Dislocation Scattering in GaN

D. C. Look
Semiconductor Research Center, Wright State University, Dayton, Ohio 45435

J. R. Sizelove
Air Force Research Laboratory, Wright-Patterson Air Force Base, Dayton, Ohio 45433
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A theory of charged-dislocation-line scattering is developed within the framework of the Boltzmann transport equation. A fit of the theory to temperature-dependent Hall-effect data in GaN gives dislocation densities which are in excellent agreement with those measured by transmission electron microscopy. This work shows that threading edge dislocations in GaN indeed are electrically active, in agreement with recent theoretical predictions. [S0031-9007(98)08378-1]

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GaN, and its related ternary compounds involving Al and In, have received much attention over the past few years because of several new applications, including blue light-emitting diodes (LEDs), blue laser diodes (LDs) [1], and high-power microwave transistors [2]. However, one of the biggest problems to overcome has been the lack of a lattice-matched substrate, since bulk GaN is very difficult to grow in large sizes. So far, the substrate of choice has been sapphire (Al_2O_3), which has a 14% lattice-size mismatch and a 34% mismatch in the thermal expansion coefficient. Thus, epitaxial growth of (0001) GaN on Al_2O_3 leads to high concentrations (typically 10^9-10^{11} cm^{-2}) of threading edge and screw dislocations which traverse vertically from the GaN/Al_2O_3 interface to the GaN surface [3–5]. It is astounding to most observers that optical devices such as LEDs and LDs will work with such a high dislocation density (N_{dis}) since, in GaAs-based LDs, a value of $N_{dis} = 10^4$ cm^{-2} is usually sufficient to prevent laser action [5]. The most common explanation advanced to explain this phenomenon is that threading dislocations in GaN must not have electronic states in the band gap, and, indeed, a recent theoretical calculation of a full-core dislocation structure seems to bear out this fact [6]. However, other calculations indicate that dislocations may well be charged; e.g., in n-type GaN, Ga vacancies [7,8] in the core, or Ga vacancies complexed with oxygen [9], should have acceptor nature. Indeed, the existence of such acceptor states seems quite plausible, since many observers note an inverse correlation between μ and N_{dis} [10]. Thus, there is some uncertainty over this issue. Recent scanning capacitance microscopy imaging of threading dislocations shows that negative charge exists near the dislocations, which could indicate acceptorlike traps [11].

Many years ago, Bonch-Bruevich and Glasko calculated the potential due to a vertical line charge as seen by electrons moving perpendicular to this line [12]. Later, Pödör [13] calculated the momentum relaxation rate arising from this potential, and obtained a mobility (apparently a "drift" mobility) after averaging over energy. However, a Hall mobility was never calculated, and other scattering mechanisms were included only approximately. Very recently, Weimann *et al.* [14] employed Pödör's relaxation rate (without any energy averaging) to obtain a mobility, and then compared their results with detailed μ vs carrier concentration n data, at various values of N_{dis}. The qualitative agreement was quite good, although quantitative agreement with hampered by the approximate nature of the mobility calculation and the fact that different samples were involved for each combination of n and N_{dis}. Also, Ng *et al.* [15] have done an analysis of μ vs T on one of the samples from this same group, but, again, they used a very approximate expression for μ. These efforts have demonstrated, for the first time, that high dislocation densities can indeed directly affect mobility in GaN. However, they lack the theoretical rigor necessary for a quantitative assessment. In this work, we begin with the Bonch-Bruevich potential, and develop an accurate mobility theory, including all relevant scattering mechanisms, within the framework of the Boltzmann transport equation. We then apply this theory to temperature-dependent μ and n data for two, well-characterized GaN/Al_2O_3 samples (A and B) grown by a group at the University of Santa Barbara, and recently discussed in the literature [3,10]. We obtain very good fits to n vs T and μ vs T for *both* samples *with no arbitrary parameters,* except for the bulk donor concentrations and energies, and the dislocation densities. Moreover, our model predicts the same dislocation densities as those which were measured earlier by transmission electron microscopy [3,10]. This theory also helps to resolve several other paradoxes in GaN research: (1) A mobility decrease, instead of the expected increase, at low values of n [14–16]; (2) higher (instead of lower) mobility with higher Si doping [17]; and (3) generally lower mobilities in GaN layers grown by molecular beam epitaxy (MBE) than in those grown by metal-organic chemical vapor deposition (MOCVD) or hydride vapor phase epitaxy (HVPE).

The screened potential energy at a large distance from a charged dislocation line was given by Bonch-Bruevich

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and Glasko [12] as

$$V(r) = \frac{e}{2\pi\varepsilon c} K_0(r/\lambda), \tag{1}$$

where e is the electronic charge, c is the lattice parameter along the (0001) direction, ε is the static dielectric constant, K_0 is a zero-order modified Bessel function, and λ is the screening parameter, given by

$$\lambda = \left(\frac{\varepsilon k_B T}{e^2 n'}\right)^{1/2}. \tag{2}$$

Here, k_B is Boltzmann's constant, and n' is the effective screening concentration, which may involve both free carriers, and bound carriers,

$$n' = n + (n + N_A)[1 - (n + N_A)/N_D], \tag{3}$$

where N_D and N_A are the *bulk* donor and acceptor concentrations (not involving acceptors on dislocations). The dislocation acceptors will remove electrons from the donors, and this fact must be included in the charge-balance equation. If the acceptors are formed by Ga atoms being removed from the dislocation core [7,8], then there will be one Ga vacancy (V_{Ga}) per c-axis distance (5.185 Å in GaN). (Of course, a V_{Ga}-O_N complex [9], in place of each V_{Ga}, would hold equally as well.) If each V_{Ga} contains one negative charge, then the charge balance equation can be written as

$$n + N_A + N_{dis}/c = \frac{N_D}{1 + n/\phi}, \tag{4}$$

where $\phi = [(g_0/g_1)N_C' \exp(\alpha/k_B)]T^{3/2}\exp(-E_D/kT)$. Here g_0 and g_1 are the degeneracies of the unoccupied and occupied donor states, respectively, N_C' is the effective conduction-band density of states at $T = 1$ K, E_{D0} is the activation energy of the donor at $T = 0$, and α is the temperature coefficient defined by $E_D = E_{D0} - \alpha T$. The quantity N_{dis} is the *arreal* concentration (m^{-2}) of threading edge dislocations, and N_{dis}/c is the *volume* (m^{-3}) concentration of the associated acceptors. If the acceptors have a charge larger than unity, then the fitted N_{dis} will be larger than the actual dislocation density.

The scattering due to dislocation-line charges is two dimensional, because only electrons moving perpendicular to the dislocation will be scattered. Thus, the relevant scattering wave vector is $\overline{q} = \overline{k}_\perp' - \overline{k}_\perp$, where $\overline{k}$ is the incoming wave vector and $\overline{k}'$ is the outgoing. The Fourier transform of the scattering potential is

$$A(\overline{q}) = \int_0^\infty \int_0^{2\pi} \frac{e^2\lambda^2}{2\pi\varepsilon c} K_0(x) e^{-iq\lambda x\cos\theta} x\, d\theta\, dx, \tag{5}$$

where $x = r/\lambda$. It turns out that, to an excellent approximation,

$$A(\overline{q}) = \frac{e^2\lambda^2}{\varepsilon c(1 + q^2\lambda^2)}, \tag{6}$$

where $q^2 = |\overline{k}_\perp' - \overline{k}_\perp|^2$. The scattering rate for electrons of wave vector $\overline{k}$ is then given by

$$S(\overline{k}) = \frac{1}{(2\pi)^2}\frac{2\pi}{\hbar}\int A^2(\overline{k},\overline{k}')(1 - \cos\theta_k) \times \delta(E_{\overline{k}_\perp} - E_{\overline{k}_\perp'})\, d\overline{k}_\perp', \tag{7}$$

where $(2\pi)^2$ is the density of states in two-dimensional k space, θ_k is the angle between $\overline{k}_\perp$ and $\overline{k}_\perp'$, E is the electron energy ($E = \hbar^2k^2/2m^*$), and the factor $(1 - \cos\theta_k)$ is an average over θ_k, necessary to determine the momentum relaxation rate. The δ function requires that $k_\perp = k_\perp'$, so that $q^2 = 2k_\perp^2(1 - \cos\theta_k)$, and also $d\overline{k}_\perp' = k_\perp'\, d\theta_k\, dk_\perp' = (m^*/\hbar^2)d\theta_k\, dE$. This integral can be calculated exactly, and then can be inverted to give a relaxation time,

$$\tau_{dis}(k) = \frac{\hbar^3\varepsilon^2c^2}{N_{dis}m^*e^4}\frac{(1 + 4\lambda^2k_\perp^2)^{3/2}}{\lambda^4}. \tag{8}$$

This is precisely the result obtained by Pödör [13], who then carried out an unspecified average over energy, and obtained a drift mobility, $\mu_{dis} = CT^{3/2}/\lambda$. In his work, μ_{dis} was roughly combined with the lattice mobility by use of Matthiessen's Rule ($\mu^{-1} = \mu_{dis}^{-1} + \mu_{latt}^{-1}$) and then compared with experiment (not involving GaN). Weimann *et al.* [14] evidently approximated $k_\perp^2$ in Eq. (8) by $2m^*kT/\hbar^2$, to get $\tau_{dis}(k)$, then set $\mu_{dis} = e\tau_{dis}/m^*$, and finally applied Matthiessen's Rule to obtain a satisfactory fit to GaN literature data, at least qualitatively. Ng *et al.* [15] used Pödör's approximate drift mobility, $\mu_{dis} = CT^{3/2}/\lambda$, and also employed Matthiessen's Rule to fit their data. The results of Weimann *et al.* and Ng *et al.* clearly demonstrate that dislocation scattering must be included in mobility analysis when $N_{dis} \gtrsim 10^8$ cm^{-2}; however, their analyses are only semiquantitative, and the effects of the various approximations are not clear. For example, the use of the drift mobility, instead of the Hall mobility, can cause a 70% error in sample B, discussed below. Also, the use of Matthiessen's Rule can easily cause a factor of 2 error. Thus, a more rigorous analysis is required to prove the scattering power of dislocations in GaN.

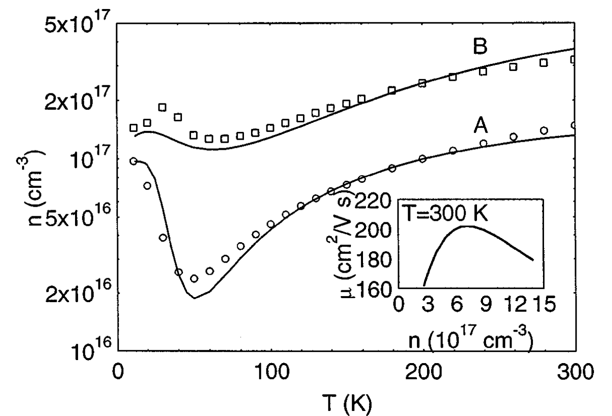

FIG. 1. Hall concentration vs temperature for samples A and B. The solid lines are theoretical fits to the data. The inset illustrates the dependence of mobility on carrier concentration for the case $N_{dis} = 2 \times 10^{10}$ cm^{-2}.

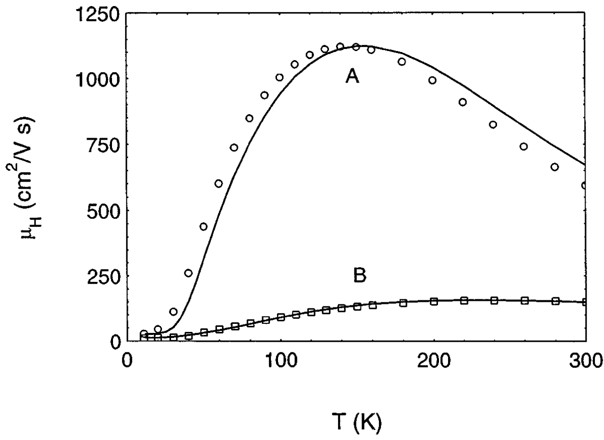

FIG. 2. Hall mobility vs temperature for samples A and B. The solid lines are theoretical fits to the data.

In this work, we have used the Boltzmann transport equation (BTE), solved by Rode's iterative method [18], to obtain an accurate solution of the Hall mobility. The BTE is solved at the magnetic field used in the experiment (5 kG). The charge-balance equation, Eq. (4), must be solved simultaneously with the BTE since μ is a function of n. The various scattering potentials included in the analysis are optical mode (polar), acoustical mode (deformation and piezoelectric), and screened coulomb (dislocations and point defects and impurities). All of the parameters for these terms come from the literature (see Ref. [19]) except for the obvious sample-dependent parameters, N_D, N_A, E_D, and N_{dis}. The data are presented in Figs. 1 and 2. Impurity-band effects are obvious at the lower temperatures, and are modeled by a simple, two-band approximation [20],

$$n_{\text{two-band}} = \frac{(n\mu_d + n_{\mathrm{ib}}\mu_{\mathrm{ib}})^2}{n\mu_d\mu_H + n_{\mathrm{ib}}\mu_{\mathrm{ib}}^2}, \tag{9}$$

$$\mu_{\text{two-band}} = \frac{n\mu_d\mu_H + n_{\mathrm{ib}}\mu_{\mathrm{ib}}^2}{n\mu_d + n_{\mathrm{ib}}\mu_{\mathrm{ib}}}, \tag{10}$$

where μ_H and μ_d are the conduction-band (cb) Hall and drift mobilities, respectively, μ_{ib} is the impurity-band (ib) mobility, n is the cb electron concentration, and $n_{\mathrm{ib}} = N_A$. Here, the unoccupied levels (of approximate concentration N_A) in the donor band may be thought of as the carriers, following Mott [21], since the empty levels are far fewer than the filled levels, especially at low temperatures where ib conduction is important. (Note that the conduction vanishes in a totally filled band.) The values of μ_{ib} are given by the data at the lowest temperature (11 K); $\mu_{\mathrm{ib}} = 27\ \mathrm{cm^2/V\,s}$ for sample A and $11\ \mathrm{cm^2/V\,s}$ for sample B. No distinction is made between Hall and drift mobilities for the impurity band, since we are only roughly modeling this region anyway, and it is further assumed that these mobilities are temperature independent, since the data of Fig. 2 clearly show this to be the case for $T < 20$ K, and the data of Fig. 1 show that impurity-band conduction rapidly loses importance for $T > 50$ K. Thus, although μ_{ib} probably has a temperature dependence above 20 K, it does not produce a critical effect on the overall fitting parameters, which are mainly determined by the higher-temperature data. The fits of Eqs. (9) and (10) to the n vs T and μ vs T data for samples A and B are shown in Figs. 1 and 2. The fits are very good, especially considering that the only fitting parameters are the sample-dependent terms: N_D, E_D, and N_{dis}. Note that N_A is not a fitting parameter, since we have assumed $N_A = n_{\mathrm{ib}}$. The fitting parameters are given in Table I. Secondary ion mass spectroscopy (SIMS) [22] data for sample A shows C at a $1 \times 10^{17}\ \mathrm{cm^{-3}}$ level and Si at a $(1-4) \times 10^{17}\ \mathrm{cm^{-3}}$ level. Thus, it is quite possible that C is the residual acceptor and Si is the residual donor. (Unfortunately, accurate SIMS data could not be obtained for sample B, because of a rough surface.) Also, the donor energies for samples A and B are reasonable for their respective concentrations. The values of N_{dis} are dependent upon the type of screening assumed, i.e., either free carriers alone (n) or both free and bound carriers (n'). An assumption of free carriers alone leads to almost exact agreement with the values of N_{dis} measured by transmission electron microscopy (TEM) [10], whereas an assumption of free-plus-bound carriers gives somewhat higher values. Note, however, that in either case, the ratio $N_{\mathrm{dis}}(B)/N_{\mathrm{dis}}(A)$ is the same as the TEM-measured ratio. Thus, our theory is in excellent agreement with independent TEM data, and clearly demonstrates that threading edge dislocations in GaN are charged.

A paradox explained by the model here is the observation by many groups that mobility *decreases* as n decreases below a concentration of about $10^{17}-10^{18}\ \mathrm{cm^{-3}}$; i.e., μ vs n goes through a maximum [14–16], in contrast to the behavior in most other semiconductors, in which μ continues to rise as n falls. The reason for this, as already pointed out by Weimann *et al.* [14] and by Ng *et al.* [15], is that dislocation scattering is strongly screened, as may be noted from the $\lambda(n)$ variation in Eq. (8). Thus, below

TABLE I. Hall-effect fitting parameters for samples A and B compared with TEM results.

Sample	Screening	N_D (cm^{-3})	N_A (cm^{-3})	E_D (meV)	N_{dis} (cm^{-2})	N_{dis} (TEM) (cm^{-2})
A	n	3.1×10^{17}	1.0×10^{17}	12	4.2×10^8	4×10^8
	n'	3.2×10^{17}	1.0×10^{17}	12	7.9×10^8	
B	n	13.5×10^{17}	1.4×10^{17}	1	2.3×10^{10}	2×10^{10}
	n'	16.6×10^{17}	1.4×10^{17}	1	3.5×10^{10}	

a certain n, dislocation scattering dominates, while above that value of n, ionized-impurity (or defect) scattering is more important. A related effect, also considered a paradox, is that Si doping *increases* μ in low-μ samples [17]. Such phenomena are illustrated in the inset of Fig. 1 for a case in which $N_{\text{dis}} = 2 \times 10^{10}\ \text{cm}^{-2}$, a typical value for GaN grown by MBE [14,15]. Here, n is varied in the model by changing N_D, as could be effected by Si doping, and N_A is set to $N_D/3$, for purposes of illustration. This curve well explains the data observed in Refs. [14–16], and helps to resolve the μ vs n paradox.

Finally, we comment on the fact that mobilities in MBE GaN are generally lower than those in MOCVD or HPVE GaN. For example, there are very few reports of $\mu(300\ \text{K}) > 400\ \text{cm}^2/\text{V s}$ in MBE samples [15], whereas values of $700-950\ \text{cm}^2/\text{V s}$ have been often reported for MOCVD and HVPE layers [10,20,23]. These high MOCVD and HVPE mobilities have been correlated with low ($<5 \times 10^8\ \text{cm}^{-2}$) N_{dis}, while some of the best MBE mobilities ($300-400\ \text{cm}^2/\text{V s}$) [15] are from samples with $N_{\text{dis}} > 5 \times 10^9\ \text{cm}^{-2}$. Thus, we believe that the most likely reason that mobilities are typically lower in MBE GaN layers is that N_{dis} is generally higher in those layers, probably due to the lower growth temperatures used in the MBE process.

In conclusion, we have developed an accurate model for charged dislocation scattering in GaN, and have applied it to temperature-dependent mobility and electron-concentration data for two samples, with low and high dislocation densities, respectively. The model fits the data remarkably well over the full temperature range for both samples, and thus appears to have general validity. Furthermore, it can help to resolve several paradoxes in the GaN literature.

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