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Piezoelectric polarization associated with dislocations in wurtzite GaN

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The piezoelectric polarization and its associated charge density are calculated for edge, screw, and mixed dislocations oriented parallel to the *c* axis in wurtzite GaN. It is shown that the polarization field generated by screw components of dislocations is divergence free, and thus does not generate electric fields. Edge dislocations produce polarization fields that have nonzero divergence only at interfaces. These characteristics minimize the electrical and optical effects of the dislocations mediated by the piezoelectric effect. © *1999 American Institute of Physics.*
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GaN and related materials are the objects of considerable research due to their emerging importance in applications ranging from light emission to microwave power amplification.[1] In most cases, epitaxial layers of GaN contain a high density of defects with dislocations, which form because of the absence of a suitable lattice-matched substrate for epitaxial growth. These dislocations are predominantly oriented parallel to the *c* axis of the material.[2] Since this is also the conventional growth direction, the density of dislocations does not decrease even with the use of thick buffer layers. Dislocations densities in typical epitaxial layers of GaN grown on sapphire or SiC substrates are in the neighborhood of $10^8-10^9\,\mathrm{cm}^{-2}$, although it has been shown that by lateral epitaxial overgrowth techniques the density of dislocations can be dramatically reduced.[3] It is of considerable importance to understand the effects of these large dislocation densities on electrical, optical, and mechanical properties of GaN materials and associated devices. The excellent performance of many nitride-based devices despite high dislocation densities suggests that the dislocations are more benign than in other III–V material systems.

One of the important effects already reported is that of dislocations on carrier scattering and doping distribution, which has been attributed to acceptor-like states associated with the dislocations.[4] Dislocations have also been implicated in the appearance of spatially varying surface potential.[5] In principle, the strain distribution associated with the dislocations may also be expected to have a pronounced influence through the piezoelectric effect, which is known to be strong in the nitride materials.[6] In this letter, we report a theoretical study of the piezoelectric effect associated with the *c*-axis oriented dislocations in wurtzite GaN, and describe the piezoelectric polarization generated by the dislocations. We show that there are no internal electric fields generated for screw dislocations. For edge dislocations, polarization charge density and electric fields are generated only in the neighborhood of interfaces. These polarization distributions produce minimal effects on electrical and optical characteristics of the materials.

For dislocations parallel to the (0001) axis (*c* axis) of wurtzite materials, the strain and stress distributions, and the piezoelectric polarization have a particularly simple form, because the elastic compliance tensor and the piezoelectric tensor are isotropic in the basal plane. For a screw dislocation with Burgers vector b_s, the distribution of displacement, u_s, can be written as column vectors[7]

$$u_s=(u_{sx},u_{sy},u_{sz})^T=\left(0,0,\frac{b_s}{2\pi}\tan^{-1}\frac{y}{x}\right)^T, \tag{1}$$

and strain, S_s, is calculated as

$$S_s=\frac{b_s}{2\pi}\frac{1}{x^2+y^2}(0,0,0,x,y,0)^T, \tag{2}$$

where z is along the direction of the dislocation and S_s is expressed in contracted matrix notation. The piezoelectric tensor for wurtzite GaN is of the form[8]

$$e=\begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix}; \tag{3}$$

so the piezoelectric polarization can be written as

$$\mathbf{P}_s=e\times S_s=\frac{b_se_{15}}{2\pi}\frac{1}{x^2+y^2}\begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}=\frac{b_se_{15}}{2\pi}\frac{1}{r}\hat{\theta}, \tag{4}$$

where (r,θ,z) is a cylindrical coordinate system and $b_s=\langle 0001\rangle$ is directed along the *c* axis, with magnitude 5.13 Å.[5,9] The form of $\mathbf{P}_s$ in the xy plane is pictured in Fig. 1. While the piezoelectric constants of the nitride materials are not known with certainty, for the calculation of numerical values, we used $e_{31}=e_{15}=-0.42\,\mathrm{C/m}^2$. These are estimates based on published values for AlN,[10] estimates for GaN,[11] and experimental results inferred from the behavior of AlGaN/GaN heterostructure field-effect transistors (HFETs).[6]

The polarization surrounding the screw dislocation is divergence free and has the same form as that of a magnetic field surrounding a conducting line. Thus, within the continuum approximation, there is no piezoelectrically induced effective charge density associated with the dislocation, ei-

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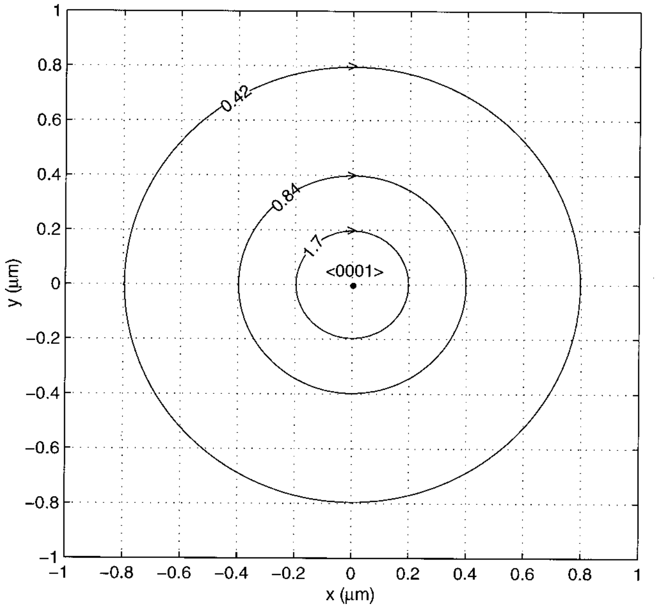

FIG. 1. Polarization vector (in 10^{-4} C/m^2) associated with a pure screw dislocation directed along the *c* axis.

ther at its core or in the surrounding bulk material. This situation differs from that encountered for representative 60° dislocations in cubic zincblende materials.[12]

For an edge dislocation with Burgers vector b_e, the corresponding displacement distribution is[7]

$$\begin{pmatrix} u_{ex} \\ u_{ey} \\ u_{ez} \end{pmatrix} = \frac{b_e}{2\pi}\,\frac{1}{4(1-\nu)}\,\frac{1}{(x^2+y^2)} \times \begin{pmatrix} 4(1-\nu)(x^2+y^2)\tan^{-1}\dfrac{y}{x}+2xy \\ -(1-2\nu)(x^2+y^2)\ln(x^2+y^2)-(x^2-y^2) \\ 0 \end{pmatrix}, \tag{5}$$

and we calculate that the strain distribution S_e is (in a cylindrical coordinate system)

$$S_e=\frac{b_e}{4\pi(1-\nu)}\,\frac{1}{r}(-(2-2\nu+\cos 2\theta)\sin\theta, \\ (2\nu+\cos 2\theta)\sin\theta,0,0,0,\cos\theta+\cos 3\theta)^T, \tag{6}$$

where $\nu=c_{12}/(c_{12}+c_{11})=0.298$,[13] and $b_e=\frac{1}{3}\langle 11\bar{2}0\rangle$ has a magnitude of 3.16 Å.[5,9] The polarization surrounding the dislocation is given by

$$\mathbf{P}_e=eS_e=\frac{b_e e_{31}}{2\pi}\,\frac{1-2\nu}{\nu-1}\,\frac{1}{r}\sin\theta\hat{z}. \tag{7}$$

The *z* component of $\mathbf{P}_e$ is illustrated in Fig. 2. The divergence of the polarization for the edge dislocation also vanishes in the bulk and at the core of the dislocation. However, at positions where the dislocations intersect a crystal surface or interface, the difference in polarizations across the interface dislocations will give rise to an effective surface charge. For example, a *c*-axis oriented edge dislocation intersecting a (0001) crystal surface will generate a surface charge density Q_s that is given approximately by

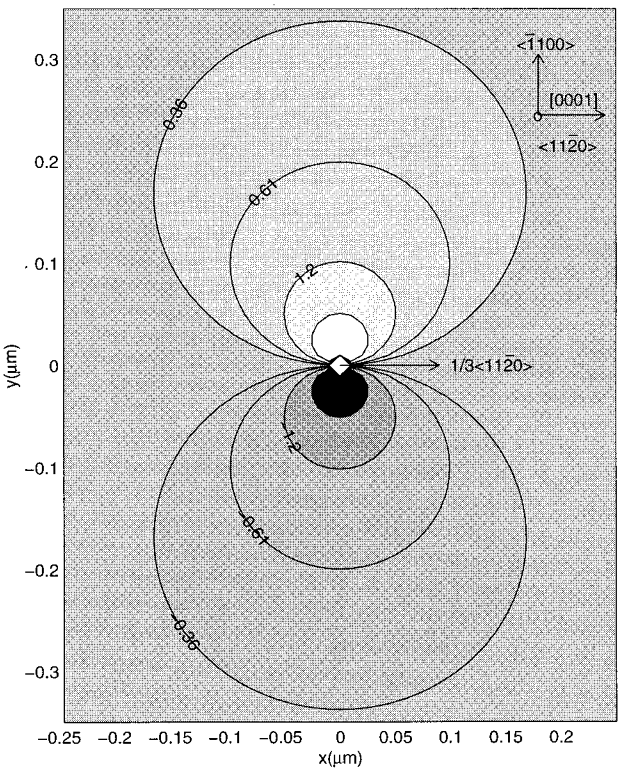

FIG. 2. Contours of constant *z* component of polarization $\mathbf{p}_e$ (in 10^{-4} C/m^2) associated with an edge dislocation directed along the *c* axis. The *xy* plane is perpendicular to the line of dislocation.

$$Q_s=p_z=\frac{b_e e_{31}}{2\pi}\,\frac{1-2\nu}{\nu-1}\,\frac{1}{r}\sin\theta. \tag{8}$$

The surface charge density can be inferred directly from the values of polarization in Fig. 2, and reaches about $10^{11}e/\text{cm}^2$ within 0.1 μm of the dislocation core. It can be expected that the piezoelectrically induced surface charge density will create electric fields in the material which will induce free charges that screen the electric fields far from the surface.

Figure 3 summarizes the dislocation geometries and resultant polarizations for edge and screw dislocations. For mixed dislocations, the strain and polarizations may be computed as a sum of screw and edge components. Thus the overall polarization field shares the divergence-free characteristic indicated above. For dislocations which are oriented in directions other than the *c* axis, the strain distributions and

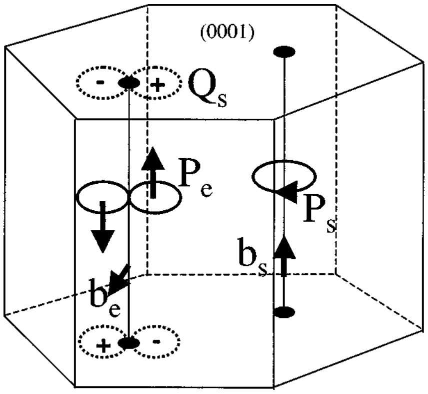

FIG. 3. Schematic diagram illustrating the dislocation geometry, associated polarizations and charge densities.

polarization fields are considerably more complex, and it may be expected that there is a nonzero divergence of the polarization in the vicinity of the dislocation.

The simple form derived for the piezoelectric polarization has important implications for assessing the effects of the dislocations on the electrical and optical properties of the materials. Our results indicate that there is minimal piezoelectric scattering of electrons and holes due to the dislocations within the bulk of the material (although there is deformation potential scattering associated with these centers, as well as, potentially, coulomb scattering from a charged core).[4] Similarly, there are no built-in electric fields that modify optical properties through the Franz–Keldysh effect. The results do suggest, however, that at surfaces and interfaces, dislocations with an edge component may produce piezoelectrically induced charges. Dislocations threading through the interface between the AlGaN barrier layer and the GaN channel layer in a HFET, for example, will produce a local charge density of the form

$$Q_s = p_{z2} - p_{z1}, \tag{9}$$

where the polarizations p_{z^2} in the AlGaN and p_{z^1} in the GaN have very similar spatial distributions but different magnitudes because of the variation in piezoelectric coefficient and ν between the two materials. These induced charge densities may reach values of up to $10^{11} e/\mathrm{cm}^2$ within a distance of 0.03–0.05 μm of the dislocation core, and will modulate the local sheet carrier density of the two-dimensional electron gas formed at the interface. The effects of the charges will thus be most important when the sheet density is lowest; for example, for gate bias in the vicinity of HFET threshold voltage.

At the surfaces of GaN crystals, edge dislocations are most likely expected to produce effective charge densities. These piezoelectrically induced charges will be shielded by free charge at surface states or in surface depletion regions. For the latter situation, the piezoelectric effect of the dislocations will lead to a modulation of the surface potential of the semiconductor. The spatially varying surface potential found by Hansen *et al.*[5] in the neighborhood of dislocations may be related to the effect just described.

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[1] See, for example, S. N. Mohammad, A. A. Salvador, and H. Morkoc, Proc. IEEE **83**, 1306 (1995); S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, Y. Sugimoto, and H. Kiyoku, Appl. Phys. Lett. **70**, 1417 (1997); S. C. Binari, K. Doverspike, G. Kelner, H. B. Dietrich, and A. E. Wickenden, Solid-State Electron. **41**, 177 (1997).

[2] X. H. Wu, L. M. Brown, D. Kapolnek, S. Keller, B. Keller, S. P. DenBaars, and J. S. Speck, J. Appl. Phys. **80**, 3228 (1996).

[3] T. S. Zheleva, O.-H. Nam, M. D. Bremser, and R. F. Davis, Appl. Phys. Lett. **71**, 2472 (1997).

[4] H. M. Ng, D. Doppalapudi, T. D. Moustakas, N. G. Weimann, and L. F. Eastman, Appl. Phys. Lett. **73**, 821 (1998).

[5] P. J. Hansen, Y. E. Strausser, A. N. Erickson, E. J. Tarsa, P. Kozodoy, E. G. Brazel, J. P. Ibbetson, U. Mishra, V. Narayanamurti, S. P. DenBaars, and J. S. Speck, Appl. Phys. Lett. **72**, 2247 (1998).

[6] E. T. Yu, G. J. Sullivan, P. M. Asbeck, C. D. Wang, D. Qiao, and S. S. Lau, Appl. Phys. Lett. **71**, 2794 (1997).

[7] J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw–Hill, New York, 1968), Chaps. 3, 13.

[8] W. G. Cady, *Piezoelectricity* (Dover, New York, 1964), Chap. VIII.

[9] V. W. L. Chin, T. L. Tansley, and T. Osotchan, J. Appl. Phys. **75**, 7365 (1994).

[10] *Landolt–Bornstein: Numerical Data and Functional Relationships in Science and Technology*, edited by O. Madelung (Springer, New York, 1982).

[11] M. A. Littlejohn, J. R. Hauser, and T. H. Glisson, Appl. Phys. Lett. **26**, 625 (1975).

[12] H. Booyens, J. S. Vermaak, and G. R. Proto, J. Appl. Phys. **48**, 3008 (1977).

[13] R. Schwarz, K. Khachaturyan, and E. Weber, Appl. Phys. Lett. **70**, 1122 (1997).