NUMERICAL CALCULATIONS OF IMPURITY SCATTERING MOBILITY IN SEMICONDUCTORS

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Novel semiconductor-base nanotechnology is gradually moving into new applications in the world economy. Semiconductor application requires increasing of investigations in the direction of their properties. The primary criterion of semiconductor suitability for use in semiconductor devices is its electrical properties, particularly current carriers mobility. Therefore, the problem connected with the explanation of the experimental results of current carriers mobility on the base of theoretical formulas is very urgent. In the present paper current carriers mobility due to ionized impurity scattering is discussed and calculated using numerical methods. Calculations have been done for different temperatures and different range of current carriers concentration in InAs.

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Introduction

An integral part of the new technologies, among them nanotechnology, are semiconductor devices. They have no alternative because of the economy in electric power consumption, compactness of the equipment on accounts of the extraordinary density of element packing in circuits, longevity, full automation, simplicity in operation, duration of activity without maintenance, high reliability, and so on. As dimensions of devices shrink to the nanometer range, the range of their applications broadens. Wherein the principle of functioning of all semiconductor devices is determined by the electrical properties of the active part of devices-semiconductor material, in particular, by the charge carriers mobility. Mobility determines the process of directed motion of charged particles in a semiconductor under the action of an electric field and gives enormous information about investigated materials. Therefore, a great practical and theoretical interest is the study of those processes that occurs when an electric field is applied to charge carriers. In this case, the charge carriers are in nonequilibrium conditions and transport phenomena arise that are related to the directional displacement of the charge carriers. There are several theoretical approaches to the study of transport phenomena.[1,2] The most common among them is the method of the Boltzmann kinetic equation, by means of which it is possible to calculate the mobility of charge carriers. An essential feature of nonequilibrium processes is that they depend substantially on the mechanism of interaction of the current carriers in the solid-state system, namely, their scattering by lattices such as atomic vibrations, impurity ions, etc.

The calculation of mobility components is needed not only in the study of the theory of semiconductors but at the explanation of the experimental results of investigated transport phenomena in semiconductors. However appropriate components of mobility are expressed by very complicated formulas and their treatment requires a lot of time. In the age of computer technology, it is reasonable and necessary to use modern software tools, a universal package for analyzing and managing databases, developing custom applications, containing a wide range of analysis procedures for use in scientific research in order to interpret the experimental results obtained with high accuracy. Therefore, the goal of our paper is to calculate impurity scattering mobility numerically.

Theoretical introduction to ionized impurity scattering

Of all possible scattering mechanisms of current carriers in semiconductors, scattering on ions of impurities practically always takes place in all semiconductors. The only exception is the very low temperatures near the temperature of the liquid helium. The electrical properties of semiconductors are determined by the presence of donor or acceptor impurities introduced into it. The reason is that impurity conductivity, as a rule, far exceeds the own conductivity of the semiconductor. The intrinsic conductivity of semiconductors is usually small, since the number of free electrons, for example, at room temperature is of the order of 10^{13}–10^{14} cm^{-3}. At the same time, the number of atoms in $1cm^3$ is ~10^{23} atoms.

Impurity centers can be atoms or ions of chemical elements embedded in the lattice of a semiconductor, excess atoms or ions implanted in the interstices of the lattice and various other defects and distortions in the crystal lattice (empty knots, cracks, shifts arising when deformations of crystals, etc.). The technique of semiconductor devices requires semiconductors both of maximum purity and doped. As the degree of doping increases, the density of the current carriers increases. At low impurity concentrations, due to the considerable distance between the impurity atoms, there is no interaction between them. Impurities form local states in the forbidden band. Because of the small number of charge carriers in the allowed band, they obey to the Boltzmann statistics. When the degree of doping is increased, the distance between impurity atoms is reduced, that leads to interaction between them, overlapping

of wave functions of charge carriers. The law of the charge carrier distribution with respect to energies in the impurity band and the allowed zones obey to the statistics somewhat between Boltzmann and Fermi–Dirac.[1–3] A substantial increase in the concentration of impurities leads to the confluence of the impurity band with the allowed band, and an allowed zone is formed.

In this case, a large concentration of charge carriers obeys to the Fermi-Dirac statistics and the gas of such particles is called degenerate. Thus, the properties of the electron gas significantly differ in undoped and doped semiconductors. The reduced Fermi level ξ defines the degeneracy criteξrion. A clear division into degenerate and non-degenerate charge carrier gases is conditional and depends on the temperature. As the temperature increases, when the intrinsic conductivity appears, the particles distribution in the electron gas will approach to Boltzmann statistics and, conversely, as the temperature decreases, the particles distribution will increasingly differ from Boltzmann's. It is interesting that in semiconductors the charge carriers gas becomes degenerate at low temperatures. It is accepted to assume with error 8 %, that $\xi = -2$ is the degeneracy boundary for charge carrier gas between degeneracy and no degeneracy state. At $\xi < -2$ the charge carrier gas is nondegenerate, at $\xi < -2$-degenerate. Different physical phenomena are differently sensitive to the form of the charge carrier distribution, and hence to the boundaries of degeneracy and will be ascribed differently by Fermi levels.

There exist many essential classical research works of Conwel and Weisskopf, Brooks–Herring (taking into account a screening effect), which considered the process of electron scattering by impurity centers in semiconductors.[4,5] However, these models are valid for charge carriers gas of noninteracting particles, which obey to the classical Maxwell-Boltzmann statistics and the charge carriers gas is non-degenerate. The impurity scattering in the case of non-degenerate charge carriers gas has been discussed by Mott.[6] However, often, impurity scattering has to be considered when it is not known when charge carriers gas is either degenerate or non-degenerate. Fortunately, there exists a Mansfield model for charge carriers scattering by impurity centers in semiconductor, which is valid for any distribution either degenerate or non-degenerate gas of current carriers in energy.[7] That is why in given work Mansfield model has been programmed.

Methodology

The expression of ionized impurity scattering mobility is:[6]

$$\mu = \frac{32\varepsilon^2 m^* (kT)^3 F_2(\xi)}{n^2 e^3 h^3 f(x)} \quad (1)$$

where

$$f(x) = \ln(x+1) - \frac{x}{x+1} \quad (2)$$

$$x = \frac{\eta (kT)^{1/2} \varepsilon_0 h}{e^2 (2m^*)^{1/2} F'_{1/2}(\overline{\eta})} \quad (3)$$

$$F'_{1/2}(\xi) = \frac{dF_{1/2}(\xi)}{d\xi} \quad (4)$$

In order to find the mobility values at different temperatures and for different concentrations of the current carriers, it is necessary first to calculate the reduced Fermi levels determined from the formula:

$$n = \frac{4\pi (2m^* kT)^{3/2} F_{1/2}(\xi)}{h^3} \quad (5)$$

where n is the charge carriers concentration, and -$F_{1/2}(\xi)$ integral Fermi.

From (5) equitation we derive:

$$F_{1/2}(\xi) = \frac{nh^3}{4\pi (2m^* kT)^{3/2}} \quad (6)$$

When the current carriers concentration is known at a given temperature and given effective mass, for finding the parameter ξ, it is necessary to solve the equation (6). For this, we transform it into:

$$F_{1/2}(\xi) - \frac{nh^3}{4\pi (2m^* kT)^{3/2}} = 0 \quad (7)$$

or

$$f(\xi) = 0 \quad (8)$$

where

$$\frac{nh^3}{4\pi (2m^* kT)^{3/2}} \equiv c, \; F_{1/2}(\xi) - c = 0, \; f(\xi) \equiv F_{1/2}(\xi) - c.$$

A solution of equation (8) gives the value of ξ parameter. We used the bisectors numerical method for the solution of (8) equitation. All programs were written in Matlab.

To calculate mobility (1) it is necessary to calculate another unknown parameter $\overline{\eta}$ which is in (3) equitation and it needs to solve transcendental equation (9) to find the value of $\overline{\eta}$:

$$(\overline{\eta} - 3) e^{\overline{\eta} - \xi} = (\overline{\eta} + 3). \quad (9)$$

After calculation of ξ parameter we can transform (9) equitation and define $\overline{\eta}$ using ξ value:

$$\xi = \overline{\eta} - \ln\left(\frac{\overline{\eta} + 3}{\overline{\eta} - 3}\right) \quad (10)$$

$$\overline{\eta} - \ln\left(\frac{\overline{\eta} + 3}{\overline{\eta} - 3}\right) - \xi = 0 \quad (11)$$

$$f(\overline{\eta}) = \overline{\eta} - \ln\left(\frac{\overline{\eta} + 3}{\overline{\eta} - 3}\right) - \xi \quad (12)$$

The root of the equation $f(\overline{\eta}) = 0$ gives the value of $\overline{\eta}$ which can be solved using the bisectors method.

The alternative way of solution of transcendental equation (9) is a graphical solution. But this method is not sufficiently accurate especially when we are interested in values of $\overline{\eta}$ at

meaning of arbitrary temperature and current carriers concentration. When solving (12) equitation, it is necessary to take into account that the equation is not defined in the region (–3, +3). These points need to be eliminated at the calculation by this method.

Results

As an example, the electrons mobility of *n*-InAs has been considered using this software. InAs is one of the semiconductors currently widely used in modern electronics and nanotechnology in the form of high-speed transistors and integrated circuits, IR photodetectors, injection lasers, among them in nanostructure of nanowires, structures with quantum dots InAs, etc. The behavior of the mobility for *n*-InAs due to scattering processes on impurity ions and its relation to temperature and doping concentration has been revealed. For this reason, there has been calculated mobility for temperatures: 77, 150, and 300 K for different values of electrons concentration in the range of 10^{16}–10^{19} cm^{-3}. When the electrons concentration changes in this interval, current carriers distribution in energy changes from non-degenerate to degenerate gas state. Results of the calculation of variation of the current carrier mobility with the concentration of electrons at different temperatures for *n*-InAs are presented in Figures 1–3.

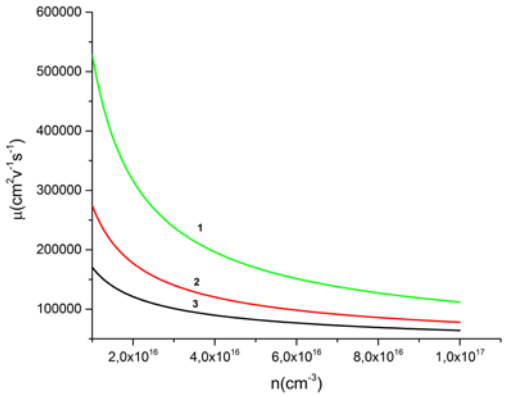

Figure 1. Calculated mobility due to scattering of electrons on impurity ions for electron concentration in the range of 10^{16}–10^{17} cm^{-3} at temperatures: 1 – 300 K, 2 – 150 K and 3 – 77 K.

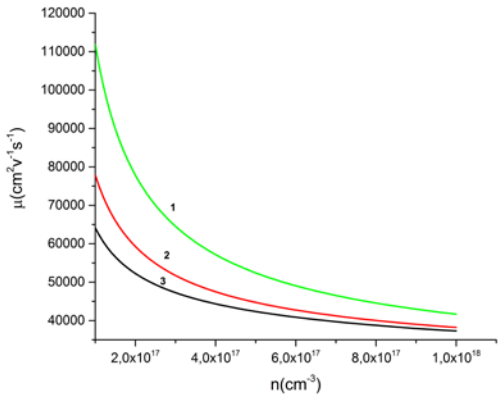

Figure 2. Calculated mobility due to scattering of electrons on impurity ions for electron concentration in the range of 10^{17}–10^{18} cm^{-3} at temperatures: 1 – 300 K, 2 – 150 K and 3 – 77 K.

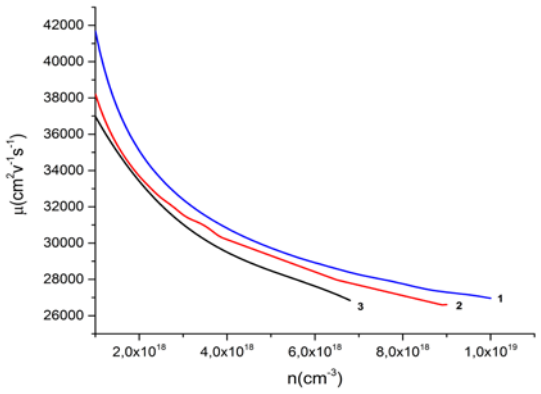

Figure 3. Calculated mobility due to scattering of electrons on impurity ions for electron concentration in the range of 10^{18}–10^{19} cm^{-3} at temperatures: 1 – 300 K, 2 – 150 K and 3 – 77 K.

It is clear that with rising temperature, mobility rises and with increasing of electrons concentration it falls. The results show that in experimental samples of InAs the impurities are all ionized in temperature range considered.[8]

The contribution of the scattering on the ionized impurity into the total scattering increases with increasing of impurity concentration. At n~$10^{17}$$cm^{-3}$ it is not still dominating. At the decrease of temperature below 300 K, the contribution of impurity ions in the scattering of carriers increases too. But with decreasing of T from 300 up to 77 K deionization of impurity levels takes place,

Comparison of experimental data of mobility in the InAs, containing an impurity in the range of 10^{16}–10^{19} cm^{-3} with the theoretical ones shows that, of all possible scattering mechanisms in InAs, the only combination of scattering on ionized impurities and optical phonons explains the experimental results in the temperature range.[8–10] The share of contribution of these scattering mechanisms into the total scattering is different at various temperatures and electrons concentration.

Conclusion

For interpreting the experimental results of current carriers mobility in semiconductors with high accuracy, there has been using modern software tools for numerical calculation of mobility due to impurity scattering. In given work model for mobility due to impurity scattering for the general case of any degree of degeneracy of the charge carriers has been programmed. The calculation has been made for the electrons mobility of *n*-InAs**.**

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