STATISTICAL- KINETIC THEORY OF CHARGE CARRIERS TRANSPORT IN SEMICONDUCTORS

BY

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Declaration

I certify that this thesis submitted for the degree of physics is the result of my own research, except master of where otherwise acknowledged, and that this thesis (or any part of the same) has not been submitted for a higher degree to any other university or institution .

Signed........................

(Amani M.K. Drabe'a)

Date..........................

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ABSTRACT

This thesis presents a semiclassical microscopic approach based on the Boltzmann transport equation for studying electrical and thermal properties of semiconductors. The relaxation-times are investigated through a microscopic model that incorporates the Boltzmann collision term with the relaxation-time approximation.

Thermal conductivity and thermal mobility are calculated as well as their temperature and density dependencies. The electronic contribution to the thermal conductivity of semiconductor materials is due to heat being transported by charge carriers, which are electrons in the n-type semiconductors or holes in the p-type material. The charge carriers also act as scattering centers for phonons and cause a reduction in lattice thermal conductivity. At temperatures sufficiently high to excite carriers across the semiconductor energy gap, the electron-hole pairs transport heat and give rise to the bipolar contribution to the thermal conductivity.

At low concentrations electrons and holes in a semiconductor do not significantly influence the thermal conductivity. Their contribution to the energy flux is typically less than the phonon contribution by a factor of 10^{-4} or less. In addition, the electron-phonon scattering does not contribute significantly to phonon relaxation and the thermal conductivity

Is much like that of an insulator . On the other hand, if the esmiconductor is heavily doped and the temperature is high the material then behaves more like a metal .

The electric thermal conductivity and the electric mobility are calculated and their temperature and density dependencies are also examined. The electronic contribution to thermal conductivity k is significant at very low doping levels but becomes increasingly important as the doping levels are increased . A good agreement with experimental and previous results is achieved. The AC conductivity exhibits also a temperature dependence.

The numerical calculation of the collision term are the most important part of the investigation. They involve three-and five-dimensional integrations evaluated by using Gaussian and Simpson's numerical methods.

To my mother and my husband

(STATISTICAL-KINETIC THEORY OF CHARGE CARRIERS TRANSPORT IN SEMICONDUCTORS)

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Chapter One

Introduction and Purpose

1.1 Introduction

A semiconductor is a crystalline solid, such as silicon (Si) or germanium (Ge), with an electrical conductivity, σ_{elc}, (typically 10^{5}-10^{-7} simens per meter) at room temperature intermediate between that of a conductor (up to 10^{9} s/m) and an insulator (as low as 10^{-15} s/m) (Broply, 1977). Besides, the electrical resistivity, ρ, values of semiconductors are also found to be intermediate between those of metals and those of insulators, generally in the ranges 10^{-4}-$10^{7}\Omega$.m at room temperature. Semiconductor elements form the fourth column in the periodic table.

As the atoms in the crystalline solid become close together, orbits of their electrons overlap and their individual energy levels are spread out into energy bands (Hagelberg, 1973). A general model for the energy levels of semiconductor consists of a series of allowed energy bands (conduction) alternating with forbidden energy bands (valence). The conduction and the valence bands are separated by an energy gap with the localized states corresponding to donor and acceptor impurities existing near the band edges. The band structure for an ideal semiconductor is shown in Figure 1.1.

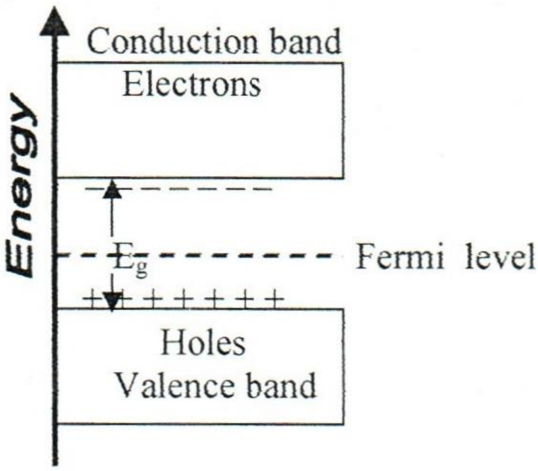


Figure 1.1. Energy level diagram for an intrinsic semiconductor. At room temperature some electrons are excited to the conduction band, leaving a hole behind. Energy levels in between the valence and conduction bands are not allowed to the electrons. The Fermi level lies at the middle of the forbidden band.

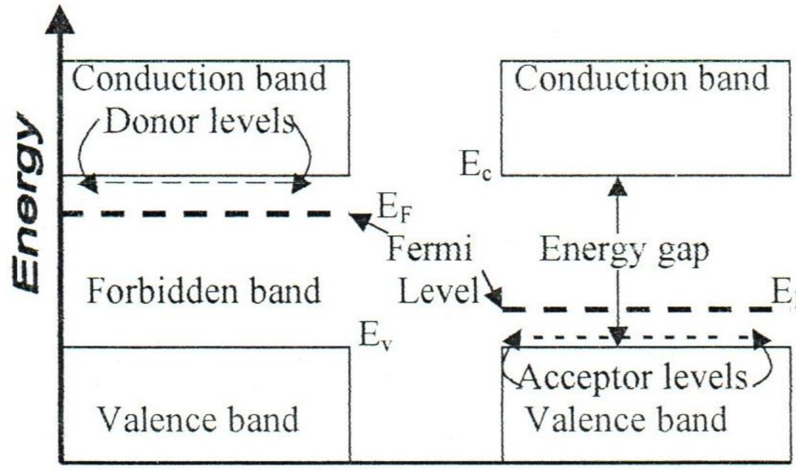
Such an arrangement of energy levels is a characteristic of semiconductors, which are insulators at 0 K and become poor conductors at some higher temperatures.

Conduction occurs in semiconductors as the result of a net movement of electrons in the conduction band and holes in the valence band, under the influence of thermal excitation or an applied electric and magnetic fields. Thermal agitation gives some electrons enough energy to jump to conduction band. The excited electrons serve as conduction electrons. Each electron raised to the conduction band leaves a vacancy, or a hole, in the valence band. The resulting holes are available for conduction in the valence band. A hole behaves as if it was an electron with a positive charge. Electrons and holes are known as charge carriers in semiconductors. The type of the charge carrier that predominates in a particular region or material is called the majority carrier, and that with the lower concentration is the minority carrier.

As the temperature is increased semiconductors become steadily better conductors because more electrons are transferred to the conduction band. The minimum energy required for moving an electron from one of the valence bands into one of the conduction bands is called the energy gap, E_g, (Kittle, 1993). In other words, the energy gap is energy between the valence and conduction band. In this case the conduction band lies a small amount of energy above the full valence band typically 1eV (Broply, 1977). Generally, the band energy for a pure semiconductor is between 0.1 and 2.5 eV. For silicon, E_g is 1.09 eV and for germanium it is 0.72 eV. These energy values are small enough for a significant number of electrons to be excited to the conduction band at room temperature.

Semiconductors are classified into intrinsic and extrinsic ones. In intrinsic semiconductors the charge carriers are electron-hole pairs resulting from thermal excitation or optical excitation and are equally divided between electrons and holes. On the other hand, in extrinsic semiconductors the type of conduction that predominates depends on the number of the impurity atom present in the valence band. Germanium and silicon atoms have a valence of four electrons, which form four covalent bonds with neighboring atoms. The structure of pure Ge crystals has the semiconductor arrangement of energy states which consists of a completely filled energy band separated from an empty higher-lying conduction level by a small energy gap, E_g, as shown in Figure 1.2.

When impurity atoms with a valence of five electrons, such as arsenic, antimony, or phosphorous is added to the lattice, an extra electron per atom available for the conduction, i.e., a single electron which is not supposed to pair with the four valence electrons of the germanium or the silicon. The n-type semiconductor is an extrinsic semiconductor doped



(a) (b)

Figure 1.2. Isolated energy level are introduced in the forbidden energy band of semiconductor by doping it with impurity atoms. (a) Donor atoms give levels just below the conduction band and raise the Fermi level above the middle of the forbidden band. (b) Acceptor atoms introduce levels just above the valence band and lower the Fermi energy below the middle of the forbidden band.

with atoms having a valence of five electrons and having electrons as