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Hsu, Leonardo

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L. Hsu, W. Walukiewicz, and E.E. Haller

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Defect Formation and Electronic Transport at AlGa_N/Ga_N Interfaces

L. Hsu^{1,2}, W. Walukiewicz¹ and E.E. Haller^{1,3}

¹Center for Advanced Materials
MATERIALS SCIENCES DIVISION
Ernest Orlando Lawrence Berkeley National Laboratory
University of California
Berkeley, California 94720

and

²Department of Physics
University of California at Berkeley
Berkeley, California 94720

and

³MSME Department
University of California at Berkeley
Berkeley, California 94720

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DEFECT FORMATION AND ELECTRONIC TRANSPORT AT $\text{AlGa}_{1-x}\text{N}/\text{GaN}$ INTERFACES

L. Hsu¹, W. Walukiewicz², and E. E. Haller^{2,3}

¹Physics Dept., Univ. of California, Berkeley, Berkeley, CA 94720 USA

²Materials Science Div., Lawrence Berkeley Nat'l Lab, Berkeley, CA 94720 USA

³MSME Dept., Univ. of California, Berkeley, Berkeley, CA 94720 USA

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Abstract. We have calculated the effects of charged defects located near a $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterointerface on the transport properties of the two dimensional electron gas confined at the interface and also determined the distribution of those defects taking into consideration the dependence of the formation energy on the Fermi level. In addition, we have investigated the effects of hydrostatic pressure on such modulation doped heterostructures and find that pressure can be used to make the determination of the properties of the two dimensional electron gas easier by eliminating parallel three dimensional conduction paths.

Introduction.

Because of its large bandgap, tunable from 3.4 to 6.2 eV, and high saturation drift velocities for electrons, $\text{Al}_x\text{Ga}_{1-x}\text{N}$ is ideally suited for high power, high temperature electronic and opto-electronic devices. Much recent research has confirmed the possibility of creating a two-dimensional electron gas (2 DEG) at a $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterointerface with low temperature mobilities greater than 7000 $\text{cm}^2/\text{V s}$ and sheet carrier concentrations of roughly $5 \times 10^{12} \text{ cm}^{-2}$ [1, 2]. In addition, the fabrication of high electron mobility transistors (HEMTs) and heterostructure field effect transistors (HFETs) with operation frequencies in the GHz range has demonstrated the potential for developing devices for high power microwave applications [3,4].

However, despite experimental progress in optimizing the parameters of such heterostructures, very little is known regarding the impurities which give rise to the 2 DEG. In particular, it is far from clear whether the 2 DEG electrons in currently grown structures originate from shallow hydrogenic impurities or from resonant donors in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$. In a previous paper, we have described the characteristics of standard $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ modulation doped heterostructures (MDHs) in which shallow donors such as Si provided the 2 DEG in the GaN well [5]. Here, we will discuss heterostructures in which the source of 2D conduction electrons are resonant donors which are responsible for n-type conductivity in nominally undoped AlGaIn. It has been shown recently that resonant donor defects which are formed in low temperature grown InP can be used to fabricate modulation defect doped InGaAs/InP heterostructures [6,7].

Electron transport.

The mobility and transport characteristics of defect-doped $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ MDHs are largely the same as those which are doped with shallow impurities with a few important differences. In contrast to MDHs doped with shallow impurities, the Fermi level of defect doped structures lies within the conduction band of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier (Fig. 1). This increase of the Fermi energy relative to impurity doped MDHs allows a more efficient transfer of electrons from the barrier into the well, especially at higher remote doping concentrations for which the Fermi energy can be more than 100 meV above the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ conduction band in regions far from the interface. This difference is illustrated in Fig. 2, in which the 2 DEG concentration is plotted as a function of the remote doping concentration for

Figure 1. Schematic representation of a $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, showing resonant donors, lowest electric subband, and Fermi level.

structures with and without a 200Å spacer of undoped $\text{Al}_x\text{Ga}_{1-x}\text{N}$. All numbers have been calculated assuming an Al fraction (x) of 15%. The 2 DEG concentration was calculated from the electrostatic equilibrium equation

$$V_0 - \frac{4\pi e^2}{\epsilon_s} N_s d - \frac{4\pi e^2}{2\epsilon_s} \frac{N_s^2}{N_I} = E_0 + \frac{\pi \hbar^2}{m^*} N_s - E_F' \quad (1)$$

Figure 2. 2D electron concentration plotted as a function of remote doping concentration for heterostructures with no (0) and a 200Å (200) spacer. The solid lines are for defect doped structures and the dashed lines are for standard MDHs.

where V_0 is the conduction band offset, N_s the 2 DEG concentration, N_I the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ defect concentration, d the spacer width, and E_F' is the Fermi level in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier. The kink in the graph for the structure with a spacer occurs at the point where the Fermi energy in the AlGaIn barrier reaches the resonant defect level and becomes pinned there. The defect level was estimated to be 475 meV above the GaN conduction band edge based on experimentally measured reductions in the carrier concentration of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ samples as a function of Al fraction [8,9,10,11].

Figures 3a and 3b show the dependence of the low temperature 2 DEG mobilities on the concentration of defects in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier as calculated by the method used in [12]. As the sheet carrier concentration is increased, ionized impurity scattering from impurities in the GaN becomes much less effective in reducing the carrier mobility due to the decreased scattering cross section of screened Coulomb potentials at high electron energies. On the other hand, scattering due to interactions

Figure 3a/3b. 2D electron mobilities plotted as a function of remote doping concentration. Also shown are the component mobilities due to alloy disorder scattering, deformation potential scattering, and scattering from remote and residual (background) donors.

with the remote donors increases because of the increasing concentration of these Coulomb centers. In addition, alloy disorder scattering becomes much more effective at limiting the mobility at high electron densities due to increased penetration of the electronic wavefunctions into the $\text{Al}_x\text{Ga}_{1-x}\text{N}$. Typical low temperature mobilities from several thousand up to a couple million cm^2/Vs in structures with a spacer are predicted by our calculations. Obtaining the highest mobilities, however, requires that the concentration of ionized impurities and defects in the GaN be kept very low ($< 10^{14} \text{ cm}^{-3}$).

Defect distribution.

In calculating the mobilities shown in Figs. 3a and 3b, it was assumed that the defect concentration was uniform throughout the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier. This would be the case if the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer were grown first. However, in all heterostructures grown so far, the GaN well is grown first and a doped $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer is grown on top of it. In such a case, one must take into consideration the fact that as the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier is grown, the electrons from these donor defects are transferred into the GaN well. This transfer of electrons to lower energy levels results in a decrease of the formation energy of the defects.

The concentration of singly charged resonant defects is given by [13]

$$N_D = N_{\text{sites}} \exp\left(\frac{-E_f}{k_B T}\right) \quad (2)$$

where N_{sites} is the concentration of possible defect sites in the crystal lattice and E_f is the defect formation energy. For positively charged (ionized) donor defects,

$$E_f = E_f^0 + E_F \quad (3)$$

where E_f^0 is the formation energy for neutral defects and E_F is the Fermi energy in the GaN well relative to the $E_d(0/+)$ charge transition state. In pure GaN,

$$E_d(0/+) = E_C + 0.475 \text{ eV} \quad (4)$$

However, for the heterostructures that we consider here,

$$E_d(0/+) = E_C + 0.475 - \Delta E \quad (5)$$

where ΔE is the conduction band offset between the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and GaN.

To calculate the concentration of defects from Eq. (2), one must know E_f^0 . The value of this parameter can be estimated from the experimentally measured carrier concentration in nominally undoped, isolated $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers, in which the electrons are assumed to originate from these resonant defects. The formation energy given in Eq. (3) can then be written as

$$E_f = E_f^0 + E_C + E_F - E_C \quad (6)$$

where E_C is the energy of the conduction band edge. Substituting (6) into Eq. (2), we find

$$N_D = N_{\text{sites}} \frac{N_C}{n} \exp\left(\frac{-E_f^0 + E_C}{k_B T}\right) \quad (7)$$

where N_C is the conduction band density of states and n is the electron concentration. If these resonant defects are the dominant donors, then $n = N_{\text{def}}$ and we obtain

$$E_f^0 + E_C = k_B T \ln\left(\frac{N_{\text{sites}} N_C}{N_{\text{def}}^2}\right) \quad (8)$$

The concentration of the donor defects depends on the growth conditions and the Al content. We have performed model calculations assuming that for $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ grown at a temperature of 1373 K, the defect concentration is roughly 10^{17} cm^{-3} [2]. Equation (8) then gives $E_f^0 + E_c \approx 2.18 \text{ eV}$ for the formation energy of the charged defects when the Fermi energy is at the conduction band edge.

To see how the formation energy and defect concentrations vary in a real heterostructure, we consider the case when $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ is grown on a pure GaN layer. Because the formation energy of these native defects depends on the Fermi energy a greater concentration of defects is expected to be found close to the interface. When the first few atomic layers of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ are grown on top of the GaN layer, the Fermi energy in the structure is well below the conduction band of the GaN due to the high growth temperature. The formation of defects in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ at this point is aided by the fact that these donor centers can transfer their electrons to the GaN, gaining an amount of energy equal to the difference between the Fermi levels in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and the GaN. This results in a substantial lowering of the formation energy for charged defects. As more layers of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ are grown, more electrons continue to be transferred to the GaN well and the Fermi energy increases, decreasing the amount of energy gained by the transfer process and causing the defect formation energy to increase. Thus, the concentration of defects incorporated into the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ also decreases.

Based on the above considerations, the variation of the charged defect formation energy and the concentration of incorporated defects is shown as a function of the distance from the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface in Fig. 4. As can be seen, the concentration of defects at the interface is enhanced by more than an order of magnitude. While this concentration of defects near the interface aids in the transfer of charge from the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier to the GaN well, it also has the effect of degrading the overall 2 DEG mobility. As can be seen from Figs.

3a and 3b, ionized impurity scattering from remote donors is often the dominant mechanism limiting the two-dimensional mobility, especially in structures with no spacer. By putting the majority of the ionized remote donors closer to the interface, the Coulomb interactions between the donors and the carriers is enhanced, causing a greater amount of carrier scattering. Although a similar effect may be expected in heterostructures doped with hydrogenic impurities, the result is much less dramatic as the formation energy of such extrinsic defects is affected much less by the location of the Fermi level.

Hydrostatic pressure.

One significant disadvantage of defect doped structures relative to those doped with hydrogenic impurities is that they are themselves highly conductive, even at low temperatures, since the carriers do not freeze out. As a consequence, if the barrier layer is grown too thick, a low mobility parallel conduction path may be formed. This additional conduction path may lead to misleading Hall effect concentration and mobility measurements as the conductivities of the two types of electrons will be mixed together. One possibility for separating the two contributions is by the application of large

Figure 4. Formation energy (top) and concentration of defects incorporated in the $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ barrier layer (bottom) as a function of distance from the interface.

hydrostatic pressures. When hydrostatic pressure is applied to GaN or $\text{Al}_x\text{Ga}_{1-x}\text{N}$, the conduction band shifts upwards in energy. On the other hand, since the defects are highly localized, their energy remains constant. This difference in behaviors makes it possible to “freeze out” any three-dimensional electrons in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier by pushing it into the forbidden gap. The concentration of two dimensional electrons in the GaN well remains relatively unchanged, as the charge transfer is governed by the actual defect concentration, which remains unchanged, and more weakly on the Fermi energy, which does not change much at low temperatures. Figure 5 shows the change in electron concentration on both sides of the interface as a function of pressure. This effect has been seen in InGaAs/InP heterostructures [7].

For the Al fraction for which Fig. 5 was calculated, a substantial amount of pressure (~ 40 kbar) is required to “freeze out” the unwanted conduction. However, in order to see this effect at lower pressure, a higher Al fraction could be used to bring the defect energy closer to the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ conduction band.

Conclusion.

We have performed calculations to determine the distribution of donor defects at the interface of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures. Due to the dependence of the formation energy of the defects on the Fermi level, we find that the defect concentration near the interface may be enhanced by more than an order of magnitude as compared to the defect concentration in isolated $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers grown under the same conditions. Although this leads to a more efficient transfer of electrons to the GaN well, the increased concentration of defects near the interface also leads to a degradation of the 2 DEG mobility due to the closer proximity of the charged defect centers. This problem could be eliminated by first growing the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier before the pure GaN layer.

Another feature of modulation doped heterostructures doped with resonant donor defects which is not found in those doped with shallow hydrogenic donors is the possible presence of an alternate conduction path in the barrier layer. As the wavefunctions of the carriers in the barrier are three dimensional in nature and have much lower mobilities than the 2 DEG, the overall effect of the additional conduction path is to increase the concentration and decrease the mobility of the electrons as calculated from Hall effect measurements. However, hydrostatic pressure can be applied to “freeze out” the undesirable three dimensional conduction path.

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Figure 5. Plot of carrier concentration in the GaN well (top) and the AlGaIn barrier (bottom) as a function of pressure.

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ONE CYCLOTRON ROAD | BERKELEY, CALIFORNIA 94720