Dislocation scattering in a two-dimensional electron gas

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(Received 17 December 1999; accepted for publication 1 February 2000)

A theory of scattering by charged dislocation lines in a two-dimensional electron gas (2DEG) is developed. The theory is directed towards understanding transport in AlGaN/GaN high-electron-mobility transistors which have a large number of line dislocations piercing through the 2DEG. The scattering time due to dislocations is derived for a 2DEG in closed form. This work identifies dislocation scattering as a mobility-limiting scattering mechanism in 2DEGs with high dislocation densities. The insensitivity of the 2DEG (as compared to bulk) to dislocation scattering is explained by the theory. © *2000 American Institute of Physics*. [S0003-6951(00)01813-1]

The last decade has witnessed a rapid development of III–V materials for a variety of optoelectronic and high power high-speed electronic devices.[1–3] The wide range of band gaps available by alloying GaN with Al and In have made it suitable for high-power, high-voltage electronic applications. AlGaN/GaN heterostructures have been an area of active research, owing to the demonstration of high power microwave high electron mobility transistors (HEMTs).[3] A good substrate, however, still remains elusive. Due to the large lattice mismatch with the present substrate of choice, sapphire, state of the art AlGaN/GaN HEMTs have[4,5] a two-dimensional electron gas (2DEG) which has $1-100\times10^8$ cm^2 line dislocations passing through it. Efforts to improve mobilities by reducing the number of dislocations have resulted in the novel growth technique of lateral epitaxial overgrowth (LEO).[6,7] Recently, Look and Sizelove[8] analyzed the effect of dislocation scattering on the mobility of three-dimensional (3D) bulk GaN. However, efforts[9–11] at explaining the observed mobilities in AlGaN/GaN 2DEGs have not considered scattering by dislocations. Surprisingly, there exists no adequate theory for dislocation scattering in a 2DEG. An effort was made to treat dislocation scattering in a AlGaAs/InGaAs/AlGaAs quantum well (QW) before the advent of AlGaN/GaN heterostructures.[12] We point out the limitations of the treatment. This letter develops the theory for the effect of dislocation scattering on transport in 2DEGs. The theory developed shows that 2DEG mobility is affected strongly by a high density of dislocations. The effect is weaker, however, than that in 3D bulk; the reasons for this are pointed out.

The system we consider is a perfect 2DEG, i.e., there is no spatial extent of carriers in the growth direction. The electrostatic potential ϕ satisfies Poisson's equation, which for the 2DEG under consideration with the Thomas Fermi approximation is[13]

$$\nabla^2\phi-2q_{\mathrm{TF}}\phi(\mathbf{r})\,\delta(z)=-\frac{4\pi\rho_{\mathrm{ext}}}{\epsilon_0\epsilon_b}. \tag{1}$$

Here ρ_{ext} is the external charge, $\epsilon_0\epsilon_b$ is the dielectric constant in the material (assumed to be same in the 2DEG and outside it), $\mathbf{r}=(x,y)$ is the in-plane vector, and $q_{\mathrm{TF}}=2/a_B^*$ is the 2D Thomas Fermi wave vector, a_B^* being the effective Bohr radius in the material. A valley degeneracy of one and spin degeneracy of two is implied. The conventional technique to arrive at the screened potential is to use the Fourier–Bessel expansion of the potential $\phi(\mathbf{r},z)=\int_0^\infty qA_q(z)J_0(qr)dq$, where J_0 is the Bessel function of order zero, and $A_q(z)$ is the Fourier–Bessel coefficient, q being the in-plane wave vector. The value of the coefficient averaged over zero spatial extent along the z axis is $A(q)=A_q(0)$. The Fourier transform of the screened 2D potential due to a point charge at a distance z from the plane of the perfect 2DEG is given by[13,14]

$$A(q)=\frac{e^2}{2\epsilon_0\epsilon_b}\cdot\frac{e^{-q|z|}}{q+q_{\mathrm{TF}}}, \tag{2}$$

where e is the electronic charge. The previous effort mentioned for quantum well dislocation scattering[12] (a) arrives at a scattering potential which models an in-plane charged impurity rather than the spatially extending dislocation line, and (b) does not consider the strong screening contribution in the highly degenerate 2DEG. We take these important factors into consideration.

A line dislocation has been shown[8,15,16] to be accurately modeled by a line of charge. Treating the line dislocation as a line of charge with charge density ρ_L (Fig. 1), we write the scattering contribution by a elementary length dz of the line charge to the screening potential as

$$dA(q)=\frac{e}{2\epsilon_0\epsilon_b}\cdot\frac{dz\rho_L e^{-q|z|}}{q+q_{TF}}. \tag{3}$$

Integrating over an infinite length of the line charge, we get the new screened potential as

$$A(q)=\frac{e}{2\epsilon_0\epsilon_b}\cdot\frac{2\rho_L}{q(q+q_{\mathrm{TF}})}. \tag{4}$$

There are N_{dis} line dislocations piercing the 2DEG per unit area. The scattering rate for a degenerate 2DEG is given by[14]

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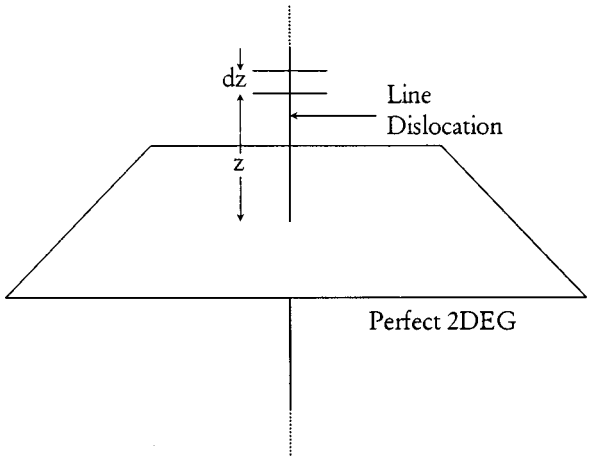

FIG. 1. Line dislocation modeled as a line of charge. The dislocation line has filled acceptor states along it. Charges on the dislocation line act as an extended remote impurity. The remote ionized impurity matrix element is integrated for all the small elemental remote impurities to account for the effect of the whole dislocation.

$$\frac{1}{\tau_{\rm dis}^{\rm 2D}} = N_{\rm dis} \cdot \left(\frac{m^*}{2\pi\hbar^3 k_F^3}\right) \cdot \int_0^{2k_F} |A(q)|^2 \frac{q^2 dq}{\sqrt{1-\left(\frac{q}{2k_F}\right)^2}}, \tag{5}$$

where $k_F = \sqrt{2\pi n_s}$ is the Fermi wave vector,[13] which depends on the 2DEG carrier concentration n_s. Using the screened potential [Eq. (4)] with the substitution $u = q/2k_F$ we get the scattering rate as

$$\frac{1}{\tau_{\rm dis}^{\rm 2D}} = \frac{N_{\rm dis} m^* e^2 \rho_L^2}{\hbar^3 \epsilon_0^2 \epsilon_b^2} \left(\frac{1}{16\pi k_F^4}\right) \cdot \int_0^1 \frac{du}{\left(u + \frac{q_{\rm TF}}{2k_F}\right)^2 \sqrt{1-u^2}}$$

$$= \frac{N_{\rm dis} m^* e^2 \rho_L^2}{\hbar^3 \epsilon_0^2 \epsilon_b^2} \cdot \frac{I\left(\frac{q_{\rm TF}}{2k_F}\right)}{16\pi k_F^4}. \tag{6}$$

The dimensionless integral $I(q_{\rm TF}/2k_F)$ can be evaluated exactly. It depends only on the 2DEG carrier concentration through the Fermi wave vector, and has an approximate $\sqrt{n_s}$ dependence. Figure 2 shows it's exact dependence on the 2DEG carrier concentration for $\epsilon_b = 10$ and $m^* = 0.228 m_0$ (for GaN). The integral is closely approximated by the relation $A \cdot (2k_F/q_{TF}) + B$, where A and B were determined to be 0.92 and -0.25, respectively. ρ_L, the line charge density is given to a very good approximation[8,15] by ef/c_0, where c_0 is the lattice spacing in the (0001) direction of wurtzite GaN, and f is the fraction of filled states, calculated by Weimann *et al*. Using this, the 2D dislocation scattering time is

$$\tau_{\rm dis}^{\rm 2D} = \frac{\hbar^3 \epsilon_0^2 \epsilon_b^2 c_0^2}{N_{\rm dis} m^* e^4 f^2} \cdot \frac{16\pi k_F^4}{I\left(\frac{q_{\rm TF}}{2k_F}\right)}$$

$$\approx \frac{\hbar^3 \epsilon_0^2 \epsilon_b^2 c_0^2}{N_{\rm dis} m^* e^4 f^2} \cdot \frac{16\pi k_F^4}{\left(\frac{1.84 k_F}{q_{\rm TF}} - 0.25\right)}. \tag{7}$$

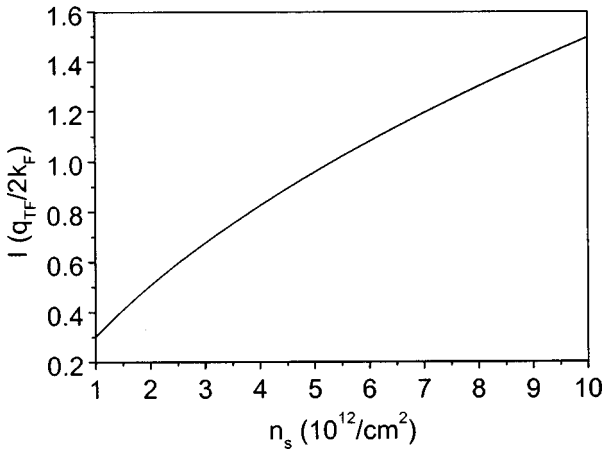

FIG. 2. Integral factor vs 2DEG carrier density. The dimensionless integral in Eq. (6) is evaluated exactly. The plot here shows it's dependence on the 2DEG carrier density for $\epsilon_b = 10$ and $m^* = 0.228 m_0$. The approximate $\sqrt{n_s}$ dependence is clearly seen.

The scattering time has an approximate $n_s^{3/2}$ dependence.

The scattering time arrived at highlights the metallic nature of the 2DEG electrons. The screening length for a 2DEG depends on $q_{\rm TF}$ and k_F. The Thomas Fermi wave vector $q_{\rm TF}$ is constant. As the free carrier density is increased, k_F increases, and λ_F, the Fermi wavelength gets shorter, leading to better screening. The 2DEG carrier density does not freeze out at low temperatures as in 3D. These factors contribute to the observed high mobilities in a 2DEG. In contrast, 3D screening and scattering is controlled by the Debye screening factor,[14] $q_D = \sqrt{e^2 n'/\epsilon k_B T}$, where n' is the effective screening concentration, involving both free and bound carriers. At low temperatures, free carriers freeze out exponentially in a semiconductor. An elongation of the Debye screening length $\lambda_D = 1/q_D$ leads to a weaker screening. In addition, the carriers are less energetic, leading to strong scattering, and hence to lower mobilities. A comparison of the dislocation scattering time in 2D [Eq. (7)] with the 3D bulk scattering time calculated recently by Look and Sizelove[8] (and also by Pödör[17]) bears out the discussion above. The result for 3D scattering time for f fractionally filled states is

$$\tau_{\rm dis}^{\rm 3D} = \frac{\hbar^3 \epsilon_0^2 \epsilon_b^2 c_0^2}{N_{\rm dis} m^* e^4 f^2} \cdot \frac{(1+4\lambda_D^2 k_\perp^2)^{\frac{3}{2}}}{\lambda_D^4} \propto \frac{(k_B T)^{\frac{3}{2}}}{\lambda_D}, \tag{8}$$

where $k_\perp$ is the wave vector for electron motion perpendicular to the dislocations, k_B is the Boltzmann constant, and T is the temperature.

2DEG mobility inhibited by dislocation scattering only, given by $\mu_{\rm dis}^{\rm 2D} = e\tau_{\rm dis}^{\rm 2D}/m^*$ is plotted in Fig. 3. Here we have assumed $f = 1$, i.e., that all the acceptor states in the dislocation are filled. Thus the mobility calculated is for the worst case. The dependence of mobility on 2DEG sheet density and dislocation density is given to an extremely good approximation by $\mu_{\rm dis}^{\rm 2D} \propto n_s^{3/2}/N_{\rm dis}$.

Our theory shows that for dislocation density of $10^{10}\,{\rm cm}^2$ and carrier densities in the $10^{12}-10^{13}\,{\rm cm}^2$ range, maximum 2DEG mobilities will be in the $10^3-10^4\,{\rm cm}^2\,{\rm V\,s}$ range. A reduction in the dislocation density to $\approx 10^8\,{\rm cm}^2$ in AlGaN/GaN HEMTs has resulted in record high mobilities

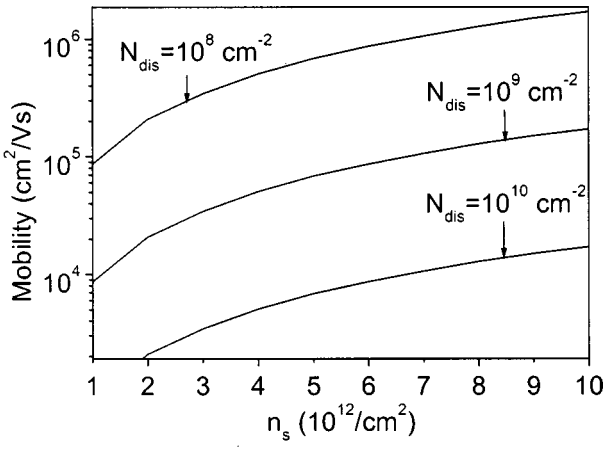

FIG. 3. Dislocation scattering inhibited 2DEG mobility. Mobilities for three different dislocation densities have been shown. Our theory predicts an approximate $n_s^{3/2}/N_{\rm dis}$ mobility dependence, which is seen in this plot. Note the strong mobility degradation at $10^{10}\,\mathrm{cm}^2$ dislocation density.

at low temperatures.[18,19] The record 2DEG mobility as of today stands at $51\,700\,\mathrm{cm}^2/\mathrm{V\,s}$, observed at 13 K with a sheet carrier density of $2.23\times10^{12}\,\mathrm{cm}^2$. By comparison, experiment and theory for a 3DEG at 13 K and carrier concentration $10^{18}\,\mathrm{cm}^3$ gives $\mu\approx100\,\mathrm{cm}^2/\mathrm{V\,s}$. The relative insensitivity of a 2DEG to dislocation scattering as compared to 3D bulk leads us to propose that modulation doped structures should be considered for replacing bulk GaN in structures infected with high dislocation densities.

In conclusion, we have developed a theory for dislocation scattering in semiconductor heterostructure 2DEGs. The theory explains the observed low temperature mobility enhancement in AlGaN/GaN HEMTs upon reduction of dislocation density. The theory finds a simple parallel to the 3D scattering theory for line dislocations, and highlights the strong screening effect by carriers in a 2DEG which helps it achieve much higher mobilities than 3D bulk values.

The authors would like to acknowledge helpful discussions with B. Heying, C. Elsass, I. Smorchkova, P. Chavarkar, J. Singh, and J. Speck.

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