2004

Effects of hydrostatic and uniaxial stress on the Schottky barrier heights of Ga-polarity and N-polarity n-GaN

Y. Liu
University of Minnesota

M. Z. Kauser
University of Minnesota

M. I. Nathan
University of Minnesota

See next page for additional authors

Liu, Y., Kauser, M.Z., Nathan, M.I., et al. Effects of hydrostatic and uniaxial stress on the Schottky barrier heights of Ga-polarity and N-polarity n-GaN. Applied Physics Letters, 84, 2112 (2004). Copyright © 2004 AIP Publishing LLC.

Authors
Y. Liu, M. Z. Kauser, M. I. Nathan, P. P. Ruden, S. Dogan, Hadis Morkoç, S. S. Park, and K. Y. Lee

APPLIED PHYSICS LETTERS VOLUME 84, NUMBER 12 22 MARCH 2004

Effects of hydrostatic and uniaxial stress on the Schottky barrier heights of Ga-polarity and N-polarity *n*-GaN

Y. Liu,[a] M. Z. Kauser, M. I. Nathan, and P. P. Ruden
Department of Electrical and Computer Engineering, University of Minnesota, Minneapolis, Minnesota 55455

S. Dogan and H. Morkoç
Department of Electrical Engineering, Virginia Commonwealth University, Richmond, Virginia 23284

S. S. Park and K. Y. Lee
Samsung Advanced Institute of Technology, P.O. Box 111, Suwon, Korea

(Received 4 December 2003; accepted 27 January 2004)

We report measurements of the Schottky barrier heights of Ni/Au contacts on Ga-polarity and N-polarity *n*-GaN under hydrostatic pressure and applied in-plane uniaxial stress. Under hydrostatic pressure the two different polarities of GaN yield significantly different rates of Schottky barrier height increase with increasing pressure. Uniaxial stress parallel to the surface affects the Schottky barrier height only minimally. The observed changes in barrier height under stress are attributed to a combination of band structure and piezoelectric effects. [DOI: 10.1063/1.1689392]

There has been much research in recent years on polarization effects in III–V nitrides due to their large piezoelectric constants and spontaneous polarization.[1] Most studies have focused on the built-in strain in nitride heterostructures,[2,3] but, in the case of GaN, the dependence of the Schottky barrier height on the polarity of the material has also been investigated.[4,5] Recently, Strittmatter *et al.*[6] studied the frequency-dependent response of Schottky diodes on *n*-GaN to a small time-dependent harmonic stress. For the small strains relevant to that work, the Schottky barrier height could be assumed to remain constant. In this letter, we report the effect of applied static hydrostatic pressure and uniaxial stress and on the Schottky barrier heights of *n*-GaN, for both Ga-polarity and N-polarity GaN.

The Ga-polarity sample was grown on a sapphire substrate by molecular beam epitaxy. The device fabrication consisted of the definition of circular Schottky contacts of 250 μm diameter that are surrounded by Ohmic contacts. The N-polarity devices were fabricated on a free-standing bulk GaN sample grown by hydride vapor phase epitaxy. These devices had sandwich geometry with 126-μm-diam Schottky contacts defined on the N-polarity surface and large area Ohmic metallization on the opposite side. Metallization for Schottky contacts consisted of Ni (300 Å)/Au (750 Å). For the Ohmic contacts it was Ti (300 Å)/Al (1000 Å)/Ti (300 Å)/Au (150 Å). Information about the apparatus for applying in-plane uniaxial stress and hydrostatic pressure can be found in an earlier letter.[7]

The forward current versus voltage characteristics of the Schottky diodes under hydrostatic pressure and uniaxial stress are shown in Figs. 1 and 2 for a Ga-polarity GaN sample, and in Fig. 3 for a N-polarity sample. The forward current of Ga-polarity samples remains almost constant under uniaxial stress, while the forward currents of both Ga-polarity and N-polarity samples shift considerably under hydrostatic pressure. The uniaxial stress data of N-polarity GaN are not available because we did not have a suitable sample with the plane parallel edges needed for that type of measurement.

To analyze the data, we consider the current to be described by a relationship based on a thermionic emission model for temperature T:

$$I = SA^* T^2 \exp(-q\phi_B/nkT)[\exp(qV_a/nkT)-1]. \quad (1)$$

Here A^*, ϕ_B, S, and n are the effective Richardson constant ($\sim$26.4 A/K^2 cm^2 for n-GaN), the Schottky barrier height (SBH), the area of the Schottky diode, and the ideality factor (IF), respectively. The latter approximately adjusts the basic thermionic emission model for image charge induced barrier lowering, thermionic field emission and, to some extent, for the effects of inhomogeneities. To compare data from devices with different ideality, we find it convenient to include n explicitly in the barrier factor, rather than to define an

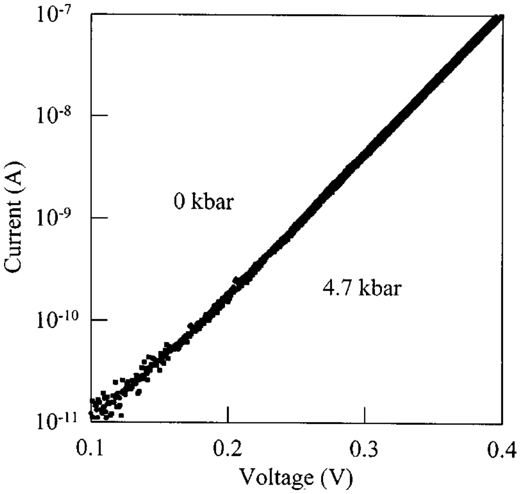

FIG. 1. Forward current–voltage characteristics of Ga-polarity Schottky diode under uniaxial stress.

---

[a] Electronic mail: ymliu@ece.umn.edu

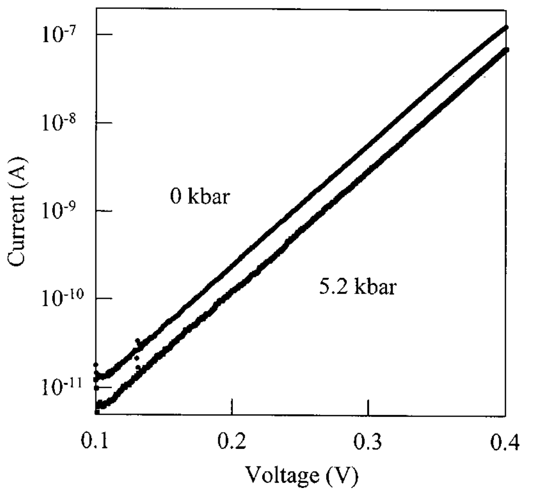

FIG. 2. Forward current–voltage characteristics of Ga-polarity Schottky diode under hydrostatic pressure.

effective SBH as ϕ_B/n.[8] Previously, these effective barrier heights were found to decrease linearly with increasing ideality factors.[9–11]

Assuming A^*, S, and T to be known accurately, ϕ_B and n can, in principle, be determined by extrapolation of the logarithm of the forward current for $qV_a \gg kT$. It is found, however, that the IFs of individual diodes show small, essentially random variations with stress. This translates into considerable uncertainty of the extrapolated SBHs. Hence, we first determine the average ideality factor $\bar{n}$ for all curves of $\ln(I(\sigma))$ versus V_a, where σ is the applied stress. Subsequently we determine

$$\ln(I(\sigma)/I(0)) \approx \Delta A^*/A^* - q\Delta\phi_B/(\bar{n}kT). \qquad (2)$$

Here, the first term denotes the change in the Richardson constant with applied stress and the second term the corresponding change in the SBH. Since the stress dependence of A^* arises only from the stress dependence of the effective mass, the first term (of order $\Delta E_g/E_g$, where E_g is the band gap) is much smaller than the second and is neglected in the following discussion.

The results are summarized in Table I and also shown in Figs. 4 and 5. The SBH change of Ga-polarity sample under uniaxial stress is small and within the statistical error, which may be estimated to be approximately $\Delta n/\bar{n}$, where Δn is the standard deviation of the random variation of the IF. The large SBH difference between two polarities observed at all stresses may be attributed to the effect of the spontaneous polarization.[4,5]

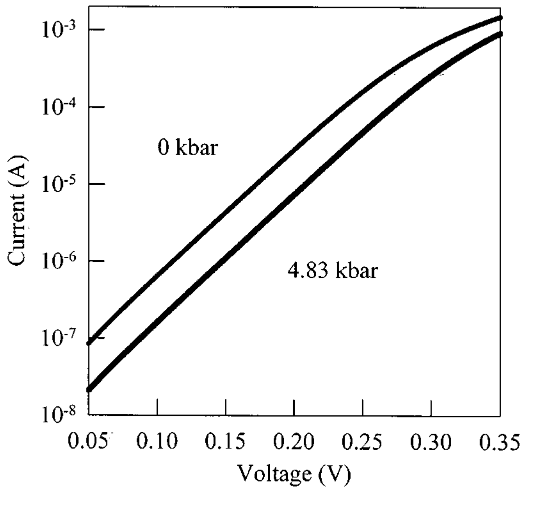

FIG. 3. Forward current–voltage characteristics of N-polarity Schottky diode under hydrostatic pressure.

TABLE I. Average ideality factors, standard deviations of ideality factors, barrier heights at zero stress, and changes of barrier heights under stress for Ga-polarity and N-polarity GaN Schottky diodes.

Schottky diodes	$\bar{n}$	Δn	ϕ_B (V)	$\Delta\phi_B$ (mV/kbar)
Ga-(hydro)	1.22	0.01	1.12	4.2
Ga-(uni)	1.20	0.01	1.12	0.0
N-(hydro)	1.006	0.001	0.62	7.1

We attribute the observed stress induced changes in the SBH to a combination of band structure and piezoelectric effects. It has been reported that the SBH of GaAs Schottky diodes shifts under hydrostatic pressure with a magnitude approximately equal to the pressure coefficient of the fundamental gap of GaAs.[12] Under uniaxial stress an additional modulation of the SBH due to piezoelectric effects was observed.[13]

Similarly, the SBH change of GaN diodes under stress can be viewed as a combination of band structure effects and piezoelectric effects. The SBH of GaN follows the Schottky model that attributes the barrier to the difference between the metal work function and the electron affinity of the semiconductor much more closely than do SBHs on GaAs or other more conventional semiconductors.[14,15] However, the effect of stress on the metal work function and on the electron affinity is not well known. On the other hand, the uniaxial symmetry of the Schottky contact structure leads us to describe the SBH change in terms of four effective deformation potential Ξ_1, Ξ_2, χ_1 and χ_2 as

$$\text{Ga-polarity:} \quad \Delta\phi_B = ((\Xi_1+\chi_1)(\epsilon_{xx}+\epsilon_{yy}) + (\Xi_2+\chi_2)\epsilon_{zz})/q, \qquad (3)$$

$$\text{N-polarity:} \quad \Delta\phi_B = ((\Xi_1-\chi_1)(\epsilon_{xx}+\epsilon_{yy}) + (\Xi_2-\chi_2)\epsilon_{zz})/q. \qquad (4)$$

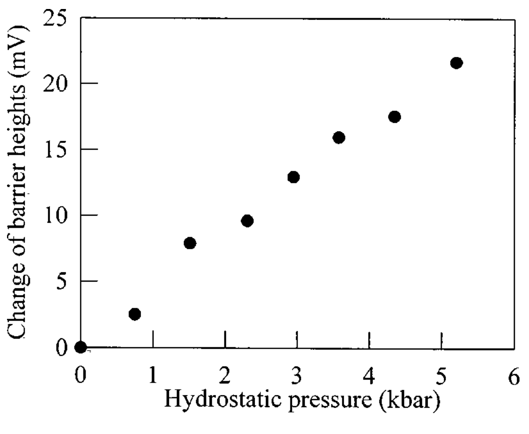

FIG. 4. Change of barrier heights of Ga-polarity Schottky diode under hydrostatic pressure.

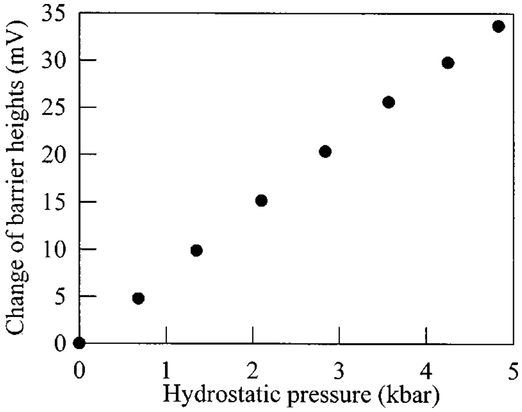

FIG. 5. Change of barrier heights of N-polarity Schottky diode under hydrostatic pressure.

Here, Ξ_1 and Ξ_2 represent the SBH change due to the change in the GaN band structure and metal work function, whereas χ_1 and χ_2 represent the change due to the polarization charge. The opposite sign of χ_1 and χ_2 in Eqs. (3) and (4) are introduced to reflect the presence of piezoelectric polarization charge of opposite sign at the Schottky interface in N-polarity samples compared to Ga-polarity samples.[2]

The areal density of the piezoelectric polarization charge in GaN is given by[2]

$$\sigma_{\mathrm{pol}} = \pm(e_{31}(\epsilon_{xx}+\epsilon_{yy})+e_{33}\epsilon_{zz})/q, \tag{5}$$

where the positive (negative) sign refers to Ga-face (N-face), and the piezoelectric coefficients e_{31} and e_{33} are -0.49 and $0.73\ \mathrm{Cm}^{-2}$, respectively. Under applied stress, the polarization charge induced at the metal–semiconductor interface either attracts or repels electrons, depending upon its polarity, thus changing the Fermi level at the interface and consequently affecting the SBH. This change in SBH to first order is proportional to σ_{pol}.[13] Hence, χ_1 and χ_2 are related to the piezoelectric coefficients:

$$\chi_1 = (e_{31}/e_{33})\chi_2. \tag{6}$$

For GaN on a sapphire substrate, the strain tensor components of uniaxial stress and hydrostatic pressure were given in previous work.[7] For free-standing GaN, they are directly related to the elastic constants of GaN. Using the elastic constants measured by Polian *et al.*[16] the calculated strain tensor elements under 10 kbar hydrostatic pressure are

$$\epsilon_{xx} = \epsilon_{yy} = -1.84\times 10^{-3}, \quad \epsilon_{zz} = -1.53\times 10^{-3}.$$

By fitting Eqs. (3), (4), and (6) with our experimental data for Ga-polarity GaN under uniaxial stress and hydrostatic pressure and N-polarity GaN under hydrostatic pressure, we obtain the effective deformation potentials, $\Xi_1 = -14.8$ eV, $\Xi_2 = -1.22$ eV, $\chi_1 = 10.4$ eV, and $\chi_2 = -15.5$ eV.

In summary, changes in Schottky barrier height were measured for Ga-polarity n-GaN under uniaxial stress and hydrostatic pressure, and N-polarity n-GaN under hydrostatic pressure. We attribute the observed increases in barrier height under compressive stress to a combination of band structure and piezoelectric effects.

The work at the University of Minnesota was supported in part by NSF-ECS.

[1] F. Bernardini, V. Fiorentini, and D. Vanderbilt, Phys. Rev. B **56**, R10 024 (1997).
[2] O. Ambacher, J. Smart, J. R. Shealy, N. G. Weismann, K. Chu, M. Murphy, W. J. Schaff, L. F. Eastman, R. Dimitrov, L. Wittmer, M. Stutzmann, W. Rieger, and J. Hilsenbeck, J. Appl. Phys. **85**, 3222 (1999).
[3] R. Cingolani, A. Botchkarev, H. Tang, H. Morkoç, G. Traetta, G. Coli, M. Lomascolo, A. Di Carlo, F. Della Sala, and P. Lugli, Phys. Rev. B **61**, 2711 (2000).
[4] U. Karrer, O. Ambacher, and M. Stutzmann, Appl. Phys. Lett. **77**, 2012 (2000).
[5] H. W. Jang, J.-H. Lee, and J.-L. Lee, Appl. Phys. Lett. **80**, 3955 (2002).
[6] R. P. Strittmatter, R. A. Beach, J. Brooke, E. J. Preisler, G. S. Picus, and T. C. McGill, J. Appl. Phys. **93**, 5675 (2003).
[7] Y. Liu, M. Z. Kauser, M. I. Nathan, P. P. Ruden, A. M. Dabiran, B. Hertog, and P. P. Chow, Appl. Phys. Lett. **81**, 3398 (2002).
[8] F. A. Padovani and G. G. Sumner, J. Appl. Phys. **36**, 3744 (1965).
[9] R. T. Tung, Phys. Rev. B **45**, 13509 (1992).
[10] R. F. Schmitsdorf, T. U. Kampen, and W. Mönch, J. Vac. Sci. Technol. B **15**, 1221 (1997).
[11] W. Mönch, J. Vac. Sci. Technol. B **17**, 1867 (1999).
[12] W. Shan, M. F. Li, P. Y. Yu, W. L. Hansen, and W. Walukiewicz, Appl. Phys. Lett. **53**, 974 (1988).
[13] K.-W. Chung, Z. Wang, J. C. Costa, F. Williamson, P. P. Ruden, and M. I. Nathan, Appl. Phys. Lett. **59**, 1191 (1991).
[14] K. M. Tracy, P. J. Hartlieb, S. Einfeldt, R. F. Davis, E. H. Hurt, and R. J. Nemanich, J. Appl. Phys. **94**, 3939 (2003).
[15] A. C. Schmitz, A. T. Ping, M. Asif Khan, Q. Chen, J. W. Yang, and I. Adesida, Semicond. Sci. Technol. **11**, 1464 (1996).
[16] A. Polian, M. Grimsditch, and I. Grzegory, J. Appl. Phys. **79**, 3343 (1996).