Vol 18 No 5, May 2009
1674-1056/2009/18(05)/2002-04

Chinese Physics B

© 2009 Chin. Phys. Soc.
and IOP Publishing Ltd

Scattering behaviour of a two-dimensional electron gas induced by Al composition fluctuation in $Al_xGa_{1-x}N$ barriers in $Al_xGa_{1-x}N$/GaN heterostructures*

Wang Yan(王 彦), Shen Bo(沈 波)†, Xu Fu-Jun(许福军), Huang Sen(黄 森), Miao Zhen-Lin(苗振林), Lin Fang(林 芳), Yang Zhi-Jian(杨志坚), and Zhang Guo-Yi(张国义)

State Key Laboratory of Artificial Microstructure and Mesoscopic Physics, School of Physics, Peking University, Beijing 100871, *China*

(Received 17 November 2008; revised manuscript received 19 December 2008)

This paper reports that cathodoluminescence (CL) measurements have been done to study the alloy fluctuation of the $Al_{0.3}Ga_{0.7}N$ layer in $Al_{0.3}Ga_{0.7}N$/GaN heterostructures. The CL images and linescanning results demonstrate the existence of compositional fluctuation of Al in the $Al_{0.3}Ga_{0.7}N$ barrier. A model using a δ-shape perturbation Hamilton function has been proposed to simulate the scattering probability of the two dimensional electron gases (2DEG) induced by Al composition fluctuation. Two factors, including conduction band fluctuation and polarization electric field variation, induced by the Al composition fluctuation have been taken into account. The scattering relaxation time induced by both factors has been estimated to be 0.31 ns and 0.0078 ns, respectively, indicating that the variation of the piezoelectric field is dominant in the scattering of the 2DEG induced by Al fluctuation.

Keywords: scattering, cathodoluminescence, fluctuation
PACC: 7210F

III-nitride semiconductors have attracted much interest during recent decades due to their applications in optoelectronic devices and microwave power devices.[1,2] $Al_xGa_{1-x}N$/GaN heterostructure field-effect transistors (HFETs) have attracted considerable attention for their promising use in high-power and high-temperature microwave electronics fields because of the unique properties of III-nitrides, including wide band gaps, high electron saturation velocities, and high critical breakdown fields.[3,4] It is a common phenomenon that composition fluctuation exists in most compounds of III-V ternary semiconductors. Up to now, many reports have focused on composition fluctuation in $In_xGa_{1-x}N$ materials.[5−9] But there are few reports on the research of composition fluctuation in $Al_xGa_{1-x}N$ alloys. Due to the large bandgap offset and polarization-induced electric field, the Al composition fluctuation will cause large conduction band fluctuation and polarization electric field variation. Both factors above will strongly influence the scattering of the two-dimensional electron gas (2DEG) in the channel, which is the basis of fabricating the HFETs. A lot of scattering behaviour has been researched by many groups, including acoustic and optical phonons, ionized impurities, alloy disorder.[10−15] However, few reports have discussed scattering behaviour induced by Al composition fluctuation.

In this study, cathodoluminescence (CL) measurements at low temperature have been done to demonstrate the existence of Al composition fluctuation in the $Al_xGa_{1-x}N$ layer. A model has been proposed to describe the Al composition fluctuation in the $Al_xGa_{1-x}N$ layer, which is used to simulate the scattering behaviour of the 2DEG in $Al_xGa_{1-x}N$/GaN heterostructures. The scattering relaxation time induced by this mechanism is finally calculated by the combination of the measurements and the model.

The $Al_xGa_{1-x}N$/GaN heterostructures for the CL measurements were grown by using metal-organic chemical vapour deposition on the (0001) surface of sapphire substrates. A nucleation GaN buffer layer was grown at 488 °C, followed by a 2.0-μm-thick unintentionally doped GaN layer deposited at 1071 °C. Then, an unintentionally doped $Al_{0.3}Ga_{0.7}N$ layer with a thickness of 30 nm was grown at 1080 °C. The composition of Al in the barrier is 0.3 according to the

*Project supported by the National Natural Science Foundation of China (Grant Nos 10774001, 60736033 and 60628402), and National Basic Research Program of China (Grant Nos 2006CB604908 and 2006CB921607).
†E-mail: bshen@pku.edu.cn

x-ray diffraction results. The measurements were performed on a Hitachi 4200 scanning microscope with a CL system (Horiba, Japan)[16] with an electron beam of 5 kV and 500 pA at 63 K on a liquid helium stage. The CL spectra were recorded in a charge-coupled device, while the monochromatic CL images were taken by a photomultiplier tube.

Figure 1 shows the CL spectrum of an $Al_{0.3}Ga_{0.7}N/GaN$ heterostructure measured at 63 K. Two peaks with different intensities are observed at the wavelengths of 363 nm and 296 nm, respectively. The stronger peak at 363 nm is from the GaN layer, while the weaker one at 296 nm is from the $Al_{0.3}Ga_{0.7}N$ layer.

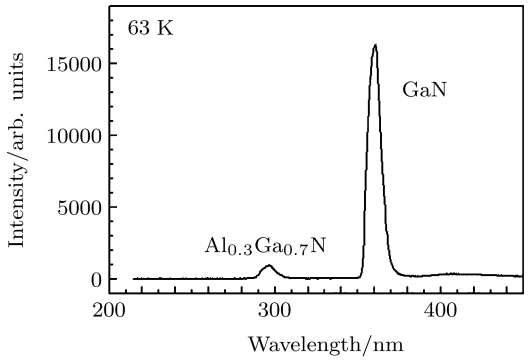


Fig.1. The CL spectrum of an $Al_{0.3}Ga_{0.7}N/GaN$ heterostructure measured at 63 K. Two peaks at 363 nm and 296 nm are corresponding to GaN and $Al_{0.3}Ga_{0.7}N$, respectively.

Figure 2 shows four images of an $Al_{0.3}Ga_{0.7}N/GaN$ heterostructure measured at 63 K. Figure 2 (a) is a normal scanning electron microscope (SEM) image, and the others are monochromatic CL images at the wavelength of 296 nm (b), 293 nm (c) and 299 nm (d), respectively. Although the SEM image shows a perfect surface, the CL ones show the fluctuation in the luminescence intensity at different locations, which are attributed to the shift of the peak position of $Al_{0.3}Ga_{0.7}N$, neglecting the strain variation in the small area.

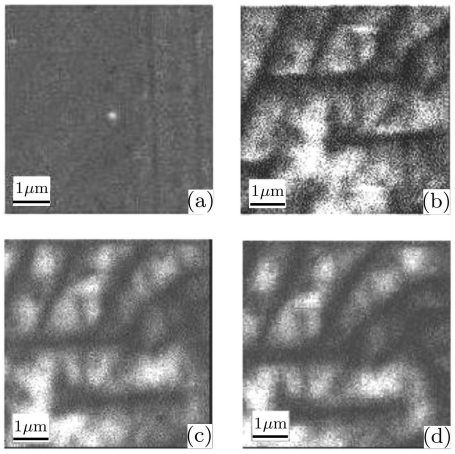


Fig.2. SEM image (a), and monochromatic CL images measured at 63 K on the same area of 6×6 μm^2 on the surface of an $Al_{0.3}Ga_{0.7}N/GaN$ heterostructure at 296 nm (b), 293 nm (c), and 299 nm (d), respectively.

Figure 3 shows a line scanning CL measurement on an $Al_{0.3}Ga_{0.7}N/GaN$ heterostructure with a scanning step of 1 μm. The results show the evident shift of the $Al_{0.3}Ga_{0.7}N$ peaks, which directly indicates the existence of Al composition fluctuation in $Al_{0.3}Ga_{0.7}N$ layer. This result is consistent with the monochromatic CL images.

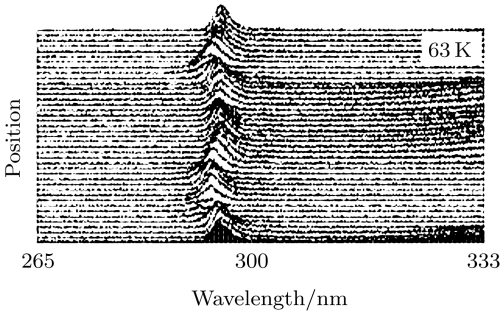


Fig.3. The CL line scanning on the surface of an $Al_{0.3}Ga_{0.7}N/GaN$ heterostructure measured at 63 K. The shift of the peak position around 296 nm is observed at different scanning locations.

A model is proposed to describe the compositional fluctuation in $Al_xGa_{1-x}N$. In a homogeneous $Al_xGa_{1-x}N$ layer, the Al composition is constant everywhere because of the periodic distribution of the Al atoms. However, once this periodicity is destroyed, which is the actual case during the growing procedure at a high temperature, there will be exhibited composition fluctuation in the alloys.

In our model, we choose a δ-shape perturbation Hamiltonian to describe the spatial Al fluctuation, as shown in Fig.4. In the two-dimensional case, it is written as

$$H' = \sum_{i,j} A_{ij}\delta(x)\delta(y), \tag{1}$$

where the parameter A_{ij} we define here will be determined in the CL experiments and the xy plane is parallel to the 2DEG plane. In an $Al_xGa_{1-x}N/GaN$ heterostructure, a plane wave function is assumed to describe the 2DEG. Thus, based on the quantum scattering theory,[17–19] the scattering matrix is defined as

$$M_{k'k} = \int \Psi_{k'} H' \Psi_k, \tag{2}$$

where ψ_k, $\psi_{k'}$ represent the incoming wavefunction and emergent wavefunction of the 2DEG, respectively. The x and y axis are totally equivalent for the 2DEG, to simplify, thus the wavefunction of the 2DEG can be written as

$$\Psi_k = \frac{1}{nx_0} \mathrm{e}^{\mathrm{i}k\cdot r}, \tag{3}$$

where $\dfrac{1}{nx_0}$ represents the normalized parameter in the given structure, x_0 is the period of the composition fluctuation in one direction, and k is the wave vector. So, $M_{k'k}$ is written as

$$\begin{aligned} M_{k'k} &= \int \Psi_{k'} H' \Psi_k \\ &= \frac{1}{n^2 x_0^2} \int_s \mathrm{e}^{\mathrm{i}(k-k')\cdot r} \sum_{i,j} A_{ij} \delta(x)\delta(y) \mathrm{d}x\mathrm{d}y \\ &= \frac{\sum\limits_{i,j} A_{ij}}{n^2 x_0^2}. \end{aligned} \tag{4}$$

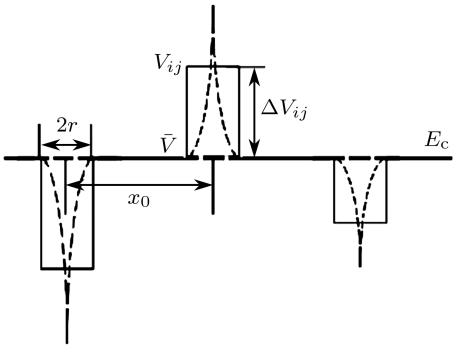


Fig.4. A proposed δ-shape perturbation Hamilton model for calculating the scattering relaxation time of the 2DEG. The parameter x_0 is the period of the δ-shape perturbation, which is also linked to the CL line scanning measurement. In order to compare this model with the experiment, the parameter $\Delta V_{ij}^* \pi r^2$ is used to replace A_{ij} in the model in the condition of the same integration.

In CL experiments on the $Al_{0.3}Ga_{0.7}N$/GaN heterostructure, further parameters can be acquired. The existing Al composition fluctuation is not a precise δ-shape perturbation as we expect. What we used here is CL measurement as a detection method by an accelerating electron beam, which has an excited area in the structures. Monte Carlo simulation has been done by Casino to describe the trajectory of electrons at 5 kV, as shown in Fig.5. The radius of the excited area r is about 100 nm based on the simulation and previous results.[20,21] In an ideal δ-shape barrier, the height trends to ∞, while the width trends to 0. The integration of δ in the whole area is 1. When the fluctuation height is ΔV_{ij} and the excited area in $Al_{0.3}Ga_{0.7}N$ is assumed as πr^2, the equivalent parameter of A_{ij} is $\Delta V^* \pi r^2$. The parameter ΔV_{ij} is determined to be $\left|V_{ij} - \overline{V}\right|$, just as shown in Fig.4. Based on the above explanation, some CL experimental parameters are introduced to the model. Thus, the scattering matrix is

$$M_{k'k} = \frac{\sum\limits_{i,j} A_{ij}}{n^2 x_0^2} = \frac{\pi r^2}{n^2 x_0^2} \sum_{ij} |\Delta V_{ij}| = \frac{\pi r^2}{x_0^2} \overline{\Delta V_{ij}}, \tag{5}$$

where the parameter $\overline{\Delta V_{ij}}$ is the statistical average parameter for all scanning points of the structure. By using the Fermi golden rule in the scattering theory, the scattering probability of the 2DEG induced by Al composition fluctuation in the $Al_xGa_{1-x}N$ layer is determined to be

$$\frac{1}{\tau_k} = \frac{2\pi}{\hbar} \frac{1}{E_k} \left|M_{k'k}\right|^2 = \frac{2\pi^3}{\hbar} \frac{1}{E_k} \frac{r^4}{x_0^4} \left|\overline{\Delta V_{ij}}\right|^2, \tag{6}$$

where $x_0 = 1$ μm is determined by the measurements. Besides, some of the parameters can be determined by the given $Al_xGa_{1-x}N$/GaN heterostructure.[22,23] By using the self-consistent Schrödinger equation and Poisson equation, at a given Al composition in an $Al_xGa_{1-x}N$/GaN heterostructure, the ground band of the 2DEG in the triangle well is given as

$$E_k(x) = \left[\frac{9\pi\hbar e^2}{8\varepsilon_0 \sqrt{8m^*(x)}} \frac{n_s(x)}{\varepsilon(x)}\right]^{2/3}, \tag{7}$$

where ε is the dielectric constant of the material, $m^* = 0.22m_0$ is the effective mass of the 2DEG, and n_s is the sheet concentration of the 2DEG.[22] In the case of 0.3 Al composition in the $Al_xGa_{1-x}N$/GaN heterostructure, the sheet concentration n_s is closed as 1.51×10^{13} cm^{-2}. The dielectric constant ε is 9.35 and the ground band energy of the 2DEG E_k is 0.36 eV.

Two scattering mechanisms induced by the Al composition fluctuation have been considered in the

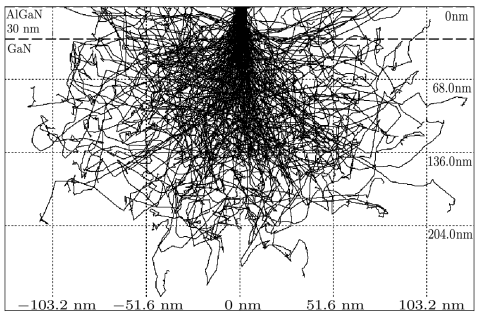


Fig.5. Monte Carlo simulation of the electron trajectory in $Al_{0.3}Ga_{0.7}N$/GaN structures at 5 kV.

$Al_xGa_{1-x}N$/GaN heterostructure, conduction band fluctuation and polarization electric field variation. Statistics of the CL line scanning has been done. An effective fluctuation magnitude of the conduction band in the $Al_{0.3}Ga_{0.7}N$ barrier is determined to be 0.011 eV, when it is assumed that 70% of the bandgap offset locates on the conduction band, based on the CL line scanning measurements. Therefore, the scattering probability of the 2DEG induced by the fluctuation of the conduction band is calculated to be 3.2×10^9 s^{-1}, and its corresponding scattering relaxation time is 0.31 ns. Moreover, based on the statistical work before, we calculate an average of composition fluctuation of Al in the $Al_{0.3}Ga_{0.7}N$ barrier in the $Al_{0.3}Ga_{0.7}N$/GaN heterostructure, the result is 0.007. By using basic equations in the calculation of the polarization filed, the variation of the polarization field induced by composition fluctuation has a magnitude of 3.6×10^4 V/cm.[23] An average of the 2DEG thickness is chosen to be 2 nm. Therefore, the variation of polarization field will lead to an effective energy variation of 0.07 eV. In this case, the scattering probability of the 2DEG induced by the variation of the polarization electric field is determined to be 1.3×10^{11} s^{-1}, and its corresponding scattering relaxation time is 0.0078 ns. Therefore, in both factors induced by Al composition fluctuation, the influence of variation of the polarization electric field is considered to be dominant. In the previous report, the scattering relaxation time influenced by the surface roughness is of the same magnitude of order as that influenced by the variation of the polarization field.[24,25]

In conclusion, the scattering behaviours of the 2DEG induced by Al composition fluctuation of the $Al_{0.3}Ga_{0.7}N$ layer in an $Al_{0.3}Ga_{0.7}N$/GaN heterostructure is investigated by means of CL measurements at low temperature and simulated by a proposed model. An average fluctuation of Al in the $Al_{0.3}Ga_{0.7}N$ barrier in the $Al_{0.3}Ga_{0.7}N$/GaN heterostructure is simulated to be 0.007. Two factors, including conduction band fluctuation and polarization electric field variation, induced by Al composition fluctuation have been taken into account. The scattering relaxation time induced by both factors has been estimated to be 0.31 ns and 0.0078 ns, respectively, which indicates that the variation of the piezoelectric field is dominant to the scattering of the 2DEG induced by the Al fluctuation.

Acknowledgement

The authors thank Prof. Takashi Sekiguchi in the National Institute for Materials Science (Japan) for the CL measurements.

References

[1] Ambacher O 1998 *J. Phys.* D **31** 2653
[2] Smart J A, Schremer A T, Weimann N G, Ambacher O, Eastman L F and Shealy J R 1999 *Appl. Phys. Lett.* **75** 388
[3] Chow T P and Tyagi R 1994 *IEEE Trans. Electron Devices* **41** 1481
[4] Khan M A, Chen Q, Yang J W, Shur M S, Dermott B T and Higgins J A 1996 *IEEE Electron Lett.* **17** 325
[5] Chang H J, Chen C H and Chen Y F 2005 *Appl. Phys. Lett.* **86** 021911
[6] Moon Y T, Kim D J, Park J S, Oh J T, Lee J M, Ok Y W, Kim H and Park S J 2001 *Appl. Phys. Lett.* **79** 599
[7] Naranjo F B, Sánchez-García M A, Calle F, Calleja E, Jenichen B and Ploog K H 2002 *Appl. Phys. Lett.* **80** 231
[8] Tabata A, Teles L K, Scolfaro L M R and Leite J R 2002 *Appl. Phys. Lett.* **80** 769
[9] Behbehani M K, Piner E L, Liu S X and El-Masry N A 1999 *Appl. Phys. Lett.* **75** 2202
[10] Walukiewicz W, Ruda H E, Lagowski J and Gatos H C 1984 *Phys. Rev.* B **30** 4571
[11] Hirakawa K and Sakaki H 1986 *Phys. Rev.* B **33** 8291
[12] Walukiewicz W, Lagowski L, Jastrzebski L, Lichtensteiger M and Gatos H C 1979 *J. Appl. Phys.* **50** 899
[13] Walukiewicz W 1992 *Semiconductor Interfaces and Microstructures* (Singapore: World Scientific)
[14] Störmer H L, Pfeiffer L N, Baldwin K W and West K 1990 *Phys. Rev.* B **41** 1278
[15] Hsu L and Walukiewicz W 1997 *Phys. Rev.* B **56** 1520
[16] Sekiguchi T, Yuan X L and Niitsuma J 2005 *Scanning* **27** 103
[17] Taylor J R 1972 *Scattering Theory: the Quantum Theory on Nonrelativistic Collisions* (New York: Wiley)
[18] Newton R G 1982 *Scattering of Waves and Particles* 2nd ed. (New York: Springer-Verlag)
[19] Narnhofer H and Thirring W 1981 *Phys. Rev.* A **23** 1688
[20] Yacobi B G and Holt D B 1990 *Cathodoluminescence Microscopy of Inorganic Solids* (New York: Plenum Press)
[21] Holt D B and Joy D C 1989 *SEM Microcharacterization of Semiconductors* (London: Academic Press)
[22] Ambacher O, Foutz B, Smart J, Shealy J R, Weimann N G, Chu K, Murphy M, Sierakowski A J, Schaff W J, Eastman L F, Dimitrov R, Mitchell A and Stutzmann M 2000 *J. Appl. Phys.* **87** 334
[23] Ambacher O, Smart J, Shealy J R, Weimann N G, Chu K, Murphy M, Schaff W J, Eastman L F, Dimitrov R, Wittmer L, Stutzmann M, Rieger W and Hilsenbeck J 1999 *J. Appl. Phys.* **85** 3222
[24] Quang D N, Tuoc V N, Tung N H, Minh N V and Phong P N 2005 *Phys. Rev.* B **72** 245303
[25] Zhang J F, Mao W, Zhang J C and Hao Y 2008 *Chin. Phys.* B **17** 2689