

Numerical calculations of the electron mobility of n-GaN

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Calculations of the electron mobility of n-type GaN have been carried out at different temperatures using the relaxation time approximation method. In this temperature range a number of possible scattering mechanisms was discussed. Neutral impurity, ionized impurity and acoustic phonon scattering types were considered. The mobility due to piezoelectric acoustic phonon scattering was assumed to be negligible at high temperatures.

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1. Introduction

III-V compound semiconductors still provide the materials basis for a number of commercial technologies and applications. Gallium Nitride (GaN) is one of III-V semiconductors that has a direct band gap and considered as important material for high-power, optoelectronics and high temperature devices. It has also a valuable application in blue light emitting diodes and blue laser diodes [1]. The importance of GaN may be due to its relatively large band gap, strong bond strength and high breakdown voltage [2,3].

GaN is normally grown by molecular beam epitaxy (MBE), metal-organic chemical vapor deposition (MOCVD) or hybrid vapor phase epitaxy (HVPE) on a substrate. GaN is usually crystallizes in the wurtzite lattice (also known as hexagonal or α -GaN). However, under certain conditions, zinc blend GaN (sometimes referred to as cubic or β -GaN) can also be grown [4].

The main problem of GaN growth is the large lattice mismatch with the substrates. The best substrates used for GaN epitaxial growth are Sapphire with 13% lattice mismatch and SiC with 4% lattice mismatch [5]. Due to the large lattice mismatch between the epitaxial GaN and the substrate, dislocations are expected to be found near the interfacial layer. This actually influences the transport properties of the semiconductor due to possible scattering with the dislocations. Far away from the interfacial layer, dislocations may not be present and the material behaves as bulk substance free of dislocations.

In GaN, above room temperature, the dominant scattering mechanism is the polar optic phonon scattering mechanism. The others are ionized impurity scattering, acoustic phonon deformation potential scattering and acoustic phonon piezoelectric scattering mechanisms [6].

As a result of being elastic process of acoustic phonon deformation potential scattering, acoustic piezoelectric scattering and ionized impurity scattering, their mobilities can be calculated by the relaxation time approach.

In this work, numerical calculations of the electron mobility as a function of temperature for GaN

semiconductor of both wurtzite and zinc blend crystal structures are carried out. The relaxation time approximation is used in the simulation. Elastic scattering processes including acoustic phonon scattering (with the two modes deformation potential and piezoelectric) and ionized impurity scattering are considered in the investigation.

2. Theory

The electron mobility is determined by solving Boltzmann equation in the relaxation time approximation as [7]

$$\mu = \frac{e\langle\tau(\varepsilon)\rangle}{m^*} \quad (1)$$

where μ is the mobility, $\langle\tau(\varepsilon)\rangle$ is the average relaxation time over the electron energies (ε), e is the electronic charge and m^* is the effective mass of the electron. The standard formula for calculating the average relaxation time is given by [8]

$$\langle\tau(\varepsilon)\rangle = \frac{e}{m^*} \frac{\int_0^\infty \tau(\varepsilon) \varepsilon^{3/2} \frac{\partial f_o}{\partial \varepsilon} d\varepsilon}{\int_0^\infty \varepsilon^{3/2} \frac{\partial f_o}{\partial \varepsilon} d\varepsilon} \quad (2)$$

where f_o is the thermal equilibrium Fermi-Dirac distribution function.

Vibrations of the ions about their equilibrium positions produce change of the energy band and thus cause the scattering of electrons. This may be considered proportional to the change in lattice spacing and can be expressed by the induced strain $\vec{\nabla} \cdot \vec{U}(r,t)$. The interaction potential for acoustic phonon is written as

$$\vec{H} = E_1 \vec{\nabla} \cdot \vec{U}(\vec{r}, t)$$

where E_1 is the deformation potential. The corresponding scattering relaxation time can be written as

$$\tau_{dp}(\varepsilon) = \frac{\pi \hbar^4 \rho s^2}{\sqrt{2} E_1^2 m^{*3/2} k T} \varepsilon^{-1/2} \quad (3)$$

where ρ is the crystal mass density, k is Boltzmann constant, \hbar is Planck's constant and s is the average speed of sound.

Electrons can suffer scattering with piezoelectric mode of acoustic lattice vibrations. In this scattering mechanism, the relaxation time due to piezoelectric potential scattering is given by

$$\tau_{pe}(\varepsilon) = \frac{2\sqrt{2}\pi\hbar^2\rho s^2 \varepsilon^2}{e^2 h_{pz}^2 m^{*1/2} k T} \varepsilon^{1/2} \quad (4)$$

where h_{pz} is the piezoelectric constant and ε is the dielectric constant of the host material.

Carriers are scattered when they encounter the electric field of an ionized impurity. The potential due to an impurity charge in a crystal is screened depending on how many free carriers are present. The relaxation time due to scattering of ionized impurities is given by [8]

Table 1. Material parameters.

Parameter	Value		Reference
	zinc blend	wurtzite	
Electron Effective mass (m^*)	0.13 m_o	0.2 m_o	[9]
Static dielectric constant (ε)	9.7	8.9	[9]
Mass density (ρ)	$6.15 \times 10^5 \text{ g/cm}^3$	$6.15 \times 10^5 \text{ g/cm}^3$	[9]
Speed of sound (s)	$6.9 \times 10^5 \text{ cm/s}$	$7.96 \times 10^5 \text{ cm/s}$	[10,11]
Deformation potential (E_1)	21.8 eV	12 eV	[12]
Piezoelectric constant (h_{pz})	0.8	0.77	[9]

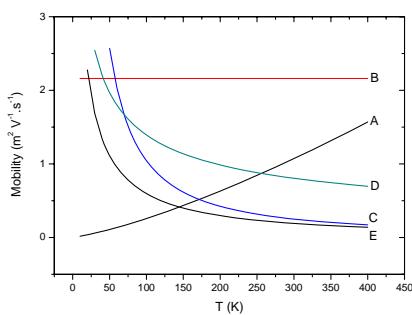


Fig. 1 Mobility versus temperature for GaN zinc blend crystal structure for different types of scattering mechanisms: ionized impurities (curve A), neutral impurities (curve B), deformation potential acoustic phonons (curve C), piezoelectric acoustic phonons (curve D) and resultant acoustic phonon scattering (curve E).

$$\tau_i(\varepsilon) = \frac{16\sqrt{2}\pi\varepsilon^2 m^{*1/2}}{N_i Z^2 e^4} F_i(\varepsilon) \quad (5)$$

where

$$F_i(\varepsilon) = \varepsilon^{3/2} \left(\ln(1 + A) - \frac{A}{1 + A} \right)^{-1}$$

and

$$A = \frac{24 \in m^* k^2}{\hbar^2 e^2 n} T^2$$

here, N_i is the concentration of the ionized impurities, and n is the density of free carriers.

3. Results and discussion

The parameters used in the calculations are shown in Table 1 for GaN with zinc blend and wurtzite crystal structures.

Fig. 1 shows the mobility versus temperature for GaN zinc blend structure in a temperature range up to 400 K for different scattering mechanisms including deformation potential acoustic phonon, piezoelectric acoustic phonon, ionized impurities and neutral impurities scattering mechanisms. In the simulations the ionized impurity concentration was taken as $4.7 \times 10^{20} \text{ m}^{-3}$ with excess carrier density of $9.5 \times 10^{19} \text{ m}^{-3}$.

The mobility due to piezoelectric acoustic phonon scattering is noticed to be greater than that of deformation potential. The combination between the two mobilities gives the effective mobility due to acoustic phonon scattering. The combination is simply given by Matthiessen's rule [7]

$$\frac{1}{\mu_{ac}} = \frac{1}{\mu_{ap}} + \frac{1}{\mu_{pe}} \quad (6)$$

The resultant mobility due to acoustic phonons is demonstrated in Fig. 1 (curve E). One can observe that it is close to the curve of deformation potential scattering at higher temperatures (curve C) and this may lead to ignoring the effect of the piezoelectric mode of acoustic phonons at high temperatures [13].

The electron mobility due to neutral impurities was also estimated. It is reported that when an electron passes

close to neutral atom, momentum can be transferred through a process in which the free electron exchanges with a bound electron on the atom. The mobility due to neutral impurity scattering is given by

$$\mu_{ni} = \frac{e^3 m^*}{80\pi N_n \epsilon \hbar^3} \quad (7)$$

where N_n is the concentration of the neutral impurities. The neutral impurity scattering process is a temperature independent and then the mobility associated to it is expected to be a constant through the material under consideration. In the case where the free carrier density is $9.5 \times 10^{19} \text{ m}^{-3}$, the density of neutral impurities is approximately $N_n = 3.8 \times 10^{20} \text{ m}^{-3}$. According to these data one can find the mobility due to neutral impurity scattering for zinc blend GaN as $2.16 \text{ m}^2/\text{V.s}$, see curve B in Fig. 1.

Fig. 2 illustrates the mobility variation with temperature for wurtzite GaN due to different types of scattering mechanisms. The same behavior as the zinc blend structure was noticed at all scattering types. The resultant mobility due to the two modes of acoustic phonon scattering was calculated. Neglecting the effect of piezoelectric scattering mechanisms at high temperatures was possible in this type of GaN structure.

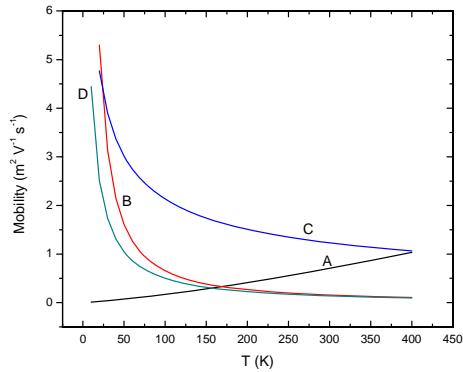


Fig. 2. Mobility versus temperature for GaN wurtzite crystal structure for different types of scattering mechanisms: ionized impurities (curve A), deformation potential acoustic phonons (curve B), piezoelectric acoustic phonons (curve C) and resultant acoustic phonon scattering (curve D).

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