Enhancement of field emission of the ZnO film by the reduced work function and the increased conductivity via hydrogen plasma treatment


1Key Lab of Semiconductor Materials Science, Institute of Semiconductors, CAS, Beijing 100083, People’s Republic of China
2Lab of Thin Film Materials, College of Materials Science and Engineering, Beijing University of Technology, Beijing 100022, People’s Republic of China

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The ZnO films deposited by magnetron sputtering were treated by H/O plasma. It is found that the field emission (FE) characteristics of the ZnO film are considerably improved after H-plasma treatment and slightly deteriorated after O-plasma treatment. The improvement of FE characteristics is attributed to the reduced work function and the increased conductivity of the ZnO:H films. Conductive atomic force microscopy was employed to investigate the effect of the plasma treatment on the nanoscale conductivity of ZnO, these findings correlate well with the FE data and facilitate a clearer description of electron emission from the ZnO:H films. © 2009 American Institute of Physics. [DOI: 10.1063/1.3167301]

ZnO is a promising candidate for applications in field emission (FE) displays because of its fascinating physical and chemical properties. In previous reports, good FE characteristics of ZnO were usually attained in ZnO nanostructures by large geometric field enhancement due to their high aspect ratios. An alternative method for improving FE characteristics is lowering work function by various surface-treatment processes, since electron emission is critically dependent on the nature of chemical species terminating the surface. Furthermore, a heavy n-type doping can also enhance FE by lifting the Fermi level and lowering the work function. Recently, it was reported that hydrogen doping significantly increased the free electron concentration and the conductivity of ZnO. On the other hand, negative electron affinity (NEA) is often observed at the surface of various wide band-gap semiconductors (e.g., diamond, boron nitride) terminated with hydrogen atoms, which allows easily for electron emission. Therefore, the introduction of hydrogen into ZnO may be one of the most potential methods for improving its FE. However, the FE characteristics of ZnO:H films were scarcely studied, and the mechanism has not yet been clearly illustrated. In this study, we report that the FE of ZnO films is enhanced by H-plasma treatment due to the reduced work function and the increased conductivity of the ZnO film.

The ZnO films were deposited on n⁺-Si (001) substrates by a conventional radio frequency (rf) magnetron sputtering. To introduce hydrogen or oxygen intentionally, the ZnO films were directly immersed in a H/O plasma in a capacitively coupled rf plasma reactor. The details of growth and treatment conditions can be found elsewhere.

The morphologies of ZnO films were characterized by Conductive atomic force microscopy (CAFM) with a NT-MDT Solver P47 using a Pt-coated Si cantilever. The current distribution image was achieved simultaneously by using the contact mode with a fixed force on the cantilever and recording the current for a fixed applied bias voltage of 8.0 V. The single point I-V curve was obtained by maintaining a constant tip/sample force and then varying the tip/sample bias voltage ranging from −10 to 10 V while measuring the cathodic current. The FE experiments were performed in an ultrahigh vacuum chamber with a base pressure better than 3 × 10⁻⁷ Pa at room temperature.

Secondary ion mass spectroscopy (SIMS) was used to investigate the distribution of hydrogen in the ZnO:H film. The depth profiles of the main elements in the ZnO:H film and Si substrate are shown in Fig. 1. It is evident that hydrogen exists in the ZnO film and diffuses into the entire film after H-plasma treatment. It has been reported that hydrogen can diffuse into ZnO films with a depth of more than several micrometers by H-plasma exposure. In the present study, the thicknesses of the ZnO films are about 1 μm, hence hydrogen can diffuse into the entire film.

As demonstrated in our previous report, the electrical properties of ZnO films were improved by H-plasma treatment. Hall measurement results show that the carrier concentration increases sharply from 10¹⁷ to 3 × 10¹⁹/cm³, and the electron mobility increases from 15 to 35 cm²/V·s after H-plasma treatment. As a result, the conductivity of the ZnO:H film is more than three orders of magnitude larger than that of the as-grown ZnO film. On the contrary, the carrier concentration and mobility of ZnO are both reduced slightly after O-plasma treatment.

FIG. 1. (Color online) SIMS depth profiles of the H-plasma treated ZnO film on Si substrate.
To demonstrate the effect of the plasma treatment on the nanoscale conductivity of ZnO, CAFM measurements were carried out for the as-grown and H/O plasma treated ZnO films, and the corresponding topography [(a), (c), and (e)] and current distribution images [(b), (d), and (f)] are shown in Fig. 2, respectively. The as-grown ZnO film shows a small and sparse current distribution, and the current intensity and density increase significantly after H-plasma treatment, whereas both of them decrease slightly after O-plasma treatment. Assuming a threshold current of 1 nA, the percentages of conductive area \( \alpha_c \) are calculated to be 2\%, 17\%, and 1.8\%, corresponding to the as-grown, the H- and O-plasma treated ZnO films, respectively. Obviously, the enhanced conductivity by H-plasma treatment leads to more channels of electron transport, thus, the increased conductive area.

The typical local current-voltage \((I-V)\) curves of these films were also measured and the results are presented in Fig. 3. As seen, the point contacts on the as-grown and O plasma-treated ZnO films result in nonlinear and rectifying \(I-V\) curves. This behavior is probably attributed to the Schottky contact created between the Pt-coated tip and the ZnO surface, since Pt has a high work function of 5.64 eV.\(^{19}\) However, the H plasma-treated ZnO film exhibits a linear \(I-V\) behavior, except for a saturated characteristic at the higher voltages that is due to the limited saturation current (\(\sim 20\) nA) of the instrument. The electron concentration of the ZnO film is high enough after H-plasma treatment, electron tunneling is a dominant transport mechanism of current flow between the ZnO film and the Pt-coated tip even though the existence of barrier between of them.\(^{20}\) As a result, the Schottky contact between the Pt-coated tip and ZnO is changed into Ohmic contact after H-plasma treatment, and much higher current flow through the Pt-coated tip and the H-plasma treated ZnO under the same bias voltage.

The electron emission characteristics of the as-grown and H/O plasma-treated ZnO films are shown in Fig. 4, respectively. Where the \(J\) and \(E\) characteristics are shown in Fig. 4(a) and the corresponding Fowler–Nordheim (F-N) plots are given in Fig. 4(b). The turn-on field \(E_{on}\) and the threshold field \(E_{th}\) are defined at an emission current density of 10 \(\mu\)A/cm\(^2\) and 1 mA/cm\(^2\), respectively, as indicated by two dashed horizontal lines in Fig. 4(a). The \(E_{on}\) and \(E_{th}\) are found to be 9.8 and 24.4 \(V/\mu m\) for the as-grown ZnO film, respectively. While the H-plasma treated ZnO film has the best FE characteristics with the lowest \(E_{on}\) of 3.6 \(V/\mu m\), and the lowest \(E_{th}\) of 12.2 \(V/\mu m\). These values are comparable with and even lower than the results attained from various ZnO nanostuctures.\(^{21,22}\) Evidently, the FE characteristics of the ZnO film are considerably improved after H-plasma treatment, while they are slightly deteriorated after O-plasma treatment (\(E_{on}=13.6\) \(V/\mu m\), \(E_{th}=24.7\) \(V/\mu m\)).

In Fig. 4(b), the FN plots show a rough linear relationship in the high-voltage range for all the samples, implying that a quantum tunneling mechanism is responsible for the emission. For the FN emission, the current density obeys the FN equation\(^{23}\)

\[
\ln \left( \frac{I}{V^2} \right) = - \frac{B \phi^3 d}{V} + \ln \left( \frac{\alpha A \beta^2}{\phi d^2} \right),
\]

where \(A\) and \(B\) are constants, \(I\) and \(\alpha\) are the emission current intensity, the effective emission area, respectively. \(\phi, d,\) and \(V\) are the work function, the distance between the anode and the cathode, and the voltage applied to the samples, respectively. The \(\beta\) is the field enhancement factor related to the surface morphology, which reflects the ability of the emitters to enhance the local electric field. The AFM images of the
ZnO films, as shown in Figs. 2(a), 2(c), and 2(e), indicate that the surface roughness and morphologies of the ZnO films treated with H/O plasma are almost similar to those of the as-grown sample. Since the morphologies of the ZnO films are not changed very much after plasma treatment, we reasonably assume that the $β$ values of the three samples are the same. Therefore, the variation in the slope $k = -B\phi^{5/2}/d$ of FN plots reflects the change in the work function $\phi$ of ZnO films since $d$ remains unchanged. According to the FN plots in Fig. 4(b), and taking the work function $\phi$ of the as-grown ZnO film as 5.3 eV, the work function $\phi$ is estimated to be 3.75 and 5.50 eV for the H- and O-plasma treated samples, respectively. In comparison with the as-grown ZnO film, the work function of the H-plasma treated sample is reduced by as much as 1.55 eV.

As mentioned previously, H-plasma treatment significantly improves the conductivity of ZnO films with much higher carrier concentration. This heavy $n$-type doping can reduce the work function of the ZnO film by up-shifting their Fermi level. This shift is estimated to be about 0.4 eV according to the relationship of electron concentration and the Fermi level.²⁵ Obviously, the smaller shift of Fermi level cannot explain the observed reduction of the work function of 1.55 eV alone. On the other hand, a lower and even NEA was usually observed at the surface terminated with hydrogen atoms for various wide band-gap semiconductors, e.g., diamond¹² and boron nitride.¹³,¹⁴ Therefore, we propose that the larger reduction of the ZnO work function mainly be attributed to the decrease of the electron affinity resulted from the H-terminated surface of ZnO.

As can be seen from Eq. (1), for a given $β$, $ϕ$, and $d$, the intercept $b = \text{ln}(a\alpha\beta^2 / \phi \delta \Phi^2)$ of FN plots reflects the variation of effective emission area $a$.²⁶ In this work, $β$ and $d$ remain uncharged and $α$ is normalized to 1 for the as-grown ZnO film. By taking the $β$ values determined from the slope above, $α$ is calculated to be 5.8 and 0.9 from the intercept of the FN plots in Fig. 4(b) for the H- and O-plasma treated samples, respectively. The effective emission area is slightly decreased after O-plasma treatment, whereas it is significantly increased after H-plasma treatment, which may be understood according to the three-step FE model.²⁴ According to the model, the emitted electrons are assumed to subject a three-step process involving internal emission, electron transport, and vacuum emission.²⁴ At the first step (internal emission), electrons are injected into the conduction band of ZnO films from $n$-$Si$ substrates. At the second step (electron transport), the injected electrons transport across the ZnO films, which is directly limited by the conductivity of the films. Moreover, at the third step (vacuum emission), the electrons emit into vacuum at the surface of the ZnO films by tunneling through a surface barrier, which depends on the local field enhancement factor and the ZnO work function. The effective emission area is determined by the three steps connected in series. In the present work, because the Si substrates are heavily doped, electrons can be easily injected from substrate to ZnO by tunneling, the influence of the internal emission on FE can be neglected. At the second step, the CAFM results show that H-plasma treatment leads to the increased conductive area, thus the most injected electrons can transport through the ZnO films. At the last step, though the field enhancement factor remains unchanged, the work function of ZnO reduces significantly after H-plasma treatment, which makes the transported electrons emit easily. Consequently, the enhanced conductivity, together with the reduced work function of ZnO:H films, leads to the increase of the effective emission area.

In conclusion, a significant enhancement of FE from the ZnO:H film has been observed, and the $E_m$ is reduced from 9.8 to 3.6 V/μm after H-plasma treatment. The improvement of FE characteristics is attributed to the reduced work function and the increased effective emission area. The increased effective emission area is related to the reduced work function and the enhanced conductivity of the ZnO:H film, while the decrease of work function is due to the lifting of the Fermi level and the H-terminated ZnO surface. Additionally, the CAFM results show that the nanoscale conductivity of ZnO:H is obviously enhanced because of tunneling emission due to H-plasma treatment.

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Photonic crystal distributed feedback quantum cascade laser fabricated with holographic technique


Electrically pumped, edge-emitting, singlemode operation of a two-dimensional photonic crystal distributed feedback (PCDFB) quantum cascade laser emitting at $\lambda \sim 7.8 \mu m$ is demonstrated. The two-beam holographic technique combined with wet-etching process is successfully used to define a square-lattice PCDFB structure on the top grating layer of the laser. This simple PC fabrication method may open exciting opportunities for the wide application of PCDFB lasers.

Introduction: Quantum cascade lasers (QCLs) are promising mid- and far-infrared light sources with a variety of applications. For potential applications, one-dimensional distributed feedback (DFB) grating and two-dimensional (2D) photonic-crystal distributed-feedback (PCDFB) structures have been employed to modulate the mode characteristic and beam quality of the lasers [1–3]. However, the fabrication of PC structures using conventional electron-beam lithography (EBL) and dry-etching process is rather complicated and time-consuming. This will be a considerable challenge for the wide application of PC devices. Here, a holographic technique [4] capable of producing a large-area periodic lattice structure with high uniformity is introduced to the fabrication of PCDFB QCLs, and singlemode operation with a sidemode suppression ratio (SMSR) above 20 dB is obtained.

Device design and fabrication: The QCL structure was grown by solid-source molecular beam epitaxy on an n-InP substrate (Si, $3 \times 10^{17}$ cm$^{-3}$). The active region consisted of 35 periods of strain-compensated $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ quantum wells and barriers, similar to [5]. The growth process started with the lower $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ waveguide layers (Si, $4 \times 10^{16}$ cm$^{-3}$, 0.4 $\mu m$), proceeded with the active layers (Si, average doping $\sim 4 \times 10^{16}$ cm$^{-3}$) and was finished by an upper $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ waveguide layer (Si, $4 \times 10^{16}$ cm$^{-3}$, 0.5 $\mu m$) and a highly $n$-doped $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ cap layer (Si, $2 \times 10^{17}$ cm$^{-3}$, 0.4 $\mu m$) on top. This cap layer was also the host layer for the grating.

The PCDFB design is based on the emission at $\lambda \sim 7.8 \mu m$ of the Fabry-Perot (F-P) lasers from the same wafer and the estimated effective index $n_e = 3.195$. We chose a square lattice, and used the first-order Bragg condition in the $\Gamma$-X direction for both the transverse and longitudinal directions of the device with a lattice constant of $\Lambda = 1.22 \mu m$. The fabrication process was started by holographically defining a square lattice grating using double-exposure of two-beam interference patterns. By a rotation angle of 90° between the two separate exposures, the holographic pattern with the square lattice was recorded on the photoresist. Fig. 1 shows the theoretical calculation result of the iso-intensity distribution of two-beam interference obtained with double exposures, and the corresponding AFM image of the lattice pattern recorded onto the photoresist. The 200 nm-deep 2D grating pattern with the circular unit cell was then transferred to the top InGaAs epilayer by wet-chemical etching in an HBr/HNO$_3$/H$_2$O solution (1:1:10). Consequently, the PCDFB structure with high uniformity and in a large area (10 $\times$ 10 mm) was obtained as shown in Fig. 2a. The PC lattice constant can be controlled by choosing an appropriate angle between the two holographic laser beams, while the hole size factor which is defined by the ratio of the hole diameter to the lattice constant, can be adjusted by controlling the exposure-time or exposure-power. The hole depth can be defined by wet etching time. Figs. 2b and c show scanning electron microscopy (SEM) pictures of the InGaAs PCDFB structure with different viewing angle and magnification. The average size factor and hole depth are about 0.9 and 200 nm, respectively. This simple PC fabrication greatly enhances the throughput of processing by reducing the time scale into a few minutes, and the results could be easily repeated.

![Fig. 1 Calculated light intensity distribution of double-exposure of two-beam interference patterns and corresponding AFM image of 2D periodic structure with square lattice](image1)

- Calculated light intensity distribution of double-exposure of two-beam interference patterns
- Corresponding AFM image of 2D periodic structure with square lattice

![Fig. 2 SEM images of etched InGaAs grating layer with top view (Fig. 2a), ×1000. (Fig. 2b), ×10000, oblique view (Fig. 2c), ×30000, before insulating and metal deposition, and (Fig. 2d) SEM image of portion of PCDFB device](image2)

![Fig. 3 Lasing spectrum of PCDFB QC laser, and light output characteristics of PCDFB device and its F-P counterpart](image3)

- Lasing spectrum
- Inset: Peak emission wavenumber of PCDFB laser with 2D lattice patterns and F-P laser against temperature
- Light output characteristics

After recording the 2D lattice structure, the wafer was processed into double channel ridge waveguide lasers of 50 $\mu m$ ridge width using contact photolithography and nonselective wet-chemical etching. A
350 nm-thick SiO2 layer was deposited for electrical insulation around the ridges. A 40 µm window was then opened on top of the ridge for current injection. After the deposition of Ti/Au (30 nm/120 nm) contact on the top layer, the wafer was then lapped down to about 150 µm, and polished for back Ti/Au (30 nm/120 nm) contact deposition. Finally, 2 mm-long laser bars were cleaved from the wafer and indium soldered to cooper heatsinks with the epilayer side up. The SEM image of a portion of the PCDFB device is shown in Fig. 2d.

Characterisation: The spectral purity of a PCDFB QC laser operated in pulsed mode (pulse width 1 µs and 5 kHz) is shown in Fig. 3a with SMSR above 20 dB in the working temperature range. The measured peak position and the full width at half maximum (FWHM) of the emission spectrum at 4 A driving current is 7.8 µm and 0.52 cm⁻¹, respectively. The later is limited by the resolution (0.5 cm⁻¹) of the spectrometer (Bruker Equinox 55). The inset of Fig. 3a shows temperature-dependent peak emission wavelengths for the 2D PCDFB device and its F-P counterpart. The tuning rate of −0.084 cm⁻¹/K for the PCDFB device is three times lower than that of the F-P laser, further proving the distributed feedback mechanism of the PC lattice structure.

Fig. 3b shows the light output characteristics of a PCDFB device and its F-P counterpart at 80 K with a duty cycle of 1%. As for the slope efficiency of 110 mW/A for its F-P counterpart, the PCDFB laser shows a smaller value of 59 mW/A. The ratio of the efficiency between the PCDFB and F-P lasers is as high as 53%, which indicates an optimised 2D PC feedback lattice structure being recorded on the grating layer of the PCDFB laser [6].

Conclusion: We have demonstrated the development of electrically pumped, edge-emitting, singlemode PCDFB QCLs by use of two-beam multi-exposure holography. Singlemode operation with an SMSR above 20 dB is obtained. Our approach with high efficiency and low cost will be of significance to the wide application of PCDFB QCLs.

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Q. Lu, W. Zhang, L. Wang, F.-Q. Liu and Z. Wang (Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People’s Republic of China)
E-mail: fqliu@red.semi.ac.cn

References
40-Gb/s Low Chirp Electroabsorption Modulator Integrated With DFB Laser

Yuanbing Cheng, Jiaoqing Pan, Yang Wang, Fan Zhou, Baojun Wang, Lingjuan Zhao, Hongliang Zhu, and Wei Wang

Abstract—A 40-Gb/s monolithically integrated transmitter containing an InGaAsP multiple-quantum-well electroabsorption modulator (EAM) with lumped electrode and a distributed-feedback semiconductor laser is demonstrated. Superior characteristics are exhibited for the device, such as low threshold current of 20 mA, over 40-dB sidemode suppression ratio at 1550 nm, and more than 30-dB dc extinction ratio when coupled into a single-mode fiber. By adopting a deep ridge waveguide and planar electrode structures combined with buried benzocyclobutene, the capacitance of the EAM is reduced to 0.18 pF and the small-signal modulation bandwidth exceeds 33 GHz. Negative chirp operation is also realized when the bias voltage is beyond 1.6 V.

Index Terms—Distributed-feedback (DFB) laser, electroabsorption modulator (EAM), 40 Gb/s, low chirp, monolithic integration, selective area growth (SAG).

I. INTRODUCTION

The growth of the Internet and associated data-driven applications has resulted in increased bandwidth demand, which necessitates the development of higher speed transmission systems. Recently, a 40-Gb/s transmission technology has been widely considered as a strong candidate for the next-generation terabit-per-second communication networks [1]. Owing to its compactness, low packaging cost, low driving voltage, and high stability, the 40-Gb/s electroabsorption modulated distributed-feedback laser (EML) has attracted much attention [2]–[6]. For EMLs used in 40-Gb/s systems, it is desirable to realize low chirp operation in addition to extending the modulation bandwidth to 40 GHz or more [7], [8]. Since the transmission distance limited by fiber dispersion is roughly inversely proportional to the square of the data rate, the chirp parameter for a 40-Gb/s electroabsorption distributed-feedback (DFB) strongly influences the data transmission, even in very short reach applications. Efficient transmission is far more difficult at a bit rate of 40 Gb/s and is found to be only 1/16 the distance achievable at 10 Gb/s. Negative or zero chirp is much preferred for EMLs because low power penalty is important to both long- and short-haul transmission. Primarily, there are three ways of controlling the chirp parameter, i.e., design of the multiple-quantum-well (MQW) core, biasing the chip voltage and control over the wavelength detuning between the DFB and electroabsorption modulator (EAM). A combination of the above approaches is, therefore, a promising approach towards achieving a practical solution to these difficulties.

Among the many ways of laser-modulator monolithic integration explored [2]–[6], selective area growth (SAG) has received great attention due to the large degree of freedom in bandgap energy control and almost 100% optical coupling achievable between the components [9]. This method allows definition of different regions of MQW bandgaps on a single masked substrate with a one-step growth process. The bandgap energy detuning depends primarily on MQW thickness growth enhancement, with small composition modulation. Desirable characteristics of the SAG methods have been already demonstrated through 10-Gb/s EMLs [4]. However, the SAG method cannot optimize the EAM and DFB respectively because of the single material growth by metal–organic chemical vapor deposition (MOCVD). Generally, the length of the EAM is reduced to less than 100 µm in order to obtain the bandwidth of 40 GHz or more, and the extinction ratio of the EAM has been sacrificed. Up to now, there are limited reports on 40-Gb/s applications using the SAG method due to rather strict and limited design margins for realizing high-performance 40-Gb/s EMLs.

Yun et al. have reported an SAG structure EML for a 40-Gb/s system by adopting a traveling-wave electrode structure in the modulator section [5]. They emphasized the package structures and characteristics of the module. In this letter, the design and fabrication of InGaAsP MQW EMLs with a simple device structure for 40-Gb/s applications are reported, in which a lumped-electrode structure is used for the EAM to avoid the fabrication complexity and stringent process tolerances in the traveling-wave electrode modulators. Low chirp operation is realized through carefully designing the MQW core material of the EAM, and the wavelength detuning between EAM and DFB.

II. DEVICE FABRICATION

Fig. 1 shows the schematic of the 40-Gb/s EML device, which is composed of a 250-µm-long DFB laser and a 100-µm-long EAM. Different active regions of laser and EAM at 1552 and 1495 nm, respectively, have been obtained by the SAG method. Device fabrication started with a deposition of 200-nm-thick SiO₂ dielectric films on the S-doped (100) InP substrates by plasma-enhanced chemical vapor deposition (PECVD). Masks were patterned along the [11] direction by conventional photolithography. Then, the SAG process was carried out on the patterned substrates. An n-InP buffer layer

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The authors are with the Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, 100083 Beijing, China (e-mail: ybcheng@semi.ac.cn,wwang@semi.ac.cn).

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and an eight-pair InGaAsP–InGaAsP MQW structure were successively grown by ultra-low-pressure MOCVD (30 mbar, 655 °C). The MQWs consist of undoped 8-nm-thick 0.7% compressive strain InGaAsP wells separated by 9-nm-thick 0.3% tensile strain In_{0.85}Ga_{0.15}As_{0.42}P_{0.58} barriers, sandwiched between 100-nm-thick lattice-matched In_{0.78}Ga_{0.22}As_{0.47}P_{0.53} optical confinement layers. It is well known that the principal mechanism of selectively grown MOCVD lies in the lateral gas phase diffusion of group-III precursors. At ultralow pressures, the reagent particles can easily diffuse out of the stagnation gas phase layer. The measured growth enhancement rate between the stripes is 20% which fits well with the lateral gas phase diffusion model [10]. A first-order grating is partially formed on the laser section by conventional holographic exposure followed by chemical etching. The exposure and dry-etching processes were controlled to achieve a grating duty factor of approximately 50% for an optimum coupling coefficient. To complete the epitaxial structure, a p-type InP cladding layer and p–i–n-InGaAs contact layer were successively grown. To ensure a small series resistance of the DFB laser and a low capacitance of the EAM, a single reverse-mesa-ridge structure has been formed by conventional photolithographic technology and etching. The EAM section was further processed into a deep mesa ridge waveguide structure by reactive ion etching to reduce the junction capacitance of the device. Electrical isolation between the laser and the modulator were realized by forming 50-μm-wide trench between them and adopting He⁺ implantation in the trench. Three steps of He⁺ implantation were used for a flat ion distribution with doses of 1 × 10¹⁴, 8 × 10¹⁴, and 5 × 10¹⁴ cm⁻² and at energies of 180, 100, and 80 keV, respectively. An isolation resistance greater than 100 kΩ was obtained. Benzocyclobutene (BCB) was used under the bonding pad to reduce the parasitic electrode pad capacitance of EAM. The scanning electron microscope (SEM) image of the ridge EAM section is shown in Fig. 2. The ridge waveguide was well protected and passivated. Thus low capacitance of the modulator (estimated to be 0.14 pF) and low leakage currents were obtained. Then, patterned Ti–Au p-electrode was formed on top of the planarized wafer. Au–Ge–Ni n-electrode was evaporated onto the backside of the device after thinning the wafer down to about 100 μm. Finally, the wafer was cleaved into device chips, and the facet of the EAM and DFB laser were antireflection and high-reflection coated with dielectric layers deposited by PECVD, respectively. A 40-GHz vector network analyzer and a calibrated receiver were applied for a high-speed measurements.

III. CHARACTERISTICS OF EML’S CHIP

The measured light output power versus current curve of a typical EML chip is shown in Fig. 3. A threshold current as low as 20 mA and an output power of 8 mW at 100 mA were achieved. A sidemode suppression ratio of more than 40 dB has been realized at an injection current of 65 mA. The divergence angles from the EAM output are 40.2°× 34.6° in the vertical and horizontal, respectively; the coupling efficiency to single-mode fiber reached 42% in the experiment. In Fig. 4, the dc extinction ratio measured using an integrating sphere is plotted as a function of the reverse bias applied to the EAM. The extinction ratio at 4-V reverse bias is estimated to be approximately 10 dB. When coupled to single-mode fiber, the dc extinction ratio at 4-V reverse bias is more than 30 dB. By adopting a deep ridge waveguide and planar electrode structures combined with buried BCB, the capacitance of the EAM is reduced to 0.18 pF. The measured relative electrical–optical (E/O) responses of the EML are shown in Fig. 5, which has been calibrated to account for the frequency response of the photodetector and high-frequency probe. The measured 3-dB bandwidth is more than 33 GHz at various reverse bias voltages, making it suitable for 40-Gb/s nonreturn-to-zero signal transmission. High-frequency oscillation with large amplitude is also seen in the figure when the frequency is beyond 35 GHz. It is limited by the high-frequency characteristics of the submount, because the S11 is greater than...
The measured extinction behavior of integrated light source with 100-μm EAM section using an integrating sphere.

The E/O responses of the EML chip at various reverse bias voltage.

The fabricated and performance of a low chirp InGaAsP–InP MQW EML for 40-Gb/s applications is presented in the letter. The SAG structure has not only simplified the fabrication process, but also realized good optical coupling. Accordingly, the potential reliability and output power of the device have been improved. In order to realize high-speed operation, a deep ridge structure combined with BCB as the ridge passivation material is adopted to reduce parasitic capacitance. A 3-dB small-signal response of more than 33 GHz is demonstrated for the EML chip, which is suitable for 40-Gb/s operation.

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Shape stability of InAs self-assembled islands on vicinal GaAs(001) substrates

S. Liang *, H.L. Zhu, W. Wang

Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, People’s Republic of China

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ABSTRACT

We have grown InAs self-assembled islands on vicinal GaAs(001) substrates. Atomic force microscopy and photoluminescence studies show that the islands have a clear bimodal size distribution. While most of the small islands whose growth is limited by the width of one multi-atomic step have compact symmetric shapes, a large fraction of the large islands limited by the width of one step plus one terrace have asymmetric shapes which are elongated along the multi-atomic step lines. These results can be attributed to the shape-related energy of the islands at different states of their growth.

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1. Introduction

Self-assembled three-dimensional islands have been intensively studied in recent years because of their unique optical and electrical properties [1,2]. However, the stochastic nature of these spontaneously formed islands makes it difficult to obtain islands with well-defined shapes and sizes, which is the main obstacle for the device application of these islands. In order to control the island morphology, it is required to understand the mechanism of island evolution.

It has been observed that the shapes of islands underwent a drastic change from symmetric dots into elongated dashes when the islands grow larger [3]. Tersoff and Tromp have proposed a theoretical model [4] in which the balance between the surface/interface energy and the elastic relaxation is the cause of the shape transition. The model has been confirmed by the study of CoSi2 growth on Si(100) substrates [5]. It was found that CoSi2 clusters grew in a square shape before a shape transition to clusters with large aspect ratios. Similar observations have also been made in other material systems such as Ge/Si [6], Au/Si [7] and InSb/InP [8]. However, up to now, there have been very few reports of island shape transitions in InAs/GaAs [9] which is recently the most promising material system for the practical use of self-assembled islands. Moreover, it is highly desirable to obtain different types of InAs/GaAs nanostructures (dots or dashes) in a controlled way for their device uses.

In this Letter, we report the growth of self-assembled InAs islands on vicinal GaAs(001) substrates. The multi-atomic steps on the substrates are found to affect the growth of InAs islands differently at different stages of their growth. While most of the small islands whose growth is limited by one multi-atomic step have symmetric shapes, a large fraction of the large islands limited by the width of one step plus one terrace have elongated shapes. These results can be attributed to the shape-related energy of the islands at different states of their growth and reflect the competition between the elastic relaxation and the surface/interface energy during the island growth in a novel way.

2. Experimental

The experiment was performed in a low pressure metal–organic chemical vapor deposition system. The substrate used in this study was epi-ready GaAs(001) with a 2° miscut angle toward the (110) facets. Prior to the deposition of InAs, a 200 nm GaAs buffer layer was first grown at 600 °C with a growth rate of 1 ML/s and a V-III ratio of 25. Under this growth condition, terraced surface with periodical multi-atomic steps was obtained by the step bunching mechanism [10]. The measured average width of the multi-atomic steps and that of the terrace are 21 and 20 nm, respectively. The islands were grown subsequently at 507 °C with an InAs deposition rate of 0.034 ML/s, a V-III ratio of 5 and an InAs coverage of 1.7 MLs. After the island formation, the sample was cooled down to below 350 °C within 5 min under the protection of AsH3 flow. The islands were characterized by atomic force microscopy (AFM) with a tapping mode in air. The photoluminescence (PL) measurements were carried out in a closed-cycle He cryostat under the excitation of the 514.5 nm line of an Ar+ laser focused onto a 0.5 mm2 spot. The luminescence spectra were detected with a Fourier transform infrared spectrometer operating with an InGaAs photodetector.

3. Results and discussion

Fig. 1a shows a typical AFM image of the InAs islands with a line in the figure showing the direction of the multi-atomic step lines. The corresponding histogram of the island base diameters perpendicular to the step lines (D⊥) is shown in Fig. 1b. Islands at different
stages of growth are formed on the substrates at the same time due to the inherent size fluctuation of the islands as well as the multi-atomic steps on the substrate. Thus, the shape evolution of the islands with their sizes can be studied. As can be seen from Fig. 1, the InAs islands have a clear bimodal size distribution and consist of a group of small islands with \(D_1\) centered around 21 nm (mode I) and a group of large islands with \(D_2\) centered around 40 nm (mode II). Another feature of the InAs islands is that the islands are formed in lines with a certain degree of space ordering which is resulted from the fact that the islands tend to nucleate on the many multi-atomic lines on the substrates [11]. Fig. 2 shows the excitation power dependent PL spectra of the sample measured at 77 K. The inset of the figure shows that the PL spectrum can be well fitted with two dominant peaks using Gaussian curves. Because the spectra have no dependence on the excitation power as can be seen from Fig. 2, the peaks of the fitted Gaussian curves are attributed to the ground state transitions from the two groups of islands.

Fig. 3a and b show the scatter plots of the aspect ratios and the heights of 60 mode I InAs islands at different possible sizes. Here the aspect ratio of an island refers to the ratio of island base diameter parallel to the multi-atomic steps (\(D_1\)) to \(D_2\). As shown in the figures, while the heights of the islands increase with \(D_2\), the aspect ratios roughly keep a constant value of 1. This indicates that most of the mode I InAs islands have compact symmetric shapes within the range of their possible sizes. Only when \(D_2\) is larger than 20 nm, can islands with aspect ratios of about 1.1 be found and they are only a small fraction of the mode I islands (about 3%). The aspect ratios of the mode II InAs islands as a function of \(D_2\) are shown in Fig. 3c. Contrary to the mode I islands, the aspect ratios of a large fraction of the mode II islands are noticeably larger than 1 when \(D_2\) is below about 58 nm. This indicates that the mode II islands can have asymmetric shapes, which are elongated along the multi-atomic steps as can been seen from Fig. 1a. As \(D_2\) increases over about 58 nm, the islands take compact shapes again as shown in Fig. 3c by their small aspect ratios. As shown in Fig. 3d, the heights of the mode II islands increase also with \(D_2\), which is similar to the mode I islands.

The growth of the quantum islands in the direction perpendicular to the step lines has been shown to be limited by the multi-atomic steps [12,13]. For our sample, the growth of the mode I islands is limited by the width of one multi-atomic step and the growth of the mode II islands is also limited, however, by the width of one step plus one terrace, as shown schematically in Fig. 4. This can be proved by the fact that the average \(D_2\) of the mode II islands is 41.2 nm which is very close to the average width of one step plus one terrace. For the mode I islands, the average \(D_1\) is nearly equal to the average width of one step. In earlier studies it has been observed that the islands can grow along the multi-atomic lines, and wire-like islands can be obtained after the sizes of the islands perpendicular to the step lines are saturated by the step width [14]. The results presented above show, however, while a large number of the mode II islands can have asymmetric shapes which are elongated along the step lines, most of the mode I islands have compact symmetric shapes.

These results can be qualitatively explained by the theoretical work of Tersoff and Tromp [4]. Considering the contributions of both the elastic relaxation and the surface/interface energy, the island energy per unit volume can be written as:

\[
E = 2\pi \left( \frac{S}{S^1} + \frac{t_1}{t_1} - \gamma \frac{t_1}{t_1} \ln \left( \frac{S}{S^1} \right) + \frac{t_1}{t_1} \ln \left( \frac{S}{S^1} \right) \right),
\]

where \(E\) is the island energy, and \(S, t_1, h\) and \(V = hst\) are the length, height and the volume of an island with other parameters being defined as in Ref. [4]. Assuming a constant \(h\), the island energy per unit volume as a function of island area was calculated for two kinds of dots with aspect ratios of 1 and 4. As shown in Fig. 5, below a certain size \(a_0\) the island energy per unit volume of an island with an elongated shape (aspect ratio of 4) is higher than that of an island with a symmetric shape (aspect ratio of 1). What is more, the \(E/V\) difference between the two kinds of islands varies with the island sizes as shown by the dashed line in the figure. Based on our AFM results we propose that the sizes of the mode I islands are at around \(a_1\), for example. When the islands are forced to take elongated shapes by the step lines, the \(E/V\) increase of the mode I islands is higher than that of the mode II islands which have larger sizes such as being at \(a_2\). Thus, the elongated mode I islands are relatively unstable than the mode II islands and tend more likely to transform to round islands through diffusion, which explains our observations showed above. A similar mechanism leads to the increase of the aspect ratios with \(D_2\) as indicated by the linear fit line in Fig. 3c. The increase of the aspect ratios reflects the decrease of the \(E/V\) difference with \(D_2\) around \(a_2\).
As can be seen from Fig. 3c and d, at a given $D$, the heights of the mode II islands grow much slower than the lateral dimensions of them along the step lines when the shape transitions occur. This meets the requirement that the heights of the islands should be kept relatively constant in Tersoff and Tromp's model [4]. The apparent increase of island height with $D$, on the other hand, indicates that islands lower their strain energy by increasing their heights before $D$ is saturated by the multi-atomic step lines. For islands with very large sizes the constraint from the multi-atomic steps becomes small and the islands tend to have symmetric shapes [14], which leads to the formation of islands with low aspect ratios when $D$ is larger than 58 nm. During the 5 min cooling period as mentioned in Section 2, a coarsening process of the islands may happen, which, however, should be much slower than for exactly oriented substrates because of the multi-atomic steps [13]. In the process, the mode II islands may grow at the expense of the mode I islands, leading to the increase of both the density and the aspect ratios of the mode II islands compared to the as-grown sample.

4. Conclusions

In summary, we have studied the size dependent shapes of InAs self-assembled islands grown on vicinal GaAs(001) substrates. It is found that with similar effects of growth limitation from the multi-atomic step lines, while most of the group of islands with small sizes have symmetric shapes, a large fraction of the group of islands with larger sizes have asymmetric shapes that are elongated along the step lines. The observations can be related to the shape-dependent energy of islands at different states of their growth.

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References

Dislocation core effect scattering in a quasitriangle potential well

Xiaoqing Xu, Xianglin Liu, Shaoyan Yang, Jianming Liu, Hongyuan Wei, Qinsheng Zhu, and Zhanguo Wang

Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People’s Republic of China

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A theory of scattering by charged dislocation lines in a quasitriangle potential well of \( \text{Al}_x\text{Ga}_{1-x} \text{N} / \text{GaN} \) heterostructures is developed. The dependence of mobility on carrier sheet density and dislocation density is obtained. The results are compared with those obtained from a perfect two-dimensional electron gas and the reason for discrepancy is given. © 2009 American Institute of Physics. [DOI: 10.1063/1.3098356]

The promising possibilities of large gap semiconductors, such as GaN, AlN, and AlGaN alloys, together with their heterostructures, for advanced photonic and electronic device applications have recently raised some attention for the experimental and theoretical studies of their transport properties.\(^1,2\) AlGaN heterostructures have been an area of active research, owing to the demonstration of high power microwave high electron mobility transistors. In practice, the layers are mainly grown by epitaxial methods such as metal-organic vapor-phase epitaxy and molecular beam epitaxy on highly lattice-mismatched sapphire substrates.\(^3,4\) GaN heterostructures have been an area of active research, owing to the demonstration of high power microwave high electron mobility transistors. In practice, the layers are mainly grown by epitaxial methods such as metal-organic vapor-phase epitaxy and molecular beam epitaxy on highly lattice-mismatched sapphire substrates.\(^3,4\) Transmission electron microscopy observation reveals, GaN is generally characterized by very large dislocation densities (typically in the range of \( 10^6 \) to \( 10^{10} \) cm\(^{-2}\)). Dislocation scattering in three-dimensional bulk GaN has been analyzed with great efforts,\(^5-7\) however, it was not so much considered in AlGaN/GaN two-dimensional electron gas (2DEG). Jena et al.\(^8\) developed a typical theory of dislocation scattering in a perfect 2DEG. He elicited the screened potential of a charged dislocation from the scattering potential of a point charge, and gave the dependence of mobility on 2DEG sheet density and dislocation density. However, a real AlGaN/GaN heterostructure has a quasitriangle potential well determined by solving the Poisson and Schrödinger equations self-consistently. Ando et al.\(^9\) and Stern and Howard\(^10\) have made efforts to bring forward the Fourier transferred potential of a point charge in both cases of zero and nonzero thickness for the charge distribution of electrons. In this paper, we deduce the Fourier transferred potential of a dislocation based on a more realistic case of a quasitriangle potential well approximation, and calculate the electron mobility in AlGaN/GaN heterostructures. Afterward, we take a comparison of our results with those obtained by Jena et al.\(^8\) from a perfect 2DEG, and attempt to give reasons for the discrepancy.

A schematic diagram of the conduction-band structure of a AlGaN/GaN heterostructure near the interface is shown in Fig. 1. In a simple case, the GaN layer (at \( z \geq 0 \)) and the AlGaN layer (at \( z \leq 0 \)) are both nominally undoped with all the electrons originating from surface states. Suppose the AlGaN barrier is grown pseudomorphically on a relaxed GaN layer, a polarization field will be present at the AlGaN/GaN interface. Thus, the electrons are confined to the triangular well at the interface, leading to a quantization of the energy-band structure into subbands. In this paper, only the ground subband is taken into consideration and the areal (2D) electron concentration is labeled as \( N_s \). The simplest approximation for the wave function \( \chi(z) \) and the charge distribution of electrons \( g(z) \) is the one made for inversion layers by Fang and Howard\(^11\)

\[ g(z) = |\chi(z)|^2 = \frac{b^3}{2} z^2 e^{-bz}, \]  

where \( b \) is the variational parameter.\(^3\)

The dielectric constants \( \varepsilon_{\text{GaN}} \) for GaN and AlN are close so we treat them uniformly in this paper. The additional electrostatic potential \( \phi \) produced by an external source is related to the charge density by Poisson’s equation. Using the charge distribution of \( g(z) \), the relation can be expressed as \(^9\)

\[ \nabla^2 \phi - 2q_e \phi(r)g(z) = -\frac{4\pi q_{\text{ext}}}{\varepsilon_0 \varepsilon_{\text{GaN}}}, \]  

where \( q_{\text{ext}} \) is the external charge density, \( r \) is the in-plane vector, and \( q_e = 2/e_B \) is the 2D Thomas Fermi wave vector, with \( e_B \) being the effective Bohr radius in the material. To find the screened Coulomb potential for our 2D system, we use a conventional Fourier–Bessel expansion for the potential \( \phi(r,z) = \int_0 \phi_q A_q(z) J_0(qr) dq \), where \( J_0 \) is the zero-order Bessel function.

FIG. 1. (Color online) Schematic diagram of the energy-band structure in a AlGaN/GaN heterostructure, showing the ground subband (\( E_g \)), Fermi energy (\( E_F \)), and the charge distribution of electrons (blue curve) in the quasitriangle well.

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\(^a\)Electronic mail: xlliu@red.semi.ac.cn.

\(^b\)Electronic mail: qszhu@semi.ac.cn.
The Fourier–Bessel transform is labeled as $\tilde{A}_q$. As in the case of a point charge located at $z = z_0$, $\tilde{A}_q$ can be divided into $\tilde{A}_qf$ (for $z_0 \approx 0$) and $\tilde{A}_qr$ (for $z_0 \approx 0$),

\[
\tilde{A}(q) = \int_{-\infty}^{0} \tilde{A}_qfdz + \int_{0}^{\infty} \tilde{A}_qrdz = \frac{e\rho_L}{2\epsilon_0\epsilon_b} \frac{P_0}{(q + q_s P_{av})q} + \begin{cases} 
\frac{e\rho_L}{2\epsilon_0\epsilon_b} \frac{1}{(q + q_s P_{av})} \frac{b^3}{(b - q)^3} & \text{for } b \neq q \\
\frac{e\rho_L}{2\epsilon_0\epsilon_b} \frac{1}{(q + q_s P_{av})} & \text{for } b = q.
\end{cases}
\]  

(6)

where $\theta$ is the deflection angle of the particles from their original direction of motion, $\nu$ is the electron velocity, and $m^*$ is the effective electron mass. Since there are $N_{\text{dis}}$ dislocation lines piercing the 2DEG per unit area, using the screened potential given by Eq. (6), the scattering rate for a degenerate 2DEG is given by

\[
\frac{1}{\tau_{\text{dis}}} = N_{\text{dis}} \cdot \frac{m^*}{2\hbar^3 v} \cdot 2 \int_{0}^{\pi} |\tilde{A}(q)|^2 (1 - \cos \theta) d\theta.
\]  

(8)

The formula for scattering rate we have obtained in Eq. (8) is essentially the same as what is used by Jena et al.,

\[
\frac{1}{\tau_{\text{dis}}} = N_{\text{dis}} \cdot \frac{m^*}{2\hbar^3 k_F} \cdot \int_{0}^{2\pi} |\tilde{A}(q)|^2 \sqrt{q^2 dq / (1 - (q/2k_F)^2)}.
\]  

(9)

In fact, Eqs. (8) and (9) are the same by transforming the integral variable $q$ in Eq. (9) into $\theta$, using the relation of $q = 2k_F \sin (\theta/2)$ with $k_F = \sqrt{2\pi N_e}$ (Ref. 9), and $N_e$ being 2DEG density. Therefore, the difference in the scattering rate can only originate from the different expressions for the potential $\tilde{A}(q)$ in the two equations. Based on $g(z)$, the function for charge distribution, we obtain

\[
g(z) = \lim_{b \to \infty} b^3 e^{-bz} = \begin{cases} 
\infty & \text{for } (z = 0), \\
0 & \text{for } (z \neq 0),
\end{cases}
\]  

(10)

\[
\tilde{A}(q) = \frac{2e^2}{2\epsilon_0\epsilon_b} \frac{P_0 e^{P_{av}}}{q + q_s P_{av}},
\]  

(4)

\[
\tilde{A}(q) = \frac{2e^2}{2\epsilon_0\epsilon_b} P(z_0).
\]  

(5)

The parameters $P_0$, $P_{av}$, and $P(z_0)$ are all functions of $q$ and $b$, and the detailed expressions for them can be referred to Ando et al.,

As a dislocation can be modeled by a line of charge, we deduce the screened dislocation potential by integrate over the dislocation line with charge density $\rho_L$.

\[
\int_{0}^{\infty} g(z)dz = \int_{0}^{\infty} \frac{b^3}{2} e^{-b} e^{P_{av}} dz = 1,
\]  

(11)

for any value of $b$, and then for any value of $N_e$, which means that the charge distribution function used for a quasitriangle well can be converted to $\tilde{A}(q)$ for a perfect 2DEG. Thus, using the limiting qualification $b \to \infty$, the parameters $P_0$, $P_{av}$, and $P(z_0)$ in Eqs. (4) and (5) can be transformed as

\[
P_0 \to 1, \quad P_{av} \to 1, \quad P(z_0) \to e^{-P_{av}},
\]  

so that $\tilde{A}(q)$ in Eq. (6) can be simplified as

\[
\tilde{A}(q) = \frac{e\rho_L}{2\epsilon_0\epsilon_b} \frac{2}{(q + q_s P_{av})q}.
\]  

(12)

which is just the screened potential for dislocation scattering in the ideal 2DEG. As discussed above, the effect of dislocation scattering on transport in a quasitriangle well can be reverted to the same as the case of a perfect 2DEG, of which the typical result has been deduced by Jena et al., Therefore, our theory developed for dislocation core effect scattering in a quasitriangle well should be more reasonable for general cases.

The 2DEG mobilities inhibited by dislocation scattering with different carrier densities and different dislocation densities are plotted in Fig. 2, where the result of Jena et al., on perfect 2DEG is also presented for a comparison. It can be seen that the result of Jena et al., is not totally the same as in his paper. That is because Jena et al., used an approximation of $\sqrt{\tau_{\text{dis}} \sim k_F^2 / (1.84 k_F / q_s - 0.25)}$, while in our study, we treat it in its original form without any approximation. It is clear that our mobilities are lower than those obtained by Jena et al., The reason is that 2DEG in a quantum well with nonzero thickness experiences weaker screening than that of the ideal 2DEG. Without regard to screening effect, as a point charge located at $z_0 < 0$, the potential felt by the electrons in a quantum well with nonzero thickness is weaker than the case of an ideal 2DEG, due to a...
larger distance between the point charge in a dislocation line and the free electrons in the quantum well, while it is stronger for $z_0 > 0$, with a smaller distance. In the case of a dislocation piercing through the 2DEG in x–y plane, the total scattering potential is uniform in both cases of electron distribution. This conclusion can also be elicited from the unscreened potential equation

$$U(q) = \frac{e\rho_s}{\varepsilon_0\varepsilon_f q^2}, \quad (13)$$

where $U(q)$ is the bare potential energy, which is obtained by integrating the unscreened point charge scattering potential $V(q) = e^2/2\varepsilon_0\varepsilon_f e^{-qz_0}/q$ over $z$ with charge density $\rho_s$. It is clear from Eq. (13) that such potential is independent of the electron distribution; therefore, the unscreened dislocation scattering potential should be the same in both cases of electron distribution. Thus, the lowering of mobilities in our result as compared with those of Jena et al. should be attributed to the weakening of screening effect. Numerical imitating using the method of least-squares reveals an approximate $N_s^{14734}$ dependence of the mobility in the typical carrier density range of $1 \times 10^{12} \div 1 \times 10^{13}$ cm$^{-2}$, and the fitting curves are also plotted in Fig. 2. Experimental data from different references are included in Fig. 2 for a comparison with our theoretical results. Theoretically, for dislocation density of $10^{10}$ cm$^{-2}$ and in the typical carrier density range we discussed, maximum electron mobility will be in the range of $10^3$–$10^4$ cm$^2$/V s, which means that dislocation scattering will be one of the dominant mechanisms when dislocation density is in the order of $10^{10}$ cm$^{-2}$. A reduction in the dislocation density to $10^8$ cm$^{-2}$ or less will effectively improve the electron mobility. Smorchkova et al. obtained a mobility of $51 \ 700$ cm$^2$/V s at 13 K in a Al$_{0.9}$Ga$_{0.1}$N/GaN heterostructure grown on sapphire with a sheet carrier density of $2.23 \times 10^{12}$ cm$^{-2}$ (symbol $\star$ in Fig. 2). It should have a dislocation density lower than $10^8$ cm$^{-2}$ based on Fig. 2. Moreover, Frayssinet et al. succeeded in obtaining a mobility of $60 \ 100$ cm$^2$/V s at 1.5 K in a Al$_{0.15}$Ga$_{0.87}$N/GaN heterostructure grown on GaN single crystal with a sheet carrier density of $2.4 \times 10^{12}$ cm$^{-2}$ (symbol $\blacktriangle$ in Fig. 2). This sample is declared to be dislocation-free in the paper of Frayssinet et al. and this mobility value is one of the highest report ever in GaN-based semiconductors. Four other samples (symbol $\Delta$ and $\nabla$ in Fig. 2) show a mobility range of $10^3$–$10^4$ cm$^2$/V s, and they may have dislocation densities in the typical range of $10^3$–$10^{10}$ cm$^{-2}$.

In conclusion, we have deduced a theory for dislocation core effect scattering in a quasitrangle Al$_{0.9}$Ga$_{0.1}$N/GaN heterostructure potential well. The dependence of mobility on carrier sheet density and dislocation density is imitated to be $N_s^{14734}/N_{dis}$ approximately in the typical 2DEG density range of $1 \times 10^{12} \div 1 \times 10^{13}$ cm$^{-2}$. The results are compared with those obtained from a perfect 2DEG, and the reason for discrepancy is attributed to the different screening effect experienced by the ideal 2DEG and the electrons in a quasitriangle well.

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Measurement of polar $C$-plane and nonpolar $A$-plane InN/ZnO heterojunctions band offsets by x-ray photoelectron spectroscopy

Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People’s Republic of China

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The valence band offsets of the wurtzite polar $C$-plane and nonpolar $A$-plane InN/ZnO heterojunctions are directly determined by x-ray photoelectron spectroscopy to be 1.76 ± 0.2 eV and 2.20 ± 0.2 eV. The heterojunctions form in the type-I straddling configuration with a conduction band offset of 0.84 ± 0.2 eV and 0.40 ± 0.2 eV. The difference of valence band offsets of them mainly attributes to the spontaneous polarization effect. Our results show important face dependence for InN/ZnO heterojunctions, and the valence band offset of $A$-plane heterojunction is more close to the “intrinsic” valence band offset. © 2009 American Institute of Physics.

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InN has been attracted remarkable interest because of its excellent theoretically predicted electrical properties and potential for application in high speed devices.1 High-quality low band gap (0.7 eV) InN could extend the wavelength range of optoelectronic devices covered by the group-III nitrides into the near infrared. With continual improvements in the growth quality of InN epitaxial layers, prospects of realizing devices based on heterostructures have advanced considerably.2 Recently ZnO has been used as an efficient buffer layer in the growth of high-quality GaN,3,4 Ikuta et al.5 reported that ZnO-buffered $\alpha$-Al$_2$O$_3$ is effective to the epitaxial growth of InN thin films and, furthermore, improve their electrical properties. Moreover, some researchers indicated that oxidation reduces the surface electron accumulation of InN film.6 So InN/ZnO heterojunction may be a promising structure for fabricating optical and electronic devices. Unfortunately, due to the lack of an inversion center leads to a charge asymmetry along the polar (0001) direction, the wurtzite ZnO and InN layers generate an internal electric field at their heterojunctions.7 Waltereit et al.8 demonstrated that the epitaxial growth of GaN/(Al,Ga)N on tetragonal LiAlO$_2$ in a nonpolar direction allows the fabrication of structures free from electrostatic fields, resulting in an improved quantum efficiency. Measurements of the valence band offsets (VBOs) are of crucial importance for the design of such devices. Moreover, the VBO of $C$-plane (polar) InN/ZnO heterojunction has been directly determined by x-ray photoelectron spectroscopy (XPS) by Zhang et al.9 Yet, there is a lack of experimental data on the interface band alignment of A-plane (nonpolar) InN/ZnO heterojunction. XPS has been demonstrated to be a direct and powerful tool for measuring the valence band discontinuities of heterojunctions.10-12 In this letter, we will present an experimental determination of the VBOs of the $C$-plane and A-plane InN/ZnO heterojunctions by XPS.

Two groups of samples were used for XPS experiments: a 270-nm-thick $C$-plane ZnO film grown on $C$-plane sapphire, a 690 nm and a 5 nm C-plane InN epitayers grown on ZnO-buffered C-plane sapphires separately; a 110-nm-thick A-plane ZnO film grown on $R$-plane sapphire, a 390 nm and a 5 nm A-plane InN epilayers grown on ZnO-buffered $R$-plane sapphire separately. The $C$-plane and A-plane ZnO in this study were grown by low-pressure metal-organic chemical vapor deposition (MOCVD), as described elsewhere.13,14 The $C$-plane and A-plane InN was grown at 520 °C by atmospheric pressure MOCVD.9 The crystal structures and epitaxial relationships were characterized using a Philips X’Pert x-ray diffraction (XRD) apparatus and high-resolution XRD measurements (Beijing Synchrotron Radiation Facility, not shown here). Both InN and ZnO films in our experiments are unintentionally n-type doped.

The XPS measurements were performed on a PHI Quantera SXM instrument with Al Kα (energy 1486.6 eV) as the x-ray radiation source, which had been carefully calibrated using work function and Fermi energy level ($E_F$). And all XPS spectra were calibrated by the C 1 s peak (284.8 eV) from contamination to compensate the charge effect.

The VBO ($\Delta E_v$) can be calculated from the formula

$$\Delta E_v = \Delta E_{CL} - (E_{InN}^{3d} - E_{VBM}^{3d}) + (E_{ZnO}^{2p} - E_{VBM}^{2p})$$

where $\Delta E_{CL}$ is the energy difference between In 3d and Zn 2p core levels (CLs) which are measured in the heterojunction sample, ($E_{InN}^{3d} - E_{VBM}^{3d}$) and ($E_{ZnO}^{2p} - E_{VBM}^{2p}$) are the InN and ZnO bulk constants of the respective thick film. Zn 2p$_{3/2}$ and In 3d XPS spectra of the two groups of samples are shown in Figs. 1(a)–1(d) and 2(a)–2(d) fitted using Shirley backgrounds and Voigt (mixed Lorentzian–Gaussian) functions, the parameters for which are shown in Table I. Since considerable accordance of the fitted line to the original measured data has been obtained, the uncertainty of the CL position should be lower than 0.03 eV, as evaluated by numerous fittings with different parameters. The Zn 2p$_{3/2}$ spectra of both the ZnO and the InN/ZnO samples were fitted by a single contribution, attributed to the bonding configurations Zn–O. However, for the In 3d spectra of both the InN and the InN/ZnO samples, additional low-intensity higher-binding-energy components were also required. In Figs. 1(b) and 2(b) these extra components are attributed to In–O bonding due to the oxide contamination when InN is present at the surface.15 In Figs. 1(d) and 2(d), they are attributed to In–O bonding at the InN/ZnO inter-

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a) Electronic mail: alyang@semi.ac.cn.

b) Electronic mail: xliu@semi.ac.cn.
InN samples are shown in Figs. 1 and 2. The valence band XPS spectra for the thick ZnO and InN samples, and InN/ZnO samples, and In 3d XPS spectra for A-plane and C-plane heterojunctions are collected from the same surface (InN surface), therefore, the surface band-bending effects can be cancelled out for the measurement of ΔE_{CL}, as was the measurement of the band offset of the InN/AlN heterojunction by others. As indicated by Zhang et al., a strain-induced piezoelectric field could be completely relaxed at the heterojunction. If this is the case, the piezoelectric polarization effect is negligible and only the spontaneous polarization effect plays an important role. The foregoing measurement results indicate that “In−O” bonding at the InN/ZnO interfaces,” accordingly, we speculate that the interface structure for C-plane heterojunction is Zn−O−In−N. Due to the existence of an internal electric field, the electrons must do more work for C-plane heterojunction. The difference of the VBOs of C-plane and A-plane heterojunctions may attribute to spontaneous polarization field. Recently, Wu et al. investigated the intrinsic band lineup (0.78 eV for the N-polarity VBO) at the InN/GaN heterojunction by using the technique of synchrotron-radiation photoelectron microscopy and spectroscopy on the in situ cleaved, nonpolar cross-sectional surface of InN/GaN heterojunction under surface flat band conditions. It is different from the VBOs previously reported by them (1.04 and 0.54 eV for In/Ga- and N-polarity cases at polar III-nitride heterointerfaces), although the In 4d and Ga 3d peaks were used in their experiment. The VBO of C-plane heterojunction determined here is approximately twice that of the value of 0.82 eV suggested by Zhang et al. Our results should be more reliable in view of the ZnO and InN valence band photoemission spectra exhibiting the expected shape for an anion 2p-dominated valence band. Also, the VBO of the C-plane of VB spectra to the base lines in order to account for the finite instrument resolution. The parameters deduced from Figs. 1 and 2 are summarized in Table I for clarity. The scatter of the data relative to the fit are estimated as an uncertainty in VBM positions of less than 0.1 eV, as also estimated from fitting with different parameters. The VBOs of C-plane and A-plane are calculated to be 1.76 ± 0.2 eV and 2.20 ± 0.2 eV by substituting those values obtained in experiments into Eq. (1).

![FIG. 1.](image1) (Color online) Zn 2p XPS spectra for C-plane (a) ZnO and (c) InN/ZnO samples, and In 3d XPS spectra for C-plane (b) InN and (d) InN/ZnO samples. Experimental data points are fitted by Voigt (mixed Lorentzian–Gaussian) lineshapes (solid lines) after the application of a Shirley background (dashed line). Also shown are valence band spectra for (e) ZnO and (f) InN. The peak and VBM positions are summarized in Table I.

![FIG. 2.](image2) (Color online) Zn 2p XPS spectra for A-plane (a) ZnO and (c) InN/ZnO samples, and In 3d XPS spectra for A-plane (b) InN and (d) InN/ZnO samples. Experimental data points are fitted by Voigt (mixed Lorentzian–Gaussian) lineshapes (solid lines) after the application of a Shirley background (dashed line). Also shown are valence band spectra for (e) ZnO and (f) InN. The peak and VBM positions are summarized in Table I.

### Table I. XPS CL spectra fitting results and VBM positions obtained by linear extrapolation of the leading edge to the extended base line of the VB spectra. The errors in the peak positions and VBM are ±0.03 and ±0.1 eV, respectively.

<table>
<thead>
<tr>
<th>Sample</th>
<th>State</th>
<th>C-plane binding energy (eV)</th>
<th>A-plane binding energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>InN</td>
<td>In 3d_{3/2} (In-N)</td>
<td>4.43 ± 0.03</td>
<td>4.43 ± 0.03</td>
</tr>
<tr>
<td></td>
<td>(In-O)</td>
<td>4.44 ± 0.04</td>
<td>4.44 ± 0.04</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>0.56 ± 0.03</td>
<td>0.39 ± 0.03</td>
</tr>
<tr>
<td>ZnO</td>
<td>Zn 2p (Zn-O)</td>
<td>1.02 ± 0.02</td>
<td>1.02 ± 0.02</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>2.43 ± 0.02</td>
<td>2.29 ± 0.02</td>
</tr>
<tr>
<td>InN/ZnO</td>
<td>In 3d_{3/2} (In-N)</td>
<td>4.43 ± 0.03</td>
<td>4.43 ± 0.03</td>
</tr>
<tr>
<td></td>
<td>(In-O)</td>
<td>4.44 ± 0.04</td>
<td>4.44 ± 0.04</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>0.56 ± 0.03</td>
<td>0.39 ± 0.03</td>
</tr>
<tr>
<td>Zn 2p (Zn-O)</td>
<td></td>
<td>1.02 ± 0.02</td>
<td>1.02 ± 0.02</td>
</tr>
</tbody>
</table>
heterojunction is very close to the value (1.95 eV) that was predicted by Veal et al.\textsuperscript{20}

Using the room temperature band gaps for ZnO and InN (3.3,\textsuperscript{13,14} and 0.7 eV,\textsuperscript{1} respectively), the InN/ZnO heterojunctions are found to have a type-I (staggered) band lineup, as shown in Fig. 3, with corresponding conduction band offsets (CBOs) of 0.84 ± 0.2 eV and 0.40 ± 0.2 eV for C-plane and A-plane heterojunctions.

In summary, the VBOs of the C-plane and A-plane InN/ZnO heterojunctions have been measured by XPS. A type-I band alignment with VBOs are 1.76 eV and 0.2 eV for C-plane and A-plane heterojunctions.

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