

Calculation of Electron Hall Mobility in GaSb, GaAs and GaN Using an Iterative Method

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Electron Hall mobility in GaSb, GaAs and GaN are calculated for different temperature, doping dependencies and compensation ratios. The two-mode nature of the polar optic phonons is considered jointly with deformation potential acoustic, piezoelectric, ionized impurity scattering. Band non-parabolicity, admixture of p functions, arbitrary degeneracy of the electron distribution, and the screening effects of free carriers on the scattering probabilities are incorporated. The Boltzmann equation is solved by an iterative method using the currently established values of material parameters. The agreement with the available experimental data is found to be satisfactory.

1. Introduction

GaSb, GaAs and GaN materials have very wide applications and have been used as various microwave devices such as field-effect transistors and for optoelectronic devices with tailored spectral response. As an aid to the device-related work, the transport coefficients of the materials need careful investigation [1-4]. Transport properties of electrons in GaSb, GaAs and GaN semiconductors can be conveniently derived by direct solution of the Boltzmann equation [5-6]. Previous applications of this technique were directed toward calculations of drift mobility in ideally pure semiconductors. There is also a considerable interest in accurate description of impure crystals, both from the experimental and the theoretical view points. In the former case, for example, one may take advantage of the sensitivity of mobility to ionized impurities in the analyses of impurity content. In the latter case, highly doped materials allow one to probe regions of the conduction band in the neighborhood of Fermi level, well above the band edge. Obviously, accurate calculation, in conjunction with the experimental data, are helpful in exposing weaknesses of the theoretical model, particularly with regard to electron scattering by ionized impurities at low temperatures. The purpose of the present paper is to calculate electron Hall mobility for various temperatures and ionized-impurity concentrations [7-9]. The formulation itself applies only to the central Γ valley conduction band. We have also considered the band non-parabolicity, admixture of p-type valence-band wave

functions, degeneracy of the electron distribution to any arbitrary degree, and the screening effects of free carriers on the scattering probabilities. All the relevant scattering mechanisms, including the two-mode nature of the polar optic phonon scattering, are taken into account. The Boltzmann equation is solved iteratively for our purpose, jointly incorporating the effects of all the scattering mechanisms. Our calculated results are compared with the available experimental data on both temperature and the free electron concentration dependence of mobility.

This paper is organized as follows. Details of the iterative model, the electron scattering mechanism which have been used and the electron mobility calculations are presented in Sec. 2 and the results of iterative calculations carried out on GaSb, GaAs and GaN structures are interpreted in Sec. 3.

2. Model details

In principle, the iterative technique gives exact numerical prediction of electron mobility in bulk semiconductors. To calculate mobility, we have to solve the Boltzmann equation to get the modified probability distribution function under the action of a steady electric field. Here, we have adopted the iterative technique for solving the Boltzmann transport equation. Under the application of a uniform electric field, the Boltzmann equation can be written as [10-13]

$$\left(\frac{e}{\hbar}\right)E \cdot \nabla_k f = \oint [s' f'(1-f) - s f(1-f')] dk \quad (1)$$

where, $f=f(k)$ and $f'=f(k')$ are the probability distribution functions and $s=s(k,k')$ and $s'=s(k',k)$ are the differential scattering rates. If the electric

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field is small, we can treat the change from the equilibrium distribution function as a perturbation which is first order in the electric field. The distribution in the presence of a sufficiently small field can be written quite generally as

$$f(k) = f_0(k) + g(k) \cos \theta \quad (2)$$

where $f_0(k)$ is the equilibrium distribution function, θ is the angle between k and E and $g(k)$ is an isotropic function of k , the function being proportional to the magnitude of the electric field. In general, contributions to the differential scattering rates come from two types of scattering processes, elastic scattering S_{el} , due to acoustic, impurity and piezoelectric phonons, and inelastic scattering S_{inel} , due to polar optic phonons

$$s(k, k') = s_{el}(k, k') + s_{inel}(k, k') \quad (3)$$

The polar phonon energy is high, especially in the case of GaAs and GaN materials [14]. Hence, this scattering process cannot be treated within the framework of Relaxation Time Approximation (RTA) because of the possibility of a significant energy exchange between the electron and the polar optic modes. In this case, S_{inel} represents transitions from the state characterized by k to k' either by emission [$S_{em}(k, k')$] or by absorption [$S_{ab}(k, k')$] of a phonon. The total elastic scattering rate will be the sum of all different scattering rates, which are considered as elastic processes, i.e., acoustic, piezoelectric and ionized impurity scattering. In the case of polar optic phonon scattering, we have to consider scattering-in rates by phonon emission and absorption as well as scattering-out rates by phonon absorption and emission. Using Boltzmann equation and considering all differential scattering rates, the factor $g(k)$ in the perturbed part of the distribution function $f(k)$ can be given by

$$g(k) = \frac{-eE \frac{\partial f_0}{\partial k} + \sum \int g' \cos \phi [s_{inel}'(1-f) + s_{inel} f] dk}{\sum \int (1 - \cos \phi) s_{el} dk + \sum \int [s_{inel}(1-f') + s_{inel}' f'] dk} \quad (4)$$

Note the first term in the denominator is simply the momentum relaxation rate for elastic scattering. It is interesting to note that if the initial distribution

is chosen to be the equilibrium distribution, for which $g(k)$ is equal zero, we get the relaxation time approximation result after the first iteration. We have found that convergence can normally be achieved after only a few iterations for small electric fields. Once $g(k)$ has been evaluated to the required accuracy, it is possible to calculate quantities such as the electron Hall mobility.

3. Results and discussion

Electron Hall mobility is an important parameter in determining the performance of semiconductor devices. Here we show the results of temperature and free electron dependence of the electron Hall mobility in bulk GaSb, GaAs and GaN materials using iteration method at low electric field applications. Important parameters used throughout the calculations are listed in Table 1, which are taken from Refs. [15,16].

Fig. 1 shows the calculated electron Hall mobility in bulk GaSb, GaAs and GaN materials as a function of temperature with free electron concentration of 10^{22} m^{-3} and with the electric field applied along one of the cubic axes.

It can be seen from the figure that the electron Hall mobilities at room temperature that we find for GaAs is $8300 \text{ cm}^2/\text{V-s}$, while those for GaSb and GaN are about 12000 and $1300 \text{ cm}^2/\text{V-s}$, respectively, for an electric field equal to 10^4 Vm^{-1} . The result plotted in Fig. 1 indicates that the electron Hall mobility of GaN is lower than other structure at all temperatures. This is largely due to the higher Γ valley effective mass in the GaN phase. Also, it can be seen that below 100 K , ionized impurity and piezoelectric scattering are the dominant forms of lattice scattering. The approximate $T^{-1/2}$ mobility dependence near 100 K signals the dominance of ionized impurity and piezoelectric scattering.

Fig. 2 shows the calculated variation of the electron Hall mobility as a function of free electron concentration for all crystal structures at room temperature. The mobility does not vary monotonically between free electron concentrations of 10^{20} m^{-3} and 10^{24} m^{-3} due to the dependence of electron scattering on free electron concentration, but shows a maximum near 10^{20} m^{-3} for all structures.

Table 1: Important parameters used in our calculations for GaSb, GaAs and GaN

Parameter	GaSb	GaAs	GaN
Band-gap (eV)	0.726	1.42	3.5
Electron effective mass (m^*)	0.041	0.063	0.18
Nonparabolicity (eV^{-1})	0.5	0.61	0.213
Static relative permittivity ϵ_0	15.7	12.5	9.5
Optical relative permittivity ϵ_∞	14.4	8.7	5.35
Density (kgm^{-3})	5610	5370	6150
Sound velocity (ms^{-1})	6070	5500	4330
Deformation potential (eV)	8.9	8.8	8.3
Piezoelectric constant (Cm^{-2})	0.08	0.05	0.375
Optical phonon energy (eV)	0.029	0.02	0.0995

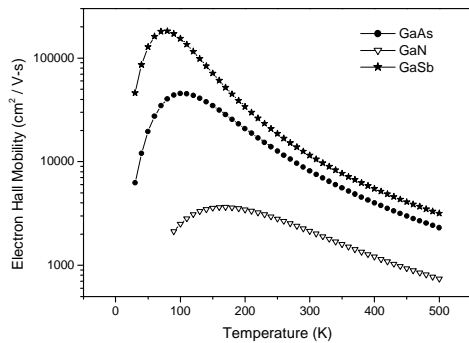


FIG 1: Electron Hall mobility versus temperature of pure intrinsic GaSb, GaAs and GaN. Impurity and piezoelectric scattering dominate the data below 100 K.

In many experimental situations, impurity concentrations are sufficiently high to limit the mobility. One can then use the mobility and free electron concentration determined by Hall measurements to calculate the donor and acceptor concentrations from figure 3. The electron Hall mobility at 300 K is plotted for several values of the compensation ratio $(N^+ + N^-)/(n + p)$. The compensation ratio equals zero for pure intrinsic material. Curves in Fig. 3, for the compensation ratio of unity, display a maximum value at $\sim 4 \times 10^{21} m^{-3}$, because the use of unity for the

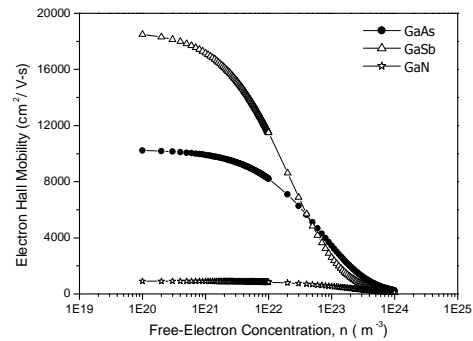


FIG 2: Calculated low-field electron Hall mobility of GaSb, GaAs and GaN as a function of different free electron concentration at room temperature.

compensation ratio ensures the presence of some acceptor impurities. Fig. 3 displays the expected experimental behavior wherein the compensation ratio increases with decreasing free electron concentration due to the presence of a fixed number of acceptor impurities.

The variation of the electron Hall mobility in GaN with temperature for various types of scattering mechanisms such as ionized impurity, acoustic phonon via deformation potential, piezoelectric scattering and polar optical phonon scattering individually.

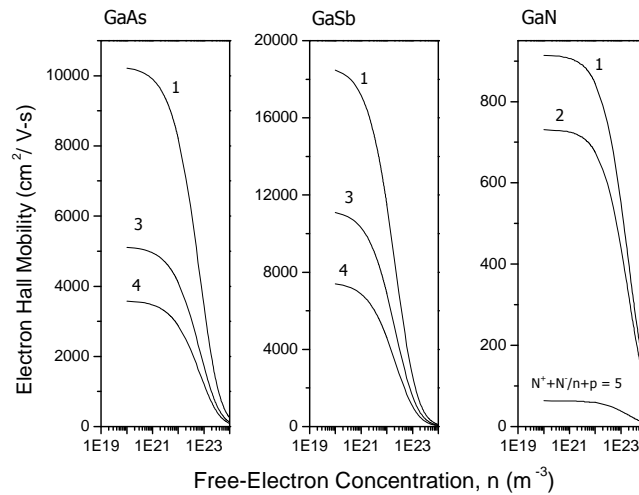


FIG. 3: Calculated low-field electron Hall mobility of GaSb, GaAs and GaN for different compensation ratios of 1, 3 and 4 for GaAs and GaSb and 1, 2 and 5 for GaN.

It is evident from this figure that at very high temperatures the mobility is limited by longitudinal optical phonon scattering, whereas the mobility varies inversely with donor concentration at low temperature, as we would expect from the foregoing discussion. The decrease in mobility at low temperature is caused in part by neutral impurity scattering. For the lowest doping concentration considered in this calculation, 10^{21} cm^{-3} , we find that the neutral impurity scattering plays a large role at low temperature because of the significant carrier freeze-out evident from Fig. 3.

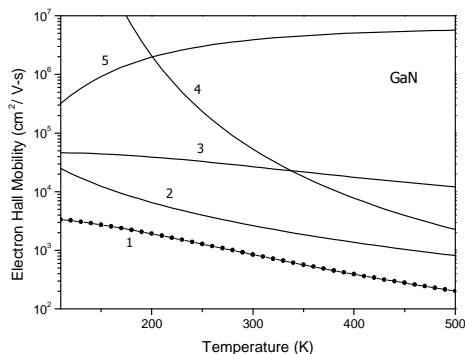


Fig. 4: Variation of electron Hall mobility with temperature for acoustic phonons via deformation potential (3), piezoelectric (2), ionized impurity (4), polar optical phonon (5) and with including all scattering processes (1) in GaN material.

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