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DISLOCATION SCATTERING-LIMITED ELECTRON MOBILITY IN WURTZITE n-TYPE GALLIUM NITRIDE

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The dislocation scattering-limited electron mobility (μ_{dis}) for wurtzite GaN was analytically calculated as a function of both temperature and carrier concentration. The calculated results indicated that μ_{dis} increases slightly by increasing the temperature in the range from 100-400 K. Moreover, as the dislocation density per unit area increases, μ_{dis} is lowered particularly at low temperatures. Calculation of the mobility as a function of carrier concentration at constant temperature showed that the dislocation limited mobility grows up when the carrier concentration increases. A large change of μ_{dis} was noticed by varying the fraction of the filled traps. The electron drift mobility was calculated considering many scattering centers, includingthe dislocation scattering mechanism. The results were compared with experimental data and it was found an agreement between the calculated electron mobility including dislocations with the experimental results particularly at low temperatures.

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Keywords: dislocation, electron mobility, filled trap, GaN.

1. Introduction

The electron mobility in semiconductors is basically determined by the existence of scattering processes. The scattering centers in the material depend on many factors such as impurity doping level, the structure of the material and the quality of growth fabrication [1].

The epitaxial growth of Gallium Nitride (GaN) on appropriate substrate is still one of the important points of research [2]. It was reported that the mismatch in the case of GaN-substrate system leads to a formation of high density dislocations in the order of $10^7 – 10^{11}$ cm^{-2} [3]. Even there is more than 12% lattice mismatch in the case of GaN and Sapphire while there is approximately 3.5% mismatch between GaN and SiC, these two substances are the most usable materials as substrates [4]. Thus, one of the important points in this field is to find a substrate where the lattice mismatch with the GaN epilayer is a minimum.

The effect of dislocation on transport properties of solids has been studied by many authors [3-13].The calculations have indicated that threading edge dislocations produce defect levels in the forbidden energy gap and constitute energy traps for the electrons.Empty trap is electrically neutral but when such trap is filled with electron, it is assumed to be negatively charged in n-type GaN and free carriers are scattered from these dislocations [4,6].

Weimann et al. [4] and Ng et al. [10] have investigated the role of dislocation in mobility. They have concluded that the decrease of the electron mobility at lower carrier concentrations is attributed to the scattering of electrons by charge threading dislocations. If the dislocations have an edge component, they introduce acceptor centers along the dislocation line which capture electrons from the conduction band in an n-type semiconductor. Other researchers have studied the temperature and impurity dependence of the electron mobility taking into account the scattering by dislocations [4,6].

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In the present work, the effect of dislocations on the electron mobility in Wurtzite GaN is discussed. Analytical calculations of the dislocation scattering-limited electron mobility are carried out as a function of temperature and carrier concentration.

2. Theoretical background

The presence of dislocations in n-GaN produces traps for electrons. Therefore, the dangling bonds through dislocations can be represented as negative line charge.The potential established by these charged dislocation traps were specified by many authors [5,7,11]. Two fundamental models have been proposed. The first model was suggested by Bonch-Bruevich and Glasko [14] and the other one by Read [15].

Bonch-Bruevich and Glasko (BG) obtained the potential at any position apart from dislocation center on the form:

$$V_{BG}(r) = \frac{1}{4\pi\varepsilon}\frac{2qf}{c}K_o\left(\frac{r}{\lambda_D}\right) \tag{1}$$

where $q$is the electronic charge, c is the basal lattice constant of wurtzite GaN, f is the fraction of filled traps$(0 \le f \le 1)$, ε is the dielectric constant of the material, K_o is the Bessel function of the second kind, the radius r being measured from the center of the dislocation, and λ_D is the Debye screening length given by;

$$\lambda_D = \sqrt{\frac{\varepsilon k_B T}{q^2 n}} \tag{2}$$

where k_B is the Boltzmann constant, T is the absolute temperature and n is the screening carrier concentration.

Podor [16] used this potential to calculate the electron drift mobility as:

$$(\mu_{dis})_{BG} = \frac{\hbar^3\varepsilon^2 c^2}{q^3 f^2 m^{*2}\lambda_D^4 N_{dis}}(1 + 4k^2\lambda_D^2)^{3/2} \tag{3}$$

where $\hbar$ is the reduced Planck's constant, m^* is the electron effective mass in GaN, k is the electron wave vector on the direction of the dislocation, and N_{dis} is the dislocation density per unit area.

Readmodel [15] assumed that the dislocation centers form a charged cylinder with effective radius R. The potential at any position $r < R$ is given by:

$$V_R(r) = \frac{1}{4\pi\varepsilon}\frac{qf}{c}\left[ln\left(\frac{R}{r}\right)^2 - 1 + \left(\frac{r}{R}\right)^2\right] \tag{4}$$

Using this potential, the dislocation scattering contribution to drift mobility is obtained as;

$$(\mu_{dis})_R = \frac{30\sqrt{2\pi}\varepsilon^2 c^2 (k_B T)^{3/2}}{q^3 N_{dis} f^2 \lambda_D \sqrt{m^*}} \tag{5}$$

The dependence of the mobility due to dislocation scattering on temperature in this model is greater than that of BG model.

3. Calculated results and discussion

The dislocation traps are not always filled. It depends on the density of dislocation and on the temperature.The dependence of the fraction of filled traps on temperature is weak, only through Fermi energy E_F. The fraction of filled traps is calculated using the following equations [8]:

$$E_T + E_F + E_o\left[3f\ln\left(\frac{f}{c\sqrt[3]{\pi N_i}}\right)\right] - 0.232\,f = 0 \tag{6}$$

$$E_o = \frac{q^2}{4\pi\varepsilon c} \tag{7}$$

$$E_F = E_g - \frac{k_B T}{q}\ln\frac{N_C}{n} \tag{8}$$

$$N_C = 2\left(\frac{2\pi m^* k_B T}{h^2}\right)^{3/2} \tag{9}$$

$$N_i = n + f\left(\frac{N_{dis}}{c}\right) \tag{10}$$

where E_T is the trap energy from the conduction band, E_o is the electrostatic energy between two charges, E_F is Fermi energy which is assigned for nondegenerate semiconductor, E_g is the energy gap for wurtzite GaN, N_C is the conduction-band effective density of states, h is Planck's constant and N_i is the density of ionized impurities.

Table 1 Material parameters of wurtzite GaN used in the calculations [8].

Parameter	Value
Electron effective mass (m^*)	$0.2\ m_o$ kg
Static dielectric constant (ε)	8.9
Average longitudinal elastic constant (C_{11})	$\mathbf{2.653 \times 10^{10}\ N/m^2}$
Basal lattice constant (c)	5.185 Å
Acoustic deformation potential ($\boldsymbol{E_d}$)	8.3 eV

Fig. 1 represents the calculated fraction of filled traps at different dislocation density as a function of carrier concentration. Calculations are made at room temperature. The parameters used in the calculation are listed in table 1. From the figure, it is noticed that the fraction of filled traps increases by increasing of the dislocation density. It is also noticed that at high carrier concentrations (greater than 10^{23} m^{-3}) the fraction of filled traps decreases by decreasing of carrier concentration. At low range, f decreases slowly by decreasing of carrier concentration and then it tends to be nearly constant particularly at high dislocation density. These results agree with that obtained by Weimann et al. [4].

The relationship between the concentration of ionized impurities and carrier concentration at different dislocation density is depicted in Fig. 2. This relationship is calculated using equation 10 at $f = 0.5$. It is concluded from the figure that all carriers are trapped in the case that the ionized impurity concentration is less than the trap density. The same relationship is plotted in Fig. 3 at different fraction of filled traps and constant dislocation density at $N_s = 10^{13}$ m^{-2}.

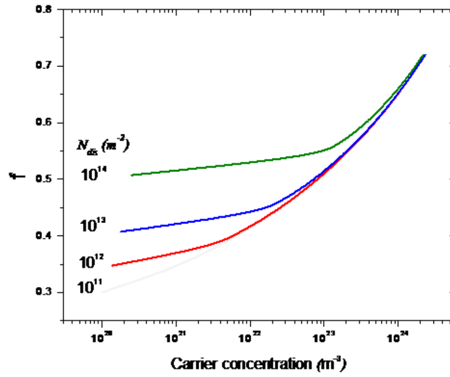

Fig. 1: The fraction of filled traps as a function of carrier concentration for n-GaN. The curves are calculated using equations (6-9) and the constants listed in table 1.

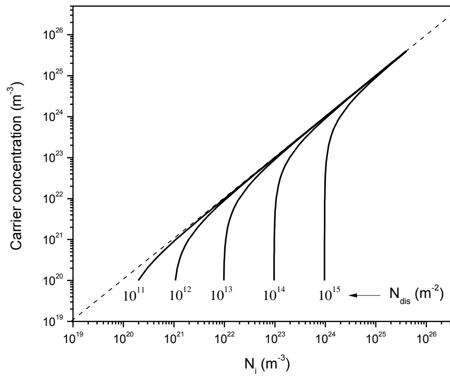

Fig. 2: Relationship between ionized impurity concentration and free carrier concentration of n-GaN at different dislocation density. The calculations are carried out using equation 10 and constants listed in table 1 at fraction of filled trap $f = 0.5$.

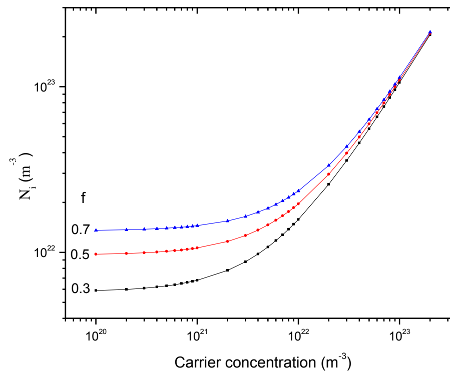

Fig. 3: Relationship between ionized impurity concentration and free carrier concentration of n-GaN at different values of the fraction of filled traps at dislocation density $N_s = 10^{13}$ m^{-2}.

The mobility due to dislocation scattering for n-type GaN using Read approach [15] is calculated using equations 2 and 5 and the parameters listed in table 1. The model of Read for mobility estimation is temperature dependent. Such dependence comes directly from equation 5 and also from the temperature dependent Debye screening length. Fig. 4 shows the calculated dislocation scattering-limited electron mobility of GaN at a different dislocation density in the

temperature range from 100 to 400 K. As the temperature is raised the mobility increases slightly, while it noticeably decreases by increasing of the dislocation density. A weak temperature dependence of μ_{dis} is recorded, but strong dislocation density dependence is assigned. This could be attributed to the fact that the dislocation traps act as Coulomb scattering centers which results in a decrease of the electron mobility [8].

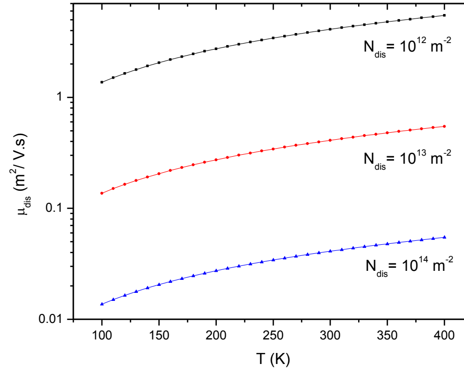

Fig. 4: Calculated dislocation scattering-limited electron mobility of GaN at a different dislocation density in the temperature range from 100 to 400 K using equations 2 and 5 and values listed in table 1.

The carrier concentration dependent electron mobility due to dislocation scattering at room temperature is depicted in Fig. 5. The calculations are carried out at two different dislocation density; 10^{13} and 10^{14} m^{-2} and fraction of filled traps = 0.5. A large increase in μ_{dis} by increasing of the carrier concentration is noticed particularly at $N_{dis} = 10^{13}$ m^{-2}. The same results are obtained in Fig. 6 where μ_{dis} versus carrier concentration is plotted at room temperature and different f but constant dislocation density.

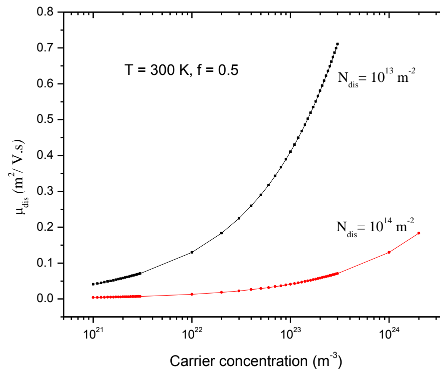

Fig. 5: Electron mobility due to dislocation scattering versus carrier concentration at room temperature and two different dislocation densities; 10^{13} and 10^{14} m^{-2}. The fraction of filled traps is taken as 0.5.

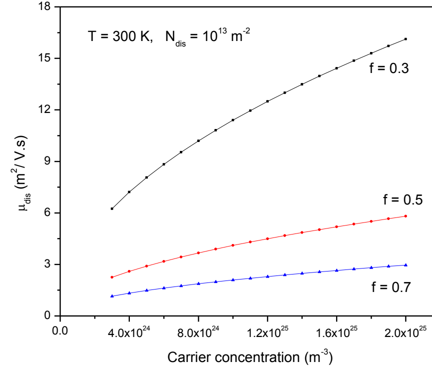

Fig. 6: Electron mobility due to dislocation scattering versus carrier concentration at room temperature and different fraction of filled traps. The dislocation density is fixed at $N_{dis} = 10^{13}$ m^{-2}

In order to investigate the influence of dislocation scattering on the electron mobility in wurtzite GaN, electron drift mobility is calculated taking into account the dislocation scattering. Many different elastic scattering mechanisms that affect the mobility are considered. These scattering sources are the ionized impurities, acoustic phonon scattering. The mobility due to ionized impurities is calculated from the expression [17];

$$\mu_i = \frac{64\pi^{1/2}\varepsilon^2(2k_BT)^{3/2}}{N_i q^3 (m^*)^{1/2}} \left\{ ln \left[1 + \left(\frac{12\pi\varepsilon k_B T}{q^2 N_i^{1/3}} \right)^2 \right] \right\}^{-1} \tag{11}$$

The acoustic phonon-limited electron mobility is calculated from the equation [17];

$$\mu_{ac} = \frac{q(8\pi)^{1/2}\hbar^4 C_{11}}{3E_d^2 (m^*)^{5/2} (k_B T)^{3/2}} \tag{12}$$

Here E_d is the acoustic deformation potential.
Using equations 5, 11 and 12, the total electron mobility μ_T is calculated from the equation:

$$\frac{1}{\mu_T} = \frac{1}{\mu_{dis}} + \frac{1}{\mu_i} + \frac{1}{\mu_{ac}} \tag{13}$$

Fig. 7 shows the plot of total electron mobility versus temperature in the range from 100 to 400 K. The line curve represents the calculations taking into consideration the dislocation scattering (equation 13). The graph is compared with the calculations neglecting the dislocation scattering (dashed curve) and experimental results obtained from Ref. [8]. Calculations of Fig. 7 are carried out at $f = 0.6$, $N_{dis} = 9 \times 10^{12}$ m^{-2} and $n = 10^{25}$ m^{-3}. The value of the dislocation density is chosen to be the same value taken in the experimental work for comparison.

Fig. 7 obtains a peak behavior of the electron mobility with room temperature value μ_T = 800 cm^2/V.s. which is in good agreement with the results obtained by authors for samples grown by metal-organic chemical vapor deposition (700-950 cm^2/V.s) [18,19]. Inspection of Fig. 7 reveals that there is a good agreement between the calculations made by this model and that of the experimental work at low temperature range (up to 150 K) and a deviation is noticed at T grater than 150 K. This may be due to that the calculations did not consider the scattering by optical phonons which play a vital role in the mobility at high temperatures.

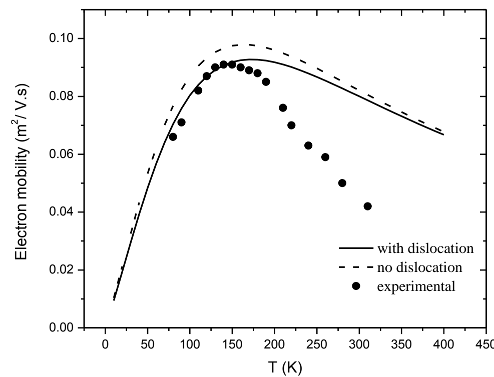

Fig. 7. Total electron mobility versus temperature in the range from 100 to 400 K. The line curve represents the calculations taking into consideration the dislocation scattering (equation 13). The dashed curve is calculations neglecting the dislocation scattering. The points represent experimental results obtained from Ref. [8]. Calculations are carried out at $f = 0.6$, $N_{dis} = 9\,x10^{12}\ m^{-2}$ and $n = 10^{25}\ m^{-3}$.

4. Conclusions

Analytical calculations of dislocation scattering-limited electron mobility was carried out for n-type wurtzite GaN in a temperature range up to 400 K using Read approximation. The mobility increases when both the fraction of filled traps and dislocation density increase. The temperature dependent total electron mobility due to scattering by ionized impurities, acoustic phonons and dislocations was found to be in a good agreement with the experimental results at low temperature range up to 150 K.

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