ON SOME ASPECTS OF ELECTRONIC TRANSPORT CHARACTERISTICS OF SEMICONDUCTOR STRUCTURES AT LOW LATTICE TEMPERATURES

THESIS SUBMITTED FOR THE DEGREE OF DOCTOR OF PHILOSOPHY (SCIENCE) JADAVPUR UNIVERSITY 2024



By
SOUMA SAHA
DEPARTMENT OF PHYSICS, JADAVPUR UNIVERSITY
KOLKATA- 700032, INDIA

যা দ্বপুর বিশ্ববিদ্যালয় কলকাতা-৭০০০৩২, ভারত



JADAVPUR UNIVERSITY KOLKATA-700 032, INDIA

FACULTY OF SCIENCE: DEPARTMENT OF PHYSICS

Dr. Subhadipta Mukhopadhyay

Professor

Department of Physics

Email: phy-smukhenjee@gmail.com

Ref No.:

Date: 11.09.2024

CERTIFICATE FROM THE SUPERVISOR

This is to certify that the thesis entitled "ON SOME ASPECTS OF ELECTRONIC TRANSPORT CHARACTERISTICS OF SEMICONDUCTOR STRUCTURES AT LOW LATTICE TEMPERATURES" submitted by Shri SOUMA SAHA, who got his name registered on 30.01.2018 for the award of Ph.D. (Science) degree of Jadavpur University, is absolutely based upon his own work under the supervision of Dr. Subhadipta Mukhopadhyay and that neither this thesis nor any part of it has been submitted for either any degree/diploma or any other academic award anywhere before.

Subhadipta Muchosadhyay

(Signature of the Supervisor with official seal)

Dr. Subhadipta Mukhopadhyay Professor Dept. of Physics Jadavpur University, Kolkata-700 032

Declaration

I hereby declare that the work embodied in the present thesis titled 'ON SOME ASPECTS OF ELECTRONIC TRANSPORT CHARACTERISTICS OF SEMICONDUCTOR STRUCTURES AT LOW LATTICE TEMPERATURES' has been carried out by me in the Department of Physics, Jadavpur University, Kolkata-700032, India. Neither this thesis nor any part of it has been submitted for any degree elsewhere.

Date: 11.09, 2024.

Souma Saha,

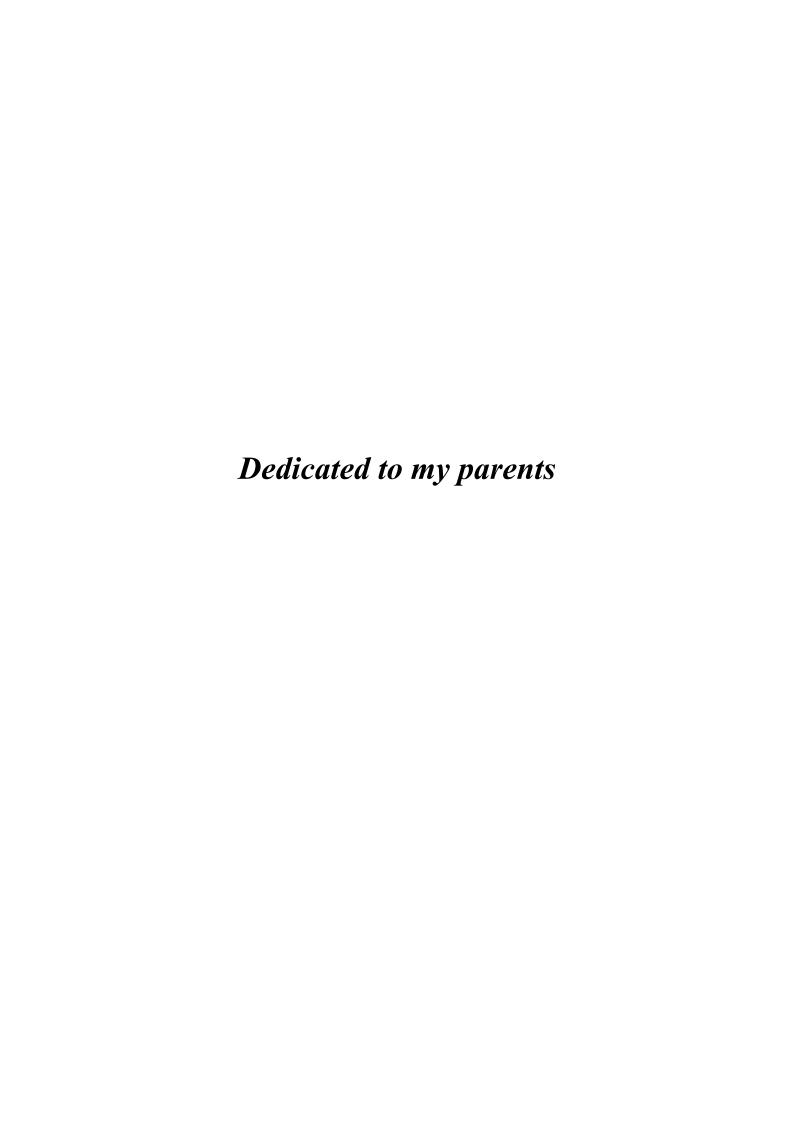
(SOUMA SAHA)

Research Scholar

Department of Physics

Jadavpur University

Kolkata-700032, India



Acknowledgement

This thesis would be absolutely incomplete without my sincere expression of gratitude to one and all who helped me in my endeavour in some way or other.

The very first one to mention is my supervisor, Dr. Subhadipta Mukhopadhyay for his invaluable guidance and support throughout my Ph.D. journey. He has guided me steadfastly throughout my research studies with her patience and knowledge, and always encouraged me to work in my own way. His untiring support through illuminating discussions and invaluable advice has inspired me to work with determination.

I thankfully acknowledge the financial support from the Government of West Bengal, India, for providing Swami Vivekananda Merit Cum Means Scholarship Scheme. I would also like to thank Jadavpur University for providing me the infrastructural support that I needed to complete this thesis.

I am also grateful to my senior lab mates Dr. A. Basu & Dr. B. Roy for helpful discussions and to my colleagues who have supported me in numerous ways, both professionally and personally. Their camaraderie and encouragement have made the long hours of my research work more bearable. The help rendered by Prof. D.P. Bhattacharya is duly acknowledged.

I am thankful to my friend Dr. Koyel Sarkar, who has been a constant source of help and support throughout this journey. I would also like to thank my friends Dr. Prosenjit Biswas, Dr. Sumit Das, Arup Paul, Chayan Sarkar, Aditya Bandyapadhayay and Lt. Rajdeep Sinha.

Finally, I would like to thank my family for their unconditional love and unwavering support throughout my academic journey. Their belief in me and my abilities has been a constant source of motivation.

Souma Saha,

SOUMA SAHA Department of Physics Jadavpur University Kolkata 700032

Contents

	Page No.
Chapter 1: Introduction, basic assumptions and scope of the thesis	01 – 21
1.1. Introduction	01
1.2. Basic assumptions	04
1.3. Concepts and specific features of low lattice temperature	07
1.4. Different types of Semiconductor Structures	11
1.5. Scope of the thesis	15
References	19
Chapter 2: Some basic physics and properties of different semiconductor structu	ires
	22 – 37
2.1. Introduction	22
2.2. Electron fundamental lengths in solids	22
2.3. (a) Wave function, energy dispersion, wave vector element	
(b) Density of states function for different structures, sub band energy,	
(c) Equilibrium carrier concentration	
(d) Current density	22
2.4. Scattering mechanisms	28
2.4.1. Classification of Scattering	29
2.4.2. Relative importance of different scattering mechanisms	31
References	35
Chapter 3: Analysis of the average energy loss rate of non-equilibrium electr	ons in the
non-degenerate sample of different III -V compound semiconductors at	low lattice
temperature	38 – 52
3.1. Introduction	38
3.2. Development	40
3.3. Results and Discussion	45

3.4. Conclusion	51
References	52
Chapter 4: Dependence of the Effective electron temperature upon the electric	field
of the non-equilibrium electrons in a non degenerate semiconductor at low l	attice
temperature 53	3 – 70
4.1. Effective electron temperature of the non-equilibrium electrons for the com-	ıbined
interaction with the acoustic and the piezoelectric phonons	53
4.1.1. Introduction	53
4.1.2. Development	54
4.2. Effective electron temperature of the non-equilibrium electrons for the com-	ibined
interaction with the acoustic and the piezoelectric phonons as well as with the 1s	to 2p
excitation and ionization of the neutral impurities	57
4.2.1. Introduction	57
4.2.2. Development	59
4.2.3. Results and Discussion	61
4.2.4. Conclusion	66
References	69
Chapter 5: Microwave harmonic generation by non ohmic ensemble of carrie	rs in
compound semiconductors at low lattice temperatures	
71	- 89
5.1. Introduction	71
5.2. Brief review of the studies on the characteristics of Harmonic Generati	on in
semiconductor structures	73
5.3. Method of calculation of the efficiency of SHG in an ensemble of 3DEG	75
5.4. Results for the dependence of the efficiency of SHG upon the biased field in	non-
equilibrium ensemble of InSb, InAs and GaSb with different lattice temperatures	77
5.4. Discussions	84
References	87

Chapter 6: Overall Conclusion of the Thesis and future direction in the relevant field

	90 – 97
6.1. The set-up considered	90
6.2. The framework used for the theoretical analysis	90
6.3. The limitations of the assumptions made	91
6.4. Overall conclusion of the thesis	94
6.5. Contemplated future direction of work in the relevant field	97

List of Symbols

List of publications

Seminar, Symposium, Conferences and Awards

Chapter 1

Introduction, Basic Assumptions and Scope of The Thesis

INTRODUCTION, BASIC ASSUMPTIONS AND SCOPE OF THE THESIS

The use of electronic gadgets has become indispensable for our daily life. The technological advancement of the process of designing and fabrication of semiconductor devices is already quite phenomenal. It is now possible to fabricate elegant quantum well devices which are not only practically more useful but are also economically more viable. This in turn has resulted in quite significant boost of the electronics industry and hence of the world economy.

The comprehension of the performance of a semiconductor device structure and subsequently to strive for its improvement, demands the knowledge of the physics of the constituent semiconductor materials the device is made of. In course of achieving such knowledge newer ideas, theories etc. have been developed. That in turn led to numerous newer devices and circuits which possesses more useful and challenging applications and paves the way for more exciting developments in this rapidly growing field. Almost insatiable demand for faster and faster devices, which again operate at smaller and smaller input power demands scaling down the device sizes. All these have led to realization of quantum-confined, low-dimensional semiconductor structures. Hence, to work in this field is a challenging task and thus inspires future worker in this field.

1.1. Introduction

Semiconductor devices have been considered as one of the most important inventions of 20th century because of their remarkable applications in modern technology and electronic goods. The physics of such devices is dependent upon the physics of the materials they are made of and their structures. In order to understand the purpose a device may serve and to know how to manipulate its performance, one should have a detailed knowledge of the electrical transport characteristics of the structures the device is made of.

The study of electronic transport in different semiconductor structures under different prevalent conditions is a traditional subject, which has been well analysed over the past few decades. Transport properties are known to underlie numerous technical applications of semiconductors. Besides, such properties are sensitive to the dispersion laws of the current carriers and the nature of the interaction of the carriers with various defects of the crystal lattice or phonons. Therefore, many conventional methods of investigating semiconducting materials are based on the study of different kinetic effects. They become especially efficient under some extreme conditions of low temperatures. Satisfactory and reliable results are obtained when an integral investigation is carried out and the conclusions of the theory of electron transport phenomena are taken into account. Though such studies in and around room temperature are well available, but the same for low temperatures are quite scarce. Of late, particularly after the discovery of Hall Effect (QHE) and Fractional Quantum Hall Effect (FQHE), the study of low temperature electrical transport in semiconductors has assumed high importance.

It is well known that in the presence of a relatively high electric field $(\vec{\varepsilon})$, the electron ensemble in a semiconductor may be significantly perturbed from the state of thermodynamic equilibrium with the lattice atoms. Since the average energy of an electron then exceeds its thermal equilibrium value, the ensemble thus assumes a field dependent effective temperature $T_e(\varepsilon)$ which exceeds the lattice temperature T_L . The high field transport characteristics of any semiconductor structure exhibits some novel features, which are not observed at the low fields [1-7]. The knowledge of the high-field features is rather important from the device point of view.

At the low lattice temperatures $T_L \le 20K$, a seemingly low electric field as low as a fraction of a volt/cm or so may turn out to be effectively high, and the high-field features

may be observed. At such low lattice temperatures, when the concentration of the neutral impurities is quite high, the presence of an effectively high field may make the amount of the loss of energy of the electrons due to the ionisation (ion.) and $1s \rightarrow 2p$ excitation (ex.) of the neutral impurities significantly large [5,6]. Moreover, under the condition when the lattice temperature is low, the average thermal energy of an electron tends to be comparable with the energy of an acoustic phonon. As such, the electron-phonon collisions thus also tend to be inelastic.

The theory of high-field transport for a non-degenerate ensemble of electrons may be developed in the effective electron temperature approximation assuming a "heated" Maxwellian energy distribution for the non-equilibrium electrons at a field dependent effective electron temperature $T_e(\varepsilon)$ of the carriers [1,5,7]. Such an approximate analysis is quite worthy, as because, it often provides data, which are useful for the device technologists.

One of the most important parameters which describes the high-field effects in a semiconductor is the average rate of loss of energy of an electron to the lattice $\langle \frac{dE_{\vec{k}}}{dt} \rangle$, \vec{k} being the wave vector of an electron with energy $E_{\vec{k}}$ [1].

The energy loss rate of the non-equilibrium electrons in a semiconductor has been analysed there using the perturbation theory, under the condition when the lattice temperature is high and for the quasi-elastic interaction of the electrons only with the deformation potential acoustic phonons. But the same analysis of the energy loss rate at the low lattice temperatures being scarce in the literature, such an analysis needs to be taken up. Moreover, the subsequent analysis of the dependence of the effective electron temperature upon the electric field for a non-degenerate ensemble of electrons in a compound semiconductor, at the low lattice temperature is also important [7].

The field dependence of the effective electron temperature may be obtained from the solution of the energy balance equation of the electron-phonon system [5,7]. The solution however, is determined by the prevalent conditions in respect of (i) the lattice temperature, (ii) the dominant interactions of the electrons with the lattice imperfections, and (iii) the concentration of the carriers etc. By solving the energy balance equation for the electron-phonon system the field dependence of T_e for a bulk semiconductor material has been theoretically obtained in [5], separately, for different interactions, under the condition, when the lattice temperature is high. Apart from that some studies have been made about the effective electron temperature characteristics, particularly the relationship of T_e with T_L considering specific devices at and around the room temperatures [8].

Such theoretical studies are beset with much mathematical difficulties. The low temperature features are either absent at higher temperatures or ignored to make an analysis easily tractable. The basic physics involved in high field effects at low temperatures is quite complicated and not yet well understood.

1.2. Basic Assumptions

In order to develop the mathematical theory of any system, often some simplifying assumptions may have to be made so that the problem becomes amenable to a solution. These assumptions need to be physically realistic so that the results that follow from the subsequent theoretical analysis can indeed describe the characteristics of the real system under the prevalent condition without significant loss of accuracy. In the present thesis, to carry out the theoretical investigations of the electrical transport parameters of an ensemble of electrons in Bulk Semiconductor structures, the principal basic assumption that have been made are pointed out in what follows now.

In a compound semiconductor which lacks inversion symmetry, the conduction electrons interact simultaneously with the intrinsic deformation potential acoustic phonons and the piezoelectric phonons along with the impurity atoms and other lattice defects. The effectiveness of each scattering mechanism depends upon the lattice temperature and the amount of doping.

At low lattice temperatures, the average thermal energy of the electrons would not be sufficient enough to excite optical mode lattice vibrations and thus the optical phonons hardly control the electron transport characteristics. The electronic collision processes which have been taken into account in the present work include that with the deformation potential acoustic phonons, the piezoelectric phonons and the ionized impurities. It may be mentioned here that the impurity scatterings may be neglected when the material is ultra-pure.

In the domain of low lattice temperatures $(T_L \le 20K)$ of interest here, the ensemble of carriers may be significantly perturbed from the state of thermodynamic equilibrium with the lattice atoms, and their average thermal energy may exceed the thermal equilibrium value K_BT_L , in the presence of a relatively weak fields, sometimes of the order of a fraction of a volt/cm. The energy distribution function of these non-equilibrium carriers can no longer be represented by the equilibrium F.D. function at a temperature T_L . In principle, the solution of BTE under these conditions may be worked out to obtain the energy distribution of the non-equilibrium electrons. But usually for an analytical solution of BTE, one needs to make some approximations which very often compromise with the accuracy of the analysis. Hence, one may take recourse to the well-known electron temperature approximation and assume that the effective temperature of the electrons T_e of the ensemble now exceeds the lattice temperature, and turns field dependent: $T_e(\varepsilon) > T_L$. The energy distribution function

may now be represented by the 'heated' F.D. distribution replacing T_L by $T_e(\varepsilon)$. The field dependence of the electron temperature $T_e(\varepsilon)$ may be calculated from the energy balance equation of the electron-phonon system [9-15].

At the low lattice temperatures, normally can hardly reach a value above some ten to hundred times the lattice temperature. Hence under this condition the electrons are confined to a short segment of the energy dispersion curve near the minimum of the lowest sub-band, where the band is assumed to be essentially parabolic, without any serious loss of accuracy. The strength of the electric field which the microstructure system is subjected to is assumed to be such, that it only changes the form of the energy distribution of the carriers and does not trigger the impact ionization process. As such, the carrier concentration essentially remains independent of the applied field.

The maximum value of the field is thus limited, so that the average crystal momentum of the carriers falls within the Brillouin zone. As such, the theoretical investigation of interest here may be carried out in the semi-classical framework. In this framework, the carriers are considered to be moving between successive collisions in accordance with the classical mechanics, while the scattering rates, in the host crystal are derived from the quantum theory.

The mechanism of interaction of the charge carriers with the lattice imperfections is assumed to be independent of the applied field, and the collisions are assumed to occur almost instantaneously, compared to the average time between two successive collisions. The scattering rates may be calculated using the first order perturbation theory, and consequently only two body interactions need to be analyzed.

A number of interactions may be simultaneously effective under any prevalent conditions of the experiment. Then in calculating the total transition probability the interaction processes are taken to be uncorrelated.

The theoretical investigations carried out here making use of all these basic assumptions would usually give the qualitative aspects of some of the characteristics of the three-dimensional structures formed at the interface of a heterostructure made of widely used compound semiconductors and mostly under the condition when the lattice temperature is low.

The concept and various features of the low lattice temperature are described in the next section.

1.3. Salient features of low temperature

The low temperature features that make such studies complicated include [16-20] -

 (i) Necessity of using true phonon distribution, as the simple equipartition approximation of Bose – Einstein's (B.E.) distribution function may hardly be assumed. The energy distribution for the phonons is

$$N_{\vec{q}(\vec{Q})} = \frac{1}{\exp\left(\frac{\hbar\omega_{\vec{q}(\vec{Q})}}{k_B T_L}\right) - 1}$$

where, \vec{q} and \vec{Q} are the three and two dimensional phonon wave vectors respectively, $\hbar = \frac{\hbar}{2\pi}$; h being the Planck's constant, $\omega_{\vec{q}(\vec{Q})}$ is the frequency of corresponding lattice wave vectors given by $\omega_{\vec{q}(\vec{Q})} = u_l q(Q)$; u_l is the acoustic velocity of the electrons; k_B the Boltzmann constant and T_L is the lattice temperature. At high temperatures, the above expression may be simplified to the well-known equipartition law i.e. [16,18]

$$N_{\vec{q}(\vec{Q})} = \frac{k_B T_L}{\hbar \omega_{\vec{q}(\vec{Q})}}$$

because of the fact that $k_B T_L \gg \hbar \omega_{\vec{q}(\vec{Q})}$ i.e. the average thermal energy of the free carriers largely exceeds the phonon energy at thermodynamic equilibrium. However, at low temperatures ($T_L \leq 20 K$), $N_{\vec{q}(\vec{Q})}$ may be approximated by Laurent expansion [21]

$$\begin{split} N_{\vec{q}(\vec{Q})} &= \sum_{m=0}^{\infty} \frac{B_m}{m!} [x(X)]^{m-1}; x(X) \leq \bar{x}(\overline{X}) \\ N_{\vec{q}(\vec{Q})} &= \exp[-x(X)]; \ x(X) > \bar{x}(\overline{X}) \end{split}$$

where x(X)is the normalized phonon wave vector given by $\frac{\hbar u_l q\left(Q\right)}{k_B T_L}$ and B_m is the Bernoulli's number [21,22,23].

In addition, at the low temperature regime, the full form of the phonon distribution function may be expressed as [24,25]

$$N_{\vec{q}(\vec{Q})} = \sum_{n=0}^{\infty} \exp \left[-\frac{(n+1)\hbar \omega_{\vec{q}(\vec{Q})}}{k_B T_L} \right] \ll 1$$

Though the phonon population at low temperatures is indeed limited, putting $N_{q(Q)} \approx 0$ seems to be an oversimplification.

(ii) Inelasticity of the electron-phonon interaction as the phonon energy becomes comparable with the average thermal energy of the electrons. Under the condition when T_L is high, the analyses neglect the phonon energy (ϵ_{ph}) compared to the electron energy (ϵ_k) . Hence, the electron-phonon collisions are treated to be elastic. The ratio $\frac{\epsilon_{ph}}{\epsilon_k}$ is of the order of $\frac{2u_1}{v_{th}}$; v_{th} being the velocity of the electron which is in thermodynamic equilibrium with the lattice. At higher temperatures, the ratio being very small, the phonon energy is indeed only a negligible fraction of the carrier energy. But with the lowering of T_L , the ratio increases, eventually making the phonon energy comparable with the electron energy. Hence, at low temperatures, the assumption that the electron-phonon collisions are elastic, can no longer be made. However, the interaction of the electron – phonon

system is assumed to be elastic even at low temperatures to overcome the mathematical difficulties in solving a problem. But such study will indeed incur some errors in the results [16,17,18,24,26].

(iii) The carrier ensemble may be non-degenerate or degenerate. But, one of the important low temperature features is the degeneracy of the carrier ensemble. At low temperatures, if the Fermi energy ε_F is not much lower than k_BT_L of the conduction band edge and the electron densities are beyond the insulator to metal transitions, the free electron ensemble in the semiconductor is to be treated as degenerate. With the increase of doping level, as the electron concentration of an n-type material exceeds the effective density of states, the Fermi level moves into the conduction band and the material seems to exhibit degeneracy. The critical concentration of the donor N_D required for the onset of degeneracy, may roughly be calculate from [16,18,27].

$$\varepsilon_{\rm F} = \frac{\hbar^2}{2m^*} (3\pi^2 N_{\rm D})^{\frac{2}{3}} > E_{\rm d}$$

where, m^* is the effective mass of an electron and E_d is the donor ionization energy. The degree of degeneracy is generally expressed in terms of $\frac{\epsilon_F}{k_B T_I}$.

- (iv) At low temperatures, the carrier ensemble being degenerate, the distribution function for the electrons should be expressed in terms of Fermi-Dirac (F.D.) distribution rather than simple Maxwellian function, which is used when the carrier ensemble is assumed to be non-degenerate.
- (v) Electrical non-linearity may set in due to significant perturbation of the electron ensemble from the state of thermodynamic equilibrium for a fraction of few volts or less at low temperatures. This will lead the electrons to be hot. Hot electron transport has become an important phenomenon for the understanding of all the modern semiconductor

devices. Such devices are categorized into two groups – the ballistic devices and the quasi-thermal devices, depending on the type of a hot electron ensemble essentially employed in their operation.

- (vi) The scattering potential due to lattice imperfections may be significantly screened, particularly in microstructures. In the absence of any potential, one may assume that the free electrons are uniformly distributed in a sample. But the electrons either collect or are removed from the region where any potential discontinuity occurs depending upon the sign of the discontinuity. This resulting space charge causes an extra potential and modifies the prevalent one thereby effectively screens its effects at large distances. This behavior of an electron ensemble describes the electrostatic screening of the electron-electron, electronlattice and electron-impurity interactions in the material. As a result, the transition probability of an electron from any state is finite for interactions with ionized impurities and piezoelectric phonons. A non-degenerate ensemble of electrons yields an inverse of screening length $\beta_s = \left[\frac{4\pi e^2 n_0}{K k_B T_L}\right]^{1/2}$, where n_0 is the free electron concentration and K is the dielectric constant of the material [28,29]. Evidently the effect of screening is felt more and more with the lowering of the lattice temperature and for higher concentrations. As the sizes of the electronic devices have become smaller and the carrier densities become larger, the role of screening has become of much importance within the devices. In addition, screening is important in many cases like in heavily doped materials when the carrier concentration becomes high or when impurity breakdown takes place at low temperatures due to impact ionization giving rise to a sharp increase in the concentration at a field of only a few volt/cm. Thus, one can hardly neglect the effect of screening when studying the electron transport in semiconducting materials at low temperatures.
- (vii) Transition from $1s \rightarrow 2p$ of the neutral impurity atoms.

(viii) At low lattice temperatures, when the ionization of the impurities in semiconductors is quite incomplete, the concentration of the neutral impurities is large. The electronic collision with the neutral impurities now changes to be inelastic, since the ionization and excitation of these impurities contribute significantly to the net energy loss of the electrons. Hence, unlike the state of high temperatures, this interaction could no longer be neglected while analyzing electron transport at low temperatures.

- (ix) Mobility becomes field dependent and non-linearity comes into play.
- (x) The structure tends to be non-ohmic.

It is apparently a formidable task to solve each part of the problem analytically at a time. As such, there remains ample scope of work with physically realistic approximations without compromising the validity of the model. In theoretical research, whenever one wants to develop a mathematical formulation for the physically realistic systems, some assumptions may have to be made very often so that the mathematical problem becomes amenable to solution. These assumptions need to be physically realistic so that the results that follow from the subsequent investigation can describe the characteristics of the real system under the prevalent condition. In the present thesis, to carry out the theoretical investigations on different semiconductor structures, we too have made some basic assumptions which identify the structure and the prevalent physical conditions.

1.4. Different semiconductor structures

Since a long time, the bulk semiconductors have been used for device applications. However, there have been remarkable developments and inventions in the field of low dimensional semiconductor structures during the last few decades. Due to the advancement of new techniques like Molecular Beam Epitaxy (MBE), Czochralski method, Bridgman-Stockbarger technique etc, it has become possible to control the growth of the materials as

per our desired dimension. One can precisely control the compositions of modern semiconductor heterostructures in the atomic scale to develop low dimensional systems that have revolutionized the physics of semiconductor device and their impact on modern information technology [16,19,20]. The importance of the microstructures lies on the fact that, it is possible to segregate impurities from the carrier ensemble, unlike the bulk semiconductors. Thus, a large carrier concentration may be realized without any associated reduction in the mobility. Whereas, in the bulk materials, the carrier concentration may be increased by increasing the concentration of the impurity, which in turn cause a decrease in the carrier mobility.

In the low dimensional structures, the free electrons lose one or more degrees of freedom when subjected to some potential barriers thereby making them confined along certain directions. Degree of such confinement may be described on comparing the sizes L_X , L_y and L_z along X, Y and Z axes respectively with the electron wavelength (λ). Different structures may be categorized as [30,31]

- 1.4.1. If $\lambda \ll L_X$, L_Y , L_Z : One gets a bulk structure. The electrons are free to move along all the three dimensions and the system is termed as three-dimensional electron gas (3DEG).
- 1.4.2. If $\lambda \cong L_Z << L_X$, L_Y : One gets a quantum well structure. The quantization of the electron motion is now along Z- axis. However, they freely move along X and Y axes. Hence, the motion of the electrons is now confined on the X-Y plane and the electrons have lost one degree of freedom. The electron ensemble is now two dimensional and termed as two-dimensional electron gas (2DEG).
- 1.4.3. If $\lambda \cong L_Z \cong L_Y \ll L_X$: One gets a quantum wire structure. The quantization of electron motion takes place along Y and Z axes. Along X axis, the electrons move

as free particles. Thus, electrons have lost two degrees of freedom and one gets a one-dimensional electron gas (1DEG).

1.4.4. If $\lambda \cong L_Z \cong L_Y \cong L_X$: One gets a quantum dot structure. The quantization of the electrons takes place along all the three axes. The electrons having lost three degrees of freedom, the ensemble is now zero-dimensional electrons gas (0DEG).

In the first few chapters, different transport properties in bulk semiconductor structure have been extensively analyzed under different prevalent conditions.

Minimization of the electronic devices is acceptable which leads to better performance. When the anticipated quantum confinement of the free electrons in semiconductor microstructures was first observed, there has been phenomenal growth of interest in the study of such structures for the last three decades or so. Subsequently, this has opened up the world of useful Low –Dimensional Structures and mesoscopic devices.

The almost insatiable demands for the growth of memory and computational capabilities and the race for increasing the processing and transmission speeds of signals, have stimulated the research studies in these areas since the advent of metal-oxide-semiconductor-field effect transistors (MOSFET) with easily controllable surface characteristics. In general, the practical realization of the mesoscopic devices and making them economically viable, have become possible because of mastering a knowledge of the physics of the constituent structures, the device is made of.

Extensive experimental and theoretical studies in the field of electronic transport in semiconductor quantum well structures have been carried out over the last few decades, since the significantly higher mobility of the free carriers could be observed in such structures. Much of these studies have been carried out at quite low temperatures. This is because the enhancement of the mobility values due to reduction of the effect of the

impurities is prominent at low temperatures. The quality of the samples can be assessed from such studies. But the studies at higher temperatures are usually relevant to the performance of the devices [32,33]. As a result of these studies, there have been lots of advancement in the Solid-State devices and experimental methods producing more and more accurate results. Without going for an elaborate review of the studies, a brief account of it may be made here. Since it is now possible to get a Si-SiO2 interface with a high degree of perfection, the bipolar devices are now being replaced by the field effect devices, for many applications. The Metal-Oxide-Semiconductor (MOS) structures having similar interfaces are now widely used in digital integrated circuits. The free carriers in the conducting channel of those structures are not provided by the usual method of doping, but by the process of inversion and depletion of the surface layer. A typical concentration of about 10¹⁶/m² in the surface layer of SiO2 gives rise to a rather strong surface electric field Es 10⁷ V/m. Such a strong field effectively quantifies the motion of the carriers in a direction perpendicular to the interface. But the electrons move freely on the interfacial surface.

One of the present authors, along with others, made the same theoretical analysis in the field of electronic transport in quantum wells of Si and some compound semiconductors, taking due account of some of the low temperature features, which are usually neglected in the studies under the condition of high temperature. Their studies include the problems of (i) the interaction of the electrons with deformation potential and piezoelectric phonons, (ii) energy loss to intravalley acoustic modes, (iii) ohmic and non-ohmic mobility characteristics, etc. The results which they obtained have been found to be interesting and significantly different from what can be obtained under the condition of high temperature, and inspire further studies in the field [34-42]. Notwithstanding such

advancement, even now there remains ample scope for work of potential interest in the field.

In the present communication, we have considered a compensated, non-degenerate semiconductor compound in the presence of a relatively high electric field, at a low lattice temperature. The effects of the inelastic interaction of the non-equilibrium electrons with the neutral impurities through the processes of $1s \rightarrow 2p$ excitation and the ionization, on the net energy loss of the electron have been assessed here. The intrinsic quasi-elastic interactions with both the acoustic phonons, the piezoelectric and the deformation potential, have also been taken into account. Then the resulting field dependence of the effective temperature of the non-equilibrium electrons has been obtained. The numerical results that follow from our analysis for the compounds like InSb, InAs and GaSb have been compared with the available experimental and other theoretical results.

1.5. Scope of the thesis

In the present thesis the theories have been developed on some aspects of the electronic transport in the bulk structures, under the condition when the lattice temperature is low. The chapter-wise orientation is as follows:

Based on the basic assumptions which have been elaborated in the paragraph 1.2 and taking due account of the specific features of the low lattice temperatures as described in the paragraph 1.3, theories have been developed on some aspects of the electron transport in the presence of an effectively high electric field. The results of the electron transport characteristics as theoretically obtained here, have been compared with available experimental data.

The aspects of the electronic transport that have been dealt with include:

- (i) The energy loss rate and the non-ohmic mobility characteristics of the electrons considering the non-degeneracy of the ensemble.
- (ii) The field dependence of the effective electron temperature characteristics of the electron ensemble taking due account of the non-degeneracy of the ensemble.
- (iii) The efficiency of the second harmonic generation of microwaves due to the electrical nonlinearity of the electron ensemble.

Chapter II:

In chapter II a brief introduction has been made on the different types of semiconductor structures and their properties. The electron fundamental length in different semiconductors have been calculated. The basic properties like the (a) wave function, energy dispersion, wave vector element, (b) density of states function for different structures, sub band energy, (c) Equilibrium carrier concentration, (d) current density have been obtained. The chapter ends with the discussions on different scattering mechanisms in semiconductor material.

Chapter III:

The purpose here is to solve the energy balance equation for the electron-phonon system for the combined interaction of the electrons with the deformation potential and piezoelectric phonons as well as the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities and thus to obtain the dependence of the average energy loss rate of an electron, in a non-degenerate ensemble of electrons upon the average electron energy. Numerical

results are obtained for Insb, InAs and GaSb. The results are analyzed in detail and compared with other available data.

Chapter IV:

Chapter IV deals with Dependence of the normalized electron temperature (T_e/T_L) upon the electric field ε at low lattice temperature T_L considering the energy loss due to all the processes of energy loss of an electron (interaction with the acoustic and the piezoelectric phonons as well as the $1s \to 2p$ excitation and ionization of the neutral impurities). Numerical results are obtained for Insb, InAs and GaSb. The results are analyzed in detail and compared with other available data. The results exhibit here that the inelastic interaction of the non-equilibrium electrons with the neutral impurities, brings in significant changes in the field dependence of the effective temperature of the non-equilibrium electrons, under the condition, when the lattice temperature is low.

Chapter V:

Chapter V deals with the generation of harmonics of the input microwave signal in the bulk structure of compound semiconductors, due to the electrical nonlinearity of current-voltage characteristics of the ensemble of the non-equilibrium electrons. The chapter starts with a brief review of the microwave harmonic generation in semiconductor structures. This is followed by the method of calculation of the efficiency of Second Harmonic Generation (SHG) in the non equilibrium ensemble of Bulk Semiconductor Structures. The numerical results for the efficiency of microwave harmonic generation of SHG upon the biased field in InSb, InAs and GaSb have been obtained at different lattice temperatures. Then a comparative discussions of the results for the different materials have been made.

Chapter VI:

Chapter VI deals with the overall conclusion of the thesis and future direction in the relevant field. The chapter contains the set up used in the theoretical calculation, the framework used for the theoretical analysis and the limitations of the assumptions made have also been discussed.

References

- [1] E.M. Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967.
- [2] B.R. Nag, Electron Transport in Compound Semiconductor, Springer, Berlin, 1980.
- [3] Z.S. Kachlishvili, Galvanomagnetic and Recombination Effects in Semiconductors in a Strong Electric Field, Phys. Stat. Sol (a) 33 (1976) 15-51.
- [4] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, A. Alberigi-Quaranta, Electron drift velocity in silicon, Phys. Rev. B 12 (1975) 2265-2284.
- [5] B.R. Nag, Theory of Electrical Transport in Semiconductors, Pergamon Press, Oxford, 1972.
- [6] Z.S. Kachlishvili, Inelastic Impurity Scattering of Hot Electrons in Semiconductors. Phys. Stat. Sol (b) 48 (1971) 65-75.
- [7] G. Bauer, Springer Tracts in Modern Physics, Vol. 74, Springer, New York, 1974.
- [8] L.F. Mao, H. Ning, C. Hu, G. Wang, Physical Modeling of Activation Energy in Organic Semiconductor Devices based on Energy and Momentum Conservations, Sci. Rep. 6 (2016) 24777.
- [9] E.M. Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967.
- [10] C. Jacoboni and L. Reggiani, Rev. Mod. Phys. 55, 645 (1983).
- [11] G. Bauer, Springer Tracts in Modern Physics, Vol. 74, Springer, New York, 1974.
- [12] F. Stern and W.E. Howard, Phys. Rev. 163, 816 (1967).
- [13] A.B. Fowler, F.F. Fang, W.E. Howard and P.J. Stiles, Phys. Rev. Lett. 16, 901 (1966).

- [14] F.F. Fang and A.B. Fowler, Phys. Rev. 169, 619 (1968).
- [15] D.J. Bishop, D.C. Tusi and R.C. Dynes, Phys. Rev. Lett. 44, 1153 (1980).
- [16] B.R.Nag, Theory of Electrical Transport in Semiconductors, Pergemon Press, Oxford,1972
- [17] B.R.Nag, Electron Transport In Compound Semiconductors, Springer, Berlin, Heidelberg, New York, 1980
- [18] E.M.Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967
- [19] C.Hamaguchi, Basic Semiconductor Physics, Springer, Berlin, Heidelberg, New York, 2010
- [20] C.Jacoboni, Theory of Electron Transport in Semiconductors, Springer-Verlag Berlin Heidelberg, 2010
- [21] Canali C., Jacoboni C, Nava F., Ottaviani G. and AlberigiQuaranta A., Phys. Rev. B 12, (1975) 2265
- [22] S. Nag and D. P. Bhattacharya, Physica E 42, 1319 (2010)
- [23] S.Nag, A.Basu, B.Das, T.R.Middya, D.P.Bhattacharya, Physica E ,Volume 72, August 2015, Pages 77-83
- [24] A. Basu, B. Das, T.R. Middya, D.P. Bhattacharya; Journal of Physics and Chemistry of Solids, Volume 100, January 2017, Pages 9–13
- [25] A. Basu, T. R. Middya, and D. P. Bhattacharya, Journal of Applied Physics 122, 2017, 105703
- [26] A. Basu, B. Das, T.R. Middya, D.P. Bhattacharya; Physica B, Volume506, 1 February 2017, Pages 65–68
- [27] S. Midday, S.Nag, D.P.Bhattacharya, Physica B 458 (2015) 18-21

- [28] F. Stern and W. E. Howard, Phys. Rev. 163, 816 (1967)
- [29] B. K. Ridley: Quantum Processes in Semiconductors, Clarendon Press, Oxford, 1993.
- [30] C. Kittel, Elementary Statistical Physics, John Wiley & Sons, Inc., New York, 1958
- [31] S.M. Sze, Physics of Semiconductor Devices, Wiley Eastern Limited, New Delhi, 1983
- [32] T. Ando, A. B. Fowler and F. Stern, Rev. Mod. Phys. 54, 437 (1982).
- [33] B. R. Nag, Physics of Quantum Well devices, Kluwer Academic Publisher Dordrecht, 2000
- [34] S. S. Paul, A. K. Ghorai, and D. P. Bhattacharya, Phys. Rev. B 48, 18268 (1993).
- [35] A. K. Ghorai and D. P. Bhattacharya, J. Appl. Phys. 80, 3130 (1996).
- [36] A. K. Ghorai and D. P. Bhattacharya, Surf. Sci. 380, 293 (1997).
- [37] S. Nag and D. P. Bhattacharya, Superlattices Microstruct. 50, 359 (2011).
- [38] D. P. Bhattacharya, S. Midday, S. Nag, and A. Biswas, Physica E 47, 264 (2013).
- [39] D. P. Bhattacharya, S. Midday, and S. Nag, Superlattices Microstruct. 72, 126 (2014).
- [40] S. Nag, A. Basu, B. Das, T. R. Middya, and D. P. Bhattacharya, Physica E 72, 77 (2015).
- [41] S. Nag and D. P. Bhattacharya, J. Phys. Chem. Solids 76, 59 (2015).
- [42] S. Nag, B. Das, A. Basu, J. Das, D. P. Bhattacharya, and C. K. Sarker, Physica E 87, 237 (2017).

Chapter 2

Some Basic Physics and Properties of Quantum Confined Semiconductor Structure

SOME BASIC PHYSICS AND PROPERTIES OF DIFFERENT SEMICONDUCTOR STRUCTURES

2.1 Introduction

Prior to making a detailed enumeration of the comprehensive theoretical analysis of some of the aspects of the electron transport characteristics of a non-equilibrium ensemble of 3DEG in a heterostructure, under the condition of low lattice temperature and at effectively high electric field, it is worth to highlight a short review of the basic physics of the structure that is under consideration here.

2.2 Electron fundamental lengths in solids

The dimensionality of a structure is determined by comparing the dimensions of the structure with the de Broglie wavelength λ of the electrons in the material. When any of the dimensions is miniaturized to the order of λ , the electronic properties of the carrier ensemble get significantly influenced. Hence, the knowledge of this fundamentally important length λ is required.

The de Broglie wavelength λ_0 for a free electron is given by $\lambda_0 = 2\pi\hbar/\sqrt{2m_0E}$, where E is the electron energy and m_0 is the mass of an electron in vacuum. As such, the de Broglie wavelength λ of an electron in the material is given by $\lambda = 2\pi\hbar/\sqrt{2m^*E}$. Since $m^* < m_0$, then $\lambda > \lambda_0$.

2.3. (a) Wave function, energy dispersion, wave vector element, (b) Density of states function for different structures, sub band energy, (c) Equilibrium carrier concentration, (d) Current density

Some of the specific electrical transport related factors which frequently occur in the present analysis are described for different structures in what follows now.

(a) Wave function, energy dispersion, wave vector element

(i) Bulk structure:

The wave function of an electron for this structure is

$$\psi_{\vec{k}}(\vec{r}) \sim exp(i\vec{k}.\vec{r})$$
 (1)

where in rectangular coordinates the wave vector may be represented as $\vec{k} = \hat{\imath}k_x + \hat{\jmath}k_y + \hat{k}k_z \text{ and } \vec{r} = \hat{\imath}x + \hat{\jmath}y + \hat{k}z.$

For the parabolic band structure

$$E_{\bar{k}} = \frac{\hbar^2}{2m^*} \left(k_x^2 + k_y^2 + k_z^2 \right) = \frac{\hbar^2 k^2}{2m^*}$$
 (2)

This proves to be a good approximation particularly near the bottom of the conduction band or the top of the valance band.

 $d\vec{k}$, the 'volume' element in three dimensional \vec{k} space given by the space between two concentric spheres of radii \vec{k} and $\vec{k}+d\vec{k}$. Thus

$$d\vec{k} = 4\pi k^2 dk \tag{3}$$

(ii) Two-dimensional structures (quantum well)

Let the quantum well be along the z-axis. The \vec{k} space is now two-dimensional: $\vec{k}=\hat{i}k_x+\hat{j}k_y$

If the well is an infinite well, the wave function of an electron now assumes a form

$$\psi_{\vec{k}}(\vec{r}) \sim \sin\left(\frac{m\pi z}{L_z}\right) exp(i\vec{k}.\vec{r})$$
 (4)

Here $\vec{k}.\vec{r} = k_x x + k_y y$.

$$E_{\vec{k}} = \frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + E_m \tag{5}$$

$$E_{\vec{k}} = \frac{\hbar^2 k^2}{2m_{\parallel}^*} + E_m, \quad m_{\parallel}^* = \left(m_1^* m_2^*\right)^{1/2} \tag{6}$$

where E_m is the mth energy eigenvalues for the well of width L_z , and is given by

$$E_{m} = \frac{m^{2}\hbar^{2}\pi^{2}}{2m_{w}^{*}L_{z}} \tag{7}$$

 m_w being the effective mass of an electron in the well. Thus, for each m one gets a subband.

 \vec{k} is now two-dimensional and the 'volume' element in the two-dimensional \vec{k} space is the annular region between two concentric circles of radii \vec{k} and $\vec{k} + d\vec{k}$. Thus

$$d\vec{k} = 2\pi k dk \tag{8}$$

(iii) One-dimensional structure (quantum wire)

Let there be two infinite quantum wells, one along the y-axis of width L_y and the other along the z-axis, of width L_z respectively.

The wave vector \vec{k} is now one-dimensional: $\vec{k} = \hat{i}k_x$.

The wave function of an electron now assumes the form

$$\psi_{\vec{k}}(\vec{r}) \sim \sin\left(\frac{n\pi y}{L_y}\right) \sin\left(\frac{m\pi z}{L_z}\right) exp(i\vec{k}.\vec{r})$$
 (9)

Here $\vec{k}.\vec{r} = k_x x$ and

$$E_{\vec{k}} = \frac{\hbar^2 k_x^2}{2m_1^*} + E_n + E_m \tag{10}$$

where E_n and E_m are respectively the nth and mth energy eigenvalues for the wells along the y and z axes respectively.

 \vec{k} is now one-dimensional, and $d\vec{k}$ is the space element between lines of lengths \vec{k} and $\vec{k} + d\vec{k}$. Thus

$$d\vec{k} = 2dk \tag{11}$$

(iv) Zero-dimensional structure (quantum dot)

In the quantum dot structure, the electrons are confined in all the three directions. As such the total energy of an electron in the quantum dot taking together all the three directions is completely discrete, having no continuous part. Hence, quantum dots are often called an artificial atom or a giant-atom.

If we take the confining potential of a quantum dot similar to that a particle in a 3D potential box, of width L_x , L_y and L_z along x, y and z directions respectively, the energy eigenvalues of an electron may be expressed as

$$E_{n_x,n_y,n_z} = \frac{\hbar^2 \pi^2}{2m^*} \left(\frac{n_x}{L_x^2} + \frac{n_y}{L_y^2} + \frac{n_z}{L_z^2} \right); \ n_x, n_y, n_z = 0, \pm 1, \pm 2...$$
 (12)

(b) Density of states function [1]

In a unit volume of a structure, the number of \vec{k} states in the "volume" element $d\vec{k}$ of the \vec{k} space for a p dimensional structure is given by [1]

$$dg = \frac{2g_v}{(2\pi)^p} d\vec{k} \tag{13}$$

where p stands for the dimensionality of the structure. It assumes the values 3, 2 and 1 respectively for the bulk, the quantum well and quantum wire structure. g_{ν} is the valley degeneracy factor. The factor 2 at the numerator takes into account the spin degeneracy. Now using energy dispersion relation $E \equiv E(\vec{k})$ for any structure, one can obtain $D(E_{\vec{k}}) = dg/dE_{\vec{k}}$. Thus $D(E_{\vec{k}})$ gives us the number of quantum states per unit energy interval. Hence, one can obtain

(i) For the bulk structure:

$$D_3(E_{\bar{k}}) = g_v \frac{\sqrt{2}}{\pi^2} \left(\frac{m^*}{\hbar^2}\right)^{3/2} E_{\bar{k}}^{1/2} \sim E_{\bar{k}}^{1/2}$$
 (14)

(ii) For the quantum well structure:

$$D_{2}\left(E_{\vec{k}}\right) = \sum_{n=0}^{\infty} \frac{g_{\nu} m_{\parallel}^{*}}{\pi \hbar^{2}} H\left(E_{\vec{k}} - E_{n}\right) \sim E_{\vec{k}}^{0}$$
(15)

where E_n is the lowest energy of the nth subband and H(x) is the Heaviside step function [2].

(iii) For the quantum wire structure:

$$D_{1}(E_{\vec{k}}) = \sum_{n_{y},n_{z}=0}^{\infty} \frac{g_{v}\sqrt{2m^{*}}}{\pi\hbar} \left(E_{\vec{k}} - E_{n_{y},n_{z}}\right)^{-1/2} H\left(E_{\vec{k}} - E_{n_{y},n_{z}}\right) \sim E_{\vec{k}}^{-1/2}$$
(16)

(iv) For the quantum dot structure:

What follows from (12) the density of states for an electron in a single quantum dot consists of a set of Dirac delta functions at the discrete allowed values of energy of the electron.

(c) Equilibrium carrier concentration [1]

The equilibrium carrier concentration n_p of a ' p ' dimensional structure may be calculated from the integral

$$n_p = \frac{2}{(2\pi)^p} \int f(\vec{k}) d\vec{k} \tag{17}$$

where $f(\vec{k})$ is the equilibrium distribution function of the carriers. Assuming F.D. distribution for $f(\vec{k})$ one can obtain

(i) For the bulk structure (p=3):

$$n_3 = 2\left(\frac{2\pi m^* K_B T}{h^2}\right)^{\frac{3}{2}} F_{\frac{1}{2}}(\eta_D) \tag{18}$$

(ii) For the quantum well structure (p=2):

$$n_2 = 2 \left(\frac{2\pi m^* K_B T}{h^2} \right) F_0(\eta_D) \tag{19}$$

(iii) For the quantum wire structure (p=1):

$$n_1 = 2\left(\frac{2\pi m^* K_B T}{h^2}\right)^{\frac{1}{2}} F_{\frac{-1}{2}}(\eta_D) \tag{20}$$

where $w=E/K_BT$, $\eta_D=E_F/K_BT$, ε_F being the Fermi energy and $F_j\left(\eta_D\right)$ is the Fermi integral of j^{th} order and is given by $F_j\left(\eta_D\right)=\frac{1}{\Gamma(j+1)}\int_0^\infty \frac{w^jdw}{1+exp(w-\eta_D)}$.

(d) Current density

The expression for the current density is given by [3]

$$\vec{J} = \frac{e}{\hbar} \int \left(\nabla_{\vec{k}} E_{\vec{k}} \right) f(\vec{k}) d\vec{k} \tag{21}$$

here $f(\vec{k})$ is the distribution function of the free carrier and may be obtained from the solution of the Boltzmann transport equation (BTE). The unknown distribution function $f(\vec{k})$ may be expanded in a series neglecting the higher order terms as [3]

$$f\left(\vec{k}\right) = f_0\left(E_{\bar{k}}\right) + \vec{k}.f_1\left(E_{\bar{k}}\right) \tag{22}$$

 $f_{\scriptscriptstyle 0}ig(E_{_{ec{k}}}ig)$ is the isotropic part of the distribution function.

Let us assume that a d.c. field of magnitude \mathcal{E} is applied to a homogeneous sample having an electron concentration of n. The force on the electron due to the applied electric field is $e\vec{\mathcal{E}}$. In the steady state the BTE in relaxation time approximation can be written as

$$\frac{e\vec{\varepsilon}}{\hbar} \cdot \nabla_{\vec{k}} f = \frac{\partial f}{\partial t} \bigg|_{coll} = -\frac{f - f_0}{\tau}$$
 (23)

where τ is the effective relaxation time of the collision. Replacing f by $f_0(E_{\vec{k}}) + \vec{k} \cdot f_1(E_{\vec{k}})$ from Eq. (22) and neglecting higher order terms in the left-hand side, we obtain

$$-\frac{\vec{k}.f_1(E_{\vec{k}})}{\tau} = \frac{e\vec{\varepsilon}}{\hbar}.\nabla_{\vec{k}}f_0 = \frac{e\vec{\varepsilon}}{\hbar}.\nabla_{\vec{k}}E_{\vec{k}}\frac{\partial f_0}{\partial E_{\vec{k}}}$$
(24)

But
$$\vec{\varepsilon}.\nabla_{\vec{k}}E_{\vec{k}} = \hbar^2\vec{\varepsilon}.\overrightarrow{M}.\vec{k} = \hbar^2\vec{k}.\overrightarrow{M}.\vec{\varepsilon}$$

Eq. (23) thus yields for
$$f_1(E_{\vec{k}}) = -\hbar e \tau (\overrightarrow{M}.\vec{\varepsilon}) \frac{\partial f_0}{\partial E_{\vec{k}}}$$

Now, replacing the value of $f(\vec{k}) = f_0(E_{\vec{k}}) - \hbar e \tau (\vec{k}.\vec{M}.\vec{\varepsilon}) \frac{\partial f_0}{\partial E_{\vec{k}}}$ in Eq. (21), we get the current density

$$\vec{J} = -e^2 \int \left(\nabla_{\vec{k}} E_{\vec{k}} \right) \left(\vec{k} \cdot \vec{M} \cdot \vec{\varepsilon} \right) \tau \frac{\partial f_0}{\partial E_{\vec{k}}} d\vec{k}$$
 (25)

When constant energy surfaces are spherical in k - space, the reciprocal effective mass tensor \overline{M} can be reduced to a scalar $1/m^*$ and the integrand may be expressed in polar coordinates with the direction of the applied field as the reference. One then obtains

$$\vec{J} = -\frac{e^2 \varepsilon}{m^*} \int \frac{\hbar^2 k^2}{m^*} \cos^2 \theta \tau \frac{\partial f_0}{\partial E_{\vec{k}}} d\vec{k}$$
 (26)

On carrying out the integral (26) one can obtain the expression for the current density.

2.4 Scattering Mechanisms

The wave function of an electron in a perfectly crystalline material is given by the stationary Bloch function. When subjected to an electric field, the drift velocity of the electron should increase indefinitely with time. But in a real crystal, the average drift velocity gets limited by the collisions, the electron may suffer with various lattice imperfections. These imperfections, whenever they occur, produce a perturbation in the periodic potential of the perfect crystal. The electron is said to be scattered whenever it interacts with any such perturbing potential and changes its wave vector and, or the energy states [4].

The dynamic imperfection is intrinsic and is produced by the thermal vibration of the lattice atoms about their equilibrium positions. On the other hand, the static imperfections arise due to the crystal defects or impurity atoms, introduced at the time of crystal growth.

If the imperfections are not much frequent and the perturbing potential due to it be small, the effects of such potential may be worked out in the framework of the time dependent perturbation theory [5].

2.4.1. Classification of Scattering

On interacting with any imperfection an electron can make a transition to a state that belongs to either the same or a different valley. As such, the transitions may be classified either as intravalley or as intervalley respectively. In case of holes, the respective transitions are called either intraband or interband. The most important sources of scattering that may cause electronic transitions include [5,6,7,8,10].

- (a) Lattice vibrations
- (b) Defects
- (c) Other carriers

(d) Interface roughness

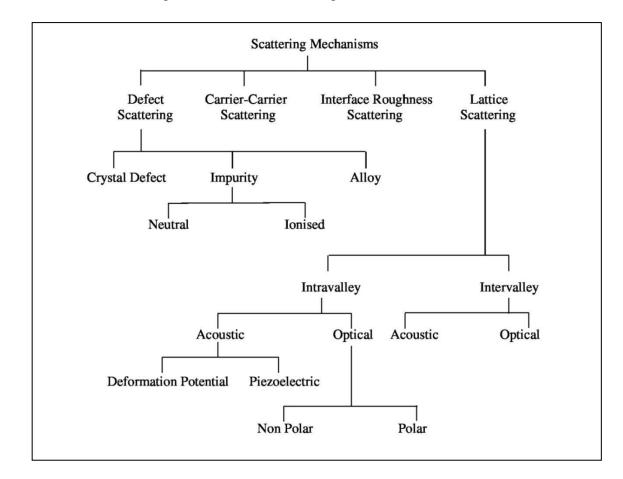
The interaction of the free charge carriers with the lattice vibrations takes place through phonons which are produced as a result of deformation of an otherwise perfect crystal. Such an interaction, typical of covalent semiconductors, is called deformation potential interaction, involving both acoustic and non-polar optical phonons. In polar materials having no inversion symmetry, however, the electrostatic potentials produced by the polarization waves due to lattice vibrations may also result in an interaction, which is either the piezoelectric interaction involving the acoustic phonons or the polar interaction that involves the optical phonons.

The lattice scattering for which the final and initial states of the electron are in the same valley in the $E-\vec{k}$ space is called intravalley scattering. In some materials with the lowest minima in the <100> or <111> directions the lattice scattering may transfer an

electron from one valley to another valley having its energy minima at the same level. Such scattering is termed as intervalley scattering.

In semiconductors, defects can arise owing to various types of dislocation in crystals and to impurity atoms. The impurity atoms may be either ionized or neutral or they may give rise to dipoles, depending upon the lattice temperature, the concentration of the impurity atoms and the compensation ratio [5,7,11]. In semiconducting alloys, the defects may also arise due to random distribution of the constituent atoms among the available lattice sites. Then the concentration of the free electrons in semiconductor is high enough, the effects of an electron changing states by collision with another free electron through their Coulomb field, may become important. Such collisions called inter-electronic or carrier- carrier collisions, become important on increasing the electron concentration. The effects of this collision may be neglected compared to the effects produced by other scattering mechanisms for concentrations of the order of 10¹³-10¹⁴ cm⁻³. Carrier-carrier scattering acting alone cannot restore a perturbed distribution of the carrier ensemble to its normal equilibrium condition. Actually, there would be a mixture of energy and momentum of electrons and that would lead to a modification of the distribution function.

In many cases, the interfaces in a semiconductor structure, like that which occurs between Si and SiO₂ in a FET or between GaAs and AlGaAs in a HEMT are not perfectly smooth. This is another type of imperfection which may constitute a major cause for scattering and is called surface roughness scattering. It is known to be effective especially at high concentration of the carriers and for low temperatures [12].



A schematic diagram of different scattering mechanisms is shown below.

2.4.2. Relative importance of different scattering mechanisms

All the scattering mechanisms as described in the previous section are not always equally important. The electronic transport characteristics of any semiconductor structure are determined by the scattering mechanisms which seem to be dominant under the prevalent experimental conditions in respect of the lattice temperature, impurity or carrier concentration etc.

The impurity atoms occupy the lattice sites as substitutional atoms and cause a perturbation in the periodic crystal potential. At very low temperatures, near 4K, these atoms remain neutral. Therefore, the neutral impurity scattering of the electrons may dominate when the lattice temperature is very low. For the high purity semiconductors, the impurity scattering can hardly play any significant role even at low temperatures. With

the increase of the lattice temperature, the impurity atoms are more and moreionized and the interaction with ionized impurity atoms tends to be important. The ionized impurity scattering is significant when the carrier concentration is high enough and the lattice temperature is not very low [13]. The field produced by an impurity atom may be assumed to be time independent and the collisions between the electrons and the impurity atoms are essentially interaction with fixed force fields. This type of collision, being elastic in nature, cannot alone limit the drift velocity of the carriers in the presence of an external electric field. As such it must be supplemented by some other scattering mechanisms which would be responsible for the dissipation of the electron energy and thus would limit the drift velocity.

Apart from these, some structural defects may be introduced during the crystal growth. They include edge dislocations and screw dislocations etc. The carriers may be scattered at these sites when charges collect there. The dislocation scattering prevails at low lattice temperature and the mobility value is affected strongly by high density of the dislocation [14-22]. However, if the crystal is properly grown, the effects of such dislocations can be neglected.

In alloys of two semiconducting compounds the dissimilarities of the constituent compounds lead to distortions in the band structure at the points where they meet. These boundaries are randomly positioned and act as individual scattering centres similar to an impurity atom. But the scattering being due to discontinuities in the band edges, the mechanism is similar to that for deformation potential acoustic scattering. For In_{0.53}Ga_{0.47}As, the alloy scattering is more dominant than impurity and surface roughness scattering at low lattice temperature [23].

The scattering due to lattice imperfections that are produced by crystal defects or impurity atoms may be controlled through improved techniques of crystal preparation.

However, the phonon scattering of the free carriers in any material, due to interaction with lattice vibrations, is intrinsic in nature and cannot be controlled like the former mechanisms.

The deformation potential scattering becomes important for relatively higher temperatures. But in high purity samples, if the carrier concentration is not high enough the deformation potential scattering may also dominate at $T_L < 20 \text{ K}$ [6,10, 24-27].

The piezoelectric scattering of the carriers is important in all compound semiconductors, particularly at low temperatures. It is, however, stronger in materials with wurtzite structure than in the materials with sphalerite structure due to the lower symmetry of the former. It may be mentioned here that due to strong piezoelectric interaction in compounds like CdS, ZnO etc. they are usually the chosen materials for acoustoelectric devices [10, 28-30].

The optic strain due to lattice vibrations produces a perturbing potential with which the carriers may interact depending upon the symmetry of the band structure. This interaction is rather weak for electrons at the Γ - point minima or for the <100> minima. Since in most of the compound semiconductors the lowest minimum is at the Γ - point, this kind of scattering is of little importance there. The aluminium and gallium and lead compounds are exceptions where the non-polar optic scattering may be important. The dipole moment resulting from the displacement of the neighbouring atoms with the opposite ionic charges gives rise to perturbing potential with which the carriers may also interact. Such scattering, termed as polar optic phonon scattering, is often the most important scattering mechanism, particularly at liquid-nitrogen or higher temperatures [10,13].

The electrical transport in semiconductor structures is determined by the dominant interactions which the free carriers may have with various static and dynamic lattice

defects in the materials. The free carriers interact with optical and intervalley phonons at the lattice temperatures above some 100K and with impurities at lower temperatures. Between these two extreme situations a range of lattice temperature exists where the free carriers in a high purity covalent semiconductor interact dominantly only with intravalley acoustic phonons through the deformation potential and in compound semiconductors having no inversion symmetry they interact dominantly with both the deformation and the piezoelectric acoustic phonons [6,9,10,13,28,31-36].

Here in the present Thesis, the various transport properties are studied considering mainly the interaction of the electrons with the deformation acoustic and the piezoelectric phonons and as well as the inelastic interaction of the non-equilibrium electrons with the neutral impurities through the processes of $1s \rightarrow 2p$ excitation and the ionization, on the net energy loss of the electrons have been assessed here under different prevalent conditions.

References

- [1] B.G. Streetman and S.K. Banerjee, *Solid State Electronic Devices*, Sixth Edition, Pearson Education, New Jersey, USA, 2006.
- [2] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Dover Publications Inc., New York, 1972.
- [3] B.R. Nag, *Theory of Electrical Transport in Semiconductors*, Pergamon Press, Oxford, 1972.
- [4] D.J. Griffiths, Instroduction to Quantum Mechanics, Prentice Hall, New Jersey, 07458
- [5] B.R. Nag, Theory of Electrical Transport in Semiconductors, Pergemon Press, Oxford,1972
- [6] E.M. Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967
- [7] C. Kittel, Elementary Statistical Physics, John Wiley & Sons, Inc., New York, 1958
- [8] S.M. Sze, Physics of Semiconductor Devices, Wiley Eastern Limited, New Delhi, 1983
- [9] T. Ando, A. B. Fowler and F. Stern, Rev. Mod. Phys. 54, 437 (1982).
- [10] B. R. Nag, Physics of Quantum Well devices, Kluwer Academic Publisher, Dordrecht, 2000
- [11] John H. Davies, The Physics of Low-Dimensional Semiconductors: An Introduction, Cambridge University Press, 1998
- [12] C.-Y. Wu and G. Thomas, Phys. Rev. B 9, 1724 (1974).
- [13] B.R.Nag, Electron Transport In Compound Semiconductors, Springer, Berlin, Heidelberg, New York, 1980
- [14] S. Gökden, A. Ilgaz, N. Balkan and S. Mazzucato, Physica E 25, 86 (2004).

- [15] D. Zanato, S. Gökden, N. Balkan, B. K. Ridley, W. J. Schaff, Semicond. Sci. Technol. 19, 427 (2004)
- [16] B. Tanatar and S-T. Chui, J. Phys.: Condens. Matter 6, L485 (1994).
- [17] H. M. Ng, D. Doppalapudi, T. D. Moustakas, N. G. Weimann and L. F. Eastman, Appl. Phys. Lett. 73, 821 (1998).
- [18] D. C. Look and J. R. Sizelove, Phys. Rev. Lett. 82, 1237 (1999).
- [19] D. Jena, A. C. Gossard and U. K. Mishra, Appl. Phys. Lett. 76, 1707 (2000).
- [20] S. Gökden, Physica E 23, 19 (2004).
- [21] J. Kundu, C. K. Sarkar and P. S. Mallick, Semicond. Phys. Quantum Electronics and Optoelectronics 10, 1 (2007).
- [22] L. Reggiani, Hot Electron Transport in Semiconductors, Springer-Verlag, Berlin, 1985.
- [23] P. K. Basu and B. R. Nag, Surf. Sci. 142, 256 (1984).
- [24] S. S. Paul, A. K. Ghorai and D. P. Bhattacharya, Phys. Rev. B 51, 5445 (1995).
- [25] A. K. Ghorai and D. P. Bhattacharya, J. Appl. Phys. 80, 3130 (1996).
- [26] S. S. Paul, A. K. Ghorai and D. P. Bhattacharya, Phys. Rev. B 48, 18268 (1993).
- [27] S. N. Patra and D. P. Bhattacharya, J. Phys. Chem. Solids 58, 829 (1997).
- [28] P. K. Basu and B. R. Nag, J. Phys. C: Solid State Phys. 14, 1519 (1981).
- [29] F. Comas, C. Trallero, H. Leon and J. Tutor, Physica B 152, 352 (1988).
- [30] D. N. Quang, V. N. Tuoc and T. D. Huan, Phys. Rev. B 68, 195316 (2003).
- [31] P. K. Basu and B. R. Nag, Phys. Rev. B 22, 4849 (1980).
- [32] C. Jacoboni and L. Reggiani, Rev. Mod. Phys. 55, 645 (1983).
- [33] H. L. Störmer, L. N. Pfeiffer, K. W. Baldwin and K. W. West, Phys. Rev. B 41, 1278 (1990).
- [34] P. K. Basu and K. Bhattacharya, J. Phys. C: Solid State Phys. 15, 5711 (1982).

[35] W. Knap, E. Borovitskaya, M. S. Shur, L. Hsu, W. Walukiewicz, E.Frayssinet, P. Lorenzini, N. Grandjean, C. Skierbiszewski, P. Prystawko, M. Leszczynski and I. Grzegory, Appl. Phys. Lett. 80, 1228 (2002).

[36] D. Chattopadhyay, Phys. Stat. Sol. (b) 135, 409 (1986).

Chapter 3

Analysis of the average energy loss rate in the non-degenerate sample of different III - V compound semiconductors at low lattice temperature

ANALYSIS OF THE AVERAGE ENERGY LOSS RATE OF NON EQUILIBRIUM ELECTRONS IN THE NON-DEGENERATE SAMPLE OF DIFFERENT III-V COMPOUND SEMICONDUCTORS AT LOW LATTICE TEMPERATURE

3.1 Introduction

It is well-known that in the presence of a relatively high electric field $(\vec{\epsilon})$, the electron ensemble in a semiconductor may be significantly perturbed from the state of thermodynamic equilibrium with the lattice atoms. Since the average energy of an electron then exceeds its thermal equilibrium value, the ensemble thus become 'hot', assuming a field dependent effective temperature $T_e(\epsilon)$ which exceeds the lattice temperature (T_L) . The high-field transport characteristics of any semiconductor structure exhibits some novel features, which are not observed at the low fields. The knowledge of the high-field features is rather important from the device point of view [1-7].

In compound semiconductors, the intrinsic acoustic vibrations of the lattice atoms produce an additional electric field that gives rise to piezoelectric scattering potential along with the deformation potential. The piezoelectric scattering is known to be quiet important in many semiconductors under the condition of relatively lower lattice temperature. Eventually, the electrical transport at low lattice temperatures is principally controlled by the combined interactions of the electrons with the piezoelectric and acoustic phonons. On the other hand, at low lattice temperatures, say when $T_L \leq 20K$, a seeming low electric field, as low as a fraction of a volt/cm or so, may turn out to be effectively high, and the high-field features of the electrical transport characteristics may be exhibited [1, 4, 6]. At such low temperatures, the ionisation of the neutral impurities is quite incomplete, and thus the concentration of the neutral impurities is rather large. Moreover, the average thermal energy of the electrons is quite small. Hence, in the presence of an effective high electric field, the amount of loss of energy of the electrons due to ionisation (ion.) and $1s \rightarrow 2p$ excitation (ex.) of the neutral

impurities is now relatively quite large. This renders the collision with the neutral impurities inelastic, at the low lattice temperatures. It is well-known that this inelastic interaction of the hot electrons now becomes the main mechanism of the dissipation of their energy [3, 4, 6].

Traditionally, the theory of high field transport is developed through solving the Boltzmann Transport equation. An analytical solution of the transport equation is beset with much mathematical difficulties, as has already been said, unless one makes simplifying approximation, which more often than not compromises with the physical validity of the results.

If the carrier concentration is large, so that the energy exchange between the carriers is much faster than that between the carriers and the lattice, the carriers share their energy ϵ mainly amongst themselves and the energy distribution for a non-degenerate ensemble of carriers may be approximated by the heated Maxwellian distribution at a field dependent carrier temperature T_e [1,2,7]. The field dependence of T_e may be obtained from the solution of the energy balance equation of the electron phonon system. Such dependence has already been obtained solely for the individual interactions, like acoustic, piezoelectric etc. [5]. To calculate the field dependence of the effective electron temperature for some combined interactions of the electrons, the energy balance equation needs to be solved afresh taking into account all the individual scatterings simultaneously.

The non-ohmic mobility characteristics $\mu(\vec{\epsilon})$ in the presence of relatively high fields may now be obtained from [1]

$$e\mu(\varepsilon)\varepsilon^2 = \sum \left(\frac{dE_{\vec{k}}}{dt}\right) \tag{i}$$

where e is the electronic charge, $\vec{\epsilon}$ is the applied electric field, and $\langle \frac{dE}{dt} \rangle$, the average energy loss rate for the same combination of interactions, that needs to be calculated taking all the individual scattering into account simultaneously.

The field dependence of the effective electron temperature may be obtained from the solution of the energy balance equation of the electron-phonon system [5, 7]. The solution however, is determined by the prevalent conditions in respect of (i) the lattice temperature, (ii) the dominant interactions of the electrons with the lattice imperfections, and (iii) the concentration of the carriers etc. By solving the energy balance equation for the electron-phonon system the field dependence of T_e for a bulk semiconductor material has been theoretically obtained in [5], separately, for different interactions, under the condition, when the lattice temperature is high. Apart from that some studies have been made about the effective electron temperature characteristics, particularly the relationship of T_e with T_L considering specific devices at and around the room temperatures [8].

In the present communication, we have considered a compensated, non-degenerate semiconductor compound in the presence of a relatively high electric field, at a low lattice temperature. The effects of the inelastic interaction of the non-equilibrium electrons with the neutral impurities, through the processes of $1s \rightarrow 2p$ excitation and the ionization, on the net energy loss of an electron have been assessed here. The intrinsic quasi-elastic interactions of the electrons, with both the acoustic phonons, the piezoelectric and the deformation potential, have also been taken into account. Then the resulting field dependence of the effective temperature of the non-equilibrium electrons has been obtained. The numerical results that follow from our analysis for the compounds like InSb, InAs and GaSb have been compared with the available experimental and other theoretical results. The results exhibit here that the inelastic interaction of the non-equilibrium electrons with the neutral impurities, brings in significant changes in the field dependence of the effective temperature of the non-equilibrium electrons, under the condition, when the lattice temperature is low.

3.2 Development

3.2.2. Energy loss rate for the combined interaction with the piezoelectric and deformation acoustic phonons.

The field dependence of the effective electron temperature being known, one can now calculate the non-ohmic mobility characteristics using (i), when the average energy loss rate of the non-equilibrium ensemble of electrons for the same combination of interactions is known.

Again starting from the perturbation theory, one may first calculate the energy loss rate of a carrier of energy E by summing over all the possible emission and absorption processes that such a carrier may undergo in making transition to and from the states $|\vec{k}+\vec{q}\rangle$ and $|\vec{k}-\vec{q}\rangle$. Then the loss rate needs to be averaged over the distribution of carrier energies. Proceeding in this way the expression for the average loss rate for the interaction with deformation acoustic phonons has already been available [1]. It takes the form

$$\label{eq:delta_ac} \langle \frac{\text{dE}}{\text{dt}} \rangle_{ac} = \frac{8\sqrt{2}}{\pi^{3/2}} \frac{{E_1}^2 \text{m}^{*5/2}}{\hbar^4 \rho} (k_B T_e)^{3/2} \left(\frac{T_L}{T_e} - 1\right) \tag{ii)}$$

Proceeding in the same manner one can get the following expression for the average loss rate for interaction with the piezoelectric phonons

$$\label{eq:pz} \left<\frac{{\rm d}E}{{\rm d}t}\right>_{\rm pz} = \frac{{\rm e}^2 K_{\rm m}^2}{2\pi^3 (2\pi)^{3/2}} \frac{{\rm u_l}^2 m^{*3/2}}{\varepsilon_{SC} \hbar^2} (k_B T_e)^{1/2} \left(\frac{T_L}{T_e} - 1\right) \tag{iii}$$

Finally, the average energy loss rate may be obtained by adding (3.8) and (3.9). Thus,

$$\langle \frac{dE}{dt} \rangle_{Combintion} = \langle \frac{dE}{dt} \rangle_{ac} + \langle \frac{dE}{dt} \rangle_{pz}$$
 (iv)

Using (iv) a relationship between $\langle \frac{dE}{dt} \rangle_{Combintion}$ and T_e can be plotted. Figure 3.1 describes the dependence of energy loss rate of the electrons upon their effective temperature in samples of InSb, InAs and GaSb, and the data is further used to determine the non-ohmic mobility for the three samples respectively.

3.2.3. Energy loss rate for the combined interaction with the piezoelectric and deformation acoustic phonons as well as with the 1s to 2p excitation and ionisaton of the neutral impurities.

We consider a non-degenerate ensemble of free electrons in an extrinsic n-type compound semiconductor which is doped with both donor and acceptor impurities at a low lattice temperature, so that the impurities are not completely ionized. Let N_D and N_A are respectively the donor and acceptor concentrations. So the total impurity concentration is $N_D + N_A$. The shallow impurity levels are very close to the band edges. At $T_L \approx 0K$, there is neither any ionization of the impurities, nor there can be any band to band transition. Thus, no free carriers are generated, and the semiconductor behaves like an insulator. However, as the lattice temperature increases from 0K, more and more ionization of the neutral impurities takes place. Thus, even though there is hardly any band to band transition, the concentration of the carriers, as well as that of the ionization impurities begins to increase from a small value, at low lattice temperatures, and the semiconductor starts conducting. The concentration of the net impurity level is given by $N = N_D - N_A$ and the compensation ratio $c = N_A/N_D$ [6]. The electric field dependence of the effective electron temperature may be obtained from the energy balance equation which may be represented by [1]

$$e\mu(\varepsilon)\varepsilon^2 = \sum \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle,$$
 (1)

where
$$\sum \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle = \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ac.} + \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{pz.} + \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ex} + \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ion}. \tag{2}$$

Here, e is the electronic charge, $\mu(\varepsilon)$ is the effective high-field mobility and it is represented by

$$\mu^{-1}(\varepsilon) = \mu_{ac}^{-1} + \mu_{pz}^{-1} + \mu_{l}^{-1} + \mu_{N}^{-1},\tag{3}$$

where μ_{ac} , μ_{pz} , μ_{I} and μ_{N} are the non-ohmic mobilities due to interaction of the electrons with the deformation potential acoustic (ac.) phonons, piezoelectric (pz.) phonons, ionized impurities (I) and the neutral (N) impurities respectively. $\left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{n}$ are the average rate of energy loss of an electron to the lattice due to nth type of such interactions.

As has already been said, the high-field distribution function f_0 of the non-degenerate ensemble of electrons may be approximated by

$$f_0 = N_0 \exp\left(\frac{-E_{\vec{k}}}{K_B T_e}\right) \tag{4}$$

 K_B being the Boltzmann constant, and the normalization constant N_0 is given by [1,5,7]

$$N_0 = \frac{n\hbar^3}{\left(2\pi m^* K_B T_e\right)^{\frac{3}{2}}}$$
, $\hbar = \frac{\hbar}{2\pi}$, h is the Planck's constant, m^* is the effective mass, n is the

concentration of the electrons.

The high field mobility can now be obtained by calculating the current density J from [5]

$$J = -\frac{e^2 \varepsilon}{m^*} \int \frac{h^2 k^2}{m^*} \cos^2 \theta \, \tau \left(E_{\vec{k}} \right) \frac{\partial f_0}{\partial E_{\vec{k}}} d\vec{k} \tag{5}$$

where, for a parabolic law of dispersion, the energy of an electron $E=\hbar^2k^2/2m^*$, $\tau\left(E_{\vec{k}}\right)$ is the relaxation time, θ is the angle between $\vec{\varepsilon}$ and $\vec{k}\cdot\vec{\varepsilon}$

Thus one can obtain,

$$\mu_{ac} = \mu_{ac}^{0} \left(\frac{T_{L}}{T_{e}}\right)^{\frac{1}{2}}; \ \mu_{pz} = \mu_{pz}^{0} \left(\frac{T_{e}}{T_{L}}\right)^{\frac{1}{2}}; \ \mu_{I} = \mu_{I}^{0} \left(\frac{T_{e}}{T_{L}}\right)^{\frac{3}{2}}, \mu_{N} = \mu_{N}^{0}$$
 (6)

 μ_{ac}^{0} , μ_{pz}^{0} , μ_{I}^{0} and μ_{N}^{0} are the low field mobilities, for the respective interactions, of the electrons with the acoustic phonons, piezoelectric phonons, ionized impurities and neutral impurities. They are given by [5]

$$\mu_{ac}^{0} = \frac{2(2\pi)^{\frac{1}{2}} e \hbar^{4} s^{2} \rho_{v}}{3E_{1}^{2} m^{*\frac{5}{2}} (K_{B} T_{L})^{\frac{3}{2}}}; \qquad \mu_{pz}^{0} = \frac{16(2\pi)^{\frac{1}{2}} \hbar^{2} \varepsilon_{sc}}{3k_{m}^{2} e m^{*\frac{3}{2}} (K_{B} T_{L})^{\frac{1}{2}}}; \qquad \mu_{I}^{0} = \frac{128(2\pi)^{\frac{1}{2}} \varepsilon_{sc}^{2} (K_{B} T_{L})^{\frac{3}{2}}}{N_{i} e^{3} m^{*\frac{1}{2}} ln \left[1 + \left(\frac{12\pi \varepsilon_{sc} K_{B} T_{L}}{e^{2} N_{i}^{\frac{1}{3}}}\right)^{2}\right]}; \qquad \text{and}$$

 $\mu_N^0 = \frac{e}{20\hbar N a_0}$; where E_1 is the deformation potential constant, s is the average acoustic velocity, ε_{sc} is the static dielectric constant, k_m is the piezoelectric coupling constant, N_i is the concentration of the ionized impurity atoms, each of charge -Ze and a_0 is the Bohr radius.

The average rate of energy losses may be obtained by the standard methods [1, 6, 9]. The expression for $\left(\frac{dE_{\vec{k}}}{dt}\right)_{ac}$ has already been worked out in [1] and is given by,

$$\left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ac} = 32es^2 \frac{\left(\left[\frac{T_e}{T_L} \right]^{\frac{3}{2}} - \left[\frac{T_e}{T_L} \right]^{\frac{1}{2}} \right)}{3\pi\mu_{ac}^0}.$$
 (7)

Following the same framework as that used in obtaining (7) we calculate here the energy loss rate for the interaction with the piezoelectric electric phonons, and obtain

$$\left\langle \frac{dE_{k}^{-}}{dt} \right\rangle_{pz} = \frac{0.254e^{2}k_{m}^{2}m^{*\frac{3}{2}}s^{2}(K_{B}T_{e})^{\frac{1}{2}}\left(1 - \frac{T_{L}}{T_{e}}\right)^{2}}{\hbar^{2}\varepsilon_{sc}} \tag{8}$$

The energy loss rate for ionization and excitation of the neutral impurities may be expressed as [6].

$$\left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ion} = A_I N E_{ion}, \tag{9}$$

$$\left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ex} = A_I N E_{ex.},\tag{10}$$

where, A_I is the excitation or the ionization coefficient, E_{ex} is the excitation energy, E_{ion} is the ionization energy. $A_I(T_e)$ may be calculated by the standard method [9] once the impact cross-section σ_I is known. There being no standard theory for σ_I available in the literature, here we make use of the widely adopted simplest assumption that the cross-section for the

impact of the energetic electrons with the neutral impurities σ_l is constant, independent of energy $E_{\vec{k}}$. Since the cross-section hardly corresponds to any physical quantity in the semiconductor, its choices by many others seem to be somewhat arbitrary and usually the value is adjusted to the experimental data, thus introducing an adjustable parameter for the analysis [10]. Hence the coefficient $A_l(T_e)$ comes out to be

$$A_I(T_e) = \sigma_I \sqrt{\frac{2K_B T_e}{m^*}} \frac{\Gamma(\alpha, x)}{\Gamma(\frac{3}{2})},\tag{11}$$

where $\Gamma(\alpha, x)$ is an incomplete gamma function [11]. Here $\alpha = 2$ and x stands for the ionization and excitation energies, which are normalized to K_BT_e .

Thus, one can calculate from (2) the average of the total rate of the energy loss of an electron by adding together the individual rates for different interactions as a function of the average energy $\langle E_{\vec{k}} \rangle = \frac{3K_BT_e}{2}$. Subsequently from (1), (3) and (6) the field dependence of the effective temperature of an electron can be known.

3.3 Results and Discussions

As an application of the above theory numerical results have now been obtained for some well-known compounds like InSb, InAs and GaSb, which are useful for the fabrication of devices. Another reason for the choice of these compounds is that, some experimental data for the effective electron temperature characteristics of these materials being available in the literature, a comparison of our theoretical results with the experimental data could be made.

The values of the material parameters for the compounds are given in Table 1. The concentration of the ionised impurities N_I in the compensated materials may be obtained from [6] $N_I = \left(\frac{2c}{1-c}\right)N$. The numerical calculations have been carried out for a constant value of the compensation ratio $c = \frac{N_A}{N_D} = 0.5$. The results which follow from the present analysis

for the three compounds, InSb, InAs and GaSb are presented in Figs. 3.1, 3.2 and 3.3 respectively. The experimental results which are available in the literature are also shown in the Figs.

As has already been said the values of the impact cross-section σ_I , which has been assumed to be a constant, independent of energy, are hardly available in the literature, except for Ge. Since it is taken to be an adjustable parameter [10], its value is so adjusted that the theoretical data obtained from the present theory, should be physically realistic and are also consistent with the experimental data. It may also be mentioned here that the effective electron temperature characteristics is not much sensitive to the changes in the chosen value of σ_I . It is seen that hardly any changes in the characteristics are affected due to the variation of the value of σ_I by an order or so. One may take note of the suitable choice for the value of σ_I from the figures for each material.

Table 1: Material parameters

Physical Parameters	InSb	InAs	GaSb
Deformation potential, E_1 (eV)	20.0	8.0	12.0
Acoustic velocity, $u_l \left(\times 10^3 \text{ m.s}^{-1} \right)$	3.7	3.83	5.06
Density, ρ_{ν} (×10 ³ kg.m ⁻³)	5.78	5.66	5.66
Static dielectric constant, ε_{sc}	17.51	14.60	15.70
Piezoelectric coupling constant, k_m	0.027	0.029	0.026
Effective mass ratio, (m^*/m_0)	0.014	0.023	0.042
Ionization energy (meV)	0.62	1.47	2.3
Excitation energy (meV)	0.47	1.10	1.74

 m_0 being the free electron mass

Before assessing the effects of the inelastic interaction of non-equilibrium electrons with the neutral impurities, let us first note the effects of intrinsic interaction with the acoustic phonons.

Comparing the curves 2 and 3 for each material it is seen that the interaction with the piezoelectric interaction makes significant contribution to the energy loss process. The loss due to the collisions with the piezoelectric phonons turns out to be comparable with the same due to collisions with the deformation acoustic phonons. Hence the effects of the interaction with the piezoelectric phonons could not be neglected in developing the present theory under the condition of low lattice temperatures.

It may be noted that the inelasticity of the collisions of electrons with the neutral impurity atoms, makes the highest contribution to the loss of energy of an electron, to the lattice atoms at any energy. However, the qualitative nature of the dependence of the average loss rate of energy of an electron on the average energy, remains more or less the same for all the three processes of energy loss, always increasing monotonically. When the effects of all the three processes are taken together, one can see from the curves 1, that the monotonic increase in the energy loss rate with the average energy $\langle E_{\vec{k}} \rangle$ tends to be significantly faster.

It thus turns out, that the loss of energy of a non-equilibrium electron due to the processes of excitation and ionisation of the neutral impurities plays quite a significant role in determining the non-ohmic characteristics of a compensated and non-degenerate semiconductor compound under the condition when lattice temperature is low. Moreover, the interaction of the electrons with the piezoelectric phonons, unlike that with the deformation potential acoustic phonons, effects the non-ohmic characteristics more and more as the lattice temperature is lowered.

We have considered here only a few well-known features of the low lattice temperature. Taking account of all of them at a time in any theoretical analysis is hardly

possible. However, the interesting results which have been obtained here, stimulate further studies in the same field. As such, there is ample scope for the refinement of the present analysis.

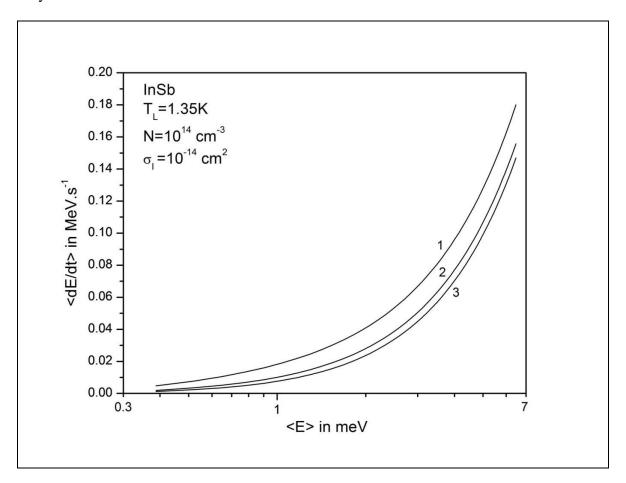


Fig.3.1 Dependence of the average energy loss rate of an electron, in a non-degenerate ensemble of electrons in InSb, upon the average electron energy $\langle E_{\vec{k}} \rangle$ at a lattice temperature T_L of 1.35K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{14}cm^{-3}$ and $10^{-14}cm^2$. The curve 1 is obtained considering all the processes of energy loss of an electron (interaction with the acoustic and the piezoelectric phonons as well as the $1s \to 2p$ excitation and ionization of the neutral impurities). The curve 2 is obtained for the combined interaction with the acoustic and the piezoelectric phonons and the curve 3 is obtained for interaction only with the acoustic phonons.

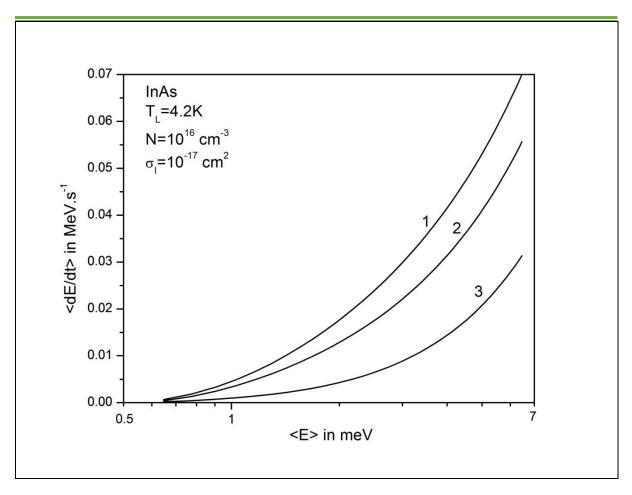


Fig.3.2 Dependence of the average energy loss rate of an electron in a non-degenerate ensemble of electrons in InAs upon the average energy $\langle E_{\vec{k}} \rangle$ at a lattice temperature of 4.2K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{16} cm^{-3}$ and $10^{-17} cm^2$ respectively. The curve 1 is obtained considering all the processes of energy loss of an electron (interaction with the acoustic and the piezoelectric phonons, as well as the $1s \to 2p$ excitation and ionization of the neutral impurities). The curve 2 is obtained for the combined interaction with the acoustic and the piezoelectric phonons, and the curve 3 is obtained for interaction only with acoustic phonons.

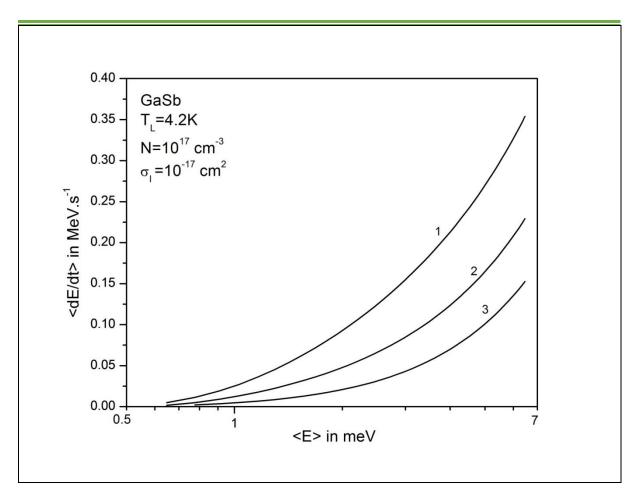


Fig.3.3 Dependence of the average energy loss rate of an electron in a non-degenerate ensemble of electrons in GaSb upon the average energy $\langle E_{\bar{k}} \rangle$ at a lattice temperature of 4.2K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{17} \, cm^{-3}$ and $10^{-17} \, cm^2$ respectively. The curve 1 is obtained considering all the processes of energy loss of an electron (interaction with the acoustic and the piezoelectric phonons, as well as the $1s \to 2p$ excitation and ionization of the neutral impurities). The curve 2 is obtained for the combined interaction with the acoustic and the piezoelectric phonons and the curve 3 is obtained for interaction only with acoustic phonons.

3.4. Conclusion

For a non-degenerate ensemble of electrons in a compensated semiconductor compound at a low lattice temperature, an analysis is made here to study the effects of the interactions of the non-equilibrium electrons with the neutral impurities on the non-ohmic characteristics of the ensemble.

Since the piezoelectric interaction is important at relatively low temperatures, and at such low temperature regime the electron ensemble in compounds like InSb or InAs which possess a low value of the effective mass, gets heated up even for a field of a fraction of a volt/cm. So, such a low field appears to be effectively high enough to perturb the electron ensemble significantly from the state of thermodynamic equilibrium with the lattice atoms. It may be seen from the figures that, when the piezoelectric interaction is considered in combination with that due the deformation acoustic phonons, significant qualitative as well as quantitative changes in the non-ohmic transport characteristics are effected over the low ranges of the electric field and the lattice temperature.

In particular, the effects of the inelastic collisions with the neutral impurity atoms due to their ionisation and $1s \rightarrow 2p$ excitation have been studied. The intrinsic interactions with the acoustic phonons, both piezoelectric and deformation potential have also been taken into account. The theory is developed for the dependence of the average rate of energy loss of an electron to the lattice, on the average energy of the electrons, and subsequently, the dependence of the effective temperature of the electrons on the electric field.

One can now conclude again from the above studies that the inelasticity of the collisions of the non-equilibrium electrons with the neutral atoms, makes the highest contribution in the process of the loss of energy of an electron of the non-equilibrium ensemble, to the lattice. This inelasticity makes the rate of loss of energy with the average energy $\langle E_{\vec{k}} \rangle$, significantly faster.

References

- [1] E.M. Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967.
- [2] B.R. Nag, Electron Transport in Compound Semiconductor, Springer, Berlin, 1980.
- [3] Z.S. Kachlishvili, Galvanomagnetic and Recombination Effects in Semiconductors in a Strong Electric Field, Phys. Stat. Sol (a) 33 (1976) 15-51.
- [4] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, A. Alberigi-Quaranta, Electron drift velocity in silicon, Phys. Rev. B 12 (1975) 2265-2284.
- [5] B.R. Nag, Theory of Electrical Transport in Semiconductors, Pergamon Press, Oxford, 1972.
- [6] Z.S. Kachlishvili, Inelastic Impurity Scattering of Hot Electrons in Semiconductors. Phys. Stat. Sol (b) 48 (1971) 65-75.
- [7] G. Bauer, Springer Tracts in Modern Physics, Vol. 74, Springer, New York, 1974.
- [8] L.F. Mao, H. Ning, C. Hu, G. Wang, Physical Modeling of Activation Energy in Organic Semiconductor Devices based on Energy and Momentum Conservations, Sci. Rep. 6 (2016) 24777.https://doi.org/10.1038/srep24777.
- [9] V.L. Bonch-Bruevich, E.G. Landsberg, Recombination Mechanisms, Phys. Stat. Sol. 29 (1) (1968) 9-43.
- [10] A. Zylbersztejn, Theory of Low-Temperature Impact Ionization in High-Purity Germanium, Phys. Rev. 127(3) (1962) 744-749.
- [11] I.S. Gradshteyn, I.M. Ryzhik, Tables of Integrals, Series, and Products, seventh ed., Academic Press, New York, 1965.

Chapter 4

Dependence of the effective electron temperature upon the electric field of the non-equilibrium electrons in a nondegenerate semiconductor at low lattice temperature DEPENDENCE OF THE EFFECTIVE ELECTRON TEMPERATURE UPON THE ELECTRIC FIELD OF THE NON-EQUILIBRIUM ELECTRONS IN A NON DEGENERATE SEMICONDUCTOR AT LOW LATTICE TEMPERATURE

4.1. Effective electron temperature of the non-equilibrium electrons for the combined interaction with the acoustic and the piezoelectric phonons

4.1.1. Introduction

To make a theoretical analysis of the transport characteristics of a material in the presence of a relatively high field at any lattice temperature, low or high, one needs to solve the Boltzmann Transport equation taking into account the various interactions of the electrons with the lattice defects. In the presence of a relatively high field, the free carriers in a semiconductor may be significantly perturbed from the state of thermodynamic equilibrium with the host lattice atoms. The critical field at which the electrons may be drifted to such a significantly perturbed state in any material increases with the increase of the lattice temperature and with the decrease of the values of the initial mobility. For example, in n-Ge, when the lattice temperature is low, say around 5K, the electrons may be so perturbed for a field of only a few Vcm⁻¹, and in InSb, when the lattice temperature is around 2K, similar perturbation may be observed for a fraction of a Vcm⁻¹. On the other hand, if the lattice temperature is raised to around room temperature, significant perturbation of the carriers requires fields of several kVcm⁻¹ in Ge and some hundred Vcm⁻¹ in InSb. Such a perturbed ensemble is known to exhibit a number of novel phenomena which are technologically important from the device point of view [1-6].

The field dependence of the effective temperature of the electrons may be calculated from the solution of the energy balance equation. The solution however, depends upon the dominant type of interaction under the prevailing condition and the band structure of the material. The interaction with the optical and intervalley phonons may be dominant for lattice temperatures above some hundred degrees. On the other hand, the interaction with the

intravalley acoustic phonons is intrinsic and may dominate along with the impurity scattering at the lower temperatures. However, the collision with impurities being elastic, the intravalley acoustic phonon scattering will dominate in determining the field dependence of the effective electron temperature in the lower temperature regime. Such field dependence has already been worked out for a non-degenerate material [1, 2, 6].

However, the III-V compounds, which lack inversion symmetry, are piezoelectric in nature. Such materials, like InSb, InAs, GaSb etc are now widely used to fabricate infrared detectors, galvanomagnetic devices, light emitting diodes respectively. The collision (coll) of the electrons with the piezoelectric phonons also makes significant contribution in controlling the electron transport in these materials at relatively lower temperatures. The interaction with high energy phonons like polar optical or intervalley phonons, do not come into consideration at low lattice temperatures of interest here [2, 7, 8]. The importance of piezoelectric interaction in controlling the ohmic transport has already been studied [9,10]. The purpose of the present communication is to carry out an analysis of the field dependence of T_e in some degenerate III-V compounds, as controlled by the combined interaction with the acoustic and piezoelectric phonons, at low lattice temperatures. The analysis has been made in the same framework as that in [7]. The numerical results obtained for InSb, InAs and GaSb are compared with other theoretical and available experimental data [7,8,11]. The results reveal the importance of the piezoelectric interaction in controlling the characteristics of the effective electron temperature in non degenerate materials, under the conditions of the low lattice temperature. Moreover it is also seen, how important is the piezoelectric interaction, in deciding the field dependence of the effective temperature of the electrons.

4.1.2. Development

The electric field dependence of the electron temperature $T_e(\varepsilon)$ for the material, under the prevailing conditions can be determined from a solution of the equation that

describes the condition of conservation of the energy of the electron-phonon system. The rate of gain of energy of the electron from the field, balances the rate of loss of energy of the energy of the electrons through collision with the lattice imperfections. The equation is symbolically written as [2]

$$\int \frac{\partial f\left(\vec{k}\right)}{\partial t} \left| Ed\vec{k} = \sum_{j} \int \frac{\partial f\left(\vec{k}\right)}{\partial t} \right|_{i} Ed\vec{k}$$

For the mixed interaction under consideration here, we can write [1, 2]

$$\left. \sum_{j} \frac{\partial f(\vec{k})}{\partial t} \right|_{j^{th}_{coll}} = \frac{\partial f}{\partial t} \Big|_{ac} + \frac{\partial f}{\partial t} \Big|_{pz}$$

where $f(\vec{k})$ is the high field distribution function of the electron in the sample of a degenerate III-V compound semiconductor under the condition of low lattice temperature, when the electron simultaneously interact with the intravalley acoustic (ac) and piezoelectric (pz) phonons, \vec{k} is the electron wave vector, $\frac{\partial f(\vec{k})}{\partial t}\Big|_{j^{\text{th}}\text{coll}}$ is the rate of change of the distribution function due to the j^{th} interaction mechanism, E, the carrier energy, is assumed to be $E_{\vec{k}} = \frac{\hbar^2 k^2}{2m^*}$ and m^* is the isotropic effective mass of the electrons. The distribution function, in the diffusion approximation may be written as (4.2).

In order to calculate $\frac{\partial f(\vec{k})}{\partial t}\Big|_{coll}$, for either of the interactions, acoustic or piezoelectric, we consider the four process of absorption and emission of a phonon of wave vector \vec{q} , corresponding to the scattering of the electrons into and out of the state $|\vec{k}\rangle$, which results in transition to and from the states $|\vec{k}+\vec{q}\rangle$ and $|\vec{k}-\vec{q}\rangle$. Using the perturbation theory one can write [1].

$$\frac{\partial f\left(\vec{k}\right)}{\partial t} \bigg|_{coll} = \frac{2\pi}{\hbar} \sum_{\vec{q}} \left[\left| \left\langle \vec{k}, N_{\vec{q}} \pm 1 \middle| H \middle| \vec{k} \pm \vec{q}, N_{\vec{q}} \right\rangle \right|^{2} \delta\left(E_{\vec{k}} - E_{\vec{k} \pm \vec{q}} \pm \hbar \omega_{\vec{q}}\right) f\left(\vec{k} \pm \vec{q}\right) \left[1 - f\left(\vec{k}\right)\right] - \left| \left\langle \vec{k} \pm \vec{q}, N_{\vec{q}} \pm 1 \middle| H \middle| \vec{k}, N_{\vec{q}} \right\rangle \right|^{2} \delta\left(E_{\vec{k} \pm \vec{q}} - E_{\vec{k}} \pm \hbar \omega_{\vec{q}}\right) f\left(\vec{k}\right) \left[1 - f\left(\vec{k} \pm \vec{q}\right)\right] \right]$$

As has already been said, $N_{\vec{q}}$ is the equilibrium distribution function of the phonons, $\omega_{\vec{q}}$ is the angular frequency of the phonon. The upper or the lower sign in the first term should be taken for the processes of emission and absorption respectively. But the same sign in the second term corresponds to the reverse process [1,2,13-17].

When the band edge shifts are linearly dependent upon the strain, one can neglect the spin exchange scattering [18]. Hence the matrix elements for the above transitions in the degenerate material remain the same as that of the non-degenerate materials.

Thus one can use [1, 2] for the acoustic interaction

$$\left| \left\langle \vec{k}, N_{\vec{q}} \pm 1 \middle| H' \middle| \vec{k} \pm \vec{q}, N_{\vec{q}} \right\rangle \right|^{2}_{ac} = \frac{E_{1}{}^{2}\hbar q}{2\rho u_{l} V} \begin{bmatrix} N_{\vec{q}} \\ N_{\vec{q}} + 1 \end{bmatrix}$$

And for the piezoelectric interaction

$$\left| \left\langle \vec{k}, N_{\vec{q}} \pm 1 \middle| H' \middle| \vec{k} \pm \vec{q}, N_{\vec{q}} \right\rangle \right|^{2}_{pz} = \frac{e^{2} \hbar q u_{l} k_{m}^{2}}{4V k^{2} \epsilon_{sc}} \begin{bmatrix} N_{\vec{q}} \\ N_{\vec{q}} + 1 \end{bmatrix}$$

where E_1 is the deformation potential constant, ρ is the density of the material. u_1 is the average acoustic velocity, V is the volume of material, e is the electronic charge, k_m is the piezoelectric coupling constant, ϵ_{sc} is the is the static dielectric constant.

Proceeding in this way the expression for the average loss rate for the interaction with deformation acoustic phonons takes the form

$$\left\langle \frac{dE}{dt} \right\rangle_{ac} = \frac{8\sqrt{2}}{\pi^{3/2}} \frac{E_1^2 m^{*5/2}}{\hbar^4 \rho} (k_B T_e)^{3/2} \left(\frac{T_L}{T_e} - 1 \right)$$
 (i)

Proceeding in the same manner one can get the following expression for the average loss rate for interaction with the piezoelectric phonons

$$\left\langle \frac{dE}{dt} \right\rangle_{pz} = \frac{e^2 K_m^2}{2\pi^3 (2\pi)^{3/2}} \frac{u_l^2 m^{*3/2}}{\epsilon_{SC} \hbar^2} (k_B T_e)^{1/2} \left(\frac{T_L}{T_e} - 1 \right)$$
 (ii)

Finally, the average energy loss rate may be obtained by adding (i) and (ii). Thus,

$$\left\langle \frac{dE}{dt} \right\rangle_{Combintion} = \left\langle \frac{dE}{dt} \right\rangle_{ac} + \left\langle \frac{dE}{dt} \right\rangle_{pz}$$
 (iii)

4.2. Effective electron temperature of the non-equilibrium electrons for the combined interaction with the acoustic and the piezoelectric phonons as well as with the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities.

4.2.1. Introduction

It is well known that in the presence of a high electric field (ε) , the electron ensemble in a semiconductor may be significantly perturbed from the state of thermodynamic equilibrium with the lattice atoms. The average energy of an electron then exceeds its thermal equilibrium value. Such an ensemble is sometimes picturized as one with a field dependent effective temperature $T_e(\varepsilon)$ that also exceeds the lattice temperature T_L . Under these conditions the material exhibits some unexpected, novel properties which are technically of much importance from the device point of view. However, the electric field at which the high field effects are exhibited in a particular material depends upon the lattice temperature. For low lattice temperatures $(T_L \le 20K)$ even a field of a fraction of volt/cm may seem to be effectively high [19, 20]. The low lattice temperature has a number of specific features, which are hardly consistent with higher lattice temperatures. In developing the theory of electron transport for the higher temperatures such low temperature features are usually ignored even when they occur in order to make the theoretical analysis easily tractable [21].

At low lattice temperatures, say when $T_L \leq 20K$, a seeming low electric field, as low as a fraction of a volt/cm or so, may turn out to be effectively high, and the high-field features

of the electrical transport characteristics may be exhibited [19, 22, 24]. At such low temperatures, the ionisation of the neutral impurities is quite incomplete, and thus the concentration of the neutral impurities is rather large. Moreover, the average thermal energy of the electrons is quite small. Hence, in the presence of an effective high electric field, the amount of loss of energy of the electrons due to ionisation (ion.) and $1s \rightarrow 2p$ excitation (ex.) of the neutral impurities is now relatively quite large. This renders the collision with the neutral impurities inelastic, at the low lattice temperatures. It is well-known that this inelastic interaction of the hot electrons now becomes the main mechanism of the dissipation of their energy [21, 22, 24].

The theory of high-field transport for a non-degenerate ensemble of electrons may be developed in the effective electron temperature approximation, assuming a "heated" Maxwellian energy distribution for the non-equilibrium electrons, at a field dependent effective electron temperature $T_e(\varepsilon)$ of the carriers [19, 23,27]. Such an approximate analysis is quite worthy, as because, it often provides data, which are useful for the device technologists.

The field dependence of the effective electron temperature may be obtained from the solution of the energy balance equation of the electron-phonon system [23,27]. The solution however, is determined by the prevalent conditions in respect of (i) the lattice temperature, (ii) the dominant interactions of the electrons with the lattice imperfections, and (iii) the concentration of the carriers etc. By solving the energy balance equation for the electron-phonon system the field dependence of T_e for a bulk semiconductor material has been theoretically obtained in [23], separately, for different interactions, under the condition, when the lattice temperature is high. Apart from that some studies have been made about the effective electron temperature characteristics, particularly the relationship of T_e with T_L considering specific devices at and around the room temperatures [26].

In the present communication, we have considered a compensated, non-degenerate semiconductor compound in the presence of a relatively high electric field, at a low lattice temperature. The effects of the inelastic interaction of the non-equilibrium electrons with the neutral impurities, through the processes of $1s \rightarrow 2p$ excitation and the ionization, on the net energy loss of an electron have been assessed here. The intrinsic quasi-elastic interactions of the electrons, with both the acoustic phonons, the piezoelectric and the deformation potential, have also been taken into account. Then the resulting field dependence of the effective temperature of the non-equilibrium electrons has been obtained. The numerical results that follow from our analysis for the compounds like InSb, InAs and GaSb have been compared with the available experimental and other theoretical results. The results exhibit here that the inelastic interaction of the non-equilibrium electrons with the neutral impurities, brings in significant changes in the field dependence of the effective temperature of the non-equilibrium electrons, under the condition, when the lattice temperature is low.

4.2.2 Development

The electric field dependence of the effective electron temperature may be obtained from the energy balance equation which may be represented by [19]

$$e\mu(\varepsilon)\varepsilon^2 = \sum \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle,$$
 (1)

$$\sum \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle = \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ac.} + \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{pz.} + \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ex} + \left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_{ion}. \tag{2}$$

Here, e is the electronic charge, $\mu(\varepsilon)$ is the effective high-field mobility and it is represented by

$$\mu^{-1}(\varepsilon) = \mu_{ac}^{-1} + \mu_{pz}^{-1} + \mu_{l}^{-1} + \mu_{N}^{-1}, \tag{3}$$

where μ_{ac} , μ_{pz} , μ_{I} and μ_{N} are the non-ohmic mobilities due to interaction of the electrons with the deformation potential acoustic (ac.) phonons, piezoelectric (pz.) phonons, ionized

impurities (I) and the neutral (N) impurities respectively. $\left\langle \frac{dE_{\vec{k}}}{dt} \right\rangle_n$ are the average rate of energy loss of an electron to the lattice due to nth type of such interactions.

As has already been said, the high-field distribution function f_0 of the non-degenerate ensemble of electrons may be approximated by

$$f_0 = N_0 \exp\left(\frac{-E_{\vec{k}}}{K_B T_e}\right) \tag{4}$$

 $K_{\scriptscriptstyle B}$ being the Boltzmann constant, and the normalization constant $N_{\scriptscriptstyle 0}$ is given by [1,5,7]

$$N_0 = \frac{n\hbar^3}{\left(2\pi m^* K_B T_e\right)^{\frac{3}{2}}}$$
, $\hbar = \frac{h}{2\pi}$, h is the Planck's constant, m^* is the effective mass, n is the

concentration of the electrons.

The high field mobility can now be obtained by calculating the current density J from [23]

$$J = -\frac{e^2 \varepsilon}{m^*} \int \frac{h^2 k^2}{m^*} \cos^2 \theta \, \tau \left(E_{\vec{k}} \right) \frac{\partial f_0}{\partial E_{\vec{k}}} d\vec{k} \tag{5}$$

where, for a parabolic law of dispersion, the energy of an electron $E = \frac{\hbar^2 k^2}{2m^*}$, $\tau(E_{\vec{k}})$ is the relaxation time, θ is the angle between $\vec{\varepsilon}$ and \vec{k} .

Thus one can obtain,

$$\mu_{ac} = \mu_{ac}^{0} \left(\frac{T_{L}}{T_{e}}\right)^{\frac{1}{2}}; \ \mu_{pz} = \mu_{pz}^{0} \left(\frac{T_{e}}{T_{L}}\right)^{\frac{1}{2}}; \ \mu_{I} = \mu_{I}^{0} \left(\frac{T_{e}}{T_{L}}\right)^{\frac{3}{2}}, \mu_{N} = \mu_{N}^{0}$$
 (6)

 μ_{ac}^{0} , μ_{pz}^{0} , μ_{I}^{0} and μ_{N}^{0} are the low field mobilities, for the respective interactions, of the electrons with the acoustic phonons, piezoelectric phonons, ionized impurities and neutral impurities. They are given by [23]

$$\mu_{ac}^{0} = \frac{2(2\pi)^{\frac{1}{2}}e\hbar^{4}s^{2}\rho_{v}}{3E_{1}^{2}m^{*\frac{5}{2}}(K_{B}T_{L})^{\frac{3}{2}}}; \qquad \mu_{pz}^{0} = \frac{16(2\pi)^{\frac{1}{2}}\hbar^{2}\varepsilon_{sc}}{3k_{m}^{2}em^{*\frac{3}{2}}(K_{B}T_{L})^{\frac{1}{2}}}; \qquad \mu_{I}^{0} = \frac{128(2\pi)^{\frac{1}{2}}\varepsilon_{sc}^{2}(K_{B}T_{L})^{\frac{3}{2}}}{N_{i}e^{3}m^{*\frac{1}{2}}ln\left[1+\left(\frac{12\pi\varepsilon_{sc}K_{B}T_{L}}{e^{2}N_{3}^{\frac{1}{2}}}\right)^{2}\right]}; \qquad \text{and}$$

 $\mu_N^0 = \frac{e}{20\hbar N a_0}$; where E_1 is the deformation potential constant, s is the average acoustic

velocity, ε_{sc} is the static dielectric constant, k_m is the piezoelectric coupling constant, N_i is the concentration of the ionized impurity atoms, each of charge -Ze and a_0 is the Bohr radius.

4.2.3 Results and Discussions

By solving the energy balance equation for the electron-phonon system in a moderately non degenerate compound semiconductor, we have obtained the electric field dependence of the effective electron temperature, under the conditions of low lattice temperatures. At the low temperatures, the electrons are dominantly scattered simultaneously by the acoustic and the piezoelectric phonons, and the electrons may get heated up at relatively low fields.

The dependence of the effective electron temperature, upon the electric field, as derived here, using the results for the energy loss rate of an electron, seems to be more complex. It may be seen from the curves 2 and 3 of the energy loss rate characteristics that for the interaction with the deformation potential acoustic phonons and for the combined interaction with the piezoelectric and the deformation potential acoustic phonons, the characteristics are qualitatively similar. From the same curves of the electron temperature characteristics, it follows that in both cases, the effective electron temperature rises monotonically with the electric field, but the rate of increase is lower for the combined interaction. Moreover, it may also be seen that the collisions with the piezoelectric phonons effect the characteristics more appreciably for the lower values of the electric field.

More importantly, it may be seen from the curve 1, how significantly does the inelasticity of the collisions with the neutral impurity bring in changes in the effective electron temperature characteristics. From Fig.4.1. it may be noted that for InSb, when the contribution of the collisions only with the phonons are taken into account, $\left(\frac{T_e}{T_L}\right)$ assumes a value, nearly 10 for a field of the order of 0.01 V/cm. Whereas, when the inelasticity of the

collisions with the neutral impurities is also taken into account, it follows from the present theory that a quite higher field, of the order of 0.6 V/cm, which is nearly 60 times higher, is now required to attain the same value of $\left(\frac{T_e}{T_L}\right)$. Apart from that, in general, the consideration of the inelasticity of the collision with the neutral impurity atoms considerably shifts the effective electron temperature characteristics towards the higher fields. Hence, to attain the same value of $\left(\frac{T_e}{T_L}\right)$, a significantly higher field is required, as the present theory reveals. This makes the theoretical curve appreciably nearer to the experimental curve for any material of interest here.

Still there are both qualitative and quantitative differences between the theoretical and experimental characteristics. This discrepancy may be ascribed to the unknown values of the material parameters for the experimental samples.

It thus turns out, that the loss of energy of a non-equilibrium electron due to the processes of excitation and ionisation of the neutral impurities plays quite a significant role in determining the non-ohmic characteristics of a compensated and non-degenerate semiconductor compound under the condition when lattice temperature is low. Moreover, the interaction of the electrons with the piezoelectric phonons, unlike that with the deformation potential acoustic phonons, effects the non-ohmic characteristics more and more as the lattice temperature is lowered.

We have considered here only a few well-known features of the low lattice temperature. Taking account of all of them at a time in any theoretical analysis is hardly possible. However, the interesting results which have been obtained here, stimulate further studies in the same field. As such, there is ample scope for the refinement of the present analysis.

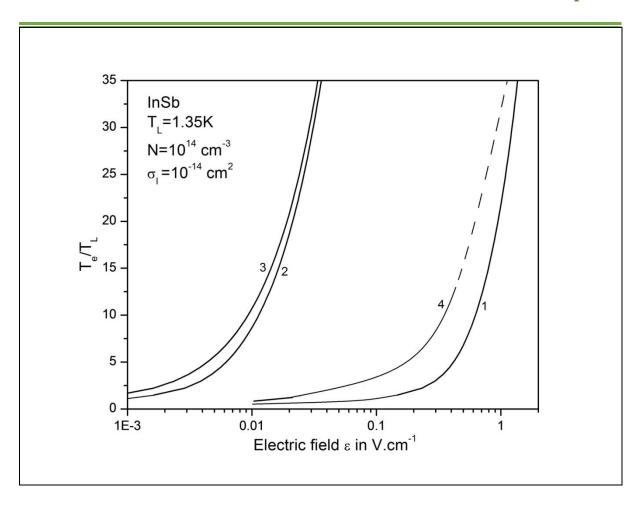


Fig.4.1 Dependence of the normalized electron temperature $\left(\frac{T_e}{T_L}\right)$ upon the electric field ε in InSb at a lattice temperature T_L of 1.35K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{14} cm^{-3}$ and $10^{-14} cm^2$ respectively. The curve 1 is obtained considering the energy loss due to all the processes of energy loss of an electron (interaction with the acoustic and the piezoelectric phonons as well as the $1s \to 2p$ excitation and ionization of the neutral impurities). The curve 2 is obtained for the combined interaction with the acoustic and the piezoelectric phonons. The curve 3 is obtained for interaction only with the acoustic phonons. The curve marked 4 is the experimental curve [27]. The dotted portion of the curve 4 is the extrapolation region for higher fields.

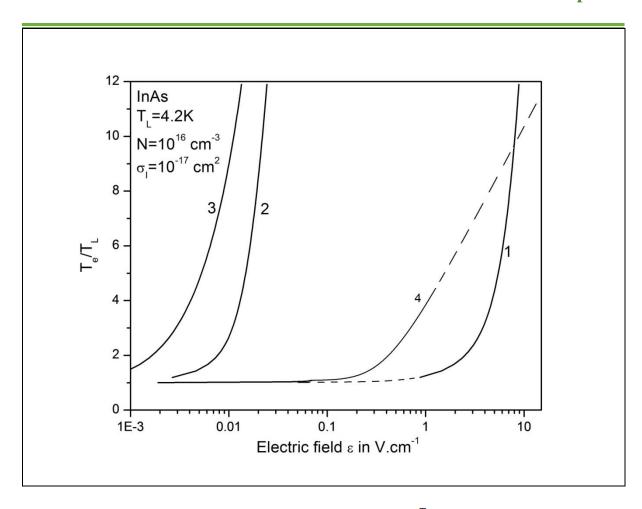


Fig.4.2 Dependence of the normalized electron temperature $(\frac{T_e}{T_L})$ upon the electric field ε in InAs at a lattice temperature T_L of 4.2K. The concentration of the neutral impurity atoms and the impact cross-section are being 10^{16} cm⁻³ and 10^{-17} cm² respectively. The curve 1 is obtained considering all the processes of energy loss (interaction with the acoustic and the piezoelectric phonons and the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities). The curve 2 is obtained for the combined interaction with the acoustic and the piezoelectric phonons, and the curve 3 is obtained for interaction only with acoustic phonons. The curve marked 4 is the experimental curve [28]. The dotted portion of the curve 4 is the extrapolation region for higher fields.

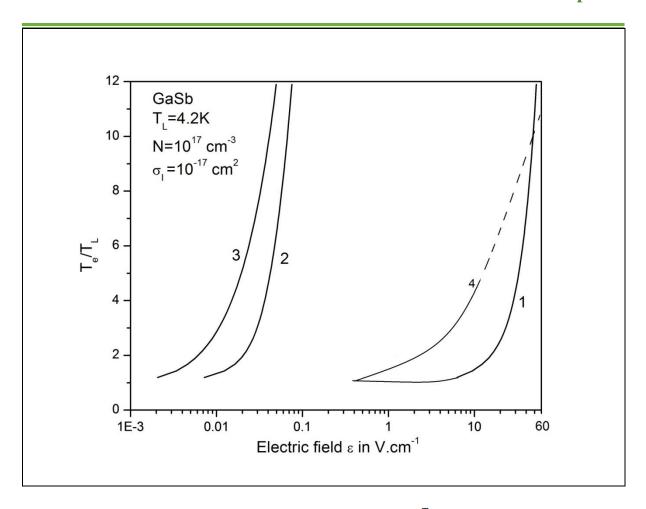


Fig.4.3 Dependence of the normalized electron temperature $(\frac{T_e}{T_L})$ upon the electric field ε in GaSb at a lattice temperature T_L of 4.2K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{17} \, cm^{-3}$ and $10^{-17} \, cm^2$ respectively. The curve 1 is obtained considering all the processes of energy loss (interaction with the acoustic and the piezoelectric phonons and the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities). The curve 2 is obtained for the combined interaction with the acoustic and the piezoelectric phonons and the curve 3 is obtained for interaction only with acoustic phonons. The curve marked 4 is the experimental curve [29,30]. The dotted portion of the curve 4 is the extrapolation region for higher fields.

Table 1: Material parameters

Physical Parameters	InSb	InAs	GaSb
Deformation potential, E_1 (eV)	20.0	8.0	12.0
Acoustic velocity, $u_l \left(\times 10^3 \text{ m.s}^{-1} \right)$	3.7	3.83	5.06
Density, ρ_{ν} (×10 ³ kg.m ⁻³)	5.78	5.66	5.66
Static dielectric constant, ε_{sc}	17.51	14.60	15.70
Piezoelectric coupling constant, k_m	0.027	0.029	0.026
Effective mass ratio, (m^*/m_0)	0.014	0.023	0.042
Ionization energy (meV)	0.62	1.47	2.3
Excitation energy (meV)	0.47	1.10	1.74

 m_0 being the free electron mass

4.2.4. Conclusion

For a non-degenerate ensemble of electrons in a compensated semiconductor compound at a low lattice temperature, an analysis is made here to study the effects of the interactions of the non-equilibrium electrons with the neutral impurities on the non-ohmic characteristics of the ensemble. In particular, the effects of the inelastic collisions with the neutral impurity atoms due to their ionisation and $1s \rightarrow 2p$ excitation have been studied. The intrinsic interactions with the acoustic phonons, both piezoelectric and deformation potential have also been taken into account. The theory is developed for the dependence of the average rate of energy loss of an electron to the lattice, on the average energy of the electrons, and subsequently, the dependence of the effective temperature of the electrons on the electric field.

The field dependence of the effective electron temperature in non degenerate semiconductors thus obtained under the conditions of low lattice temperature seems to be quite complex. It may also be seen from the figures that, when the interaction with the

piezoelectric phonons is also considered apart from that with the deformation acoustic phonons, significant qualitative as well as quantitative changes in the electron temperature characteristics are affected over the lower ranges of the electric field and of the lattice temperature. The non degenerate ensemble of electrons now interacting simultaneously with both the intravalley acoustic and the piezoelectric phonons at low lattice temperatures, gets heated up for even smaller values of the electric field due to the intrinsic unstable feature of the piezoelectric interaction. However, at higher fields, the characteristics for the combined interaction tend to that due to the acoustic interaction only, as the importance of the piezoelectric interaction reduces more and more. This picture continues till the lattice temperature and the field is high enough so that the interaction with the polar optical phonons begins to be more and more important. Thus, the effects of the piezoelectric scattering of electrons under the condition of low lattice temperature in controlling the field dependent effective temperature characteristics are revealed.

At low temperature, the average thermal energy of the electrons may become comparable with the phonon energy. As such, the electron-phonon collision becomes inelastic. Moreover, the equipartition approximation for the phonon distribution is hardly valid at low temperatures where the true phonon distribution needs to be taken into account. Since the materials which we have considered here, are assumed to be non degenerate, the electron concentration is quite high.

Fig. 4.1 exhibits that the electronic interaction with the piezoelectric phonon makes comparable contribution in determining the effective electron temperature characteristics of a compound semiconductor at low lattice temperature. But above all, the contribution of the process of excitation and ionization of the neutral impurities seem to be much more under the prevalent conditions of interest here. The values of the parameters of the experimental samples are not quoted in [24]. As such, the little discrepancy observed between the net

theoretical results which consider the electronic interaction with the acoustic and the piezoelectric phonon as well as the energy loss due to excitation and ionization of neutral impurities, and the experimental characteristics may be ascribed due to the unknown parameter values of the experimental sample. The results which have been obtained here being interesting, inspires further work taking due account of such low temperatures features.

One can now conclude again from the above studies that the inelasticity of the collisions of the non-equilibrium electrons with the neutral atoms, makes the highest contribution in the process of the loss of energy of an electron of the non-equilibrium ensemble, to the lattice. This inelasticity makes the rate of loss of energy with the average energy $\langle E_{\vec{k}} \rangle$, significantly faster. The rate of increase of the effective temperature of the electrons with the electric field now turns out to be lower. Moreover, the collision with the piezoelectric phonons effects the electron temperature characteristics more appreciably for the lower values of the electric field.

Moreover, the database resulting from such theoretical studies on the hot electron characteristics in non-degenerate compound semiconductors under the condition of low lattice temperature would be of importance for the device technologist.

References:

- [1] E. M. Conwell, High Field Transport in Semiconductors ,Academic Press, New York (1967).
- [2] B. R. Nag, Theory of Electrical Transport in Semiconductors, Pergamon Press, Oxford (1972).
- [3] S. H. Koenig, R. D. Brown and W. Schillinger, Phys. Rev. 128 1668 (1962).
- [4] A. Zylbersztjn, Phys. Rev. 127 744 (1962).
- [5] Z. S. Kachlishvili, Phys. Stat. Sol. (a) 33 15 (1976).
- [6] G.Bauer, Springer Tracts in Modern Physics 74, Springer, Berlin, Heidelberg, New York (1974).
- [7] B. Das, A. Basu, J. Das, D.P. Bhattacharya, Phys. B 474 21 (2015).
- [8] G. Bauer, Springer Tracts in Modern Physics Springer, Berlin, Heidelberg, New York (1974).
- [9] P.K. Basu, B.R. Nag, Phys. Rev. B 22 4849 (1980).
- [10] P.K. Basu, B.R. Nag, J. Phys. C: Solid State Phys. 14 1519 (1981).
- [11] B. Das, A. Basu, J. Das, D.P. Bhattacharya, Can. J. Phys. 95 167 (2017).
- [12] J.P. Maneval, A. Zylbersztein, H.F. Budd, Phys. Rev. Letters 23 848 (1969).
- [13] M. S. Sodha and B. M. Gupta, Phys Rev. B 1 3993 (1970).
- [14] S.Midday, D.P. Bhattacharya, Physica B 458 18 (2015).
- [15] S.Midday, D.P. Bhattacharya, Phys. Scr. 83 025702 (2011).
- [16] S.N.Patra, D.P. Bhattacharya, Physica B 325 17 (2003).
- [17] S.N.Patra, D.P. Bhattacharya, Physical Review B 52 4651 (1995).
- [18] W. Shockley, Electrons and Holes in Semiconductors, Van Nostrand, Princeton, N.J (1950).
- [19] E.M. Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967.

- [20] B.R. Nag, Electron Transport in Compound Semiconductor, Springer, Berlin, 1980.
- [21] Z.S. Kachlishvili, Galvanomagnetic and Recombination Effects in Semiconductors in a Strong Electric Field, Phys. Stat. Sol (a) 33 (1976) 15-51.
- [22] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, A. Alberigi-Quaranta, Electron drift velocity in silicon, Phys. Rev. B 12 (1975) 2265-2284.
- [23] B.R. Nag, Theory of Electrical Transport in Semiconductors, Pergamon Press, Oxford, 1972.
- [24] Z.S. Kachlishvili, Inelastic Impurity Scattering of Hot Electrons in Semiconductors. Phys. Stat. Sol (b) 48 (1971) 65-75.
- [25] G. Bauer, Springer Tracts in Modern Physics, Vol. 74, Springer, New York, 1974.
- [26] L.F. Mao, H. Ning, C. Hu, G. Wang, Physical Modeling of Activation Energy in Organic Semiconductor Devices based on Energy and Momentum Conservations, Sci. Rep. 6 (2016) 24777.
- [27] W. Szymanska, J.P. Maneaval, Energy exchange between hot electrons and lattice in InSb, Sol. Stat. Comm. 8 (1970) 879-883.
- [28] G. Bauer, H. Kahlert, Low-Temperature Non-Ohmic Galvanomagnetic Effects in Degenerate n-Type InAs, Phys. Rev. B5 (1972) 566-579.
- [29] H. Kahlert, G. Bauer, Hot-Electron-Phonon Interaction in the Non parabolic Conduction Band of Degenerate InSb at 4.2 K, Phys. Rev. B.7 (1973) 2670-2682.
- [30] G. Bauer, H. Kahlert, Hot electron Shubnikov-de Haas effect in n-InSb, J. Phys. C.6 (1973) 1253-1265.

Chapter 5

Microwave Harmonic Generation by Non Ohmic Ensemble of Carriers in Compound Semiconductors at Low Lattice Temperatures

MICROWAVE HARMONIC GENERATION BY NON OHMIC ENSEMBLE OF CARRIERS IN COMPOUND SEMICONDUCTORS AT LOW LATTICE TEMPERATURES

5.1. Introduction

It is well-known that in the presence of a relatively high electric field $(\vec{\varepsilon})$, the electron ensemble in a semiconductor may be significantly perturbed from the state of thermodynamic equilibrium with the lattice atoms. Since the average energy of an electron then exceeds its thermal equilibrium value, the ensemble thus becomes 'hot', assuming a field dependent effective temperature $T_e(\varepsilon)$ which exceeds the lattice temperature T_L . The high-field transport characteristics of any semiconductor structure exhibits some novel features, which are not observed at the low fields. The knowledge of the high-field features is rather important from the device point of view [1-7].

Nonlinearity of the current-voltage characteristics in a semiconductor structure may be exhibited at relatively high electric field. When the lattice temperature is low $(T_L \leq 20K)$, a few volt/cm can cause the nonlinearity of the current-voltage characteristics. At effectively high electric field, the electron mobility μ and sometimes, the concentration of the electron ensemble n in semiconductor structures may turn field dependent. This results in the electrical nonlinearity of the current-voltage characteristics of the structure. Higher harmonics of the input frequency may be generated through such nonlinearity. The analysis of the characteristics of the generated harmonics is important from the viewpoints of characterization and design of various semiconductor devices.

This electrical nonlinearity may be exploited for the generation of higher harmonics in the semiconductor structure when a microwave field is applied in conjunction with the d.c. bias field. The output at higher harmonics can be conveniently controlled by varying the d.c. field in some cases.

The cause of the electrical nonlinearity under the high-field condition is usually attributed to the field dependence of the mobility of the non-equilibrium carriers. However, at low lattice temperatures, the electrical nonlinearity sometimes may also occur due to the impact ionization of the impurity atoms by the energetic non-equilibrium electrons, and to their thermal recombination. The ionization and recombination probabilities are dependent upon the carrier energy, hence upon the electric field. As a result, the dynamical equilibrium between the free electrons and the ionization and recombination centres may shift as the effective electron temperature exceeds that of the lattice atoms in the presence of a convincingly high electric field. Hence, the concentration n of the free electrons may also turn field dependent, thus causing additional nonlinearity in the $\vec{J} - \vec{\varepsilon}$ characteristics. Thus, in general, the electrical conductivity in the presence of a high electric field may be represented as $\sigma(\varepsilon) = n(\varepsilon)e\mu(\varepsilon)$ [1,7,8,9,10].

The reports on studies of the efficiency of second harmonic generation (SHG) due to electrical nonlinearity of the bulk semiconductor structures are available in the literature [11-18]. Though in such studies the efficiency of the SHG have been reported considering only the deformation potential acoustic scattering of the carriers neglecting all other major scattering which are relevant at low lattice temperature.

In the present communication, we report the efficiency of SHG due to electrical nonlinearity of carriers in compound semiconductor at a low lattice temperature. The predominant electronic interaction of the carriers at low lattice temperature which have been considered are deformation potential acoustic phonons scattering, piezoelectric acoustic phonons scattering, ionized and neutral impurities scattering. The ensemble exhibits electrical nonlinearity when subjected to an effectively high bias field ε_0 . When an a.c. field of microwave frequency $f(\omega/2\pi)$, ω being the angular frequency) is superimposed at the

input, current harmonics of higher frequencies may be generated at the output due to the nonlinear $J-\varepsilon$ characteristics of the ensemble.

We make an attempt here to analyze the dependence of the efficiency of generation of the second harmonic current upon the bias field in compound semiconductor at the low lattice temperature. The efficiency characteristics of Second harmonic generation are obtained foe some widely used compounds like InSb, InAs, and GaSb.

As we shall see presently, that such an analysis requires the knowledge of the dependence of the non-ohmic mobility and also of its first and second order derivatives upon the bias field ε for the electron ensemble under consideration here. The required high-field mobility characteristics of the similar ensemble in compound semiconductor, under the identical conditions of interest here have already been obtained by the present authors in an earlier communication [19]. Hence, we make use of the results which have been reported in [19], for the present analysis, in order to obtain the $\eta - \varepsilon_0$ characteristics for the same well known semiconductor structures under various conditions in respect of the lattice temperature and the concentration n of the ensemble.

5.2 Brief review of the studies on the characteristics of Harmonic Generation in semiconductor structures

Seeger [20] has performed an experiment on the microwave frequency multiplication in Ge around room temperature at power levels of several kilowatt. For a fundamental frequency of 9.4 GHz, he has observed a yield of about 1% of third harmonic power. The result is in conformity with the calculations based on the observed deviation from the Ohm's law. Kobayashi et. al. [21] has performed the same experiment also at room temperature and at liquid nitrogen temperature.

For a theoretical analysis of the second harmonic generation (SHG) in a nondegenerate bulk semiconductor, P.K. Kaw has considered the d.c. electric field of arbitrary strength and made use of the Boltzmann transport equation technique to describe the motion of the carriers inside the material [22]. The carriers have been assumed to be scattered only through the acoustic mode lattice vibrations. For sufficiently strong d.c. fields, the generated second harmonic has been found to decrease with the increase of the d.c. fields obeying the simple power law. Moreover, for some optimum value of the d.c. field the generation seems to be more efficient.

It has been shown by Das that the efficiency of SHG arising from the nonlinear current-voltage characteristics should be derivable from a direct perturbation of the characteristics around the biased voltage [23]. It has been pointed out that this different derivation of the results is of preeminent practical importance as one can now easily calculate the efficiency from the experimental d.c. $J - \varepsilon_0$ characteristics for any material, thus considerably simplifying the estimation in actual experiment.

Chattopadhyay and Nag have developed an approximate theory for the third harmonic generation in GaAs which is subjected to a large high frequency sinusoidal electric field [24]. The ratio of the third harmonic to the fundamental frequency currents has been found to be 0.22 and 0.15 for a field of amplitude 6.7 KV/cm at the fundamental frequencies of 100 GHz and 450 GHz respectively.

The generation of the second harmonic of high frequency electromagnetic waves in anisotropic semiconductors has been theoretically investigated by Sodha and Gupta. D.C. electric fields of arbitrary strength has been considered and it has been assumed that the acoustic, nonpolar optical phonon and intervalley scatterings are the dominant type of scattering under the prevailing conditions of interest there. It has been observed that when the frequency of the wave is much greater than the effective collision frequency (i.e., the I.R. region), the generated second harmonic is proportional to the applied d.c. field [25]. This is in contrast to the range of microwave frequency when the generation is most efficient at some

optimum d.c. field. The calculation of the anisotropy and the magnitude of the efficiency of SHG for the [100], [110] and [111] directions have been reported, in the case of bulk structure of n-Ge.

Yamamoto and Iwasawa have made an estimation of the efficiency of SHG in nonpolar, non-degenerate semiconductor, assuming a hyperbolic equation for the nonlinear velocity-electric-field relations in the temperature range between 77 and 300*K* [26]. Their calculation has predicted a maximum efficiency of about 5% in n-Ge and n-Si for some optimum bias field.

It has been shown by Mukhopadhyay et. al. that II-VI compound semiconductors seem to be more suitable for harmonic generation under the high-field condition than the elemental semiconductors or the III-V compound semiconductors [27-29].

5.3. Method of calculation of the efficiency of SHG in an ensemble of 3DEG

We consider a non-degenerate ensemble of free electrons in an extrinsic n-type compound semiconductor which is doped with both donor and acceptor impurities at a low lattice temperature, so that the impurities are not completely ionized. Let N_D and N_A are respectively the donor and acceptor concentrations. So, the total impurity concentration is $N_D + N_A$. The shallow impurity levels are very close to the band edges. At $T_L \approx 0K$, there is neither any ionization of the impurities, nor there can be any band to band transition. Thus, no free carriers are generated, and the semiconductor behaves like an insulator. However, as the lattice temperature increases from 0K, more and more ionization of the neutral impurities takes place. Thus, even though there is hardly any band to band transition, the concentration of the carriers, as well as that of the ionization impurities begins to increase from a small value, at low lattice temperatures, and the semiconductor starts conducting. The concentration of the net impurity level is given by $N = N_D - N_A$ and the compensation ratio $c = \frac{N_A}{N_D}$ [6].

The ensemble exhibits electrical nonlinearity when subjected to an effectively high bias field ε_0 . When an a.c. field of microwave frequency $f (= \frac{\omega}{2\pi}, \ \omega$ being the angular frequency) is superimposed at the input. The current harmonics of higher frequencies may be generated at the output due to the nonlinear $J - \varepsilon_0$ characteristics of the ensemble.

Let us consider the electrical nonlinearity of a non-degenerate ensemble of electrons in bulk structure of a compound semiconductor at a low lattice temperature. The ensemble is biased with a high d.c. electric field ε_0 . When a microwave electric field of amplitude ε_1 and of angular frequency ω , is also applied in the same direction as that of ε_0 , then the total field ε at any instant t may be written as

$$\varepsilon = \varepsilon_0 + \varepsilon_1 \exp(-i\omega t). \tag{1}$$

The resultant current density J due to the electrical nonlinearity of the ensemble may then be expressed as

$$J = \sum_{m=0}^{\infty} J_m \exp(-im\omega t), \tag{2}$$

where $J_{\scriptscriptstyle m}$ is the amplitude of the mth harmonic.

The effective momentum relaxation time $(\tau_m)_{eff}$ for the combined interaction of the electrons with the deformation potential acoustic and the piezoelectric phonons, at the low lattice temperatures of interest here is $\sim 10^{-12}$ sec. It is well known that the energy relaxation time $\tau_e \sim \left(\frac{u_{th}}{u_l}\right)^2 \tau_m$, where u_{th} is the average thermal velocity of the electrons and u_l is the acoustic velocity [1]. When the lattice temperature is low, τ_e is almost of the same order as that of τ_m . So, at the microwave frequency around the x-band, $\omega \tau_e < 1$ [11]. Thus, the relaxation time being quite small, the free carriers can follow the input microwave signal quite exactly. Hence, one can derive the characteristics of SHG due to the electrical

nonlinearity of the structure, from a direct perturbation of the d.c. $J - \varepsilon_0$ characteristics, around the bias field [12].

By definition, the efficiency η of the second harmonic generation, is given by the ratio $\frac{|J_2|}{|J_1|}$, where J_1 and J_2 are respectively the fundamental and the second harmonic components of the current density. Hence while calculating the efficiency of generation of the second harmonic current, the series for J in (3) may be truncated at m=2.

If the input microwave field is small ($\varepsilon_1 \ll \varepsilon_0$), then neglecting the higher order terms one can obtain

$$\eta = \frac{\varepsilon_1 \varepsilon_0 D^2 \sigma(\varepsilon_0) + 2\varepsilon_1 D \sigma(\varepsilon_0)}{4[\varepsilon_0 D \sigma(\varepsilon_0) + \sigma(\varepsilon_0)]},\tag{3}$$

Here the operator $D \equiv \frac{d}{d\varepsilon_0}$ and $\sigma(\varepsilon_0)$ is the field dependent conductivity. Considering only small portion of non-linearity in current density due to the non-ohmic mobility, field dependent of conductivity can be written as

$$\sigma(\varepsilon_0) = en\mu(\varepsilon_0), \tag{5}$$

where e the electronic charge, n the carrier concentration and $\mu(\varepsilon_0)$ the field dependent of non-equilibrium carrier mobility.

5.4 Results for the dependence of the efficiency of SHG upon the biased field in non-equilibrium ensemble of InSb, InAs and GaSb with different lattice temperatures.

The theory is now used to investigate the characteristics of the efficiency of SHG for the non-degenerate ensembles of InSb, InAs and GaSb under various conditions, in respect of the lattice temperature T_L .

It follows from (4) and (5) that the results for the $\eta - \varepsilon_0$ characteristics evolve collectively from the field dependences of the factors like the non-ohmic mobility $\mu(\varepsilon_0)$ and

its first and second order derivatives $\frac{d\mu(\varepsilon_0)}{d\varepsilon_0}$ and $\frac{d^2\mu(\varepsilon_0)}{d\varepsilon_0^2}$. As such, the field dependence of

the derivatives of the mobility could hardly be calculated analytically. Hence, we take recourse to the numerical technique of finite differences [30,31] to calculate these derivatives.

These factors, viz. the non-ohmic mobility and its two derivatives are entangled in the expression (4) for the efficiency η , in such a way, that it is hardly possible to single out any specific aspect of the resultant $\eta - \varepsilon_0$ characteristics, that may have been produced solely by any of these three factors alone. However, it may be expected that all the complexities exhibited by the non-ohmic mobility characteristics and by its derivatives would make the $\eta - \varepsilon_0$ characteristics quite complex under any contemplated conditions.

Figures 5.1, 5.2 and 5.3 depict $\eta - \varepsilon_0$ characteristics for the non-degenerate ensembles of 3DEG of some widely used compounds like InSb, InAs, and GaSb. The numerical values of η for any ε_0 are obtained here using the values of the material parameters given in Table 1. The calculations have been carried out for $\frac{\varepsilon_1}{\varepsilon_0} = 0.1$. The maximum error involved in the numerical calculation of the derivates of $\mu(\varepsilon_0)$ has been estimated to be less than 0.5%.

The characteristics are obtained for various conditions, in respect of the dominant interaction of the carriers viz. Acoustic, piezoelectric, excitation and ionisation of neutral impurities and the lattice temperatures at 1.35k and 4.2k. The results are shown by the curves in Figures 5.1, 5.2, and 5.3 respectively for the non-degenerate ensembles on the surfaces of InSb, InAs, and GaSb. The curves are obtained considering all the processes of an electron (interaction with the acoustic and the piezoelectric phonons as well as the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities). The curves are drawn for different lattice temperatures T_L .

It is important to mention here that the d.c. bias field that may turn out to be effectively high and is thus able to set in the electrical nonlinearity in a semiconductor structure, depends upon the lattice temperature T_L . It is well-known that the electrical nonlinearity in InSb, InAs and GaSb may be exhibited at the low lattice temperatures $(T_L \le 20K)$, for d.c. bias fields of the order of a fraction of volt/cm.

Table 1: Material parameters

Physical Parameters	InSb	InAs	GaSb
Deformation potential, E_1 (eV)	20.0	8.0	12.0
Acoustic velocity, $u_l \left(\times 10^3 \text{ m.s}^{-1} \right)$	3.7	3.83	5.06
Density, ρ_{v} (×10 ³ kg.m ⁻³)	5.78	5.66	5.66
Static dielectric constant, ε_{sc}	17.51	14.60	15.70
Piezoelectric coupling constant, k_m	0.027	0.029	0.026
Effective mass ratio, (m^*/m_0)	0.014	0.023	0.042
Ionization energy (meV)	0.62	1.47	2.3
Excitation energy (meV)	0.47	1.10	1.74

 m_0 being the free electron mass

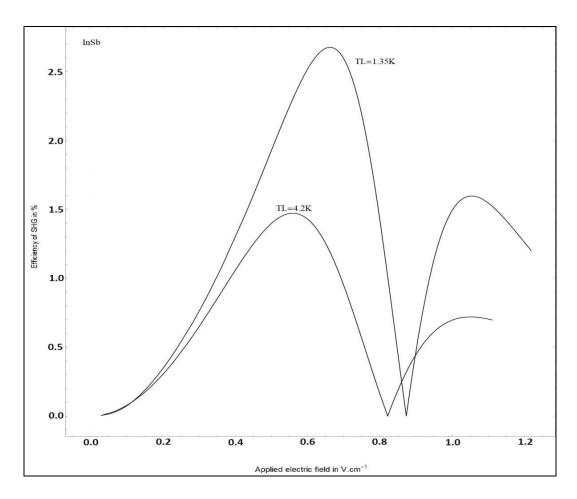


Figure 5.1 Dependence of the efficiency of SHG η upon the bias field ε_0 of a non-equilibrium ensemble of 3DEG of InSb at the lattice temperature of 1.35K and 4.2k. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{14} \, cm^{-3}$ and $10^{-14} \, cm^2$. The curves are obtained considering all the processes of an electron (interaction with the acoustic and the piezoelectric phonons as well as the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities).

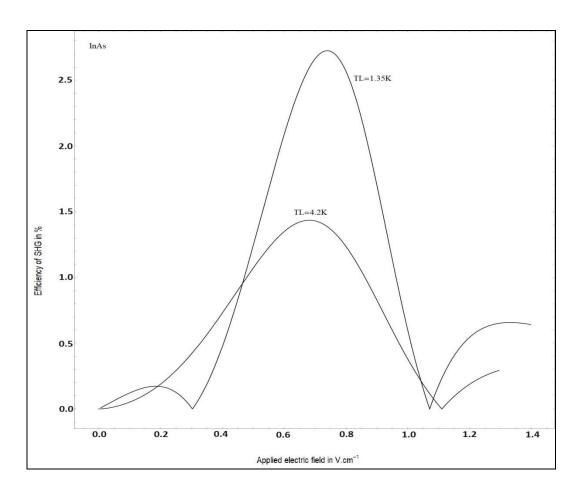


Figure 5.2 Dependence of the efficiency of SHG η upon the bias field ε_0 of a non-equilibrium ensemble of 3DEG of InAs at the lattice temperature of 1.35K and 4.2K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{16} \, cm^{-3}$ and $10^{-17} \, cm^2$. The curves are obtained considering all the processes of an electron (interaction with the acoustic and the piezoelectric phonons as well as the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities).

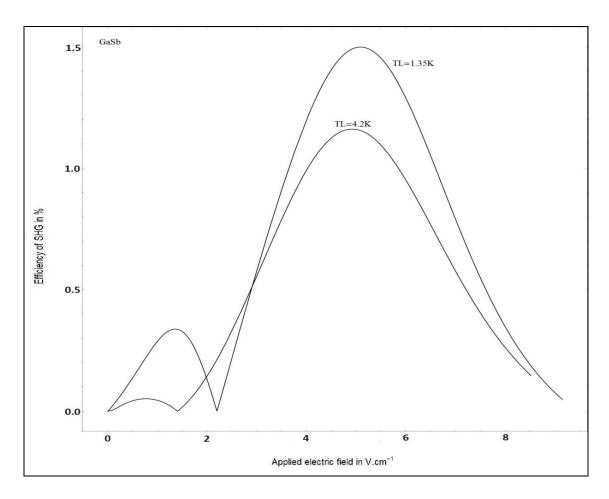


Figure 5.3 Dependence of the efficiency of SHG η upon the bias field ε_0 of a non-equilibrium ensemble of 3DEG of GaSb at the lattice temperature of 1.35K and 4.2K. The concentration of the neutral impurity atoms and the impact cross-section are being $10^{17} \, cm^{-3}$ and $10^{-17} \, cm^2$ respectively. The curves are obtained considering all the processes of an electron (interaction with the acoustic and the piezoelectric phonons and the $1s \rightarrow 2p$ excitation and ionization of the neutral impurities).

5.5 Discussions

The effects of some of the low-temperature features, like that of the non-degeneracy of the electron ensemble, and the combined interactions with acoustic phonons, piezoelectric phonons, neutral and ionized interactions, on the characteristics of the microwave harmonic generation for the above-mentioned compounds, may be observed from the present study.

It may be seen from the figures that the $\eta - \varepsilon_0$ characteristics which follow from the present analysis for the non equilibrium ensembles of 3DEG Structures of interest here seem to be quite interesting.

Generally speaking, for the non-degenerate layers, the efficiency η , in the low-field regime, slowly increases with ε_0 for any compound, irrespective of the prevalent conditions. However, the rate of increase of η at any lattice temperature is different for the different materials. Again, for the layer of any material, the rate of increase of η is also susceptible to changes with the change of the lattice temperatures.

As ε_0 increases, the characteristics turn out to be more and more complex. Moreover, the widely different values of E_1 , k_m , and m^* , make the characteristics significantly different of different materials at higher fields. The effects of the contemplated low temperature features on the field dependence of η of the semiconductor structures of any material can be revealed from a comparison of the different curves for the corresponding material.

The material parameters for InSb are not much different from those of InAs. The electrical nonlinearity in these materials is exhibited starting from a field, which is of the order of a small fraction of a volt/cm at the lattice temperatures of 1.35K and 4.2K. A small

regime of the nonlinearity up to a few tenths of a *volt/cm* for the material of InSb and up to a few *volt/cm* for the material of InAs have been considered here. In order to make the discussion more comprehensive, the results of the three compounds InSb, InAs, and GaSb may be compared.

From the Figures. 5.1, 5.2 and 5.3, it may be noted that the consideration of the degeneracy of the layers brings in significant qualitative, as well as quantitative changes in the $\eta - \varepsilon_0$ characteristics of the layer of any material, irrespective of the type of interaction of the electrons, either only with the deformation potential acoustic phonons or for the case of combined interactions.

Now the efficiency starts increasing with the field quite slowly, then the rate of increase picks up and for higher fields, the efficiency eventually tends to a saturation value. This saturation value is almost same for the layers of InSb and InAs and different for the layers of GaSb.

It seems quite pertinent to mention here that the $\eta - \varepsilon_0$ characteristics of the non-degenerate ensembles for the combined scattering of the electrons also exhibit a few extrema usually at the lower fields. The values of the maximum efficiency are the highest for the wells of InSb and InAs, and the same is lower for GaSb. As the field increases, the rate of increase of η with ε_0 decreases and eventually η tends to a saturation value. The saturation value of η under this condition is the highest for the layer of InSb and for the layer of GaAs the saturation value is little less than that of InSb layer.

On comparing the Figures. 5.1, 5.2 and 5.3, one can note that some little variation of the lattice temperature results in quite perceptible qualitative as well as quantitative changes in the $\eta - \varepsilon_0$ characteristics of the layers of any material. The results that are obtained here,

could not be compared with the experimental data, as there is a dearth of the same in the literature.

The present approximate analysis shows that, the efficiency of second harmonic generation, η of a small input signal at the microwave frequency due to the electrical nonlinearity of a 3DEG non equilibrium ensemble of a compound semiconductor structures at the low lattice temperatures depends upon the d.c. field in a quite complex manner. However, the results seem to be interesting and prompt further work through the refinement of the present analysis.

References

- [1] E.M. Conwell, High Field Transport in Semiconductors, Academic Press, New York, 1967.
- [2] B.R. Nag, Electron Transport in Compound Semiconductor, Springer, Berlin, 1980.
- [3] Z.S. Kachlishvili, Galvanomagnetic and Recombination Effects in Semiconductors in a Strong Electric Field, Phys. Stat. Sol (a) 33 (1976) 15-51.
- [4] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, A. Alberigi-Quaranta, Electron drift velocity in silicon, Phys. Rev. B 12 (1975) 2265-2284.
- [5] B.R. Nag, Theory of Electrical Transport in Semiconductors, Pergamon Press, Oxford, 1972.
- [6] Z.S. Kachlishvili, Inelastic Impurity Scattering of Hot Electrons in Semiconductors. Phys. Stat. Sol (b) 48 (1971) 65-75.
- [7] G. Bauer, Springer Tracts in Modern Physics, Vol. 74, Springer, New York, 1974.
- [8] C. Jacoboni, *Theory of Electron Transport in Semiconductors*, Springer Series in Solid Sate Sciences, Vol. 165, Springer, Berlin, Heidelberg, 2010.
- [9] V.L. Bonch-Bruevich and E.G. Landsberg, Phys. Stat. Sol. 29, 9 (1968).
- [10] Z.S. Kachlishvili, Phys. Stat. Sol. (a) 33, 15 (1976).
- [11] P.K. Kaw, Optimum second-harmonic generation in nondegenerate semiconductors using dc electric fields, J. Appl. Phys. 40 (1969) 793-797.
- [12] P. Das, Second-harmonic generation due to hot electrons in semiconductors, J. Appl. Phys. 40 (1969) 4206-4207.
- [13] S.S. Paul, D.P. Bhattacharya, Effect of recombination of the non-equilibrium carriers on the high frequency generation in semiconductors, Solid State Commun. 56 (1985) 527-529.

- [14] S.S. Paul, D.P. Bhattacharya, Harmonic generation in nondegenerate semiconductors at low lattice temperature, J. Appl. Phys. 64 (1988) 4554-4561.
- [15] T.K. Pramanik, D.P. Bhattacharya, Cross-section for impact ionisation in semiconductors, Solid State Commun. 59 (1986) 737-739.
- [16] T.K. Pramanik, D.P. Bhattacharya, Harmonic generation of microwaves in semiconductors in the presence of deep repulsive traps, J. Appl. Phys. 69 (1991) 2555-2560.
- [17] S.N. Patra, D.P. Bhattacharya, Microwave harmonics due to hot electrons in a magnetic field, J. Phys. Chem. Solids 57 (1996) 165-170.
- [18] S.N. Patra, D.P. Bhattacharya, Harmonic generation of microwaves in semiconductors in a magnetic field, Physica B 216 (1995) 121-124.
- [19] B. Roy, S. Bhattacharyya, D.P. Bhattacharya, Energy loss rate and non-ohmic characteristics of a degenerate surface layer of compound semiconductors at low lattice temperatures, Physica E 126 (2021) 114465.
- [20] K. Seeger, J. Appl. Phys. 34, 1608 (1963).
- [21] S. Kobayashi, S. Yabuki and M. Akoi, Jpn. J. Appl. Phys. 2, 127 (1963).
- [22] P.K. Kaw, J. Appl. Phys. 40, 793 (1969).
- [23] P. Das, J. Appl. Phys. 40, 4206 (1969).
- [24] D. Chattopadhyay and B.R. Nag, Int. J. Electronics 27, 443 (1969).
- [25] M.S. Sodha and B.M. Gupta, Phys. Stat. Sol. 37, 311 (1970).
- [26] H. Yamamoto and H. Iwasawa, Proc. IEEE 61, 504 (1973).
- [27] D. Mukhopadhyay and S. Dey, Proc. IEEE 68, 746 (1980).
- [28] D. Mukhopadhyay and S. Dey, Czech J. Phys. B 30, 469 (1980).
- [29] A. Choudhury and D. Mukhopadhyay, Phys. Stat. Sol. (b) 113, K49 (1982).

- [30] J.B. Scarborough, *Numerical Mathematical Analysis*, sixth ed., Oxford & IBH Publishing, 2005.
- [31] C.F. Gerald, P.O. Wheatley, *Applied Numerical Analysis*, seventh ed., Pearson, India, 2008.

Chapter 6

Overall Conclusion of The Thesis and Future Direction in The Relevant Field

OVERALL CONCLUSION OF THE THESIS AND FUTURE DIRECTION IN THE RELEVANT FIELD

For the sake of completeness of the thesis, prior to drawing up the overall conclusion from the analysis made here, a brief discussion is warranted in respect of: (a) the setup considered, (b) the framework used for the theoretical analysis, (c) the limitations of the assumptions made etc. This is precisely what follows now. Finally, the thesis ends after referring to the future direction of work in the relevant field.

6.1. The set-up considered

The setup that has been considered in the present thesis, consists of some sufficiently long samples of three-dimensional structures of well-known compound semiconductors.

The dimensionality of a structure is determined by comparing the geometrical sizes along the x, y and z axes respectively with the de Broglie wavelength λ of the electrons in the material. In the three-dimensional structures under consideration, the dimension of the structure along the x, y and z axes are quite large compared to mean free path of the electron. Hence the electrons in the ensemble there move freely on the x-y-z interface plane, and there been ample space for interaction with the prevalent lattice imperfections, the probability of of the scattering of the electrons is not at all scarce.

Considering such a structure of 3DEG, the thesis deals with the theoretical analysis of some aspects of electrical transport characteristics of the non-equilibrium ensemble of electrons. The results thus obtain have been reported and detailed discussion for each aspect have been made.

6.2. The framework used for the theoretical analysis

Although the framework of Boltzmann Transport Equation (BTE) is not free from well-known reservations in respect, of its validity, the theoretical studies on the electron transport characteristics of semiconductor structures are mostly made using the same

framework. The foremost justification for the use of this framework lies in the good agreement that is observed between the theoretical results obtainable from this framework with the experimental data. It is well known that the framework of BTE has been successfully used by many while studying electrical transport in 3DEG.

The electron mobility is defined in the usual way. Based on all these, the theoretical analysis, which has been carried out in the present thesis uses the same framework BTE.

It may be recalled once again that the set-up of our consideration in the present thesis is a sufficiently long sample of 3DEG.

6.3. The limitations of the assumptions made

For the theoretical analysis of a problem related to any set-up, some simplifying assumptions are usually made so as to make the problem amenable to a solution. The problem considered in the present thesis is indeed no exception. It remains to be seen how much the assumptions made here are physically valid, so that the results that follow from the analysis can really describe the characteristics of the actual system under the prevalent conditions, without any significant loss of accuracy. Some of the basic assumptions which have been made here may be pointed out next, mentioning the limitations of validity for each.

It may be recalled that for the analysis made in the present thesis, the lattice temperature TL is mostly assumed to be low: $TL \leq 20K$. It may be pointed out that under certain conditions, some other lattice temperatures have been needed to be considered. The framework of the Boltzmann transport equation has been used for the set-up under consideration.

The regime of the low lattice temperature has a number of conspicuously valid features. Some of the features have been considered for the analysis carried out in the present thesis. From the literature one may see that at the low lattice temperatures these features are

either overlooked or are ignored altogether for the mathematical simplicity of the theoretical analysis.

The electric field dependence of the effective electron temperature of the ensemble $T_e(\varepsilon)$, when calculated from the energy balance equation of the electron-phonon system, shows that $T_e(\varepsilon)$ can hardly reach a value above some ten to hundred times T_L . Hence one can validly assume that the electrons are confined to a short segment of the energy dispersion curve, near the minimum of the lowest sub band, where the band may be taken to be parabolic. The strength of the field is assumed to be such that it only changes the energy distribution of the electrons of the ensemble and can hardly trigger the process of impact ionization. As such, the assumptions for the constancy of the electron concentration remain valid. The strength of the electric field to which the set-up is subjected is assumed to be low enough, so that the average crystal momentum of the carriers falls within the first Brillouin zone. Hence it is validly assumed that the theoretical analysis may be carried out in the semi classical fabric.

The specific features of the low lattice temperatures include:

- (a) The widely used simple equipartition approximation for the phonon population is hardly valid in the low temperature regime of interest here, since the average thermal energy of the free electrons under the equilibrium condition is much less than the phonon energy. Hence the true phonon distribution may be validly used replacing the equipartition approximation.
- (b) It is well known that the ratio of the phonon energy to the average thermal energy of the electrons is $\sim \frac{2u_l}{u_{th}}$. But at the low lattice temperatures, when the phonon energy tends to be comparable with the electron energy, the electron-phonon interaction cannot be validly assumed to be elastic. Hence the contribution of the phonon energy must be taken into account in the energy balance equation of the electron-phonon system to make it valid.

- (c) Under the condition, when the lattice temperature is low, and the carrier concentration is high enough, it is no longer valid to assume that the electron ensemble is non-degenerate. As the lattice temperature is lowered more and more and the concentration is made higher and higher, one can validly assume that the ensemble tends to be degenerate. The level of degeneracy is decided by the value of the normalized Fermi energy η_D (= E_F/K_BT_L). Obviously, a lower value of the layer concentration may be sufficient enough to attain the same level of degeneracy at sufficiently low lattice temperatures.
- (d) The perturbing potentials, arising out of the lattice imperfections is known to be screened by the electrons of the ensemble. It is not valid that the effects of the screening of the carriers can always be neglected in the theoretical studies. When the carrier concentration is high and the lattice temperature is low, one can validly assume that the effects of screening turn up to be significant. Hence such screening should be taken into account for the development of the transport theory.
- (e) It is well known that when developing the theory of the transport characteristics of 3DEG of compound semiconductors at the regime of low lattice temperature, the interaction with the piezoelectric phonons dominates more in controlling the characteristics than what the interaction with the deformation potential acoustic phonon does.
- (d) Apart from that, at the low lattice temperatures one can validly take into account the inelasticity due to such interaction of the electrons as with the impurities that causes 1s \rightarrow 2 p Excitation.

It may be pointed out here that due to mathematical complexity, it is hardly possible to take into account these low temperature features all at a time while developing the theoretical analysis. Sometime each feature needs to be taken up separately.

6.4. Overall conclusion of the thesis

The theoretical analysis carried out in the present thesis considers a non-degenerate ensemble of electrons in a compensated semiconductor compound at a low lattice temperature, an analysis is made here to study the effects of the interactions of the non-equilibrium electrons with the neutral impurities on the non-ohmic characteristics of the ensemble. In particular, the effects of the inelastic collisions with the neutral impurity atoms due to their ionisation and $1s \rightarrow 2$ p excitation have been studied. The intrinsic interactions with the acoustic phonons, both piezoelectric and deformation potential have also been taken into account. The theory is developed for the dependence of the average rate of energy loss of an electron to the lattice, on the average energy of the electrons, and subsequently, the dependence of the effective temperature of the electrons on the electric field. The lattice temperature TL is primarily assumed to be low $(T_L \leq 20K)$. The prevalent conditions sometimes made it necessary to assume some other higher lattice temperatures.

The characteristics of the high-field electron transport coefficients in the considered semiconductor structure under the prevalent conditions have been obtained in the widely familiar framework of heated Fermi-Dirac or Maxwellian distribution at a field dependent effective temperature of the carriers. From the literature one can note that the results obtained from such a theoretical analysis are mostly known to agree well what the experiments predict.

The preeminent objective of the present theoretical analysis at the low lattice temperatures, is to assess the effects of the low-temperature features on the different aspects of the electrical transport characteristics of the semiconductor structures of consideration here.

The theoretical analysis made here, on taking into account various electron-lattice imperfections reveal the changed behaviors of the electrons in these structures at the low lattice temperatures, and that in turn, suggests their implications for the device fabrications.

The foundation work containing the discussions on the carrier concentration, scattering mechanisms, phenomenon of screening and the concept of modulation doping etc. has been carried out in Chapters I and II. After that, the main analysis containing the electron temperature characteristics, the energy loss rates, the non-ohmic mobility and the microwave harmonic generation characteristics have been developed in Chapters III, IV and V. The analysis there has provided a broader understanding of the electron dynamics in the semiconductor structure under consideration here.

From the detailed calculations, the numerical results which have been obtained for some well- known structures provide valuable knowledge about the behavior of the electrons in the structures of different materials.

The Chapter V includes the study of the generation characteristics of the second harmonic of the input microwave signal in the Bulk structures of compound semiconductors, due to the electrical non-linearity of the current density-electric field characteristics of the non-equilibrium ensemble of the 3DEG compound semiconductors. The presentation of the numerical results for different materials at different lattice temperatures, the text facilitates a comparative analysis and thus enhances the degree of understanding of the microwave behaviour in semiconductor structure.

One can now conclude again from the above studies that the inelasticity of the collisions of the non-equilibrium electrons with the neutral atoms, makes the highest contribution in the process of the loss of energy of an electron of the non-equilibrium ensemble, to the lattice. This inelasticity makes the rate of loss of energy with the average energy, significantly faster. The rate of increase of the effective temperature of the electrons with the electric field now turns out to be lower. Moreover, the collision with the piezoelectric phonons effects the electron temperature characteristics more appreciably for the lower values of the electric field.

Through some comprehensive examination of the temperature and electric field dependences, the text underscores the critical role of these features for the device fabrication and thus assigns the theoretical knowledge for the practical implications.

The high-field electron transport coefficients of the non-equilibrium ensemble of 3DEG, which is confined to the bulk structures of different compound semiconductors at various lattice temperatures have been obtained numerically sometime by others, using the values of the material parameters quoted in the standard references. The values of these material parameters can be quite different under different prevalent conditions of the experiments. This results in deviations from the experimental observations, though there may be some qualitative agreement. Here lie the limitations of the numerical analysis. Moreover, at the low lattice temperatures an apparently low electric field, sometimes, as low as a few mV/cm, may turn up to be effectively high and hence may make the structure exhibit high-field characteristics.

Still there are both qualitative and quantitative differences between the theoretical and experimental characteristics. This discrepancy may be ascribed to the unknown values of the material parameters for the experimental samples.

In conclusion, it thus turns out, that the loss of energy of a non-equilibrium electron due to the processes of excitation and ionisation of the neutral impurities play quite a significant role in determining the non-ohmic characteristics of a compensated and non-degenerate semiconductor compound under the condition when lattice temperature is low. Moreover, the interaction of the electrons with the piezoelectric phonons, unlike with the deformation potential acoustic phonons, effects the non-ohmic characteristics more and more as the lattice temperature is lowered.

We have considered here only a few well-known features of the low lattice temperature. Taking account of all of them at a time in any theoretical analysis is hardly

possible. However, the interesting results which have been obtained here, stimulate further studies in the same field. As such, there is ample scope for the refinement of the present analysis.

6.5. Contemplated future direction of work in the relevant field

The analysis which has been carried out in the present thesis and the noteworthy results obtained thereof, obviously inspire further work in the vast relevant field.

First of all, it has already been said that the preeminent objective of the theoretical analysis, as has been made in the present thesis, is to assess the effects of the conspicuous low-temperature features on the different aspects of the electrical transport characteristics of a non-equilibrium and non-degenerate ensemble of 3DEG of some well-known compound semiconductors. Only some of the low lattice temperature features have so far been taken into account. It transpires that these features which are usually, either overlooked or are ignored altogether, actually bring in significant and interesting changes in the electrical transport characteristics of the set-up. It is also known that all the low-temperature features can hardly be taken into account all at a time. Hence, as a continuation of the present work, it remains to be seen how do the rest of the low-temperature features, which so long have not been taken into consideration in the present thesis, would change the electrical transport characteristics of the set-up considered here.

Obviously, such an analysis would provide technologically important database. This in turn helps improving the performance of the existing devices and may also lead to the development of new devices altogether.

LIST OF SYMBOLS

a lattice constant

ac Acoustic

A surface area

 $A_i(z)$ Airy function of first kind

b variational parameter associated with Fang-Howard wave function

bg background impurities \vec{B} applied magnetic field

 B_m Bernoulli number

 $B_i(z)$ Airy function of second kind

d width of the layer of lattice atoms with which the electrons can interact

 d_s spacer layer width

deg Degenerate

 $D_n\left(arepsilon_{ec{k}}
ight)$ density of states function of electrons in the nth dimensional structure

e electronic charge

eff Effective

 E_1 deformation potential

 $E_1(z)$ exponential integral function

 $ec{arepsilon}$ applied electric field

 ε_s surface electric field

 \mathcal{E}_0 high d.c. electric field

 \mathcal{E}_1 amplitude of microwave electric field

f frequency of the a.c. microwave field

 $f(\vec{k})$ carrier distribution function in wave vector space

 $f_0 \left(ec{k}
ight)$ isotropic part of the distribution function of the electrons

 $f_0(E_{\vec{k}})$ Fermi-Dirac distribution function

 $f_0^n(E_{\vec{k}})$ nth derivative of the Fermi function with respect to the electron energy

$F_1(q)$	form factor for the supplementary material
$F_2(q)$	form factor for the core material
$F_{j}(x)$	Fermi integral of j th order
g_{v}, n_{v}	valley degeneracy factor
$G(q_z)$	form factor
h	Planck's constant
\hbar	reduced Planck's constant
H(x)	Heaviside step function
H'	perturbing potential
$ec{J}$	current density
${\pmb J}_m$	amplitude of the m th harmonic
$oldsymbol{J}_1$	fundamental component of current density
${J}_2$	second harmonic component of current density
k_{m}	piezoelectric coupling constant
\vec{k}	in-plane wave vector of a carrier before scattering
$ec{k}$ '	in-plane wave vector of a carrier after scattering
k_x , k_y , k_z	components of \vec{k} along x , y and z directions respectively
$K_{\scriptscriptstyle B}$	Boltzmann constant
L_x, L_y, L_z	dimensions of the semiconductor structure along x , y and z directions
	respectively
m_0	free mass of an electron
m^*	effective mass of an electron
m_1, m_2	effective mass of an electron along x and y directions respectively
$m_{ }^*$	effective mass of an electron parallel to the surface
m_{\perp}^{*}	effective mass of an electron perpendicular to the surface
\overrightarrow{M}	reciprocal effective mass tensor of an electron
$M\left(\vec{k},\vec{k}'\right)$	matrix element for scattering by crystal imperfections
non-deg, nd	non-degenerate

 N_c effective density of states in the conduction band

 N_i , n_{2D} , n surface layer concentration

 N_i^B background ionized impurities density

 N_i^r remote ionized impurities density

 $N_{\vec{q}}, N_{\vec{o}}$ phonon population

pz Piezoelectric

 $P(E_{\vec{k}})$ net scattering rate of an electron

 $P_i(E_{\vec{k}})$ scattering rates of an electron for the ith scattering

 \vec{q} two-dimensional phonon wave vector

 \overrightarrow{Q} three-dimensional phonon wave vector

 q_z transverse component of phonon wave vector

 \vec{r} position vector

rm remote impurities sr surface roughness

 $S(\vec{q})$ screening factor

 T_e effective electron temperature

 T_L lattice temperature

 u_l average acoustic velocity

 u_{th} average thermal velocity of an electron in thermodynamic equilibrium

 $(=E_{\vec{k}}/K_{\scriptscriptstyle B}T_{\scriptscriptstyle L})$

 $X = \left(=\hbar\omega_{\overline{O}}/K_{\scriptscriptstyle B}T_{\scriptscriptstyle L}\right)$, normalized phonon wave vector

 α screening length

 $\beta_1 \qquad \left(=1-K_BT_L/E_F\right)$

 $\beta_2 \qquad \left(=1+K_BT_L/E_F\right)$

 γ_n roots of the equation $A_i(-\gamma_n) = 0$

 $\delta(x)$ Dirac delta function

average height of the roughness in the z-direction Δ $E_{\vec{\imath}}$ energy of a carrier in the wave vector state \vec{k} before scattering energy of a carrier in the wave vector state \vec{k} ' after scattering $E_{\vec{k}}$ $E_{\scriptscriptstyle F}$ Fermi energy E_{ϱ} energy bandgap E_{e} $(=K_{\scriptscriptstyle R}T_{\scriptscriptstyle \varrho})$ $(=K_BT_L)$ E_L E_{ph} phonon energy energy eigenvalue of the nth subband E_n energy of the lowest subband E_0 permittivity of the material \in_{sc} η efficiency of second harmonic generation $(=\varepsilon_F/K_BT_L)$, normalized Fermi energy $\eta_{\scriptscriptstyle D}$ de Broglie wavelength λ de Broglie wavelength of free electron λ_0 spatial extent of the roughness in the direction parallel to the interface Λ θ angle between \vec{k} and \vec{E} $\theta_{\!\scriptscriptstyle ec k}$ angle between the states \vec{k} and \vec{k} ' $heta_{ec{k}ec{q}}$ angle between \vec{k} and \vec{q} $\mu_{\it eff}$ effective mobility μ_0 low-field mobility $(\mu_0)_{ac}$ low-field mobility for interaction with the deformation potential acoustic phonons low-field mobility for interaction with the piezoelectric acoustic phonons $\mu(\varepsilon)$ high-field mobility ρ_{v} volume mass density

electrical conductivity

 σ

 $au, au_{\it eff}$ effective relaxation time of the collision

 τ_e energy relaxation time

 τ_m momentum relaxation time

 $\tau_n = \left(= \tau_{acm} / \tau_{pzm} \right)$

 $\phi(z)$ surface potential

 $\psi_{\vec{k}}$ wave function of the electron

 $\psi_{1e},\;\psi_{2e}$ wave functions of the ground state and next higher energy state of the

electron respectively

 $\Psi_{F-H}(z)$ Fang-Howard wave function

 ω angular frequency

 $\omega_{\scriptscriptstyle B}$ $\left(=eB/m_{\scriptscriptstyle \parallel}^*\right)$ cyclotron resonance frequency

 $\omega_{ec{q}}$ frequency of lattice vibration for any wave vector \vec{q}

 $\omega_{\!\scriptscriptstyle ec{Q}}$ frequency of lattice vibration for any wave vector \overrightarrow{Q}

List of Publications

LIST OF PUBLICATIONS

- [1] **S. Saha,** S. Mukhopadhyay, D. P. Bhattacharya, Effects of inelastic interaction of the non-equilibrium electrons with the neutral impurities on the non-ohmic characteristics of a compensated semiconductor compound at Low Lattice Temperatures, *Physica B: Condensed Matter*, 608 (2021) 412758.
- [2] **S. Saha,** S. Mukhopadhyay, D. P. Bhattacharya, Effect of Energy Loss due to 1s-2p Excitation and Ionization of Neutral Impurites on the Non-Ohmic Characteristics of a Compound Semiconductor at Low Lattice Temperature, *Das N.R., Sarkar S. (eds) Computers and Devices for Communication. CODEC 2019. Lecture Notes in Networks and Systems, Vol 147. Springer, Singapore.*
- [3] S. Saha, B. Roy, A. Basu, S. Mukhopadhyay, Microwave Harmonic Generation by Non Ohmic Ensemble of Carriers in Compound Semiconductors at Low Lattice Temperatures (Communicated).

Seminar, Symposium, Conferences and Awards

Conference/Seminar attended

- [1] National Conference on Condensed Matter Physics 'Condensed Matter Days-2019' (CMDAYS19) at Department of Physics, Vidyasagar University, Midnapore-721102, West Bengal, India held on August 29-31, 2019 at Vidyasagar University, Midnapore, West Bengal, India
- [2] 7th International Conference on Computers and Devices for Communication (CODEC-2019) Organized by Institute of Radio Physics and Electronics, University of Calcutta. Held on 19-20 December, 2019 at Hotel Vivanta, Kolkata, India.