C_p)\Delta n^3. \tag{4.40}$$

Thus, at **high injection levels**, the Auger recombination rate exhibits a **cubic dependence** on the excess carrier density.

Total Auger Recombination Rate

The total Auger recombination rate across all energy states can be written as:

$$R_{\text{Auger,total}} = \int_{E_g}^{\infty} C(E)n(E)p(E)(n(E) + p(E))dE. \tag{4.41}$$

Implications for GaSb-Based Devices

- GaSb has a relatively small bandgap ($E_g \approx 0.726$ eV), making Auger recombination a dominant loss mechanism at high injection levels.
- At low injection levels, Auger recombination is less significant compared to radiative recombination.
- At high injection levels, Auger recombination dominates, leading to efficiency droop in LEDs and high-threshold currents in lasers.
- Suppressing Auger recombination through material engineering or device design is critical for improving efficiency in GaSb-based infrared photonics.

For precise calculations, numerical simulations using **Density Functional Theory (DFT)** or empirical fitting models are recommended.

Table 4.8: Auger recombination rate with respect to injection level

Injection Level (cm^{-3})	Auger Recombination Rate ($\text{cm}^{-3}s^{-1}$)
1.00×10^{12}	8.66×10^{6}
2.00×10^{17}	1.60×10^{22}
4.00×10^{17}	1.28×10^{23}
6.00×10^{17}	4.32×10^{23}
8.00×10^{17}	1.02×10^{24}

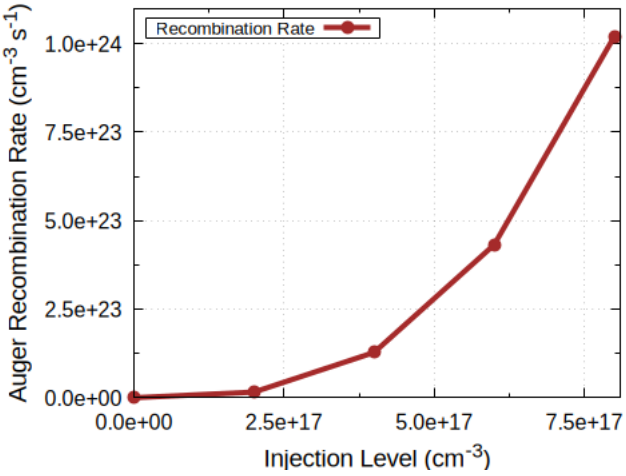

Figure 4.8: Relation between carrier injection level and Auger recombination rate

4.5 Recombinationlifetime of GaSb

4.5.1 Radiative Recombination lifetime of GaSb

The radiative lifetime of GaSb were calculated by performing Van Roosbroeck Shockley calculation for a series of plausible parameters. In this case the band gap energy of GaSb and temperature were kept constant. The computational calculation shows that the carrier lifetime of radiative recombination process of GaSb were decreased from 0.07692sec to 0.31μ sec, this makes agreement with idea that the carrier lifetime were equal to 0.009sec at the intrinsic carrier concentration level of GaSb which is experimentally be around $4.3 \times 10^12 cm^{-3}$ and 0.37μ sec at $10^{17} cm^{-3}$ carrier concentration. The carrier concentration grids are shown in Table 10. Moreover as it is observed in Figure 10 the carrier lifetime were decreases from the order of microseconds to nanoseconds. The radiative recombination lifetime is a key parameter in semiconductor physics, defining how long excess carriers persist before recombining. It is given by the inverse of the radiative recombination rate.

The radiative recombination rate in GaSb follows the van Roosbroeck–Shockley model:

$$R_{\text{rad}} = Bnp, \tag{4.42}$$

where:

- R_{rad} is the radiative recombination rate (number of recombinations per unit volume per second).
- B is the radiative recombination coefficient.
- n and p are the electron and hole concentrations.

The radiative recombination lifetime τ_{rad} is defined as:

$$\tau_{\text{rad}} = \frac{\Delta n}{R_{\text{rad}}}. \tag{4.43}$$

Intrinsic Semiconductor ($n = p = n_i + \Delta n$)

For an intrinsic semiconductor, where carrier densities are approximately equal:

$$\tau_{\text{rad,int}} = \frac{1}{B(n_i + \Delta n)}. \tag{4.44}$$

At low excess carrier concentrations ($\Delta n \ll n_i$):

$$\tau_{\text{rad,int}} \approx \frac{1}{Bn_i}. \tag{4.45}$$

At high excess carrier concentrations ($\Delta n \gg n_i$):

$$\tau_{\text{rad,int}} \approx \frac{1}{B\Delta n}. \tag{4.46}$$

Doped Semiconductor (Low-Injection Condition, $\Delta n \ll N_d, N_a$)

For an **n-type** semiconductor, where $n \approx N_d$ and $p = n_i^2/N_d$:

$$\tau_{\text{rad},n} = \frac{1}{BN_d}. \tag{4.47}$$

For a **p-type** semiconductor, where $p \approx N_a$ and $n = n_i^2/N_a$:

$$\tau_{\text{rad},p} = \frac{1}{BN_a}. \tag{4.48}$$

High-Injection Condition ($\Delta n \gg N_d, N_a$)

At high injection levels, where $n \approx p \approx \Delta n$:

$$\tau_{\text{rad,high}} = \frac{1}{B\Delta n}. \tag{4.49}$$

Total Radiative Lifetime Expression

In general, the radiative lifetime as a function of carrier concentration is:

$$\tau_{\text{rad}}(n) = \frac{1}{B(n + p)}. \tag{4.50}$$

- GaSb has a relatively small bandgap ($E_g \approx 0.726$ eV), leading to a high intrinsic carrier concentration at room temperature.
- In low-injection regimes, the radiative lifetime is determined by doping concentration.
- In high-injection conditions, the radiative lifetime decreases as carrier concentration increases.

- Shorter radiative lifetimes at high injection impact the performance of LEDs and laser diodes by increasing spontaneous emission rates.

For precise calculations, numerical simulations using **Density Functional Theory (DFT)** or empirical fitting models are recommended.

Table 4.9: Results of radiative recombination lifetime with respect to carrier concentration

Carrier Concentration (cm^{-3})	Radiative Lifetime (s)
1.00×10^{12}	0.076923
3.98×10^{12}	0.019322
1.58×10^{13}	0.004854
3.10×10^{13}	0.001219
2.51×10^{14}	0.000306
1.00×10^{15}	7.69×10^{-5}
3.98×10^{15}	1.93×10^{-5}
1.58×10^{16}	4.85×10^{-6}
6.31×10^{16}	1.22×10^{-6}
2.51×10^{17}	3.06×10^{-7}
1.00×10^{18}	7.69×10^{-8}

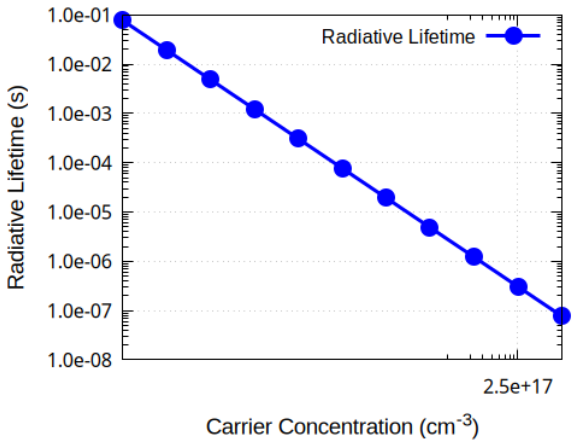

Figure 4.9: Radiative recombination lifetime with respect to carrier concentration.

4.5.2 Auger Recombination Lifetime for GaSb

The Auger recombination lifetime for intrinsic GaSb were calculated by using Van Roosbroeck Shockley calculation for a series of plausible parameters. The band gap energy and temperature were kept constant, The computational calculation shows that the carrier lifetime of Auger recombination process of GaSb were decreased from approximately around quarter past of 9

o'clock(33333.33sec) to 33.33nsec. This makes agreement with the result that were investigated by science journals. The carrier concentration grids are given in Table 11 below. Moreover as it is observed in Figure 11 the carrier lifetime were decreases from the order of tenth of thousands of seconds to nanoseconds.

Auger recombination is a non-radiative recombination process where the energy released from electron-hole recombination is transferred to another free carrier. This process is dominant in materials with small bandgaps, such as GaSb, particularly at high carrier concentrations.

The Auger recombination rate in GaSb follows the van Roosbroeck–Shockley model:

$$R_{\text{Auger}} = C_n n^2 p + C_p n p^2, \tag{4.51}$$

where:

- R_{Auger} is the Auger recombination rate (number of recombinations per unit volume per second).
- C_n and C_p are the Auger recombination coefficients.
- n and p are the electron and hole concentrations.

The Auger recombination lifetime τ_{Auger} is defined as:

$$\tau_{\text{Auger}} = \frac{\Delta n}{R_{\text{Auger}}}. \tag{4.52}$$

Intrinsic Semiconductor ($n = p = n_i + \Delta n$)

For an intrinsic semiconductor, where carrier densities are approximately equal:

$$\tau_{\text{Auger,int}} = \frac{1}{(C_n + C_p)(n_i + \Delta n)^2}. \tag{4.53}$$

At low excess carrier concentrations ($\Delta n \ll n_i$):

$$\tau_{\text{Auger,int}} \approx \frac{1}{(C_n + C_p) n_i^2}. \tag{4.54}$$

At high excess carrier concentrations ($\Delta n \gg n_i$):

$$\tau_{\text{Auger,int}} \approx \frac{1}{(C_n + C_p) \Delta n^2}. \tag{4.55}$$

Doped Semiconductor (Low-Injection Condition, $\Delta n \ll N_d, N_a$)

For an **n-type** semiconductor, where $n \approx N_d$ and $p = n_i^2 / N_d$:

$$\tau_{\text{Auger},n} = \frac{1}{C_n N_d^2}. \tag{4.56}$$

For a **p-type** semiconductor, where $p \approx N_a$ and $n = n_i^2 / N_a$:

$$\tau_{\text{Auger},p} = \frac{1}{C_p N_a^2}. \tag{4.57}$$

High-Injection Condition ($\Delta n \gg N_d, N_a$)
At high injection levels, where $n \approx p \approx \Delta n$:

$$\tau_{\text{Auger,high}} = \frac{1}{(C_n + C_p)\Delta n^2}. \tag{4.58}$$

Total Auger Lifetime Expression
In general, the Auger recombination lifetime as a function of carrier concentration is:

$$\tau_{\text{Auger}}(n) = \frac{1}{C_n n^2 + C_p p^2}. \tag{4.59}$$

- GaSb has a relatively small bandgap ($E_g \approx 0.726$ eV), making Auger recombination significant at high carrier concentrations.
- At low injection levels, Auger recombination is negligible compared to radiative recombination.
- At high injection levels, Auger recombination dominates, leading to efficiency droop in LEDs and increased threshold currents in lasers.
- The Auger recombination lifetime decreases as carrier concentration increases, significantly impacting device performance.
- Reducing Auger recombination through material engineering or device design (e.g., strain engineering, bandgap optimization) is crucial for improving efficiency.

For precise calculations, numerical simulations using **Density Functional Theory (DFT)** or empirical fitting models are recommended.

Table 4.10: results of recombination lifetime of GaSb through Auger recombination process with respect to carrier concentration

Carrier Concentration (cm^{-3})	Auger Lifetime (s)
1.00×10^{12}	33333.33
3.98×10^{12}	2103.191
1.58×10^{13}	132.7024
6.31×10^{13}	8.372955
2.51×10^{14}	0.528298
1.00×10^{15}	0.033333
3.98×10^{15}	0.002103
1.58×10^{16}	0.000133
6.31×10^{16}	8.37×10^{-6}
2.51×10^{17}	5.28×10^{-7}
1.00×10^{18}	3.33×10^{-8}

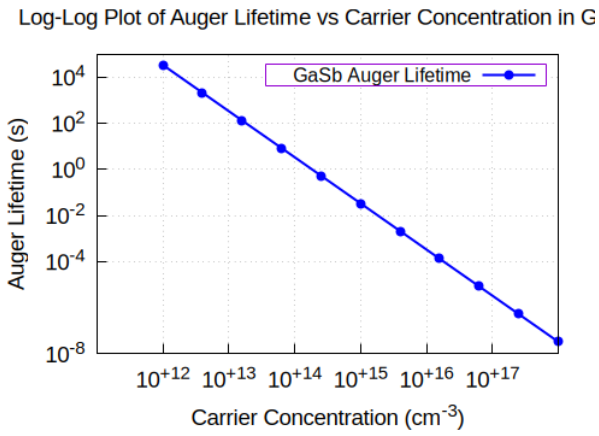

Figure 4.10: Carrier recombination lifetime of GaSb through Auger recombination process with respect to carrier concentrations

Chapter 5

Conclusion and recommendation

5.1 conclusion

The recombination lifetime of GaSb through different recombination process were investigated within the framework of Van Roosbroeck Shockley method. All calculations have been done with the help of mathimatica Wolfram programming language (software). The band gap energy calculated as a function of wave vector k and the grid respectively by keeping the parameters constant. The recombination rates of gallium antimonide (GaSb) were plotted and the corresponding grids were shown by using both radiative and auger recombination mechanisms. All of GaSb recombination rate dependencies were analyzed. The carrier recombination lifetimes of intrinsic GaSb (Gallium Antimonide) is achieved in both radiative recombination process and Auger recombination process. Radiative recombination lifetime is typically longer than Auger recombination lifetime in case of intrinsic GaSb.At higher carrier densities (e.g under doping or excitation), Auger recombination process become more dominant than radiative recombination process.

5.2 Recommendation

I recommend that the recombination life time characterizes the semiconductor devices. Since it is very essential in opto-electronic devices the Auger recombination process is the most important mechanism in the recombination of gallium antimonide. Thus the carrier life time of gallium antimonide is shorter in auger recombination process than radiative recombination. Lastly I recommend that auger recombination process is very important for high injection level of gallium antimonide.

Bibliography

[1] Neamen, D.A., *Semiconductor Physics and Devices: Basic Principles*, 4th Edition, 2003.

[2] K.B. McAfee, Jr., D.M. Gay, R.S. Hozack, R.A. Laudise, G. Schwartz, W.A. Sunder, J. Cryst. Growth 76, 263 (1986).

[3] N. Ashcroft and N. Mermin, *Solid State Physics*, Cengage Learning, Singapore, 1976.

[4] Govind P. Agrawal and Niloy K. Dutta, *Semiconductor Lasers*.

[5] C. Kittel and P. McEuen, *Introduction to Solid State Physics*, Wiley, New York, NY, USA, 1996 second ed., New York, 1993.

[6] Y. Yu, P. Manuel Cardona, *Fundamentals of Semiconductors*, 4th edition, Springer-Verlag Berlin Heidelberg, New York, 2010.

[7] J. Nelson, *The Physics of Solar Cells*, Imperial College Press, 2003.

[8] V. K. Khanna, "Physical understanding and technological control of carrier lifetimes in semiconductor materials and devices: a critique of conceptual development, state of the art, and applications," *Progress in Quantum Electronics*, vol. 29, no. 2, pp. 59–163, 2005.

[9] P. V. Jayaweera, S. G. Matsik, A. G. Perera, Y. Paltiel, A. Sher, Appl. Phys. Lett. 90 (2007) 111109.

[10] R. A. Laudise, *J. Cryst. Growth* 65, 3-23 (1983).

[11] F. Donald Bloss, *An Introduction to Crystallography and Crystal Chemistry*, Holt, Rinehart and Winston, New York, 1971.

[12] D.A. Porter, K.E. Easterling, *Phase Transformations in Metals and Alloys*, 2nd Edition, Stanley Thornes, London, 2000.

[13] S. Sheng, *Semiconductor Physical Electronics*, 2nd edition, 2006, p. 87,141.

[14] A. Cuevas, D. Macdonald, "Measuring and interpreting the lifetime of silicon wafers," *Solar Energy* 76, 255–262, 2004.

[15] S.M. Sze and M.K. Lee, *Semiconductor Devices: Physics and Technology*, 3rd Edition, John Wiley Sons, New York, 2012, p. 56.

[16] E. F. Schubert, *Light-Emitting Diodes*, 2nd Edition, New York, 2006, p. 48-56.

[17] J. S. Blakemore, *Semiconductor Statistics*, Pergamon Press, New York, 1962, p. 200.

[18] R. N. Hall, *Phys. Rev.* 87, 387 (1952).

[19] A. R. Beattie and P. T. Landsberg, *Proc. Roy. Soc. London Ser. A* 16, 249 (1959).

[20] P. T. Landsberg and A. F. W. Willoughby (eds.), *Solid State Electronics* 21, 1273 (1978).

[21] Green, Martin A., *Solar Cells: Operating Principles, Technology, and System Applications*, Englewood Cliffs: Prentice-Hall, Inc., 1982.

[22] Bernard, M. G. A., and G. Duraffourg, *Phys. Status Solidi*, 1, 699 (1961).

[23] Lasher, G., and F. Stern, *Phys. Rev.* 133, A553 (1964).

[24] Kane, E. O., *J. Phys. Chem. Solids* 1, 249 (1957).

[25] Joyce, W. B., and R. W. Dixon, *Appl. Phys. Lett.* 31, 354 (1977).

[26] Blakemore, J. S., *Solid State Physics*, 2nd Edition, Chap. 4, p. 382, New York: University of Cambridge, 1985.

[27] Z. Lu, Y. Jiang, W. I. Wang, M. C. Teich, and R. M. Osgood, Jr., *J. Vac. Sci. Technol.* B10, 1856 (1992).

[28] K. M. Schirm, P. Soukiassian, P. S. Mangat, Z. Hurych, L. Soonckindt, and J. J. Bonnet, *J. Vac. Sci. Technol.* B10, 1867 (1992).