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Citation: Journal of Applied Physics **95**, 1843 (2004); doi: 10.1063/1.1641148
View online: http://dx.doi.org/10.1063/1.1641148
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/95/4?ver=pdfcov
Published by the AIP Publishing

# Formation of a quasi-two-dimensional electron gas in GaN/$Al_xGa_{1-x}N$ heterostructures with diffuse interfaces

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(Received 6 June 2003; accepted 21 November 2003)

Calculations of the electronic energy levels and the distribution of the quasi-two-dimensional electron gas (Q2DEG) at the GaN/$Al_xGa_{1-x}N$ interface that take into account the graded nature of the interface are presented in this article. Mapping of the interface using scanning transmission electron microscopy annular dark-field imaging, the changes in the N *K*-edge and the integrated intensity of the Al $L_{2,3}$-edge revealed that the interface can be up to 20 Å wide. Self-consistent calculations in the local density approximation estimate the sensitivity of the Q2DEG formed at the interface to various parameters, including the width of the interface, the concentration of bound charge, ambient temperature, and the geometrical sizes of the structure. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1641148]

## I. INTRODUCTION

It is already well established that the polarization difference (piezoelectric and spontaneous) at the GaN/$Al_xGa_{1-x}N$ heterointerface gives rise to a positive bound charge. This bound charge [which plays the role of doping in conventional III–V-compound-based systems with a high-density two-dimensional electron gas (2DEG)] deforms the band structure so that high carrier concentrations form at the interfaces.[1,2] This results in a quasi-2DEG (Q2DEG) with a high mobility without intentionally doping heterostructures.[3]

Theoretical studies[4,5] of such GaN/AlGaN structures show that the mobility of the Q2D electrons is primarily limited by phonon scattering of the carriers at room temperature, whereas at low temperatures it is limited by alloy disorder and interface roughness scattering. Both mechanisms are sensitive to the distribution of the Q2DEG relative to the interface: the closer to the interface the Q2D electrons are, the stronger is the scattering. These observations also strongly stress the importance of accurate positioning of the Q2DEG with respect to the interface.

Despite the existence of extensive research on the GaN/$Al_xGa_{1-x}N$ structures conducted in the past several years, questions still remain unanswered: *What is the nature of the interface and how does it affect the concentration and distribution of the 2*DEG? It is clear that the electronic energy levels and the resulting distribution of the Q2DEG formed at the GaN/$Al_xGa_{1-x}N$ heterointerface should depend on whether the interface is sharp or diffuse.[6]

In this article, we report observation of wurtzite GaN/$Al_{0.25}Ga_{0.75}N$ heterointerfaces using scanning transmission electron microscopy (STEM). Annular dark-field (ADF) images of these interfaces obtained in STEM provide evidence that the interfaces are diffuse. Using ADF imaging and electron energy-loss spectroscopy (EELS) measurements of the Al $L_{2,3}$-edge and N *K*-edge across the interface, we observed that these interfaces can be up to 20 Å wide. Since this is commensurate with the width of the Q2DEG, questions immediately arise concerning the effects of this on the results of calculations based on the sharp interface model. Accordingly, we adapt Stern's model[6] of self-consistent calculations in the local density approximation (LDA) and incorporating bound charge to describe the formation of the Q2DEG at GaN/$Al_xGa_{1-x}N$ interfaces. We present its dependence on critical parameters, such as the width of the interface, the concentration of bound charge, ambient temperature, and the geometrical sizes of the structure.

## II. EXPERIMENT

The wurtzite GaN/$Al_{0.25}Ga_{0.75}N$ heterostructures studied in this article have been deposited on sapphire substrates on which ~200 Å AlN nucleation layers are grown in the molecular-beam epitaxy system. Layers of 1 $\mu$m GaN and 30 nm $Al_{0.25}Ga_{0.75}N$ were grown on this AlN buffer. The measured mobility of the Q2DEG at room temperature was 1152 $cm^2/V\,s$ with a sheet carrier density of $1.04\times10^{13}\,cm^{-2}$. A cross-sectional electron transparent sample for the STEM was prepared by standard tripod polishing techniques,[7] and ion milling was eschewed to prevent extra surface damage. Because of differences in the polishing rates of sapphire and GaN/$Al_{0.25}Ga_{0.75}N$ and the very fragile nature of GaN and $Al_{0.25}Ga_{0.75}N$, it was necessary to add a protection layer to the heterostructure before polishing. In this case, a piece of Si was used.

All measurements reported in this article were performed with the Cornell VG HB501 STEM, which has a

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field-emission gun and is equipped with a single-electron-sensitive ADF detector[8] and a parallel electron energy-loss spectrometer. The energy resolution of the spectrometer is 0.7 eV over an energy range of 0 to 2 keV. ADF images, which are sensitive to the atomic number ($Z$) and the thickness of the sample, provide information about the thickness variation of the sample and also the composition change at the atomic level. The minimum probe size of the STEM beam is ~2.1 Å, and the spatial and energy drifts are 0.3 nm/min (or less depending on conditions) and 0.03 eV/min respectively.

Extremely good alignment of the interface relative to the incident electron beam is essential in interface experiments of this type. Hence, electron diffraction was used for the initial alignment of the interface region of the sample with the zone axis, bringing the growth plane parallel to the incident e-beam. In wurtzite $GaN/Al_{0.25}Ga_{0.75}N$ heterostructures, the growth plane is the basal plane; that is, the plane perpendicular to the $c$ axis. The critical step is alignment of the basal plane parallel to the beam, thus giving later flexibility in orientations within that plane. The contrast of the periodic feature induced by composition variation in $Al_{0.25}Ga_{0.75}N$ in the direction of the $c$ axis (and detectable only after initial alignment) was then used to minimize the interface broadening on further tilt adjustment.

Another important factor is beam broadening inside the sample, caused primarily by elastic scattering of incident electrons and by the divergence of the focused beam (the convergence semi-angle of the STEM electron beam is ~10 mrad). The contribution in beam spreading caused by scattering can be estimated.[9] In our case of ~500 Å specimen thickness and ~15 mrad collection semi-angle, the estimated mean beam broadening is ~5 Å.

Since a long acquisition time is desirable to achieve low-noise EELS measurements, we also perform damage experiments on GaN and $Al_{0.25}Ga_{0.75}N$ under the same conditions as the remainder of the experiments to estimate an acquisition time sufficient to permit the collection of relatively low-noise spectra that are also relatively free of damage. For this sample, we found that N $K$-edge spectra do not show any detectable damage until after at least 7 s of acquisition time. Therefore, in all further measurements of N $K$-edge and Al $L$-edge spectra, we used 5 s as the upper limit for spectrum acquisition time. Small sample drifts (≃3 Å) during EELS measurements were corrected by recording and comparing ADF images of the specimen before and after spectra acquisition.

Several $GaN/Al_{0.25}Ga_{0.75}N$ interfaces were studied and were found to be diffuse. Figure 1(a) shows an ADF image of one interface, where the probing path is also indicated (dashed line). Since aluminum is present only on one side of the heterointerface, we measured the profile of the intensity of the Al $L$-edge across the interface [see Fig. 1(c)]. As expected, no Al signal was detected in the bulk GaN region. At a certain interfacial point, the intensity of the Al $L$-edge becomes significant and then increases up to a point where it equals the intensity of the Al $L$-edge in bulk $Al_{0.25}Ga_{0.75}N$. In these measurements, the interface was mapped by stepping the probe from the GaN to the $Al_{0.25}Ga_{0.75}N$. The solid line in Fig. 1(c) is the ADF intensity at the same location.

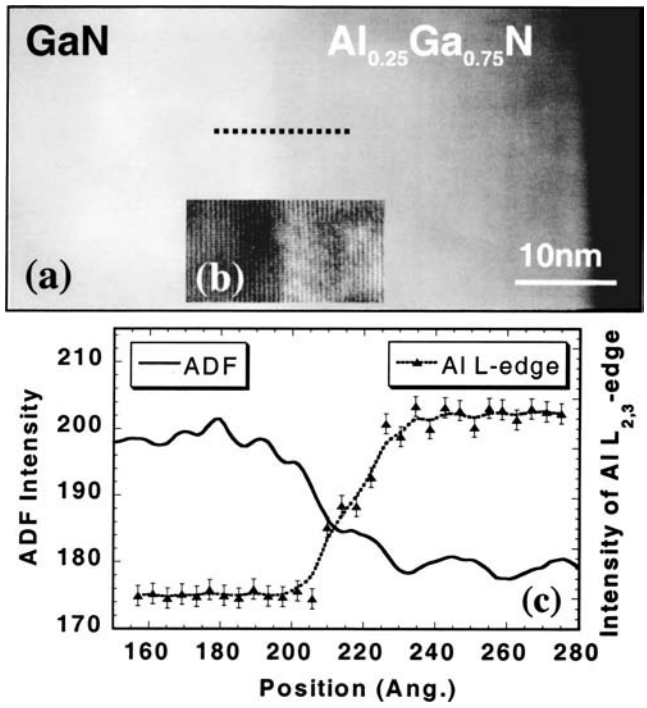


FIG. 1. (a) ADF image of $GaN/Al_{0.25}Ga_{0.75}N$ heterointerface with (b) high-resolution TEM image of the same interface obtained using a JEOL 4000EX TEM. Dashed line shows the points from GaN to $Al_{0.25}Ga_{0.75}N$ where spectra were recorded. (c) ADF intensity and Al $L_{2,3}$-edge integrated intensity across $GaN/Al_{0.25}Ga_{0.75}N$ heterointerface.

Next, the interface was examined with a step size of ~4 Å across the interface by measuring changes in the N $K$-edge. With this step size, six steps are required to cross an entire interface. The results are presented in Fig. 2. On careful examination, the spectrum of the N $K$-edge at one end has all the characteristic features of bulk GaN, while at the other, the spectrum has all the characteristic features of bulk $Al_{0.25}Ga_{0.75}N$.[10] Two interfacial spectra are presented in Fig. 2, and, as we can see, a gradual transition from GaN to $Al_{0.25}Ga_{0.75}N$ takes place. Mapping the interface by examining the alteration in the N $K$-edge spectra, the integrated intensity of Al $L_{2,3}$-edge, and the ADF intensity, reveals the diffuse nature of the heterointerface and determines the physical width to be 20 Å.[11]

## III. CALCULATIONS

A one-dimensional Schrödinger equation for one-electron systems in an effective potential can be applied to describe the energy levels and distribution of Q2DEG in the $GaN/Al_xGa_{1-x}N$ structures. Within an effective-mass approximation the Schrödinger equation has the form[12]

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m_c^*(z)}\frac{d\psi_i(z)}{dz}+V(z)\psi_i(z)=E_i\psi_i(z), \qquad (1)$$

where the effective potential energy is given by

$$V(z)=V_b(z)-e\phi(z)+V_{\mathrm{xc}}(z)+V_{\mathrm{im}}(z). \qquad (2)$$

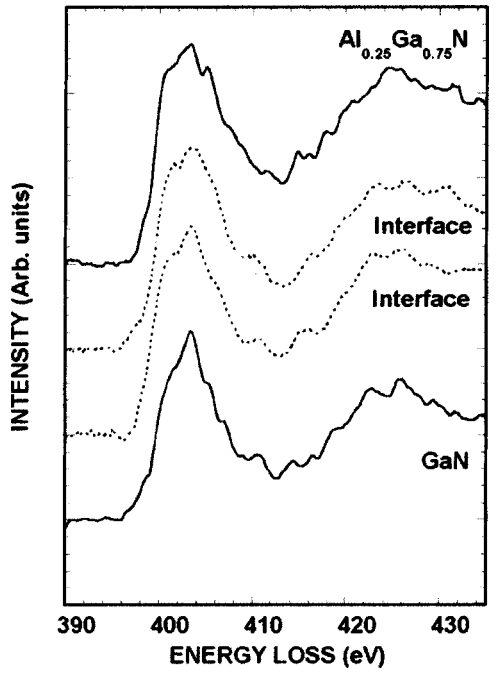


FIG. 2. N *K*-edge from EELS measurements across the $GaN/Al_{0.25}Ga_{0.75}N$ interface. Top and bottom spectra correspond to N *K*-edges in $Al_{0.25}Ga_{0.75}N$ and GaN. The dashed lines are the spectra at interfacial points. Other interfacial spectra are omitted.

In Eq. (2), $V_b(z)$ is the potential energy associated with the discontinuity of the conduction band of the heterojunction [for the AlN/GaN interface, see Fig. 3(a), where $z>0$ is GaN and $z<0$ AlN]. The second term in Eq. (2) is the electrostatic potential, which can be obtained from Poisson's equation

$$\frac{d}{dz}\epsilon(z)\frac{d\phi(z)}{dz}=-\left\{\rho_b(z)-e\sum_i N_i\left|\psi_i(z)\right|^2\right\}, \tag{3}$$

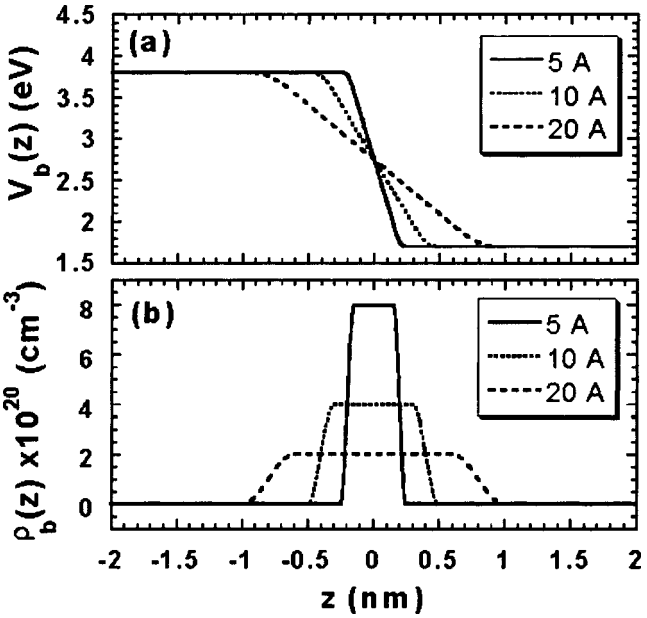


FIG. 3. The gradual changes of parameters at the AlN/GaN heterointerface: (a) potential associated with a discontinuity of the conduction band and (b) distribution of positive bound charge induced by gradient of polarization $\rho_b(z)$. The region $z>0$ is GaN and $z<0$ is AlN.

where the occupation (the number of electrons per unit area) of the *i*th subband $N_i$ is given by

$$N_i=\frac{m_c^* k_B T}{\pi\hbar^2}\ln\left[1+\exp\left[\frac{E_F-E_i}{k_B T}\right]\right], \tag{4}$$

and the polarization-induced positive bound charge is $\rho_b(z)=-\nabla\cdot\mathbf{P}$.

The last two terms in Eq. (2), $V_{xc}(z)$ and $V_{im}(z)$, are the exchange-correlation and image potentials respectively. To compute the exchange-correlation potential, the LDA was applied.[13] In calculations of $V_{xc}(z)$, the local effective mass $m_c^*(z)$ and dielectric constant $\epsilon(z)$ were used. The image potential $V_{im}(z)$, caused by the presence of two materials with different dielectric constants, is calculated using the method described by Stern.[14]

The finite width of the interface is incorporated into the problem by introducing gradual changes in the potential energy[15] $V_b(z)$, effective mass[16,17] $m_c^*(z)$, and dielectric constant[1,18] $\epsilon(z)$ across the interface. To evaluate the values at the interface, we linearly interpolate $V_b(z)$, $m_c^*(z)$, and $\epsilon(z)$ between their values in the GaN and $Al_xGa_{1-x}N$ with rounded corners.[6] The rounding removes artificial discontinuities, which create singularities in their first derivatives. In our calculations, only 20% of the total width was used for rounding (see Fig. 3). Here, we assumed that for the interfacial region, the effective-mass approximation is valid and that the local dielectric constant can be used. The same interpolation function was used to characterize the changes in the polarizations at the interface. As a result, the polarization-induced positive bound charge distribution in the structure has the form presented in Fig. 3(b).

By extending the results of Martin *et al.*[15] to arbitrary composition *x*, the discontinuity of the conduction band $V_b(z)$ can be approximated as $\Delta E_c=0.75\Delta E_g$, where the difference in the bandgaps of two materials $\Delta E_g$ can be expressed as[19]

$$\Delta E_g=x(E_g^{AlN}-E_g^{GaN})-x(1-x)b, \tag{5}$$

where $b$ is $1.0\pm0.3$ eV.

Self-consistent solutions of Eqs. (1)–(4) were generated by a standard iteration procedure starting with some trial charge distribution. In solving Poisson's Eq. (3), the imposed boundary conditions were: (i) the conduction band at the GaN/substrate boundary is at $E_c^{GaN}$ with the Fermi level set at the midgap of GaN and (ii) the Schottky barrier at the $Al_xGa_{1-x}N$ surface is pinned at $e\Phi_b$.[1]

## IV. RESULTS AND DISCUSSION

We begin with the AlN/GaN heterostructure as an extreme case of $Al_xGa_{1-x}N/GaN$. The values of the potential energy $V_b$ and the polarization-induced bound charge used in the calculations are the same as in Fig. 3. The structure considered was a 300-Å-thick AlN barrier layer on 1 $\mu$m GaN buffer layer. The pinning of the Schottky barrier at the AlN surface was 2.14 eV with the Fermi level set at $E_F=0$ eV, and the ambient temperature set at $T=300$ K. The results of the calculations for three interface widths are presented in Table I and Fig. 4. Here, only values of the ground state $E_0$

TABLE I. The energy levels, concentration of the Q2DEG and its average position from the center of interface and fractional occupation (in %) in GaN calculated for the AlN/GaN heterointerface. The values of the ground state energy $E_0$ and first two excited states are relative to $E_F=0$ eV.

| Interface width [Å] | $E_0$ [eV] | $E_{10}$ [eV] | $E_{20}$ [eV] | $n$ [$10^{13}$ cm$^{-2}$] | $\langle z\rangle$ [Å] | % in GaN |
|---|---|---|---|---|---|---|
| $d=5$ | −0.220 | 0.313 | 0.365 | 3.10 | 8.7 | 85.5 |
| $d=5$ (no $V_{xc}$) | (−0.215) | (0.259) | (0.313) | | | |
| $d=10$ | −0.218 | 0.310 | 0.371 | 3.09 | 9.5 | 73.5 |
| $d=20$ | −0.217 | 0.299 | 0.363 | 3.07 | 11.3 | 51.0 |
| $d=20$ (no $V_{xc}$) | (−0.212) | (0.252) | (0.307) | | | |

and first two excited states $E_{10}=E_1-E_0$ and $E_{20}=E_2-E_0$ are presented. As we see from Fig. 4, the profile of the conduction band is very sensitive to the width of the interface (for example, the minimum value of the conduction band changes from −0.750 eV for 5 Å interface and to −0.544 eV for 20 Å), while the concentration $n$ of the Q2DEG is not affected that strongly. On the other hand, there is a shift in the average distance of electrons from the center of the interface $\langle z\rangle$ [$\langle z\rangle=N^{-1}\int zn(z)dz$] from 8.6 to 11.3 Å. It should be noted that only the energy of the ground state $E_0$ is below the Fermi level and, as a result, the major contribution to the spatial distribution of the Q2D electrons comes from this state. The values of $\langle z\rangle$ and the distributions of the Q2DEGs also indicate that, while in the case of a 5 Å interface the electron gas is primarily located in GaN (85.5%), in the case of a 20 Å interface, only 51.0% is in GaN. This result indicates that 49.0% of the Q2D electrons are either in AlN or in the interfacial region, being subject to additional strong interface roughness or to alloy scattering.

Corrections to the energy levels due to $V_{xc}(z)$ are also presented in Table I. As we see, with $V_{xc}(z)$, all levels are shifted down, with pronounced corrections to the ground state. Due to small differences in the dielectric constants, the effects of the image potential in AlN/GaN are small and within the accuracy of the calculations, and are therefore neglected in succeeding calculations.[20]

For a given composition of $Al_xGa_{1-x}N$ and geometrical sizes of the structure, the temperature and potential drop in the $Al_xGa_{1-x}N$ barrier layer are parameters that can potentially affect the Q2DEG. For the AlN/GaN heterostructure, dependence of the energy levels and $\langle z\rangle$ on temperature is studied. With increasing temperature, $\langle z\rangle$ changes, shifting electrons more into the GaN side of the interface. A slight increase in the difference of the ground state energies between the 5 and 20 Å interfaces is also observed. Calculations show that the density of the Q2D electrons stays almost unchanged over a temperature range from 50 to 1000 K, even though there are significant changes in the energy levels and the shift in $\langle z\rangle$ (for example, for the 20 Å interface $E_0$ changes from −0.221 to −0.192 eV).

The effect of the potential drop in the $Al_xGa_{1-x}N$ barrier layer can be introduced into the calculations in two ways, by varying the value of the potential at the Schottky barrier or by keeping the Schottky barrier unchanged and varying the thickness of the $Al_xGa_{1-x}N$ layer. The results of calculations for the AlN/GaN structure with the 20 Å interface are presented in Fig. 5. Here, we used the value 2.14 eV for the Schottky barrier height in all cases. The changes in the thickness of the AlN layer from 100 to 450 Å (corresponding to a change of the Schottky barrier height from 1.77 to 4.28 eV with a constant 300 Å AlN layer) do not significantly affect the Q2DEG. With further reduction of the AlN thickness (≤100 Å), the ground level moves up and, as a result, the concentration of the electron gas decreases. A considerable change in structure occurs only for very small thicknesses (<50 Å). These results stress the presence of limitations on the size of the barrier: barriers that are too thin will significantly reduce concentration of the Q2D electrons.

The next step was consideration of the $Al_xGa_{1-x}N$/GaN heterostructures with different compositions. Calculations for compositions $x=0.4$ and $x=0.25$ ($x=0.25$ corresponds to

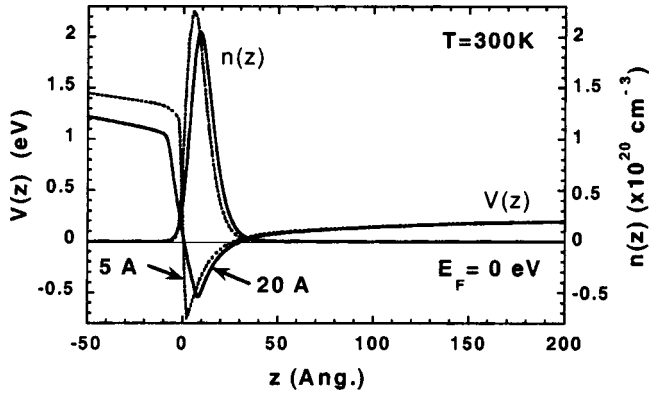


FIG. 4. Conduction band profile and distribution of Q2DEG at AlN/GaN interface for 5 and 20 Å interface widths calculated at $T=300$ K with a 300 Å AlN layer. In calculations, $\Delta E_c=2.29$ eV, $e\Phi_b=2.14$ eV, $m_c^*(GaN)=0.2m_0$, and $m_c^*(AlN)=0.48m_0$.

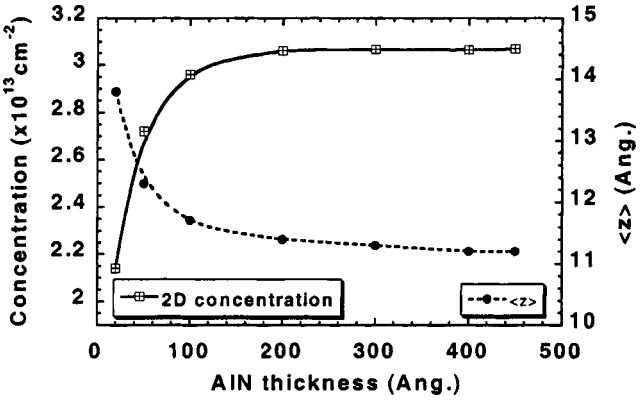


FIG. 5. Dependence of the concentration of the electron gas and $\langle z\rangle$ on the AlN barrier thickness.

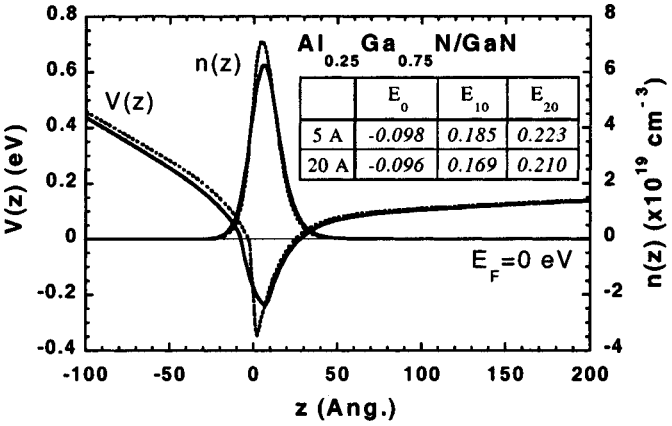


FIG. 6. Conduction band profile, distribution of the electron gas and energy levels for the $Al_{0.25}Ga_{0.75}N/GaN$ heterostructure with 5 and 20 Å interface widths calculated at $T=300$ K and a 300 Å $Al_{0.25}Ga_{0.75}N$ layer. In calculations, the following parameters were used: $\Delta E_c=0.38$ eV, $e\Phi_b=1.16$ eV, and for $Al_{0.25}Ga_{0.75}N$ layer, $m_c^*=0.27m_0$.

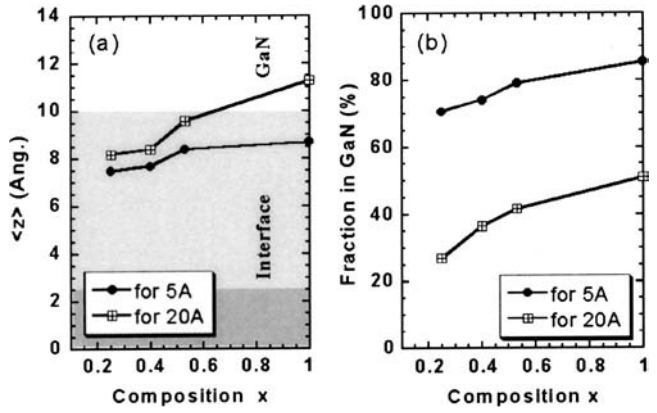


FIG. 8. (a) Dependence of the average distance of the Q2D electrons from the center of the interface for heterostructures with 5 and 20 Å interface widths (dark gray indicates 5 Å interface region and light gray 20 Å). (b) Fractional occupation of the GaN side of the heterointerface by electron gas calculated for two interface widths.

the heterostructures studied in the experiments) were also performed. The results for the $Al_{0.25}Ga_{0.75}N/GaN$ structure are presented in Fig. 6, where, for a polarization-induced bound charge of $1.50\times10^{13}\,cm^{-2}$, the concentrations of the Q2DEG were found to be $1.40\times10^{13}$ and $1.41\times10^{13}\,cm^{-2}$ for the interface widths 5 and 20 Å, respectively. These results again indicate that the size of the interface width does not significantly affect the concentration of the Q2D electrons. On the other hand, the distribution of electrons is still quite different for two cases. For example, in $Al_{0.25}Ga_{0.75}N/GaN$ with a 20 Å interface the fraction of electrons in GaN is only 36.9%. This means that 73.1% of the Q2D electrons, which are either in $Al_{0.25}Ga_{0.75}N$ or in the interfacial region, will now experience strong alloy disorder and/or interface roughness scattering.

Figure 7 summarizes the dependence of the concentration of the Q2DEG on the induced positive charge for two interface widths. Straight lines with slopes $\alpha=0.99$ and $\alpha=0.98$ (for 5 and 20 Å interfaces, respectively) fit to points

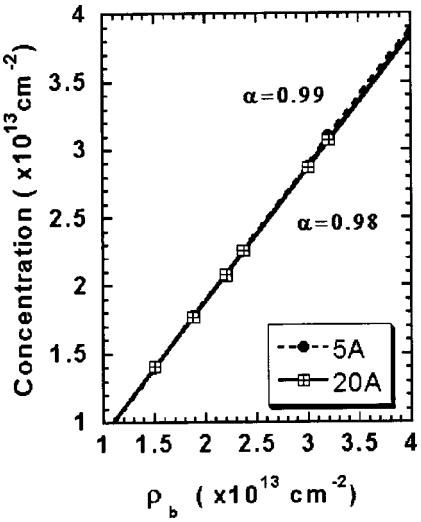


FIG. 7. Dependence of the concentration of the Q2DEG on the concentration of positive charge at the interface for 5 and 20 Å interface widths.

obtained for different compositions. This type of behavior suggests that the concentration of the Q2DEG depends primarily on the total positive charge at the interface. The distribution of electrons, on the other hand, has a more complex dependence on the parameters of the structure. For example, the bigger the conduction band discontinuity, the smaller are the tails of $|\psi_i|^2$ penetrating into $Al_xGa_{1-x}N$ region. The interface width also affects the distribution of electrons. Figure 8 shows that, while the electron gas is primarily located in the GaN side of the heterostructure for a 5-Å-wide interface, for a 20 Å interface, a significant fraction of the electrons are in the interfacial region for a wide range of compositions. As can be seen here for compositions up to $x=0.6$, only $<45\%$ of the electrons are in GaN. This linear dependence can be used for a quick and reliable estimate of the concentration of the Q2D electrons if the density of the positive bound charge is known.

The results of our calculation were also compared with some of the experimental measurements existing in the literature. Concentrations of the Q2DEG obtained here for compositions $x=0.25$ and 0.4 are in good correspondence with measured values.[1] Strong dependence of the concentration of the Q2DEG on AlN thickness in AlN/GaN heterostructures (for small thicknesses) predicted by calculations (see Fig. 5) has also been observed experimentally by Smorchkova *et al.*[21] We should note here that for very small thicknesses of the AlN layer, the concentration also becomes sensitive to other parameters, such as the degree of relaxation or the interface width. For example, in calculations we assumed AlN is completely relaxed ($r=1$) and $\rho_b=3.2\times10^{13}\,cm^{-2}$. However, within the range of acceptable relaxation $r=1$ to $r=0.4$, the positive bound charge can have values from $\rho_b=3.2\times10^{13}$ to $5.1\times10^{13}\,cm^{-2}$ and, therefore, can result in higher concentrations for Q2DEG.

## V. CONCLUSION

A STEM study of the interface by mapping changes of the N $K$-edge, the integrated intensity of Al $L_{2,3}$-edge, and the intensity of the ADF signal showed that $Al_xGa_{1-x}N/GaN$

interfaces can be up to 20 Å wide. Detailed calculations of the electronic energy levels and distribution of the Q2D electron gas were then carried out for undoped GaN/$Al_xGa_{1-x}N$ heterostructures with graded interfaces for different compositions $x$.

The results of the calculation predict that (i) the total concentration of the Q2D electrons is primarily governed by the polarization-induced positive charge; (ii) the dependence is linear ($n=0.985\times\rho_b$), which can be used to estimate the concentration of the Q2D electrons when the density of bound charge is known; (iii) the distribution of carriers and energy levels of the Q2DEG are sensitive to interface width (for example, for composition $x=0.25$, only 36.9% of the Q2D electrons are in GaN region), and therefore, must be taken into account in calculations of mobility, especially at low temperatures, and (iv) the size of the barrier can impose limitations in achieving high-concentration Q2DEGs—for example, if the thickness of the AlN barrier is reduced to about 20 Å, then the concentration of the Q2D electrons will be reduced by a factor of 2 (assuming the potential of the Schottky barrier is kept same). Thus, while there are similarities between the characteristics of the sharp and diffuse interfaces, there are also differences in details that may be significant in the appropriate circumstances.

Good agreement of the values calculated here for the concentration of Q2DEG with the experimental data indicates that the model applied here correctly describes the formation of the Q2DEG for different compositions of the $Al_xGa_{1-x}N$ layer and its dependence on the AlN thickness.

## ACKNOWLEDGMENTS

This work is supported by Office of Naval Research Contract No. N00014-99-10714, under the direction of Dr. C. E. C. Wood. One of the authors (K. A. M.) would also like to thank Dr. T. Arias for helpful discussions.

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[12] Here, we assumed that the effective-mass tensor is diagonal and its elements are equal: $m^*_{c1}(z)=m^*_{c2}(z)=m^*_{c2}(z)$. This is a good approximation for the effective mass around conduction band minima in direct band materials such as the ones we consider: GaN and AlGaN.
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