Effect of scattering by strain fields surrounding edge dislocations on electron transport in two-dimensional electron gases

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We present a theory of deformation potential carrier scattering of two-dimensional electron gases from the strain fields surrounding edge dislocations. The scattering rate is evaluated in closed form without any fitting parameters. The result is directed towards understanding mobility limiting scattering mechanisms for two-dimensional electron gases at AlGaN/GaN heterointerfaces. © *2002 American Institute of Physics*. [DOI: 10.1063/1.1429758]

Many years ago, the effect of "cold working" on metallic resistivity was studied in detail.[1–4] Cold working is a technique of introducing a controlled amount of dislocations by deformation; the study showed that metallic conductivity is reduced by scattering of conduction electrons from strain fields that develop around dislocations. The effect of strain fields on electronic energy levels and charge transport in semiconductors is a widely studied topic, assuming special importance in the problems of lattice scattering and optical transitions in strained heterostructures.

Localized strain fields exist around point and extended defects in semiconductors. Traditionally in electronic transport theory one considers charge scattering by Coulombic interaction of mobile carriers with charged defects; strain fields associated with defects are generally neglected. This approximation is justified for substitutional donors/acceptors, for example, since the lattice distortion around them is minimal. However, as our work shows for dislocations, which may or may not be charged, the strain fields can contribute substantially to scattering of mobile carriers in semiconductors, just as in metals. Electron-strain field interaction will affect transport properties for vacancies/interstitials as well; we do not consider them in this work.

The effect of dislocation scattering on transport in two-dimensional electron gases (2 DEG) has received renewed attention recently owing to its significance in the technologically important AlGaN/GaN high electron mobility transistors. The dislocation scattering effect on 2DEG transport in AlGaN/GaN heterostructures has been recently studied assuming Coulombic scattering from a charged dislocation core.[5] In this work, we solve the general problem of the effect of scattering from the strain field surrounding edge dislocations for a 2DEG. We derive the scattering rate in a closed form which can be used for easy evaluation. We examine its importance by applying the results for the AlGaN/GaN system. It is important to note that this form of scattering arises *even if the dislocation core is uncharged*.

Dislocations set up a strain field around them with atoms displaced from their equilibrium positions in a perfect crystal. The band extrema [conduction band (CB) minimum, valence band (VB) maximum] shift under influence of the strain fields. The magnitude of spatial variation of the band extrema to linear order in strain is given by the deformation potential theorem of Bardeen and Shockley.[6]

We start with a suitable model for behavior of quantum well band edges in the presence of a localized strain field, such as around a dislocation. We assume a flat quantum well, with no built-in fields, which houses a 2DEG.[7] Our work deals with electron transport; the problem of hole transport can be formulated in a similar fashion. The effect of a strain in the quantum well is to shift the conduction and valence band edges. The shift in the conduction band edge was shown by Chuang[8] to be

$$\Delta E_C = a_C Tr(\epsilon), \tag{1}$$

where a_C is the conduction band deformation potential, and $Tr(\epsilon)=\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}=\delta\Omega/\Omega$ is the trace of the strain matrix. The trace is also equal to the fractional change in the volume of unit cells ($\delta\Omega/\Omega$).

In our model, we assume dislocations with their axes perpendicular to the quantum well plane. We also assume that the 2DEG is perfect, which means there is no z direction spread along the growth axis. Considering a realistic 2DEG would require incorporation of form factors, perfect 2DEG is chosen for simplicity. As an electron in the 2DEG approaches a dislocation, it experiences a potential due the strain around the dislocation, which causes scattering (see Fig. 1 for a schematic). The strain distribution radially outward from an edge dislocation is well known.[9] Combined with Eq. (1) we get the necessary perturbing potential responsible for electron scattering

$$\delta V = \Delta E_C = a_C Tr(\epsilon) = -\frac{a_C b_e}{2\pi}\frac{1-2\gamma}{1-\gamma}\frac{\sin(\theta)}{r}. \tag{2}$$

Here b_e is the magnitude of the Burgers vector of the edge dislocation, and γ is the Poisson's ratio for the crystal. The term $\epsilon_{zz}=0$ for an edge dislocation, and nonzero for a screw dislocation. For a screw dislocation in a cubic crystal, the strain field has purely shear strain, causing no dilatation/compression of the unit cells. This means there can be no deformation potential scattering for screw dislocations in cubic crystals. However, for uniaxial crystals such as GaN, the argument does not hold, and there is a deformation potential

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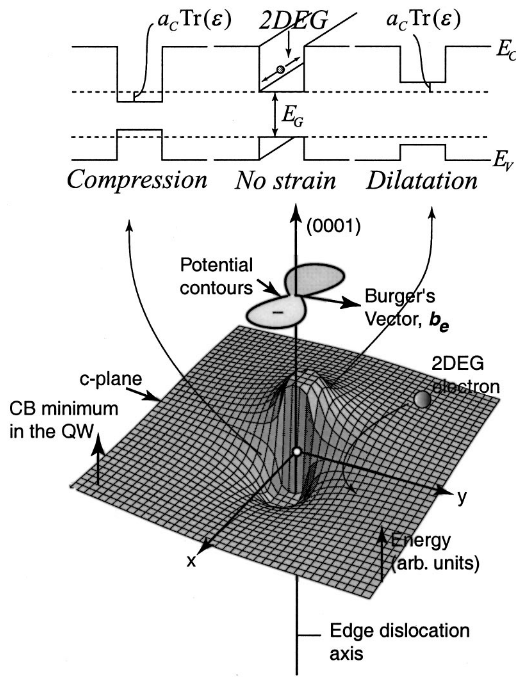

FIG. 1. The band electron experiences the depicted CB minimum fluctuation caused by strain fields around an edge dislocation. Strain is anisotropic, with maximum strain in directions perpendicular to the Burgers vector. The energy is in arbitrary units.

coupling even for screw dislocations for bulk transport. We limit ourselves to the simpler case of edge dislocations.

The matrix element of the perturbation for scattering of a 2DEG electron from state $|\mathbf{k_i}\rangle$ to state $|\mathbf{k_f}\rangle$ is needed for evaluating scattering rates in the Born approximation. Position space representations of the states are given by plane waves

$$\langle r|k_{i,f}\rangle = \frac{1}{\sqrt{S}} e^{i\mathbf{k_{i,f}}\cdot\mathbf{r}}. \tag{3}$$

Here $\mathbf{k_{i,f}}$ are the two-dimensional (2D) wave vectors of the initial (i) and final (f) states, $\mathbf{r}$ is the 2D space coordinate, and S is the macroscopic 2D area. The wave vectors of the initial and final states are both perpendicular to the dislocation axis. The matrix element $\langle \mathbf{k_f}|\delta V(r,\theta)|\mathbf{k_i}\rangle$ is given by the 2D Fourier transform of the scattering potential (the Born approximation)[10]

$$\delta V(q,\phi) = \int e^{i(\mathbf{k_i}-\mathbf{k_f})\cdot\mathbf{r}} \delta V(\mathbf{r}) d^2r = \frac{b_e a_C}{2\pi S} \frac{1-2\gamma}{1-\gamma} \frac{\sin(\phi)}{q}, \tag{4}$$

where $q=|\mathbf{k_f}-\mathbf{k_i}|$ and ϕ is the angle between $\mathbf{q}$ and $\mathbf{b_e}$, the Burgers vector. For taking into account the screening of this perturbation by mobile charges, the matrix element is scaled by the Lindhard dielectric function in the long-wavelength limit $\epsilon(q)=1+q_{\mathrm{TF}}/q$, where $q_{\mathrm{TF}}=2/a_B^*$ is the Thomas–Fermi wave vector (a_B^* is the effective Bohr radius in the semiconductor). Summing the square of the matrix element over all scatterers in the dilute scatterers limit requires an average of the angular dependence over random orientations of the Burgers vectors for different dislocations; averaging

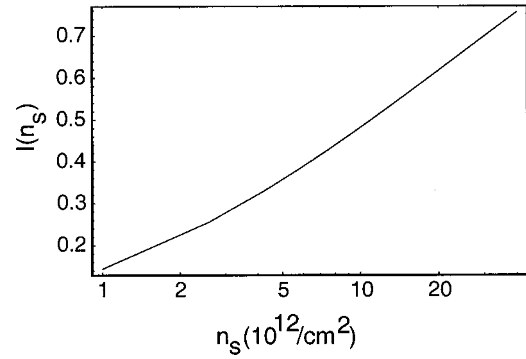

FIG. 2. Plot of the dependence of the dimensionless integral $I(n_s)$ on the 2DEG sheet density n_s.

yields $\langle \sin^2(\phi)\rangle = 1/2$. Transport scattering rate is found by Fermi's golden rule; for scattering into the single final state $\mathbf{k_f}$, the rate is given by

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} |\delta V(q)|^2 \delta(E_{\mathbf{k_i}} - E_{\mathbf{k_f}}), \tag{5}$$

where τ is the scattering rate, $\hbar$ is the reduced Planck's constant, and the δ function is a statement of the elastic nature of scattering, conserving energy between the initial ($E_{\mathbf{k_i}}$) and final ($E_{\mathbf{k_f}}$) states.

To find the ensemble rate, we sum over all the available final states in the 2D density of states, and evaluate the transport scattering rate[11]

$$\frac{1}{\tau_{\mathrm{tr}}} = \frac{N_{\mathrm{disl}} m^* b_e^2 a_C^2}{2\pi k_F^2 \hbar^3} \left(\frac{1-2\gamma}{1-\gamma}\right)^2 \underbrace{\int_0^1 \frac{u^2}{(u+\frac{q_{TF}}{2k_F})^2\sqrt{1-u^2}} du}_{I(n_s)}. \tag{6}$$

Here, N_{disl} is the 2D density of threading edge dislocations, m^* is the effective mass of conduction electrons in the 2DEG, and $k_F = \sqrt{2\pi n_s}$ is the Fermi wave vector (n_s being the 2DEG electron sheet density).

The dimensionless integral $I(n_s)$ is dependent only on the sheet density n_s, and can be evaluated explicitly. Since the expression is long and does not contain any extra information, we plot the dependence of the integral factor on the sheet density in Fig. 2. Finally, we arrive at the dislocation strain field scattering limited electron mobility given by the Drude result $\mu = e\tau_{\mathrm{disl}}^{\mathrm{strain}}/m^*$

$$\mu_{\mathrm{disl}}^{\mathrm{strain}} = \frac{2e\hbar^3\pi k_F^2}{N_{\mathrm{disl}} m^{*2} b_e^2 a_C^2} \left(\frac{1-\gamma}{1-2\gamma}\right)^2 \frac{1}{I(n_s)}. \tag{7}$$

We now apply this general result to the particular case of AlGaN/GaN 2DEGs. Quantities needed for a numerical evaluation are the magnitude of the Burgers vector $b_e = a_0 = 3.189$ Å, the conduction electron effective mass $m^* = 0.2m_0$ (m_0 is free electron mass), Poisson's ratio for the crystal, $\gamma = 0.3$,[9] and the conduction band deformation potential a_C.

For uniaxial crystals such as the wurtzite crystal (III–V nitride crystals belong to this group), the second rank deformation potential tensor Ξ_{ij} has two independent components, Ξ_1 and Ξ_2 at the Γ point in the E-k diagram. The

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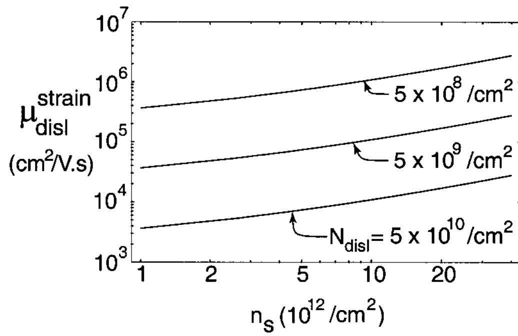

FIG. 3. Plot of AlGaN/GaN 2DEG mobility limited only by strain field scattering from dislocations. Three dislocation densities typical to III–V nitride heterostructures are used for the calculation.

volume change (compression or dilatation) leads to a shift in the band gap

$$\Delta E_G = \Xi_1 \epsilon_{zz} + \Xi_2 \underbrace{(\epsilon_{xx} + \epsilon_{yy})}_{\epsilon_\perp} , \quad (8)$$

where $\Xi_1 = a_1 = -6.5\,\text{eV}$ and $\Xi_2 = a_2 = -11.8\,\text{eV}$ for GaN.[12] For an edge dislocation, there is no strain along the z (0001) axis ($\epsilon_{zz} = 0$); thus only Ξ_2 will be required in our analysis. The deformation potential has contributions from both the CB and the VB, $\Xi_2 = \Xi_2^{\text{CB}} + \Xi_2^{\text{VB}}$. We require only the conduction band deformation potential for our calculation. Separate experimental values of the conduction and valence band deformation potentials are not available for GaN at present. We use an approximation of $a_C = \Xi_2^{\text{CB}} = -8.0\,\text{eV}$ (and $\Xi_2^{\text{VB}} = -3.8\,\text{eV}$) for numerical estimates. This split in CB and VB deformation potentials is assumed following the general trend of other III–V semiconductor deformation potentials.[12]

We are now in a position to estimate dislocation strain field scattering limited electron mobility for AlGaN/GaN quantum wells. The presence of a 2DEG at a AlGaN/GaN heterointerface in the absence of intentional modulation dopants has been demonstrated. Such 2DEGs have typical sheet densities $n_s = 10^{12}-10^{13}/\text{cm}^2$ depending on the epilayer structure and composition. Typical dislocation densities range from $N_{\text{disl}} = 10^7/\text{cm}^2$ to $N_{\text{disl}} = 10^{11}/\text{cm}^2$, depending on the growth conditions. Both edge and screw-type dislocations have been observed; our theory is applicable for edge dislocations only. We calculate the edge-dislocation strain field scattering limited electron mobility for a range of 2DEG sheet densities and dislocation densities $N_{\text{disl}} = 5 \times (10^8, 10^9, 10^{10}/\text{cm}^2)$. The results are shown in Fig. 3.

Note that the plot shows the effect of scattering from strain fields of dislocations *alone*. Since experimentally measured Hall mobility has contributions from many other scattering mechanisms, we can gauge only the relative importance of this form of scattering by comparing with experimental results. A full evaluation of various scattering rates and how strain field scattering compares with other scattering mechanisms will be published as a separate work.

A number of points can, nevertheless, be made from Fig. 3. This form of scattering seriously affects low temperature transport properties when the dislocation density is high ($N_{\text{disl}} \approx 10^{10}/\text{cm}^2$) and the 2DEG density is low ($n_s \approx 10^{12}/\text{cm}^2$). In fact, the highest reported low temperature mobilities for AlGaN/GaN 2DEGs ($\mu = 75\,000\,\text{cm}^2/\text{V}\cdot\text{s}$, $n_s = 10^{12}/\text{cm}^2$[13] and $\mu = 51\,700\,\text{cm}^2/\text{V}\cdot\text{s}$, $n_s = 2.23 \times 10^{12}/\text{cm}^2$)[14] exceeds the mobility limits posed by strain field scattering by dislocations of a density $N_{\text{disl}} \approx 10^{10}/\text{cm}^2$; thus verifying that the dislocation densities in such samples is lower. Another point of interest is the dilution of this form of scattering at high 2DEG densities; high dislocation densities should pose little problem in achieving superior transport properties for 2DEGs with $n_s \geq 10^{13}/\text{cm}^2$.

In addition to deformation potential scattering from the strain fields and charge core scattering,[5] there is also a possibility of piezoelectric fields associated with dislocations in noncentrosymmetric crystals as GaN. However, we expect this form of scattering to be negligible.[9] The effect of screw dislocations on transport in uniaxial crystals is a more subtle question, and we do not deal with it here.

The question of maximum allowable dislocation densities without hampering transport properties is an important question for device applications. Existing theoretical studies of transport of 2DEGs at AlGaN/GaN heterojunctions[15,16] neglect dislocation scattering effects on electron mobility. Inclusion of deformation potential scattering and charged core scattering by dislocations will present a comprehensive and more realistic picture of transport in such structures.

In conclusion, we demonstrated that strain fields surrounding dislocations affect measured electron transport properties in a 2DEG. We derived 2DEG scattering rates for deformation potential scattering from strain fields of edge dislocations. The theoretical results were applied to the case of III–V nitride 2DEGs.

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