

## Strained $M$ -plane GaN for the realization of polarization-sensitive photodetectors

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We theoretically investigate the oscillator strengths of the three band-edge transitions and the resulting polarization anisotropy of the absorption coefficient for an  $M$ -plane ( $[1\bar{1}00]$  oriented) GaN film as a function of an arbitrary in-plane strain. Light incident normally on an  $M$ -plane film can be completely polarized parallel or perpendicular to the unique  $c$  axis of wurtzite GaN. We show that for a particular range of  $M$ -plane strain, both the wavelength range, over which the polarization anisotropy in the absorption occurs, and its magnitude are enhanced. Consequently, strained  $M$ -plane GaN becomes a promising candidate for realizing polarization-sensitive photodetectors. For such an application, we also determine the strain dependence of the operating wavelength characteristics. © 2002 American Institute of Physics. [DOI: 10.1063/1.1517408]

Several applications require the detection of the state of polarization of an incident polarized light beam, for which one generally uses a combination of a detector and an external polarizing element, such as sheet polarizers and prisms. This is inconvenient for large-scale integration including magneto-optical readout and optical computation based on polarization-coded logic, both from the point of view of economics and mechanical aspects such as size and alignment. A better solution would be a detector, which is intrinsically sensitive to optical polarization. The usual group IV and III–V semiconductor detectors do not show any significant in-plane anisotropy in their optical absorption coefficient ( $\alpha$ ) due to their cubic crystal structure, which has high symmetry. Chemically etched surface corrugations have been used to create an artificial polarization anisotropy. With these, polarization-sensitive photodetectors (PSPDs) have been realized for infrared applications.<sup>1</sup> Ordered  $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$  alloys have also been used, taking advantage of the difference in  $\alpha$  for light linearly polarized along the  $[011]$  and  $[01\bar{1}]$  directions ( $\Delta\alpha \approx 4 \times 10^3 \text{ cm}^{-1}$  over a 13 nm range around 670 nm).<sup>2</sup> Several devices, such as polarization-sensitive detectors, threshold switches, and reset–set flip flops, have been demonstrated using this material.<sup>2,3</sup> However, higher-density magneto-optical storage and readout require shorter operating wavelengths. A limitation of  $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$  is the narrow range of its operating wavelength. This is because Cu–Pt<sub>B</sub>-type alloy ordering and the resulting polarization anisotropy in  $\alpha$  becomes weaker, if a higher Ga concentration is used to increase the band-gap energy.

Semiconductors, which intrinsically have a low-symmetry crystal structure such as the wurtzite (WZ) structure, are another possible solution. In recent years, there have been significant advances in WZ-GaN opto-electronic device technology. However, currently, all such devices are based on  $C$ -plane ( $[0001]$  oriented) GaN films (cf. Fig. 1), which

do not show any significant in-plane optical polarization anisotropy. In contrast,  $M$ -plane ( $[1\bar{1}00]$  oriented) films,<sup>4</sup> which have lower symmetry, may have greater potential for PSPD applications.  $M$ -plane films, in which electrostatic fields due to spontaneous and piezoelectric polarization are absent, have recently been of great interest in the context of obtaining quantum-well-based light emitters with higher quantum efficiency.<sup>4</sup> Due to the combination of a large mismatch in lattice constants and thermal expansion coefficients between GaN and commonly used substrates, even thick GaN films are usually strained. Since strain affects the electronic band structure (EBS), it further modifies the polarization selection rules for optical absorption. Experimental evidence for  $M$ -plane strain-induced EBS modification was recently reported.<sup>5,6</sup>

In this letter, we theoretically study the influence of  $M$ -plane strain on the EBS of GaN, with special emphasis on the oscillator strengths and the resulting polarization properties of the three band-edge transitions. Based on these results, we demonstrate how strained  $M$ -plane GaN could be used for PSPD applications.

WZ-GaN has three closely spaced valence bands (VBs) at the Brillouin-zone center (BZC). The conduction band (CB) is constructed from  $s$  orbitals with spherically symmetric  $|S\rangle$ -type wave functions. The VBs are constructed from  $p$  orbitals with wave functions having a mixture of  $|X\rangle$ -,  $|Y\rangle$ -, and  $|Z\rangle$ -type symmetry.<sup>7</sup> The  $c$  axis defines the  $z$  direction. Strain drastically modifies the polarization properties of the three transitions between the CB and the three VBs that con-

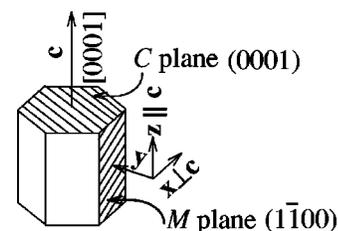


FIG. 1. Schematic diagram of the  $C$  and  $M$  planes of a WZ-GaN unit cell and the choice of coordinates.

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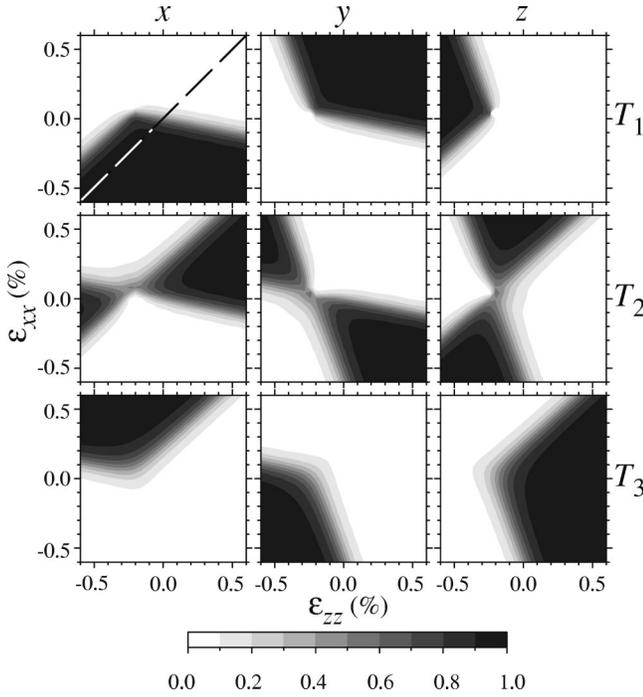


FIG. 2. Calculated relative magnitude (gray scale) of the oscillator strength components  $f_{i\beta}$  ( $i=1,2,3$ , and  $\beta=x,y,z$ ) vs  $M$ -plane strain  $\epsilon_{xx}$  and  $\epsilon_{zz}$  for the three band-edge transitions  $T_i$  of WZ-GaN. The dashed line in the first plot shows the isotropic  $M$ -plane strain trajectory  $\epsilon_{xx} = \epsilon_{zz}$ .

tribute to  $\alpha$ . Therefore, it is not possible to identify such transitions in terms of the  $A$ ,  $B$ , and  $C$  excitons of unstrained GaN, so we adopt the nomenclature  $T_i$  ( $i=1,2,3$ ) in order of decreasing transition wavelength  $\lambda_i$ . The main parameters that determine the polarization anisotropy in  $\alpha$  are the three polarization components ( $\beta=x,y,z$ ) of the oscillator strength  $f_{i\beta}$  for each  $T_i$ . Strain induces a mixing of the VB states and modifies  $f_{i\beta}$ . We have adopted the  $\mathbf{k}\cdot\mathbf{p}$  approach to determine the effect of strain<sup>8</sup> on the CB and VB states at the BZC. For VB states, the Bir–Pikus Hamiltonian<sup>9</sup> ( $6\times 6$  matrix  $H^{\text{VB}}$ ) was diagonalized. The oscillator strengths  $f_{i\beta}$  were obtained from momentum matrix elements of the type  $|\langle\Psi^{\text{CB}}|p_\beta|\Psi_i^{\text{VB}}\rangle|^2$ . Here,  $|\Psi^{\text{CB}}\rangle=|S\rangle$  and  $|\Psi_i^{\text{VB}}\rangle=a_{ix}|X\rangle+a_{iy}|Y\rangle+a_{iz}|Z\rangle$  represent the orbital part of the CB and VB wave functions, respectively. The complex coefficients  $a_{i\beta}$  are obtained by determining the eigenvectors of  $H^{\text{VB}}$ .<sup>6</sup> The values of  $|\langle S|p_x|X\rangle|^2$ ,  $|\langle S|p_y|Y\rangle|^2$ , and  $|\langle S|p_z|Z\rangle|^2$  are normalized to the same value according to Ref. 10. To obtain absolute values for the absorption-edge wavelengths, we considered all relevant EBS parameters<sup>11</sup> based on previously reported experimental results.<sup>6,12</sup> The elastic constants were taken from Ref. 13. Experimental studies on an  $M$ -plane GaN film grown on  $\text{LiAlO}_2$  have revealed asymmetric in-plane strain values  $\epsilon_{xx}=-0.56\%$  and  $\epsilon_{zz}=-0.31\%$ .<sup>5</sup> We, therefore, extended our calculations to an arbitrary in-plane strain in the range  $|\epsilon_{xx}|$  and  $|\epsilon_{zz}|\leq 0.6\%$ .

Figure 2 shows the calculated strain dependence of the relative  $f_{i\beta}$  magnitudes as gray-scale plots. As the plots indicate, the  $f_{i\beta}$  obey the following two sum rules

$$f_{ix}+f_{iy}+f_{iz}=1, \quad (1)$$

$$f_{1\beta}+f_{2\beta}+f_{3\beta}=1. \quad (2)$$

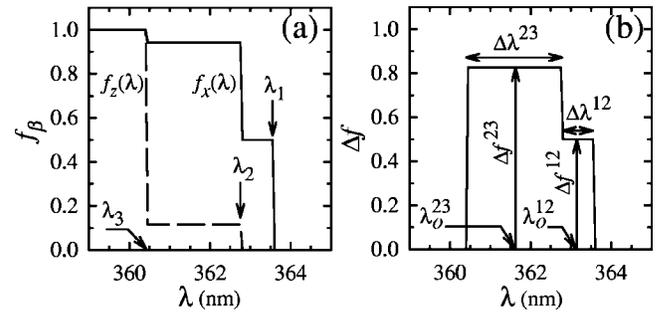


FIG. 3. (a) Oscillator strength contribution  $f_i(\lambda)$  and  $f_z(\lambda)$  vs wavelength for the three band-edge transitions  $T_i$  ( $i=1,2,3$ ) labeled by the corresponding transition wavelengths  $\lambda_i$  in unstrained GaN at 295 K. (b) Wavelength dependence of the in-plane polarization anisotropy  $\Delta f=f_x(\lambda)-f_z(\lambda)$ . The terms  $\Delta f^{ij}$ ,  $\Delta\lambda^{ij}$ , and  $\lambda_o^{ij}$  are also indicated.

These results reveal that  $M$ -plane strain can lead to dominantly  $x$ -,  $y$ -, or  $z$ -polarized transitions. In particular, even for isotropic strain ( $\epsilon_{xx}=\epsilon_{zz}$ ) in an  $M$ -plane film, the existence of a purely  $x$ - or  $y$ -polarized transition is possible. This is a consequence of the strain-induced broken symmetry in the  $x$ - $y$  plane,<sup>6,14</sup> i.e., the plane perpendicular to the  $c$  axis.

Each  $T_i$  has an onset at  $\lambda_i$  and continues for  $\lambda<\lambda_i$ . Taking this into account, we plot, in Fig. 3(a), the  $x$ -component  $f_x(\lambda)$  and  $z$ -component  $f_z(\lambda)$  of the oscillator strength near the band edge of unstrained GaN at 295 K. Due to excitonic effects, we considered a redshift in  $\lambda_i$ , but neglected a resonant increase in  $f_x(\lambda)$  and  $f_z(\lambda)$  around the band gap. For an  $M$ -plane GaN film,  $\alpha(\lambda)$  is proportional to  $f_x(\lambda)$  and  $f_z(\lambda)$ , when the electric-field vector  $\mathbf{E}$  of a normally incident light beam is polarized  $\perp c(\mathbf{E}||\mathbf{x})$  and  $||c(\mathbf{E}||\mathbf{z})$ , respectively. The difference  $\Delta f=f_x(\lambda)-f_z(\lambda)$  [cf. Fig. 3(b)] is nonzero over a wavelength range  $\Delta\lambda$ , which results in a polarization-dependent change in  $\alpha$ . This property of  $M$ -plane GaN can be utilized to build a PSPD.

$\Delta f$  and  $\Delta\lambda$  are the two important figures of merit for PSPD applications. Both parameters must be large for a suitable material for PSPD applications. A uniform  $\Delta f$  over a large  $\Delta\lambda$  also ensures a lower-temperature sensitivity. Again, taking GaN as an example, we now discuss how strain affects  $\Delta f$  and  $\Delta\lambda$ . For  $\lambda<\lambda_3$ , all three transitions contribute to  $\alpha(\lambda)$ . However, due to Eq. (2), we get  $\Delta f=\sum_{i=1}^3[f_{ix}-f_{iz}]=0$ . Therefore, a significant polarization anisotropy in  $\alpha$  can exist only for  $\lambda>\lambda_3$ , i.e., between  $\lambda_1$  and  $\lambda_3$ . We identify three regimes in this wavelength range. Regime I is the range between  $\lambda_1$  and  $\lambda_2$ . Here, only  $T_1$  contributes to  $\alpha$  so that  $\Delta f=\Delta f^{12}=|f_{1x}-f_{1z}|$ . The strain values, for which  $\Delta f^{12}$  is high, are depicted by the darker regions of the gray-scale plot in Fig. 4(a). In the regions marked  $x$  ( $z$ ),  $\alpha$  will be high for  $\mathbf{E}||\mathbf{x}$  ( $\mathbf{E}||\mathbf{z}$ ). For a strain value with a large  $\Delta f^{12}$ , one can determine, from the adjacent contour plots, the central operating wavelength  $\lambda_o=\lambda_o^{12}=(\lambda_1+\lambda_2)/2$  and the operating range  $\Delta\lambda=\Delta\lambda^{12}=\lambda_1-\lambda_2$  for PSPD applications. Regime II corresponds to wavelengths between  $\lambda_2$  and  $\lambda_3$ . Here, in general, both  $T_1$  and  $T_2$  contribute to  $\alpha$  so that  $\Delta f=\Delta f^{23}=|f_{1x}+f_{2x}-f_{1z}-f_{2z}|$ . The strain values, for which  $\Delta f^{23}$  is high, are shown by the darker regions of the gray-scale plot in Fig. 4(b). Here,  $\lambda_o=\lambda_o^{23}=(\lambda_2+\lambda_3)/2$  and  $\Delta\lambda=\Delta\lambda^{23}=\lambda_2-\lambda_3$  (cf. adjacent contour plots). For strain values, where  $\Delta f\approx 1$  in regime II, but  $\Delta f\approx 0$  in regime I, we find that  $f_{1y}\approx 1$  so that according to Eq. (1)  $f_{1x}\approx 0$  and  $f_{1z}$

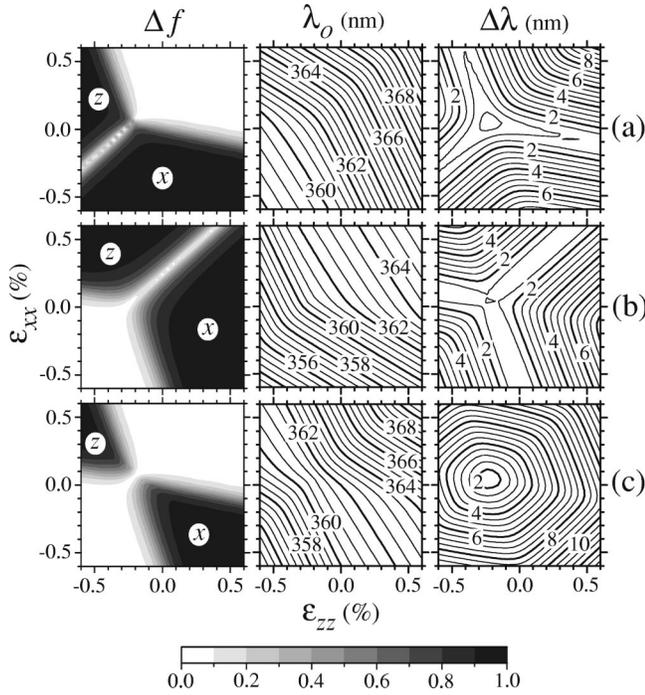


FIG. 4.  $\Delta f$  (left-hand side),  $\lambda_o$  (center), and  $\Delta\lambda$  (right-hand side) as a function of  $M$ -plane strain  $\varepsilon_{xx}$  and  $\varepsilon_{zz}$  for the three regimes for PSPD application of strained  $M$ -plane GaN. (a) regime I between  $\lambda_1$  and  $\lambda_2$ , where  $\Delta f = \Delta f^{12}$ ,  $\lambda_o = \lambda_o^{12}$ , and  $\Delta\lambda = \Delta\lambda^{12}$ ; (b) regime II between  $\lambda_2$  and  $\lambda_3$ , where  $\Delta f = \Delta f^{23}$ ,  $\lambda_o = \lambda_o^{23}$ , and  $\Delta\lambda = \Delta\lambda^{23}$ ; and (c) regime III between  $\lambda_1$  and  $\lambda_3$ , where  $\Delta f$  is taken to be the smaller of the two amongst  $\Delta f^{12}$  and  $\Delta f^{23}$ ,  $\lambda_o = \lambda_o^{13}$ , and  $\Delta\lambda = \Delta\lambda^{13}$ . In the dark regions marked  $x$  ( $z$ ), absorption is high for  $E||x$  ( $E||z$ ).

$\approx 0$  (cf. Fig. 2). Therefore, for such strain values,  $T_1$  does not contribute to  $\alpha$ , and  $\lambda_2$  defines the effective optical band gap of the  $M$ -plane film.

Note that there are strain values, for which both  $\Delta f^{12}$  and  $\Delta f^{23}$  are large. Therefore, a large and uniform polarization anisotropy in  $\alpha$  can exist for these strain values from  $\lambda_1$  up to  $\lambda_3$ . We call this regime III, in which we take  $\Delta f$  to be the smaller of the two values  $\Delta f^{12}$  and  $\Delta f^{23}$ . This represents the minimum anisotropy attainable over the whole range between  $\lambda_1$  and  $\lambda_3$ . The strain dependence of  $\Delta f$  in regime III is shown by the gray-scale plot in Fig. 4(c). The adjacent contour plots show  $\lambda_o = \lambda_o^{13} = (\lambda_1 + \lambda_3)/2$  and  $\Delta\lambda = \Delta\lambda^{13} = \lambda_1 - \lambda_3$ . The reason that one can achieve  $\Delta f \approx 1$  between  $\lambda_1$  and  $\lambda_2$  as well as between  $\lambda_2$  and  $\lambda_3$  is because for these strain values  $f_{2y} \approx 1$  [cf. Fig. 2]. Then according to Eq. (1),  $f_{2x} \approx 0$  and  $f_{2z} \approx 0$  so that even between  $\lambda_2$  and  $\lambda_3$ , it is essentially  $\Delta f^{12}$  that determines  $\Delta f$ , i.e.,  $T_2$  does not contribute to  $\alpha$  of the  $M$ -plane film. Interestingly, for the strain values  $\varepsilon_{xx} = 0.04\%$  and  $\varepsilon_{zz} = -0.24\%$ , where  $\Delta\lambda$  becomes minimal, the EBS modification due to  $M$ -plane strain cancels the energy splitting between the top two VBs at the BZC so that  $\Delta\lambda^{12} = 0$ . The band structure at the BZC is then similar to the one of an unstrained zinc-blende crystal and, likewise at this point, there is no in-plane polarization anisotropy ( $\Delta f^{12}$  and  $\Delta f^{23}$  are both zero).

Table I lists typically attainable values of  $\Delta f$  and  $\Delta\lambda$ . We see that relatively small values of strain enhance both  $\Delta f$  and  $\Delta\lambda$ . Although an in-plane polarization anisotropy in  $\alpha$  is also possible for  $C$ -plane films with a large anisotropic strain, such films are best grown on substrates such as sapphire and

TABLE I. The magnitude  $\Delta f$  of the polarization anisotropy in oscillator strength and the wavelength range  $\Delta\lambda$ , over which it exists, for some typical  $M$ -plane strain values.

Overall strain state	Regime	$\varepsilon_{xx}$	$\varepsilon_{zz}$	$\Delta f$	$\Delta\lambda$ (nm)
Unstrained	I	0.0%	0.0%	0.5	0.8
Unstrained	II	0.0%	0.0%	0.83	2.3
Compressive	I	-0.3%	-0.2%	0.96	3.4
Tensile	II	0.2%	0.3%	0.93	3.2
Antisymmetric	III	-0.2%	0.2%	0.95	6.2

SiC with hexagonal symmetry, resulting in isotropic strain. However, because of the difference in lattice constants and thermal expansion coefficients along  $x$  and  $z$ ,  $M$ -plane films invariably experience asymmetric strain, and it may even be possible to achieve antisymmetric in-plane strain as required for regime III (cf. Table I) with an appropriate choice of substrate. An important point is that, unlike for ordered  $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ -alloy-based PSPDs,  $\lambda_o$  can be varied for  $M$ -plane GaN over a much larger wavelength range simply by alloying it with either In or Al to change the energy gap. Also, in comparison, an order of magnitude larger  $\Delta\alpha \approx 5 \times 10^4 \text{ cm}^{-1}$  for  $\Delta f \approx 0.9$  can be obtained with strained  $M$ -plane nitride films. However, since the deformation potentials vary with alloy composition, the aforementioned calculation has to be repeated for each composition in order to estimate the PSPD operational characteristics.

To summarize, we have theoretically determined the polarization properties of the three fundamental band-edge transitions of GaN as a function of an arbitrary strain in the  $M$  plane. The results reveal that the in-plane polarization anisotropy in  $\alpha$  is enhanced with strain, even for small values of in-plane strain. This makes strained  $M$ -plane GaN useful for realizing PSPDs. We have also determined the strain dependence of the operating wavelength characteristics for such an application.

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