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Effect of dislocation scattering on electron mobility in GaN

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ABSTRACT

This paper presents the calculation of electron mobility of GaN at various temperatures using Relaxation Time Approximation (RTA) method. The effect of dislocation scattering on electron mobility in GaN is studied. We have discussed about the role of important scattering mechanisms in GaN. The electron mobility values thus obtained are compared with other available experimental and theoretical results.

Keywords: Dislocation Scattering; Electron Mobility; Galium Nitride; Scattering

1. INTRODUCTION

Gallium Nitride, a direct bandgap semiconductor, has emerged as an important material for high-power, optoelectronic as well as for high temperature devices because of its large bandgap (3.4 eV), strong bond strength (2.3 eV/bond) and high breakdown voltage (3×10^6 V/cm) [1]. Recently the material has become more popular because of several new applications including blue light emitting diodes and blue laser diodes [2]. GaN is normally grown either by metal-organic chemical vapor deposition (MOCVD), molecular beam epitaxy (MBE) or hybrid vapor phase epitaxy (HVPE) on sapphire (Al_2O_3) or SiC substrate with large lattice mismatch. The most commonly used substrate is Al_2O_3 with 13.8% lattice mismatch and SiC substrate with 4% lattice mismatch. The large lattice mismatch with the substrate produces large amount of dislocation at the interfacial layer resulting very poor interface characteristic. As one moves away from the interfacial layer, the dislocation density decreases very fast. This means whole GaN epilayer consists of two layers which was suggested by D. C. Look *et al*. [3]. In order to calculate the mobility in n-type GaN, we have considered the two layer model. For bulk layer away from the interface the dominant scattering mechanisms are considered to be acoustic phonon scattering via deformation potential, piezoelectric coupling and non phonon scattering such as ionized impurity scattering and the neutral impurity scattering. On the contrary, the dominant scattering mechanism near the interfacial region is assumed to be dislocation scattering only. The electrical transport properties of the entire GaN epilayer would be influenced by dislocation scattering dominant near the interfacial region. Electron mobility in GaN and the effect of dislocation scattering on electron mobility in GaN were studied earlier by many researchers [3-7]. In this paper, we have considered all the important scattering mechanisms of GaN in more detail using RTA to obtain electron mobility and we have also shown the difference between the electron mobility with and without dislocation scattering.

2. THEORY

Solution of Boltzmann equation using RTA gives electron mobility as,

$$\mu = \frac{e\langle\tau\rangle}{m^*} \tag{1}$$

where, $\langle\tau\rangle$, is average relaxation time over the electron energies, μ is mobility and m^* is the effective mass of electron. The expressions of relaxation time and mobility caused by different scattering mechanisms are given in the following sections.

2.1. Ionized Impurity Scattering

The amount of scattering due to electrostatic forces between the carrier and the ionized impurity depends on the interaction time and the number of impurities. Larger impurity concentrations result in a lower mobility [8]. The standard formula for calculating the average relaxation time is

$$\langle\tau_{ii}(E)\rangle = \frac{e}{m^*}\frac{\int_0^\infty \tau_{ii}(E)E^{3/2}\frac{df_0}{dE}dE}{\int_0^\infty E^{3/2}\frac{df_0}{dE}dE} \tag{2}$$

Hence the mobility associated with ionized impurity

scattering is

$$\mu_{ii} = \frac{128\sqrt{2}\pi^{1/2}\varepsilon^2 (kT)^{3/2}}{N_I Z^2 e^3 m^{*1/2}\left[\ln(1+y) - y/(1+y)\right]} \quad (3)$$

where, $y = \dfrac{24\varepsilon m^* (KT)^2}{\hbar^2 e^2 n}$

2.2. Neutral Impurity Scattering

When an electron passes close to neutral atom, its momentum is transferred through a process in which the free electrons exchange with a bound electron on the atom. The relaxation time can be written as [9]

$$\tau_{ni}(E) = \frac{m^*}{20 N_n \hbar a_0} \quad (4)$$

The mobility associated with neutral impurity scattering is

$$\mu_{ni} = \frac{e}{20 N_n \hbar a_0} = \frac{e^3 m^*}{80\pi N_n \hbar^3 \varepsilon} \quad (5)$$

where, a_0 and N_n are the effective Bhor radius of donor and concentration of neutral impurities respectively.

2.3. Acoustic Phonon: Deformation Potential Scattering

The acoustic mode lattice vibration induces changes in lattice spacing, which vary the band gap from point to point. Since the crystal deforms at these points, the potential is called deformation potential. The corresponding relaxation time can be written as [10]

$$\tau_{dp}(E) = \frac{\pi\hbar^4 \rho s^2}{\sqrt{2} E_1^2 m^{*3/2} kT} E^{-1/2} \quad (6)$$

where ρ is crystal density, S is average velocity of sound and e_1 is deformation potential.

The mobility associated with deformation potential scattering is calculated as

$$\mu_{dp} = \frac{e\langle \tau_{dp} \rangle}{m^*} = \frac{2\sqrt{2}\pi^{1/2}\hbar^4 \rho s^2 e}{3E_1^2 m^{*5/2} (kT)^{1/2}} \quad (7)$$

For GaN acoustic deformation potential is 9.2 eV. [8].

2.4. Acoustic Phonon: Piezoelectric Scattering

The relaxation time is [10]

$$\tau_{pe}(E) = \frac{2\sqrt{2}\pi\hbar^2 \rho s^2}{(e h_{pz}/\varepsilon)^2 m^{*1/2} kT} E^{1/2} \quad (8)$$

where, $p = \left[\dfrac{h_{pz}^2}{\rho s^2 E}\right]$, Piezoelectric coupling co-efficient, hpz is the piezoelectric constant.

The mobility associated with Piezoelectric scattering is calculated as

$$\mu_{pe} = \frac{e\langle \tau_{pe}(E) \rangle}{m^*} = \frac{16\sqrt{2}\pi^{1/2}\varepsilon^2 \rho s^2 \hbar^2}{3e h_{pz}^2 m^{*3/2} (kT)^{1/2}} \quad (9)$$

At 300 K, the piezoelectric potential scattering rate is about five times smaller than the deformation potential rate [8].

2.5. Optical Phonon: Polar Scattering

For this scattering, τ is a function of the perturbation strength not a function of energy of the electrons. The relaxation time is [11]

$$\tau_{po}(E) = 2^{3/2}\pi \frac{\hbar^2 \left(e^{T_D/T} - 1\right) \chi(T_D/T)}{e^2 (kT_D) m^{*1/2} \left(\varepsilon_\infty^{-1} - \varepsilon^{-1}\right)} E^{1/2} \quad (10)$$

The corresponding mobility is calculated as

$$\mu_{po} = \frac{2^{9/2}\pi^{1/2}\hbar^2 (kT)^{1/2} \chi(T_D/T)}{3e(kT_D) m^{*3/2} \left(\varepsilon_\infty^{-1} - \varepsilon^{-1}\right)} E^{1/2} \quad (11)$$

where

$$\chi(T_D/T) = \frac{3\pi^{1/2}}{8}\left[\frac{T_D}{T}\right]$$

The mobility values are limited by the lattice phonon scatterings such as polar optical phonon scattering, acoustic-mode deformation potential scattering and piezoelectric potential scattering.

2.6. Dislocation Scattering

The major problem of GaN is unavailability of a lattice-matched substrate. The epitaxial growth of GaN on Al_2O_3 has a 13.8% lattice mismatch and a 34% mismatch in the thermal expansion coefficient. Dislocations are typically formed due to the large lattice mismatch of GaN with the substrates on which it is epitaxially grown (SiC and Sapphire). The relaxation time is [6]

$$\tau = \frac{8\varepsilon^2 a^2 m^{*2}}{N e^4 f^2 \lambda_D} \left(v_t^2 + \hbar^2/4m^{*2}\lambda_D^2\right)^{3/2} \quad (12)$$

where V_t is the component of V perpendicular to dislocation line, "a" is the distance between imperfection centers along the dislocation line and "f" is their occupation probability.

The mobility is calculated from the average equilib-

rium distribution function as,

$$\mu_{dis} = \frac{30\sqrt{2\pi}\varepsilon^2 a^2 \left(K_B T\right)^{3/2}}{e^3 f^2 \lambda_D m^{*1/2} N} \quad (13)$$

Since the reciprocal values of relaxation time resulting from different physical mechanisms are additive, the scattering caused by the change of dislocation in n-type semiconductors gives the dominant effect below the room temperature.

3. RESULTS AND DISCUSSION

Electron mobility considering various types of scattering mechanisms such as ionized impurity, neutral impurity, acoustic phonon via potential deformation, piezoelectric, polar optical phonon and dislocation scattering is calculated at different temperatures. **Table 1** shows the material parameters of n-type GaN used in our work. The dislocation density is 10^{15} m^{-2} and carrier concentrations in bulk and interfacial layers are taken as 1.3×10^{17} m^{-3}, 7×10^{24} m^{-3} respectively.

Figure 1 shows the variation of electron mobility with temperature for various types of scattering mechanisms. It is found that the acoustic phonon via deformation potential scattering plays a significant role in electron mobility calculation whereas the role of neutral impurity scattering is negligible. This agrees to the conclusions made by C. Erginsoy [9]. Ionized impurity scatterings dominate at low temperature whereas the lattice scattering dominate at high temperature and the corresponding mobility values are shown in **Figure 1**.

We have further investigated the temperature dependence of electron mobility to verify the dislocation scattering model. **Figure 2** shows the influence of dislocation scattering on the electron mobility in GaN. It is found that dislocation scatterings have minimum influence on electron mobility at low temperature. But however, the overall effect of dislocation scattering on electron mobility in GaN is not negligible which agree qualitatively with other experimental results [6]. The mobility approaches a $T^{-3/2}$ dependence due to phonon scattering at high temperature but at low temperature, the mobility is increasing monotonically with temperature depending on a $T^{-3/2}$ due to impurity scattering. Our results agree also with F. Djeffal *et al.* [19] who have calculated electron mobility at various temperature upto 800 K.

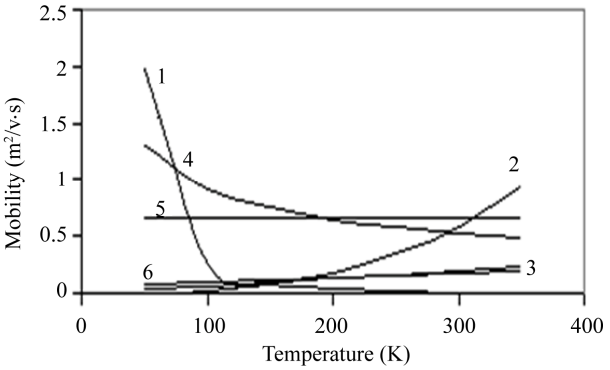

Figure 1. Variation of electron mobility with temperature for 1) acoustic phonon via deformation potential, 2) ionized impurity, 3) polar optical phonon, 4) piezoelectric potential, 5) neutral impurity and 6) dislocation scatterings. The dislocation density is 1015 m^{-2} and the carrier concentrations in bulk and interfacial layers are taken as 1.3×10^{17} m^{-3}, 7×10^{24} m^{-3} respectively.

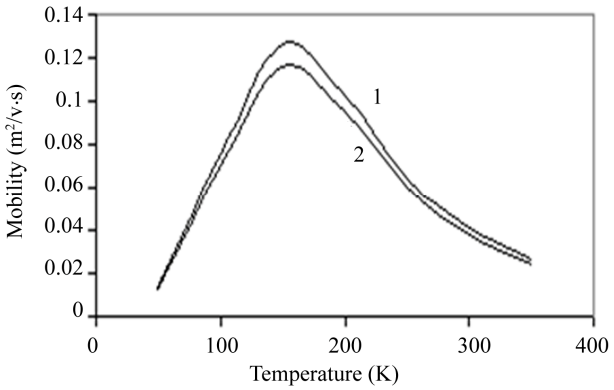

Figure 2. Variation of electron mobility with temperature in two-layer model considering 1) without Dislocation Scattering and 2) with Dislocation Scattering.

4. CONCLUSIONS

The electron mobility values in GaN obtained in this paper will be useful to study the conductivity characteristics of the devices based on this material. Scientists and Device engineers are always worried about the lattice mismatch in GaN crystal which reduces of efficiency of GaN based devices but sufficient study of this lattice

Table 1. GaN parameters used for mobility calculation.

Symbol	ε_∞	ε	T_{po}	ρ	S	h_{pz}	E_1	m^*
Value	5.47 ε_0	10.4 ε_0	1044 K	6.1×10^3 Kg·m^{-3}	6.59×10^3 m·s^{-1}	0.5 (0.375 - 0.6)	9.2 eV	0.22 m_0
Ref.	[12]	[13]	[14]	[15]	[14]	[16]	[17]	[18]

mismatch and the consequence of these studies can help them to obtain an accurate theoretical model.

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