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Numerical analysis of impact of stress in passivation films on electrical properties in AlGaN/GaN heterostructures

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Abstract: The impact of forces due to the difference in mechanical stresses between the Schottky contacts and passivation films on the electrical properties of (0001) AlGaN/GaN Schottky diodes is numerically analyzed in the framework of the edge force model. The compressive (tensile) passivation films induce negative (positive) piezoelectric charges below the Schottky contacts in the GaN channels and bring forth onsets of the concentration of two-dimensional electron gas at shallower (deeper) bias voltages. The change in the bias voltages at the onset due to edge forces of $\pm 0.5\,\mathrm{GPa}\cdot\mu\mathrm{m}$ is 1 or 2 V for diodes with 0.5-μm Schottky contacts. This indicates that passivation films with the designed stress play a crucial role in controlling the threshold voltages of AlGaN/GaN HEMTs.

Keywords: GaN, HEMTs, threshold voltage, edge force, piezoelectric effects, passivation film
Classification: Electron devices, circuits, and systems

References

[1] Y. Uemoto, M. Hikita, H. Ueno, H. Matsuo, H. Ishida, M. Yanagihara, T. Ueda, T. Tanaka, and D. Ueda, "Gate Injection Transistor (GIT)—A Normally-Off AlGaN/GaN Power Transistor Using Conductivity Modulation," *IEEE Trans. Electron Devices*, vol. 54, no. 12, pp. 3393–3399, Dec. 2007.
[2] T. Oka and T. Nozawa, "AlGaN/GaN Recessed MIS-Gate HFET With High-Threshold-Voltage Normally-Off Operation for Power Electronics Applications," *IEEE Electron Device Lett.*, vol. 29, no. 7, pp. 668–670, July 2008.
[3] T. Mizutani, M. Ito, S. Kishimoto, and F. Nakamura, "AlGaN/GaN HEMTs with Thin InGaN Cap Layer for Normally Off Operation," *IEEE Electron Device Lett.*, vol. 28, no. 7, pp. 549–551, July 2007.
[4] M. Hiroki, N. Maeda, and T. Kobayashi, "Electrical properties and device characteristics of InAlN/AlGaN/AlN/GaN heterostructure field ef-

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Published July 25, 2009

fect transistors,” *Physica Status Solidi (c)*, vol. 6, no. 52, pp. S1056–S1060, June 2009.

[5] T. Onodera and H. Nishi, “Theoretical Study of the Piezoelectric Effect on GaAs MESFET’s on (100), (011), and $(\bar{1}\bar{1}\bar{1})$Ga, and (111)As Substrates,” *IEEE Trans. Electron Devices*, vol. 36, no. 9, pp. 1580–1585, Sept. 1989.

[6] R. A. Davies, D. Z. Bazley, S. K. Jones, H. A. Lovekin, W. A. Phillips, R. H. Wallis, J. C. Birbeck, T. Martin, and M. J. Uren, “The gate-length dependent performance of AlGaN/GaN HFETs with silicon nitride passivation,” *Proc. 2000 8th IEEE Int. Symp. on High Performance Electron Devices for Microwave and Optoelectronic Appl.*, Glaskow, UK, pp. 76–81, Nov. 2000.

[7] S. G. Lekhnitskii, *Anisotropic Plates*, translated from the second Russian edition by S. W. Tsai and T. Cheron, Gordon and Breach Science Publishers, New York-London-Paris, 1968.

[8] C. E. Murray, “Mechanics of edge effects in anisotropic thin film/substrate systems,” *J. Appl. Phys.*, vol. 100, no. 10, 103532, Nov. 2006.

[9] E. Y. Chang, G. T. Cibuzar, and K. P. Pande, “Passivation of GaAs FET’s with PECVD Silicon Nitride Films of Different Stress States,” *IEEE Trans. Electron Devices*, vol. 35, no. 9, pp. 1412–1418, Sept. 1988.

[10] O. Ambacher, J. Smart, J. R. Shealy, N. G. Weimann, K. Chu, M. Murphy, W. J. Schaff, L. F. Eastman, R. Dimitrov, L. Wittmer, M. Stutzmann, W. Rieger, and J. Hilsenbeck, “Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in N- and Ga-face AlGaN/GaN heterostructures,” *J. Appl. Phys.*, vol. 85, no. 6, pp. 3222–3233, March 1999.

1 Introduction

Due to their high breakdown voltage and excellent transport properties, AlGaN/GaN HEMTs are promising devices for high-frequency and high-power applications. HEMTs with shallower or positive threshold voltages V_{th}’s have been eagerly sought so as to fully exploit their potential. A variety of structures for realizing such HEMTs, such as *p*-type doped gates [1], MIS-like heterostructures [2], InGaAs-cap layers [3], and stressed InAlN barriers [4], have been explored.

It was shown that V_{th} in GaAs MESFETs largely changed when the mechanical stress of their passivation films was varied. The change in V_{th} was explained by a scheme in which the difference in stresses between gate (Schottky) contacts and the adjacent media (the passivation films for the present) (i) caused the concentration of mechanical forces at the edges of gate contacts on semiconductor surfaces (edge force), (ii) induced the non-uniform stress and hence piezoelectric charges in the MESFET channels, and (iii) shifted the V_{th} [5]. It was reported that V_{th} in AlGaN/GaN HEMTs was shifted by means of a similar mechanism [3, 6].

In this paper, we numerically analyze the impact of the stress in passivation films on the electrical properties of Schottky diodes formed on (0001) AlGaN/GaN heterostructures. We employ the edge force model with the

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anisotropic characteristics of the elastic properties in group-III nitrides explicitly considered [7, 8]. The surface of heterostructures is assumed to be covered by group-III element layers. We focus on the relation between the concentration of two-dimensional electron gas (2DEG) in the GaN channels and the bias voltage V_b and quantitatively estimate the resultant change in the V_{th} of AlGaN/GaN HEMTs.

2 Method

We consider Schottky diodes on unintentionally-doped AlGaN/GaN heterostructures with Schottky contact lengths of 0.5 and 1.0 μm. The separation between the Schottky and ohmic contacts is 1.0 μm. The thicknesses of AlGaN and GaN layers are 20 nm and 2 μm, respectively. The Al content in the AlGaN layers is preset to 0.25. The concentration of residual donors in the GaN layer is assumed to be $1 \times 10^{15}\,\mathrm{cm}^{-3}$. The concentration of 2DEG in the unbiased heterostructure is assumed to be $1 \times 10^{13}\,\mathrm{cm}^{-2}$. We place acceptor-like surface states on the surface of the AlGaN layers. Their density is assumed to be $1 \times 10^{13}\,\mathrm{cm}^{-2}\mathrm{eV}^{-1}$.

In considering the situation that the stress of Shottky contacts is negligibly small in comparison with that of passivation films, the edge force p is approximately given by the product of the stress (σ_f) and thickness (d_f) of passivation films [5]: $p \approx \sigma_f d_f$. The sign of p is negative (positive) for the compressive (tensile) stress in passivation films. It is noteworthy that the stress in SiN films, which have been widely used for passivating the surface of AlGaN/GaN HEMTs, can be made either compressive or tensile by properly choosing conditions of deposition [9].

The edge force induces stress σ_{ij} in heterostructures, where σ_{ij} is the (i, j) component of stress tensors. The coordinates along the horizontal (Shottky-to-ohmic) and vertical directions are denoted as x_1 and x_3, respectively. We estimate the spatial distribution of σ_{ij}'s by using the stress function formalism [7, 8]. The concentration of piezoelectric charges due to the edge force, minus the divergence of the polarizability P induced by σ_{ij}'s, is obtained by

$$-\mathrm{div}P = \frac{e_{15}}{C_{44}}\sigma_{13,1} - \frac{-e_{31}C_{33} + e_{33}C_{13}}{C_{11}C_{33} - C_{13}^2}\sigma_{11,3} - \frac{e_{31}C_{13} - e_{33}C_{11}}{C_{11}C_{33} - C_{13}^2}\sigma_{33,3}, \quad (1)$$

where $\sigma_{ij,k}$ is the x_k-derivative of σ_{ij}, e_{ij} and C_{ij} are the piezoelectric constancts and the elastic compliances of GaN, respectively. Next, we numerically solve the Poisson equation of the heterostructure with these piezoelectric charges considered and obtain the band structure and the distribution of 2DEG.

We assume for simplicity that the piezoelectric constants and elastic compliances of AlGaN are the same as those of GaN. In addition, we ignore the quantum-mechanical characteristics of 2DEG. Values of parameters used in the analysis are taken from a literature [10].

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3 Results and discussions

The spatial distributions of piezoelectric charges in half of the 0.5- and 1.0-μm Schottky diodes for $p = -0.5\,\text{GPa} \cdot \mu\text{m}$ are shown in Figs. 1 (a) and (b), respectively. Note that p of $-0.5\,\text{GPa} \cdot \mu\text{m}$ corresponds to 1-μm thick passivation films with a compressive stress of 0.5 GPa. The edge force p is loaded at the position $x_1 = 0.25$ (0.5) μm in the 0.5-μm (1.0-μm) Schottky diodes (one edge of the Schottky contacts). The direction of p is shown by an arrow in the figures. The interface between the AlGaN and GaN layers ($x_3 = -20\,\text{nm}$) is shown by dashed lines.

Negative charges with a concentration of $\sim 10^{17}$ or $10^{18}\,\text{cm}^{-3}$ emerge in the heterostructure below the center of the 0.5-μm Schottky diode ($x_1 = 0\,\mu\text{m}$). The concentration decreases with increasing the Schottky contact length. In addition, the concentration of the piezoelectric charges diverges to $\pm\infty$ in the vicinity of the edges of Schottky contacts.

Figure 2 (a) compares profiles of the conduction-band edge E_C at the center of the 0.5-μm Schottky diode for $p = 0$ and $-0.5\,\text{GPa} \cdot \mu\text{m}$. The origin in the energy axis corresponds to the Fermi energy. The concentration of 2DEG at this position n_s for each case is also shown. The value of n_s changes from 10.03×10^{12} to $6.67 \times 10^{12}\,\text{cm}^{-2}$ when the edge force is loaded.

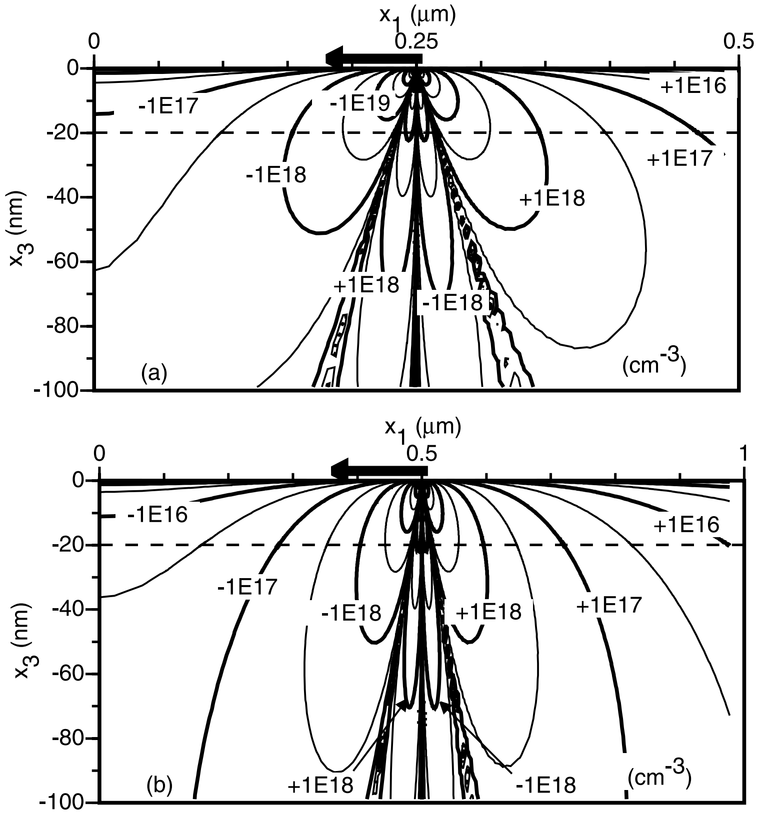

Fig. 1. The concentration of piezoelectric charges induced in the 0.5- (a) and 1.0 (b)-μm Schottky diode for the edge force $p = -0.5\,\text{GPa} \cdot \mu\text{m}$. The direction of p is also shown. The dashed lines at $x_3 = 20\,\text{nm}$ show the AlGaN/GaN heterointerface.

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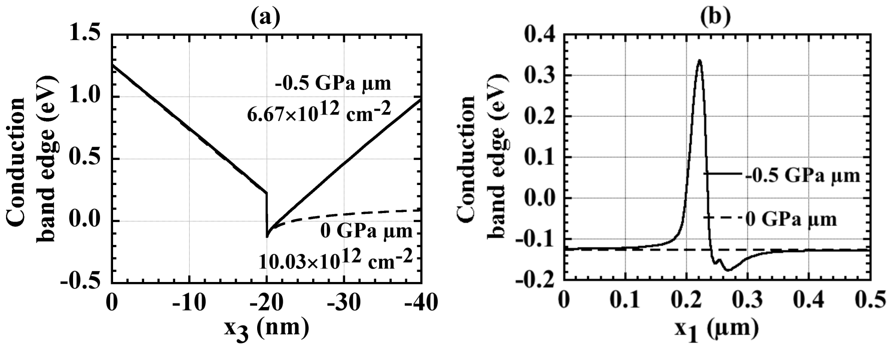

Fig. 2. (a) The profile of the conduction-band edge at the center of the unbiased 0.5-μm Shottky contact for $p = 0$ and $-0.5\,\mathrm{GPa} \cdot \mu\mathrm{m}$. The concentration of 2DEG at this position for each band profile is also shown. (b) The profile of the conduction-band edge at the AlGaN/GaN interface of the unbiased 0.5-μm Shottky contact for $p = 0$ and $-0.5\,\mathrm{GPa} \cdot \mu\mathrm{m}$.

Figure 2 (b) shows the profiles of E_C at the AlGaN/GaN interface of the 0.5-μm Schottky diode. The profile for $p = -0.5\,\mathrm{GPa} \cdot \mu\mathrm{m}$ exhibits a sharp peak around the edges of Schottky contacts, which suggests that the 2DEG be depleted there.

This peak is attributable to the anomalous spatial variation in the concentration of the piezoelectric charges shown in Fig. 1. Note that the anomaly of the piezoelectric charge concentration is due to the singularity of the stress at the edges, which inevitably occurs in the framework of the edge force model [8]. In real systems, however, such a peak may not be observed since elastic deformations are likely to occur both in the heterostructures and passivation films, so that the stress in the heterostructures should be relaxed. Measurements of channel potentials in AlGaN/GaN interfaces around the edges of Schottky contacts may provide useful informations related to this issue. Anyhow the results obtained here indicate that the piezoelectric charges play a crucial role in modulating the electrical properties of AlGaN/GaN Schottky diodes.

Figure 3 (a) shows the dependence of n_s on V_b for the 0.5-μm Schottky diode with different values of p between 0.5 and $-0.5\,\mathrm{GPa} \cdot \mu\mathrm{m}$. We find that n_s changes almost linearly with V_b for each p. The changes in the bias voltage at the onset of n_s V_{onset} due to the edge force are shown in Fig. 3 (b) for the 0.5- and 1.0-μm Schottky diodes. In the 0.5-μm Schottky diode V_{onset} increases (gets shallower) by $\approx 1.2\,\mathrm{V}$ when p changes from 0 to $-0.5\,\mathrm{GPa} \cdot \mu\mathrm{m}$. It decreases (gets deeper) by $\approx 1.8\,\mathrm{V}$ when p changes from 0 to $0.5\,\mathrm{GPa} \cdot \mu\mathrm{m}$. Values of V_{onset} in diodes with longer Schottky contacts are less sensitive to the edge forces, as expected from the fact that the concentration of the piezoelectric charges is smaller in diodes with longer Schottky contacts.

Given that V_{onset} in Shottky diodes is likely to provide a measure of the V_{th} of HEMTs, the achieved results indicate that the V_{th} of AlGaN/GaN

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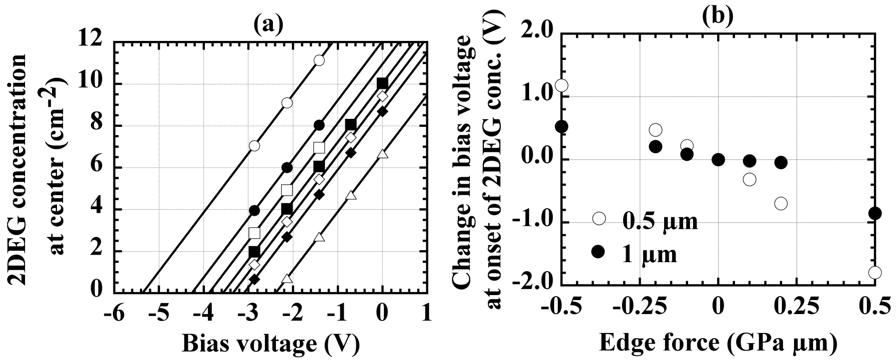

Fig. 3. (a) Relationships between the 2DEG concentration at the center of the 0.5-μm Schottky contact and bias voltage for edge forces of 0.5, 0.2, 0.1, 0, -0.1, -0.2, and -0.5 GPa $\cdot$ μm (from top to bottom). (b) The change in the bias voltage at the onset of the 2DEG concentration due to the edge force in the 0.5- and 1.0-μm Shottky diodes.

HEMTs is sensitive to the stress in the passivation films. They also suggest that the V_{th} may be trimmed by designing the stress and thickness of passivation films in HEMTs. More practically, thick passivation films with compressive stress may be useful for realizing HEMTs with shallower or positive V_{th}'s.

4 Conclusion

We numerically analyzed the impact of the stress in passivation films on the electrical properties of Schottky diodes on (0001) AlGaN/GaN heterostructures by using the edge force model. For passivation films with compressive (tensile) stress, the edge forces induced negative (positive) piezoelectric charges below the Schottky contacts in the heterostructures, which brought forth onsets of the concentration of two-dimensional electron gas at shallower (deeper) bias voltages. The change in the bias voltage at the onset due to edge forces of ±0.5 GPa $\cdot$ μm is 1 or 2 V for diodes with 0.5-μm Schottky contacts. The influence of the edge force on the onset was more marked for diodes with shorter Shottky contacts. These results suggest that passivation films with the designed stress are applicable for controlling the threshold voltages of AlGaN/GaN HEMTs.

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