Conduction band offset at the InN/GaN heterojunction

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The conduction-band offset between GaN and InN is experimentally determined. InN/*n*-type GaN isotype heterojunctions grown by molecular beam epitaxy are observed to exhibit Schottky-junction like behavior based on rectifying vertical current flow. From capacitance-voltage measurements on the heterojunction, the Schottky barrier height is found to be ~0.94 eV. The photocurrent spectroscopy measurement by backside illumination reveals an energy barrier height of 0.95 eV across the heterojunction, consistent with the capacitance measurement. By combining electrical transport, capacitance-voltage, and photocurrent spectroscopy measurement results, the conduction band offset between InN and GaN is estimated to be $\Delta E_C = 1.68 \pm 0.1$ eV. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2821378]

In the past few years, InN has attracted enormous interest since the band gap of InN has been found to be around ~0.7 eV.[1] Because the band gaps of the nitride semiconductor family (AlN, GaN, InN, and their alloys) cover the entire solar spectrum, they are possible candidates for multispectral photodetectors and high efficiency multijunction solar cells. In many possible applications of InN, the band alignments dictate carrier transport and confinement properties.

The theoretical conduction band offset (ΔE_C) between GaN and InN has been calculated to be 2.3 eV.[2] By x-ray photoemission spectroscopy, $\Delta E_V \sim 0.5$ eV was reported.[3] From optical studies of InN/InGaN multiple quantum wells, Ohashi *et al.* have extracted the ΔE_V to be 0.9 eV.[4] By synchrotron-radiation photoelectron spectroscopy, the ΔE_V between InN and GaN was measured to be 1.04 and 0.54 eV for In/Ga- and N-polar heterojunctions, respectively.[5] There is a clear discrepancy between the theoretical and experimental band offsets. One vertical transport study in InN/GaN heterojunctions has set a *lower bound* on the conduction band offset to be 1.4 eV.[6] In this work, the band offset between InN and GaN is experimentally measured using *C-V* measurements and photocurrent spectroscopy, and a charge-control model is used to explain the experimental results via band diagrams.

InN epitaxial films were grown on *n*-type (Si-) doped GaN substrates in a Vecco Gen 930 molecular beam epitaxy system. Details of the growth procedure have been discussed in an earlier work.[7] Hall-effect measurement showed that the nominally undoped InN grown on semi-insulating GaN substrates had bulk electron concentrations of 3×10^{18} cm^{-3} and mobilities in excess of 1000 cm^2/V s at room temperature. For the band-offset measurements, starting from a *n*-type Si-dope GaN substrate ($N_D \sim 4.1 \times 10^{18}$ cm^{-3}), four structures (A, B, C, and D) with different GaN buffer layers were grown, followed by a 200-nm-thick InN layer. In structure A, a 320 nm nominally undoped GaN buffer layer was used. For structures B and C, 160-nm-thick *n*-type GaN layers with doping of 4×10^{17} and 7.7×10^{17} cm^{-3}, respectively, were grown. For structure D, no GaN buffer was grown. After the growth, a mesa was fabricated by reactive ion etching using Cl_2 gas with a rf power of 100 W. Diode structures with junction areas varying from 50×50 to 400×400 μm^2 were fabricated. Then a 20/200 nm Al/Au layer was deposited by e-beam evaporation to form unannealed Ohmic contacts to both the InN and the *n*-type GaN layers. The device structure is shown in Fig. 1(a). When vertical current-voltage (*I-V*) measurements were performed, all diodes exhibited rectifying behavior which indicates a Schottky-barrier like interface between InN and *n*-type GaN, as illustrated by the band diagram sketched in Fig. 1(b). The *I-V* characteristic of a diode from structure A is shown in Fig. 1(c). The diodes from structures B, C, and D show increasing reverse-bias leakage currents, indicating the presence of tunnel currents across thin depletion regions in GaN layers. The barrier height obtained by fitting *I-V* curves using the same method as the work of Chen *et al.*[6] is ~0.5 eV with ideality factor $n \sim 1.7$. The large ideality factor ($n > 1$) clearly indicates the presence of tunneling and leakage through dislocations and other defects. Similar phenomena has been observed in InAs/AlSb heterojunctions.[9,10] For these reasons, *I-V* measurement is expected to yield unreliable results compared with capacitance voltage (*C-V*) measurements in the determination of band offsets. The rectifying nature of the junction affords enough dynamic range for reliable *C-V* measurements.

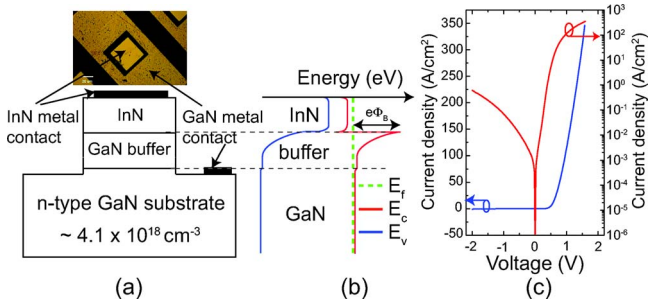

FIG. 1. (Color online) (a) The device structure of InN/*n*-GaN Schottky diode and (b) corresponding band diagram. (c) *I-V* measurement of the Schottky diode from structure A.

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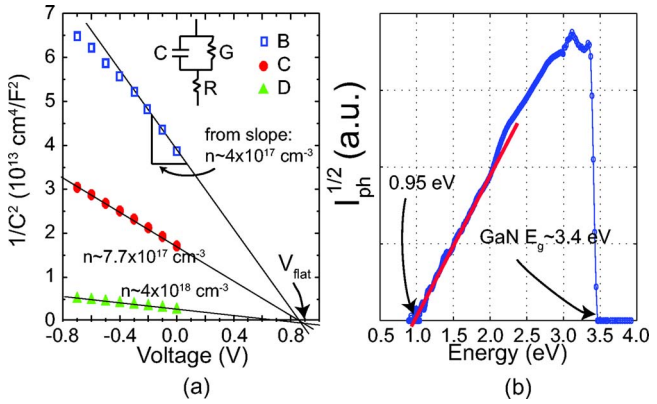

FIG. 2. (Color online) (a) *C-V* measurements of InN/*n*-GaN diodes. (b) square root of photocurrent vs photon energy.

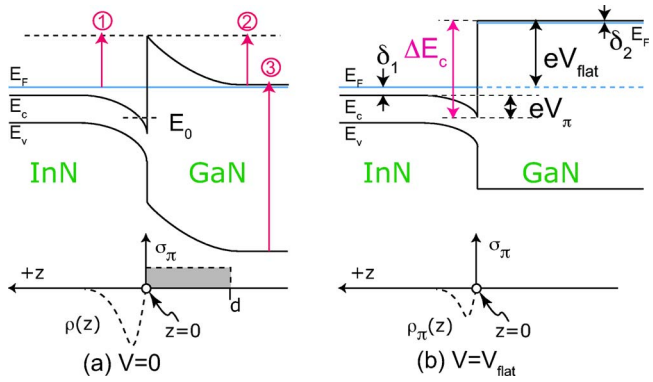

FIG. 3. (Color online) The band alignment and charge diagram of InN and *n*-GaN at (a) no bias and (b) $V=V_{\mathrm{flat}}$. In the photocurrent spectroscopy, possible optically introduced transitions for the InN/GaN heterojunction are plotted in (a).

C-V measurements were performed on the heterojuncitions from 1 kHz to 100 MHz. The junction capacitance was extracted using an equivalent circuit of the form shown in the insert of Fig. 2(a). The measured $1/C^2-V$ curves for three diodes (structures B, C, and D) are plotted in Fig. 2(a). For a Schottky diode, the *C-V* relationship can be expressed as[8] $1/C^2 \approx (2/e\varepsilon_{\mathrm{GaN}}N_D)\times(V-V_{\mathrm{bi}}-k_BT/e)$, where e is the electron charge, $\varepsilon_{\mathrm{GaN}}=9.7\varepsilon_0$ is the dielectric constant of GaN, C is the capacitance per unit area, N_D is the doping density in GaN, T is the temperature, k_B is the Boltzmann constant, V_{bi} is the built-in diffusion potential, and V is the applied voltage. At forward bias the depletion width in GaN decreases, increasing the junction capacitance, and leading to an intercept in the $1/C^2-V$ plot at $V=V_{\mathrm{flat}}=V_{\mathrm{bi}}-kT/e$. This *C-V* intercept method should be used with care since it is an approximation for isotype heterojunctions, especially when the applied voltage divides between the two sides of the heterojunction.[9,10] As shown in Fig. 2(a), the capacitance data yields a linear $1/C^2$ dependence on the voltage for three distinct samples with varying GaN doping levels. Therefore, the approximation is justified. A *constant* capacitance was observed in the nominally undoped GaN buffer layer sample (structure A), indicating that the buffer layer was completely depleted. This sample was used primarily for a consistency check, and is not discussed further in this work.

The Schottky barrier height can be written as $e\phi_B=eV_{\mathrm{bi}}+(E_c-E_F)_{\mathrm{GaN}}$, where E_c and E_F are the conduction band edge and Fermi level in the flat band region of GaN. For the diodes on structure B, $e\phi_B$ is found to be ~0.94 eV, from Fig. 2(a). Photocurrent spectroscopy is a direct way to verify electrically measured Schottky barrier heights.[10] Such a measurement was performed on a 200×200 μm^2 heterojunction (structure B) using backside illumination. The measured photocurrent versus photon energy is plotted in Fig. 2(b). According to Fowler's theory,[11] the relationship between the photocurrent per photon I_{ph}, and the incident photon energy ($h\nu$) is given by $I_{\mathrm{ph}}\propto(h\nu-e\phi_B)^2$. The barrier height, therefore, can be obtained from the straight line intercept of the $\sqrt{I_{\mathrm{ph}}}$ versus $h\nu$ plot. This barrier height is measured to be 0.95 eV, which is close to the *C-V* measurement result. With backside illumination, the photocurrent cuts off for $h\nu>E_G^{\mathrm{GaN}}=3.4$ eV, as observed in Fig. 2(b).

To relate these measurement results to the band alignment between InN and GaN, schematic conduction band diagrams of the InN/*n*-GaN heterojunction are shown in Fig. 3 for two cases $V=0$ and $V=V_{\mathrm{flat}}$ (conceptual case), along with charges that are formed at the interface. The polarization dipole due to the wurtzite structure for the InN/GaN heterojunction is shown as a positive sheet charge σ_π at the interface, and a corresponding two-dimensional electron gas $\rho_\pi(z)$. The important thing is that with applied forward bias, the charge dipole formed between the positive depletion region in GaN and the corresponding excess charge in InN can be removed, but the polarization dipole cannot. Therefore, the polarization dipole makes the band diagram at $V=V_{\mathrm{flat}}$ appear as shown in Fig. 3(b), leading directly to the relation

$$\Delta E_c = eV_{\mathrm{flat}} + \delta_1 + \delta_2 + eV_\pi, \tag{1}$$

where eV_π is the band bending in InN due to the polarization-induced electron accumulation layer, δ_1 is the energy (E_F-E_c) in the flatband neutral region of InN, and δ_2 is the energy (E_c-E_F) in the flatband neutral region of GaN. V_{flat} is directly determined from *C-V* data [Fig. 2(a)], and calculations of other three components are discussed below.

The bulk carrier density in InN determined from the Hall effect measurement is $\sim3\times10^{18}$ cm^{-3}, therefore δ_1 can be obtained from ordinary carrier statistics. Since InN is a narrow bandgap semiconductor, $k\cdot p$ theory[12] can be used to describe the nonparabolic conduction band $E(k)$ of InN

$$E(k)[E(k)+E_g] = \frac{\hbar^2k^2}{2m^*_{\mathrm{InN}}}E_g, \tag{2}$$

where k is the wavevector, $m^*_{\mathrm{InN}}=0.04m_0$ is the band edge ($k=0$) electron effective mass,[13] and $E_g=0.65$ eV is the band gap of InN. The conduction band DOS is derived as $g(E)=[8\pi k^2/(2\pi)^3]dk/dE$, and the total electron concentration is given by $n=\int_{E_c}^{\infty}g(E)f(E)dE$, where $f(E)$ is the Fermi-Dirac distribution function. A numerical solution yields $\delta_1=0.147$ eV.

The band bending (eV_π) on the InN side is due to the electron accumulation $\rho_\pi(z)$, introduced by the polarization dipole σ_π. From charge neutrality, $\int_0^\infty\rho(z)dz=-\sigma_\pi$. Due to the large barrier at the InN/GaN heterojunction, the excess electron density variation should be similar to that of a two-dimensional electron gas. Thus, the spatial distribution of the accumulated electrons in InN is well described by a Fang-Howard function $\psi(z)$,[14]

TABLE I. InN and GaN band offset calculations. $\Delta E_c^{\star}$: without considering the shift in the band bending in InN from defects in InN near the InN/GaN interface. ΔE_c: after estimating the band bending due to charged dislocations in InN near the InN/GaN interface (unit: eV).

Device	δ_1	δ_2	V_π	eV_{flat}	$\Delta E_c^{\star}$	ΔE_c
B	0.147	0.04	0.43	0.9	1.52	1.73±0.05
C	0.147	0.02	0.43	0.89	1.49	1.70±0.05
D	0.147	−0.02	0.43	0.85	1.41	1.63±0.05

$$\rho_\pi(z) = \sigma_\pi |\psi(z)|^2 = \sigma_\pi \left(\frac{b^3}{2}\right) z^2 e^{-bz}, \tag{3}$$

where $b=[33e^2 m^*_{\text{InN}} \sigma_\pi/(8\varepsilon_{\text{InN}}\hbar^2)]^{1/3}$.[15] Due to the large lattice mismatch between InN and GaN (~11%), the critical thickness of InN is close to a monolayer, and the InN is relaxed. Then, the polarization sheet charge at the interface is equal to the difference in spontaneous polarization between GaN and InN. For Ga(In)-polar crystals, we get a positive polarization sheet charge $\sigma_\pi = |P^{\text{sp}}_{\text{InN}} - P^{\text{sp}}_{\text{GaN}}| \sim 7\times 10^{12}$ /cm^2. The band bending eV_π in the InN accumulation region can then be calculated by integrating the Poisson equation. This results in $eV_\pi = 0.425$ eV.

Using the Maxwell-Boltzman approximation, δ_2 were calculated to be 0.04, 0.02, and −0.02 eV for structures B, C, and D respectively. The *C-V* measurement data and calculated results are listed in Table I. Without considering charged defects at interface, the conduction band offset between InN and GaN ($\Delta E_c^{\star}$) is found to be ~1.47±0.05 eV. The presence of the charged dislocations of density ($N_{\text{dis}} \sim 4\times 10^{11}$ cm^{-2}) at the InN/GaN interface[16] can alter the electron density in the accumulation layer at the heterojunction.[17] The experimental difficulty in determining the exact charge on dislocations at the heterojunction limits the accuracy of this measurement of the band offset. However, a reasonable estimate of the effect of dislocations can be obtained from the electrostatics. Within a few nanometers near the interface (d=4–6 nm), the change in the electron sheet density is given by $N_{\text{dis}} d/c$, where c=5.63 Å is the c-lattice constant of InN, assuming one charge per dangling bond in a unit cell. It is reasonable to assume these electrons obey the Fang-Howard distribution [Eq. (3)], thus, we can employ a similar treatment as calculating V_π. The resulting shift in the band-bending in InN due to the dislocation charge is calculated (by integrating the Poisson equation) to be 0.17–0.26 eV. Thus, based on above analysis, the conduction band offset of InN and GaN is estimated to be $\Delta E_c \sim 1.68\pm 0.1$ eV.

In summary, *n-n* isotype InN/GaN Schottky diodes were fabricated, and characterized by *I-V*, *C-V*, and photocurrent spectroscopy. The conduction band offset between InN and GaN was extracted to be $\Delta E_c \sim 1.68\pm 0.1$ eV, and the corresponding valence band offset is $\Delta E_v \sim 1.07$ eV. This ΔE_v is close to recent reported values of 0.9–1.05 eV [by x-ray photoelectron spectroscopy[4,18] (XPS)] and 1.04 eV (by photoelectron spectroscopy[5]), but higher than a previous XPS result of 0.5 eV[3] and theoretical calculation of 0.45 eV.[2] The conduction band offset (~1.68 eV) is consistent with a previous report where the authors implied that ΔE_c is larger than 1.4 eV.[6] The measured conduction band offset should prove useful for heterostructure device design.

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