Deformation potential scattering from dislocations in III-V nitride quantum wells

Debdeep Jena* and U. K. Mishra
Department of Electrical and Computer Engineering
University of California, Santa Barbara
CA, 93106

We present a theory of deformation potential carrier scattering of two-dimensional electron gases from the strain fields surrounding dislocations. The results are applied to study the transport characteristics in III-V nitride two-dimensional electron gases in Al(Ga)N/GaN quantum wells. A hypothetical charged core has been associated as the only scattering potential for analyzing experimental results for transport studies of the nitrides; we critically examine this assumption in light of our results of strain field scattering. By computing the effect of all possible scattering mechanisms we gauge the importance of strain field scattering from dislocations.

Many years ago, the effect of ‘cold working’ on metallic resistivity was studied in detail. Cold working is a technique of introducing 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 is 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.

Dislocation scattering effect on two-dimensional electron gas (2DEG) transport in AlGaN/GaN heterostructures has been recently studied assuming coulombic scattering from a charged dislocation core. In this work, we solve the general problem of the effect of scattering from the strain field surrounding edge dislocations for a 2DEG. We examine it’s 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.

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. 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 to be

\[ \Delta E_C = a_C \text{Tr}(\epsilon) \]  (1)

where \( a_C \) is the conduction band deformation potential, and \( \text{Tr}(\epsilon) = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} = \delta\Omega/\Omega \) 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 Figure[1] for a schematic). The strain distribution radially outward from an edge dislocation is well known. Combined with Equation [1] we get the necessary perturbing potential responsible for electron scattering.

*email: djena@engineering.ucsb.edu
\[ \delta V = \Delta E_C = a_C T r (\epsilon) = -\frac{a_C b_c}{2\pi} \frac{1 - 2\gamma \sin(\theta)}{1 - \gamma} r. \]  

(2)

Here \( b_c \) is the magnitude of the burger’s vector of the edge dislocation, and \( \gamma \) is the Poisson’s ratio for the crystal. \( \epsilon_{zz} = 0 \) 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 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 \( |k_i\rangle \) to state \( |k_f\rangle \) is needed for evaluating scattering rates in the Born approximation. Position space representations of the states are given by plane waves

\[ <r|k_{i,f}> = \frac{1}{\sqrt{S}} e^{i k_{i,f} \cdot r}. \]  

(3)

Here \( k_{i,f} \) are the 2D wavevectors of the initial (i) and final (f) states, \( r \) is the 2D space coordinate, and \( S \) is the macroscopic 2D area. The wavevectors of the initial and final states are both perpendicular to the dislocation axis. The matrix element \( <k_f|\delta V(r, \theta)|k_i> \) is given by the 2D Fourier transform of the scattering potential (the Born approximation)[4]

\[ \delta V(q, \phi) = \int e^{i(k_i-k_f) \cdot r} \delta V(r) d^2 r = \frac{b_c a_C}{2\pi S} \frac{1 - 2\gamma \sin(\phi)}{1 - \gamma} q, \]  

(4)

where \( q = |k_f - k_i| \) and \( \phi \) is the angle between \( q \) and \( b_c \), the Burger’s vector. For taking into account screening of this perturbation by mobile charges, the matrix element is scaled by the Lindhard dielectric function in the long-wavelength limit \( \epsilon(q) = 1 + \frac{2\pi}{q} \), where \( q_{TF} = a_B^{2d} \) is the Thomas-Fermi wavevector (\( a_B^{2d} \) 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 burger’s vectors for different dislocations; averaging yields \( <\sin^2(\phi)> = \frac{1}{2} \). Transport scattering rate is found by Fermi’s golden rule; for scattering into the single final state \( k_f \), the rate is given by

\[ \frac{1}{\tau} = \frac{2\pi}{\hbar} |\delta V(q)|^2 \delta(E_{k_i} - E_{k_f}), \]  

(5)

where \( \tau \) is the scattering rate, \( \hbar \) is the reduced Planck’s constant, and the \( \delta \) function is a statement of the elastic nature of scattering, conserving energy between the initial (\( E_{k_i} \)) and final (\( E_{k_f} \)) 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[3]

\[ \frac{1}{\tau_{str}} = \frac{N_{disl} m^* b_c^2 a_B^{2d}}{2\pi k_F^2 \hbar^3 \sigma_{C}^2} \left[ 1 - \frac{2\gamma}{1 - \gamma} \right]^2 \int_0^{1} \frac{u^2}{(u + \frac{2\pi}{k_F})^2 \sqrt{1 - u^2}} I(n_s) du. \]  

(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 wavevector (\( n_s \) 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 Figure[2]. Finally, we arrive at the dislocation strain field scattering limited electron mobility given by the Drude result \( \mu = e \tau_{str} / m^* \)

\[ \mu_{str} = \frac{2e\hbar^3 \pi k_F^2}{N_{disl} m^* b_c^2 a_B^{2d}} \left[ 1 - \frac{2\gamma}{1 - 2\gamma} \right] \frac{1}{I(n_s)}. \]  

(7)

Quantities needed for a numerical evaluation are the magnitude of the Burger’s vector \( b_c = a_0 = 3.189 \text{Å}, \) the conduction electron effective mass \( m^* = 0.2 m_0 \) (\( m_0 \) is free electron mass), Poisson’s ratio for the crystal, \( \gamma = 0.4 \), and the conduction band deformation potential \( a_c \).

For uniaxial crystals such as the wurtzite crystal, the second rank deformation potential tensor \( \Xi_{ij} \) has two independent components, \( \Xi_1 \) and \( \Xi_2 \) at the \( \Gamma \) point in the E-k diagram. The volume change (compression or dilatation) leads to a shift in the band gap.
\[ \Delta E_G = \Xi_1 \varepsilon_{zz} + \Xi_2 (\varepsilon_{xx} + \varepsilon_{yy}) \]  

(8)

Where \( \Xi_1 = a_1 = -6.5 \text{eV} \) and \( \Xi_2 = a_2 = -11.8 \text{eV} \) for GaN. For an edge dislocation, there is no strain along the \( z \) (0001) axis (\( \varepsilon_{zz} = 0 \)); thus only \( \Xi_2 \) will be required in our analysis. The deformation potential has contributions from both the CB and the VB, \( \Xi_2 = \Xi_2^C + \Xi_2^B \). 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 \( a_C = \Xi_2^C = -8.0 \text{eV} \) (and \( \Xi_2^B = -3.8 \text{eV} \)) for numerical estimates. This split in CB and VB deformation potentials is assumed following the general trend of other III-V semiconductor deformation potentials.

We now apply the derived results to 2DEGs at AlGaN/GaN heterojunctions. To do a comparison of the different scattering mechanisms, we plot mobility limited by each scattering mechanism for a range of 2DEG densities in Figure[3]. The total low temperature mobility is evaluated by Matheissen’s rule (\( \mu_{\text{tot}} = \sum_i \mu_i^{-1} \), \( \mu_i \) being mobilities limited by individual scattering mechanisms). In the same plot, we plot the highest reported 2DEG mobilities in Al(Ga)N/GaN 2DEGs\[13\]. The calculation was done for background impurity concentration \( 10^{16}/\text{cm}^3 \), remote (surface) donor density equal to the 2DEG density\[15\], interface roughness characterized by island of height \( \Delta = 5 \text{Å} \) and correlation length \( L = 10 \text{Å} \), and charged core filling factor \( f = 0.33 \). The barrier alloy concentration was 9%.

It is evident that scattering at high carrier densities is dominated by alloy scattering, and in the absence of an alloy barrier, interface roughness scattering. There is a noticeable jump in mobility at higher 2DEG densities in passing from an AlGaN (empty circles) to AlN barrier (filled circles), marking the removal of alloy scattering.

However, at low carrier densities, dislocation scattering dominates electron transport properties. Even for an uncharged dislocation core, the strain field-deformation potential scattering is large enough to limit low temperature electron mobilities. In Figure[4], we plot total mobilities calculated for three different dislocation densities \( N_{\text{dil}} = 5 \times (10^9, 10^9, 10^{10})/\text{cm}^2 \). It is important to note that dislocation scattering (be it from a charged core or from the strain field) is much stronger than charged impurity scattering for impurity and dislocation densities typical in the III-V nitrides.

In addition to the deformation potential scattering from the strain fields, there is also a possibility of piezoelectric fields associated with dislocations in non-centrosymmetric crystals as GaN. However, we expect this form of scattering to be negligible\[16\]. The effect of screw dislocations on transport in uniaxial crystals is a more subtle question, and we postpone it for a future work.

In conclusion, we demonstrated that strain fields surrounding dislocations affect measured electron transport properties in a 2DEG. We derived 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. By comparison with all low-temperature scattering mechanisms, the importance of dislocation scattering (originating from strain fields as well as charged cores) was highlighted.

The authors would like to thank P. Waltereit, J. Singh, A. C. Gossard, and J. Speck for useful discussions. The authors acknowledge funding assistance from J. Zolper (ONR-IMPACT), C. Wood (ONR-POLARIS) and G. Witt (AFOSR).

1. J. S. Koehler, Phys. Rev. 75, 106 (1949).
2. J. K. Mackenzie and E. H. Sondheimer, Phys. Rev. 77, 264 (1950).
3. R. Landauer, Phys. Rev. 82, 520 (1951).
4. D. L. Dexter, Phys. Rev. 86, 779 (1952).
5. D. Jena, A. C. Gossard, and U. K. Mishra, Appl. Phys. Lett. 76, 1707 (2000).
6. J. Bardeen and W. Shockley, Phys. Rev. 80, 72 (1950).
7. This assumption does not hold for III-V nitrides, which have strong polarization fields in QWs. However, the assumption introduces negligible error, since we assume a perfect 2DEG.
8. S. L. Chuang, Phys. Rev. B 43, 9649 (1991).
9. C. Shi, P. M. Asbeck, and E. T. Yu Appl. Phys. Lett. 74, 573 (1999).
10. J. M. Ziman, Electrons and phonons (Oxford University Press, Oxford, 2001), p.230.
11. J. H. Davies, The Physics of Low Dimensional Semiconductors (Cambridge University Press, Cambridge, 1998), p.357.
12. I. Vurgaftman et. al., J. Appl. Phys. 89, 5815 (2001).
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 Burger’s vector. The energy is in arbitrary units.

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

FIG. 3. Contribution of different scattering processes to low temperature electron mobility. There is a good match of theoretically predicted mobility given by the broken line and the experimentally measured mobility. Experimental results for AlGaN/GaN 2DEGs are plotted as empty circles, and for AlN/GaN layers as filled circles. Dislocation scattering is dominant at low 2DEG densities.

FIG. 4. The effect of strain field scattering limited electron mobility in an Al(Ga)N/GaN 2DEG as a function of the sheet density for three different dislocation densities, $N_{\text{disl}} = 5 \times (10^8, 10^9, 10^{10})/\text{cm}^2$. 

---

13 M. Manfra, private communication.
14 I. P. Smorchkova et al., J. Appl. Phys. 86, 4520 (1999).
15 J. P. Ibbetson et. al., Appl. Phys. Lett. 77, 250 (2000).
Figure 1
D. Jena and U. K. Mishra
Figure 2

D. Jena and U. K. Mishra
Figure 3
D. Jena and U. K. Mishra
Figure 4
D. Jena and U. K. Mishra