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COMMUNICATIONS

Spatially-resolved photoluminescence studies of V-shaped pits on $Al_{0.16}Ga_{0.84}N$

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We have studied optical properties of V-shaped pits on $Al_{0.16}Ga_{0.84}N$. The microphotoluminescence spectrum from the pit center shows a broader and stronger emission at 350 nm than the near-band-edge emission at 336 nm from nonpit regions. The results indicated specific defect levels associated with the V-shaped pits. Furthermore, after using atomic force microscopy to probe the surface electrical potential with a conductive tip, the pit's potential was ~0.2 V lower than its surrounding region. A simplified energy diagram is tentatively proposed to interpret our observation.
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Nitride-based materials have been drawing considerable interest in recent years for wide-bandgap emitting applications.[1,2] Among them, the AlGaN compound is even important for white light illuminination, high electron mobility transistors, and photodetectors.[3,4] However, there are some unclear mechanisms relating to how the structural and compositional inhomogeneities in the alloy affect optical properties. For example, further study is needed to determine whether threading dislocations act as nonradiative recombination centers or enhance the compositional fluctuation that induces localized exciton states to give strong emission. Thus, the optical and electrical studies of defects on AlGaN are still very important. In the early work of InGaN, Pozina *et al.*[5] found that V pits might influence the photoluminescence (PL) spectra and photocarriers strongly localize in the disordered surface region, possibly associated with V pits. V pits also give rise to a low-energy shoulder in the PL spectra.[6] Recently, Pécz *et al.*[7] observed V-shaped surface pits on AlGaN different from those on InGaN; namely, the presence of segregated Al atoms within V pits. Although similar V pits have been observed in AlGaN, their optical properties have not been studied in detail. To understand the microscopic optical properties associated with the V pit distribution of AlGaN alloys, the microphotoluminescence spectrum (μ-PL) is a very well-suited optical characterization technique. In this letter, we present experimental results of AlGaN, particularly the PL behavior of V pits. Spatially resolved μ-PL and atomic force microscope (AFM) measurements were used to investigate the photocarrier recombination mechanisms. A model is tentatively proposed to interpret the observed diffusion and transition behavior of photoexcited carriers.

The $Al_{0.16}Ga_{0.84}N$ film was grown on the (0001) sapphire substrate at 1120 °C by using low-pressure metalorganic vapor phase epitaxy. Prior to growth, a GaN nucleation layer of 250 Å was first deposited at 520 °C, followed by a 1120 °C, 2-μm-thick GaN buffer layer. The Al, Ga, and N precursors were trimethylaluminum, trimethylgallium, and ammonia (NH_3), with flow rates of 20, 10, and 5000 sccm, respectively. An AFM (Solver P47H) combined with scanning Kelvin measurements (SKM) mode was employed for the surface potential measurements. The tip with 35 nm radius of curvature is sputtered with Pt. Details of SKM measurements can be found in other reports.[8,9] For room temperature μ-PL measurements, a He-Cd laser (Omnichrome 2074) operating at 325 nm was used for above bandgap excitation and was focused to a spot size of ~1.5 μm by a microscope objective (100×, 0.5 numerical aperture). The signals were collected by the same objective lens into a monochromator (ARC-500) and a photomultiplier tube (Hamamatsu R-955) for detection.

The AlGaN surface is usually rough and contains various defects on it, including many V-shaped pits. As shown in Fig. 1, the AFM picture displays one such pit whose cross section is 1.5 μm wide and 1 μm deep. From the operational principle of SKM, the tip feels an electrostatic force of the cantilever tip and the sample surface such that

$$F_z(\omega) = -[(V_0 - \varphi_{x,y})V_1 \sin(\omega t)](\partial C/\partial z),$$

by adjusting the dc bias voltage so that the tip feels no force. The local surface potential of sample at position (x,y) $\varphi_{x,y}$ can then be obtained. $\varphi_{x,y}$ corresponds to the work function difference between the tip metal and sample; that is, $\varphi_{x,y} = \varphi_{tip} - \varphi_{AlGaN}$, where φ_{tip} is the work function of tip (5.6 eV), and $\varphi_{AlGaN} = \chi_{AlGaN} + \xi$ is the difference between the

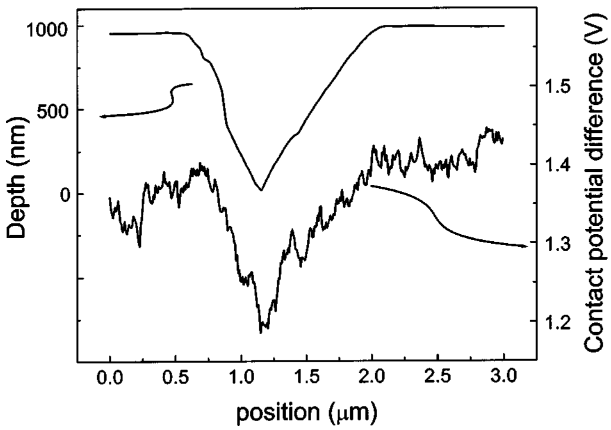

FIG. 1. AFM measured the cross-sectional image and potential depth profile of the V pit.

Fermi level and vacuum level, in which χ_{AlGaN} is the electron affinity (3.4 eV) and ξ is the energy difference between the Fermi level and conduction band. Thus, one can deduce the Fermi level at any position from $\varphi_{x,y}$. After scanning the surface electrical potential across the V pit along its diagonal line and the flat region, we measured a potential difference between them as large as 0.2 ± 0.05 V (see Fig. 1). For our AlGaN sample, the Fermi level at V-pit center is apparently lower than that at nonpit region by $\sim$0.2 eV.

To investigate the behavior of photoexcited carriers and the mechanisms of transition associated with V pit, we have spatially probed its PL signals at room temperature and observed another transition. Figure 2 shows a series of μ-PL spectra taken at different locations along a dihedral direction across the V pit. The position label indicates the approximate distance from the V pit. We can see that the spectra are dominated by the near-band-edge emission (I_{nbe}) at 336 nm as the laser spot moves far away the V pit. When it is focused on the V pit, the most significant change in the μ-PL spectra is the appearance of another broad peak at 350 nm. Obviously, this strong and prominent structure is only related

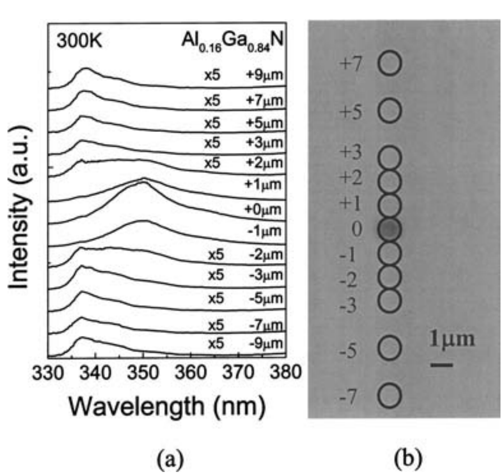

FIG. 2. (a) The spectrally resolved μ-PL spectra obtained at different locations near a V pit on the sample. (b) Peak positions of μ-PL spectra observed at the same excitation positions on the $Al_{0.16}Ga_{0.84}N$ where circles show the region probing by a He-Cd laser as in (a).

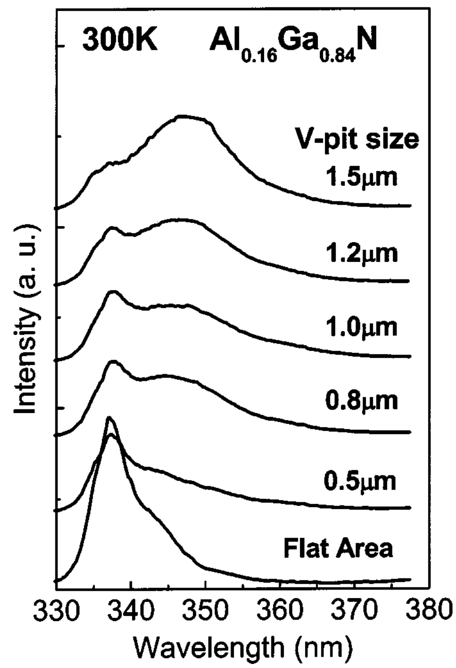

FIG. 3. The μ-PL spectra of different sizes from 0.5 to 1.5 μm.

to the V pit. Note that, although the I_{nbe} emission is still present at 336 nm, it is so weak that is submerged in the broad 350 nm band. In reported literature of the V pit in AlGaN and InGaN, people claimed that the Al and In are segregated and form Al-rich and In-rich regions.[5–7,10,11] However, the presence of both I_{nbe} and 350 nm line indicates that the Al-rich behavior does not appear in our sample. Considering the shear stress in the V pit due to different basal lattice constant (biaxial), the piezoelectric field may cause the redshift feature, between the original state of finite-skewed triangular potential.[12–14] However, if this were the case, the redshift of I_{nbe} should be dependent on the pit size. We have examined the different V-pit sizes from 0.5 to 1.5 μm and hardly found any significant shift for the I_{nbe} line as shown in Fig. 3.

According to Jenkins *et al.*[15] and Tansley *et al.*,[16] one triplet level of the native nitrogen vacancy at $\sim$30 meV below the conduction band and V_{Ga} level at $\sim$136 meV above the valence band in GaN were predicted. Concerning the origin of the broad 350 nm band, we believe that the V pit is related to accumulated native defects (namely, Ga vacancy V_{Ga}). Our AFM results appear to give evidence of the V_{Ga} level. Inside the V pit, a potential difference of $\sim$0.2 V lower than that at nonpit region is observed. It is likely that acceptor levels inside the V pit effectively lower the Fermi level. Because the native V_{Ga} levels are known to lie deep within the gap, it is reasonable to infer that the 350 nm emission in our sample can be attributed to the $V_N^+ - V_{Ga}^-$ complexes inside V pits.

Furthermore, we address the issue as to whether the PL intensity is affected by the V pit. For comparison, Figs. 4(a)–4(c) show the spatial μ-PL intensity distribution at the I_{nbe} (336 nm), V-pit-related line (350 nm), and their ratios, respectively. At the V-pit center, we have observed a rather intense peak for the 350 nm emission and noticed that the

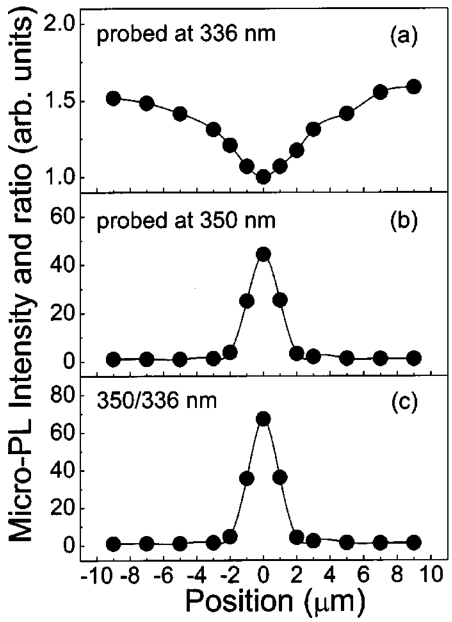

FIG. 4. Intensity distribution obtained for the ratio of (a) near band edge and 350 nm, (b) detecting at 350 nm, and (c) near band edge with various probe positions. Each intensity profile was normalized by the μ-PL intensity with the weakest one.

I_{nbe} of AlGaN is nearly quenched. Since the inferred Fermi level is lower inside the V-pit than that in the nonpit region, the electron concentration is thus less. Another probable reason is that the V pit is associated with a large amount of accumulated V_{Ga} defects, so that electrons are trapped by V_{Ga} inside the V pit. Thus, it is inferred that more states, which are not occupied by electrons, are available in the V pit, and are efficient for relaxing excess carriers to suppress the I_{nbe} line in $Al_{0.16}Ga_{0.84}N$. We believe that the origin of the enhanced V-pit-related emission is due to the deep gap states formed by V_{Ga}.

Based on the available data, we proceed to propose a schematic energy diagram. The native shallow donor level (native defect V_N) is responsible for the I_{nbe} of AlGaN. At the V pit, another level located at $\sim$0.136 eV above the valence band is formed that contributes to the strong emission around 350 nm line. The width of this defect-related level is 76 meV. In addition, from the AFM measurements, the deduced Fermi level at the V pit is $\sim$0.2 eV below that at nonpit region in $Al_{0.16}Ga_{0.84}N$.

In summary, we have examined the V-shaped pit on AlGaN by using the μ-PL and AFM. The results showed that a specific defect-related band is introduced inside the V-pit region that gives rise to a dominant feature in μ-PL spectra. In addition, the V-pit-related levels are efficient relaxation channels for photoexcited carriers so that the new broader emission peak is enhanced significantly and the I_{nbe} is suppressed. The AFM measurements provide a further evidence of the lowered Fermi level in the V pit of $Al_{0.16}Ga_{0.84}N$.

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