Fermi edge singularity observed in GaN/AlGaN heterointerfaces

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We observe sharp spectral lines, at energies which are higher than the bulk GaN band gap, in the photoluminescence and photoluminescence excitation spectra of GaN/AlGaN heterointerfaces grown by molecular beam epitaxy. The spectra and their temperature dependence are in accord with the Fermi edge singularity expected for two dimensional electron gas systems. The associated localized hole energy in the AlGaN interface side was extracted directly from the spectra. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3147869]

It is well established that in AlGaN/GaN single heterostructures (SHs) a two dimensional electron gas (2DEG) is formed on the GaN side of the interface.[1] This 2DEG results from the presence of considerably large piezoelectric and spontaneous polarizations at the heterojunction.[1] The polarization induced electric charge depends on various parameters, such as the lattice mismatch strain,[2] the gradient in the alloy composition close to the interface,[3] and the density of electronic traps due to dislocations or surface states.[4] Therefore, in reality, the electronic transport, as well as the optical properties of the system are derived not only from the intrinsic behavior of the 2DEG, but also from the method of growth, e.g., metal organic chemical vapor deposition (MOCVD) or molecular beam epitaxy (MBE), as described below.

Photoluminescence (PL) studies of MOCVD grown SHs reveal emission in the energy range at, or slightly below, the bulk GaN band gap.[5–7] This emission is assigned to optical transitions between electronic states which are spatially located at the AlGaN/GaN 2DEG interface to localized states or to free hole continuum states which extend far into the GaN region, away from the AlGaN/GaN interface. On the other hand, in a modulation doped MBE grown $Al_{0.09}Ga_{0.91}N$ SHs, broad ($\approx$100 meV) and asymmetric emission band at energies $\approx$100 meV above the bulk GaN band gap was observed.[8] The spectral shape of this band and its temperature dependence led the authors of Ref. 8 to attribute this band to optical transitions associated with the 2DEG formed in the SH interface. In particular, they attributed the enhancement in the higher energy side of the spectral band to the expected Fermi edge singularity.[9] This interpretation, however, was challenged by Monemar *et al.*,[10] who suggested that the observed PL band is due to extrinsic centers related to bulk AlGaN.

Here, we report on the PL and PL excitation (PLE) spectra of MBE grown $Al_xGa_{1-x}N/GaN$ SHs. In both PL and PLE spectra we observe a narrow ($\approx$30 meV) peak at energies which are considerably higher than the bulk GaN band gap. We show quantitatively, using a relatively simple model, that the spectral shapes of the emission (PL) and the absorption (PLE), and their temperature dependencies are in accord with optical transitions, which originate from the 2DEG interfaces of the SHs. In particular, we show that the energy of the spectral enhancement toward the higher energy side of the emission and absorption spectra agree with the Fermi energy of the SH's 2DEG, as deduced from its measured carrier density. We thereby deduce that it is, indeed, due to the effect of the singularity at the Fermi energy edge.

The AlGaN/GaN SH samples were grown by radio-frequency plasma assisted MBE on a $\approx$2 μm layer of unintentionally doped, *n*-type, (0001) oriented MOCVD grown GaN on a sapphire substrate.[11] Each of the SH samples is composed of $\approx$2 μm thick GaN layer and $\approx$30 nm thick $Al_xGa_{1-x}N$ layer. PL and PLE studies on two SH samples are reported here. Both samples are unintentionally doped. The nominal Al content in sample A and B is $x=0.17$ and $x=0.13$, respectively. A 2DEG carrier sheet density of $n_{2D} \approx 6\times10^{12}$ cm^{-2} (sample A, $x=0.17$) was extracted from Shubnikov–de-Haas magneto-oscillation measurements at 4.2 K.

For the optical studies, the samples were mounted on a cold finger cryostat and were excited by a xenon lamp whose light was dispersed by a 0.275 m monochromator. The emitted light was dispersed by a 0.25 m monochromator and detected by a UV enhanced charge coupled device camera.

The PL spectra of the two SH samples measured at 4.2 K are shown in Fig. 1 (solid lines). The spectra are composed of the known narrow PL line at $\approx$3.48 eV (marked GaN), due to electron hole recombination in bulk GaN,[5] and a higher energy broad asymmetric band (marked HE) with a relatively narrow band superimposed on its high energy tail (marked FES). Figure 1 shows that both the HE and FES emission bands are common to the two samples studied, while their energy is composition dependent. In order to characterize these three bands we have measured the PLE spectra while monitoring each one of the three PL bands. In the following we turn our attention to sample A only. The PLE spectra for sample A ($x=0.17$) is shown in Fig. 1 (dotted lines). One clearly sees that the three PLE spectra differ from each other, testifying that the PL spectral features originate from different, unrelated, absorption-recombination pro-

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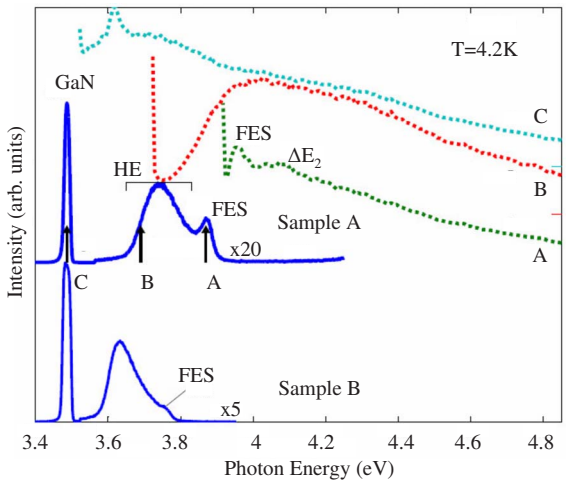

FIG. 1. (Color online) PL and PLE spectra of the MBE grown samples. The solid lines represent the PL spectra of sample A (top) and sample B (bottom). GaN, HE and FES refer to the spectral features discussed in the text. The dotted lines (marked A, B, and C) represent the PLE spectra of sample A monitored, respectively, at the positions A, B, C marked by arrows on the PL spectrum.

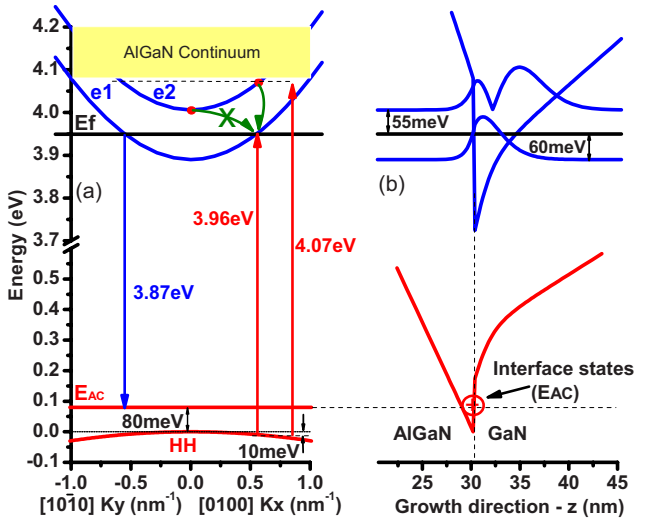

FIG. 3. (Color online) (a) Calculated dispersion curves for the two electron sublevels $E_1(k_\parallel)$, $E_2(k_\parallel)$ and the heavy hole level $E_{HH}(k_\parallel, k_z=0)$ in the three-dimensional bulk AlGaN layer. The vertical and downward arrows represent the relevant optical transitions discussed in the text. (b) Schematic description of the conduction and valence band potential profiles close to the AlGaN/GaN interface. The calculated 2DEG probability of distribution at E_1 and E_2 are overlaid on the potential profile. Also indicated by $\oplus$ sign is the position and energy of the hole trap E_{AC}.

cesses. The PLE spectrum of the GaN band (dotted line curve C), shows a blueshifted narrow band, monotonically decreasing toward higher energies. This spectral feature is interpreted as due to absorption into the bulk GaN layer.[12] Similarly, the PLE spectrum of the HE band (dotted line curve B), also shows a broader blueshifted band, which monotonically decreases toward high energies. Since the PL HE band is energetically quite close to the $Al_{0.17}Ga_{0.83}N$ layer's band gap, we ascribe it to recombination of electrons and holes at extrinsic recombination centers within the $Al_{0.17}Ga_{0.83}N$ region. The much larger width of the HE band ($\approx$100 meV) is typical for ternary materials, where the emission and absorption spectra are inhomogeneously broadened by disorder induced potential fluctuations.[13]

The PLE spectrum (dotted line curve A) of the narrow FES PL line (peaked at 3.87 eV in this sample) is clearly distinguished from the other two spectra. It shows a narrow peak (at 3.96 eV) blueshifted from the PL FES peak by $\approx$90 meV, followed by a wider peak at ΔE_2=4.07 eV, where the PLE intensity is enhanced. The temperature dependence of the FES PL and PLE spectra from sample A is shown in Fig. 2. We note that the FES PL and PLE peaks

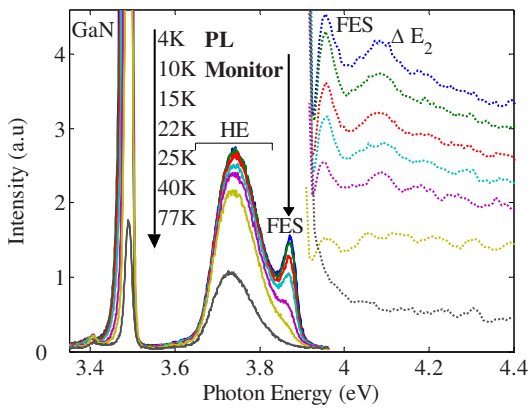

FIG. 2. (Color online) PL (solid lines) and PLE (dotted lines) spectra of sample A for various temperatures. GaN, HE, and FES refer to the spectral features discussed in the text. The PL was monitored at the FES peak.

intensity sharply decrease as the temperature increases, disappearing altogether at temperatures above $\approx$40 K, while the HE band retains more than 20% of its low temperature intensity even at 77 K. These observations clearly indicate that the HE and FES spectral features are not related. The origin of the FES band, which is the main subject of this letter, is further discussed below.

We argue that the spectral shape of the FES line in the PL and in the PLE spectra and its unique temperature dependence unambiguously indicate that it stems from optical transitions associating electrons at the GaN 2DEG Fermi energy. The optical transitions between these electrons and holes at the bulk AlGaN valence band give rise to the FES line in the PLE spectrum, while transitions to holes, which are localized by shallow SH interfacial centers at the AlGaN side, give rise to FES line in the PL spectrum.[9] Indeed, "band gap states" due to traps close ($\approx$60 meV) to the AlGaN valence band were observed using capacitance deep level optical spectroscopy in MBE grown AlGaN/GaN heterostructures.[14–16] These possibly donor like traps[16] are neutral at thermal equilibrium in the dark. Upon photoexcitation, a 2DEG electron radiatively recombines with a trapped photoexcited hole. This results in the FES spectral feature observed in the PL spectrum.

In Fig. 3(a) we schematically describe these absorption and recombination processes. The figure describes two electronic subbands and localized hole states. The diagram displays the 8×8 $k\cdot p$ calculated dispersion of the two electron sublevels $E_1(k_\parallel)$, $E_2(k_\parallel)$ and the heavy hole level $E_{HH}(k_\parallel, k_z=0)$ in the 3D bulk AlGaN layer. The downward arrow denotes photon emission due to a transition from the 2DEG electron gas to the localized hole at E_{AC}. The two upward arrows denote optical excitations due to transitions from the AlGaN valence band at $E_{HH}(k_\parallel=k_F)$, $k_Z=k(E_1)$ to $E_1(k_\parallel=k_F)$, and from $E_{HH}(k_\parallel=k_F)$, $k_Z=k(E_2)$ to $E_2(k_\parallel=k_F)$.

In Fig. 3(a) the FES PL transition energy is the energy difference E_F-E_{AC}, where E_{AC} is the localized trap energy.

This transition energy is ≈90 meV lower than the FES transition observed in the PLE spectrum (Fig. 1 dotted line curve A). The reason for this Stokes-like difference can be easily understood if one recalls that absorption (PLE) probes the density of available states for optical excitations, while emission (PL) probes the actual occupation of the states at the recombination time. Since optical transitions conserve momentum, the transition energy observed in the PLE spectrum reflects the energy difference between the energy of 2DEG electrons at the Fermi crystal momentum (k_F) to free holes having the same crystal momentum. The ≈90 meV difference is made up of the sum of E_{AC} and the heavy hole energy at $k=k_F$, $E_{HH}(k_F)$. From the measured electron density of 6×10^{12} cm^{-2}, assuming an electron effective mass of $m^*=0.2m_e$,[17] we find $E_F-E_1\approx60$ meV. Using an 8×8 $k\cdot p$ band structure calculation for the AlGaN, we find $E_{HH}(k=0)-E_{HH}(k_F)\approx10$ meV, thus yielding for the localized hole energy $E_{AC}-E_{HH}(k=0)\approx80$ meV. Such a hole trap is in line with the ≈60 meV trap energy reported earlier for MBE grown AlGaN SHs.[14,16]

The above discussion accounts also for the second peak in the PLE spectra (Figs. 1 and 2). While the FES line is the highest energy in the PL spectrum, it is the onset energy for the PLE spectrum. This is true simply because at lower electron energies all the available states are occupied and photogeneration is impossible. The FES PLE peak manifests the enhancement in oscillator strength for optical absorption occurring just at the electron Fermi energy E_F for the 2DEG system. Absorption into empty higher energy states is possible. The relative strength of the absorption into these states reflects the joint density of states for optical transitions into these states. Since the density of states is energy independent for a 2D system, the absorption at energies above the enhanced FES peak is as seen in Fig. 2. This reduction ends with a second peak at energies which permit optical excitations into the second, SH 2DEG energy level, E_2 (k_F).

In order to calculate the SH energy band structure we used a self-consistent Schroedinger and Poisson solver.[18] Figure 3(b) shows a schematic description of the conduction and valence band potential profiles close to the AlGaN/GaN interface. The calculated 2DEG probability of distribution at E_1 and E_2 are overlaid on the potential profile. Also indicated by ⊕ sign are the position and energy of the hole trap, E_{AC}. Using a Schottky barrier of ≈1.9 eV,[18] the solver yielded the energy band structure displayed in Fig. 3(b). In particular, for sample A, $E_2-E_F\approx55$ meV.

Photons that have enough energy to generate zero momentum holes and E_2 electrons are absorbed by populating either E_1 or E_2 electronic states. However, E_2 electrons having momentum smaller than k_F will not relax into the E_1 level, since such relaxation requires an increase in their momentum above k_F [the situation is schematically described in Fig. 3(a)]. Therefore, these photons do not contribute to the PLE spectrum (monitored at the PL FES peak). As the energy of excitation increases, the in-plane crystal momentum of photoexcited electrons at E_2 approaches k_F. Hence, scattering of these electrons to empty states at $E_1(k_F)$ is more favorable. This gives rise to a second enhancement in the FES PLE spectrum observed at 4.07 eV (ΔE_2 in Figs. 1 and 2), due to FES enhancement in scattering. The temperature dependence of the intensity and the width of the peaks clearly demonstrate that they are related to FES enhanced scattering processes.

In conclusion, a sharp peak in both the PL and PLE spectra was observed significantly above the GaN band gap in MBE grown GaN/AlGaN single heterostructures. The spectral position, the spectral shape, and the strong temperature dependence of this high-energy spectral feature establish that it is due to enhancement in the optical transition involving electronic states near the 2DEG Fermi edge. This establishes the first unambiguous experimental observation of the so called "Fermi edge singularity" in an AlGaN/GaN 2DEG. In addition, our work confirms the existence of near band gap defects in the disordered AlGaN layers grown by MBE.

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