Role of strain in polarization switching in semipolar InGaN/GaN quantum wells

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The effect of strain on the valence-band structure of $(11\bar{2}2)$ semipolar InGaN grown on GaN substrates is studied. A $\mathbf{k}\cdot\mathbf{p}$ analysis reveals that anisotropic strain in the *c*-plane and shear strain are crucial for deciding the ordering of the two topmost valence bands. The shear-strain deformation potential D_6 is calculated for GaN and InN using density functional theory with the Heyd–Scuseria–Ernzerhof hybrid functional [J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. **124**, 219906 (2006)]. Using our deformation potentials and assuming a pseudomorphically strained structure, no polarization switching is observed. We investigate the role of partial strain relaxation in the observed polarization switching. © *2010 American Institute of Physics*.
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Indium gallium nitride (InGaN) alloys are already widely used as commercial light emitters.[1,2] For high efficiency devices semipolar or nonpolar quantum-well orientations have been proposed. In these orientations the effect of spontaneous and piezoelectric polarization is reduced and thereby the carrier overlap increased.[3–5] Growth of InGaN on GaN along semipolar or nonpolar directions leads to different strain conditions than the conventional growth along the *c*-direction. This affects the splitting of the uppermost valence bands and hence the polarization of the emitted light. A corresponding optical anisotropy has already been observed for both nonpolar[6–8] and semipolar[9–14] devices. This raises the question of how to *control* the polarization of the emitted light, which is not only of scientific interest but also of technical importance for the performance of light-emitting diodes and laser diodes.

Recently, polarization switching has been reported for semipolar InGaN grown on a $(11\bar{2}2)$ GaN substrate.[11,12] The dominant polarization direction of emission was found to switch from $[1\bar{1}00]$ (perpendicular to the *c*-axis) to $[\bar{1}\bar{1}23]$ when the In concentration was increased above 30% but the mechanism responsible for the change in polarization could not be identified. Other experimental studies have found no evidence of polarization switching, however. Under high excitation power density the sign of the polarization ratio of InGaN/GaN was found to remain unchanged even at high In content.[13,14] Why the polarization ratio is affected by the excitation power density also remains unclear.

The following three factors critically influence the band structure of InGaN quantum wells (QW) and therefore the polarization of the emitted light: indium concentration, strain, and quantum confinement. Based on $\mathbf{k}\cdot\mathbf{p}$ modeling Yamaguchi[15] predicted that the QW thickness would strongly affect the polarization. This seems qualitatively consistent with the results of Masui *et al.*,[12] who observed an enhancement in optical polarization for thinner QWs. However, in Yamaguchi's work the magnitude of this quantum confinement effect is very sensitive to the choice of Luttinger parameters[16] and can range from 2 to 20 meV for 2 nm thick QWs. Ueda *et al.*,[11] on the other hand, found no appreciable QW thickness effect. They proposed strain to be the dominant factor, and derived a large shear-strain deformation potential of $D_6=-8.8$ eV from their measurements.[11]

Strain in $(11\bar{2}2)$ semipolar InGaN grown on GaN substrates is characterized by shear strain and anisotropic strain in the *c* plane. In this work, we calculate the effect of shear strain on the band structure of GaN and InN from first principles. We have previously reported a consistent set of strain deformation potentials D_1 to D_5 for the group-III nitrides,[17] which is completed by the D_6 values reported here. With these deformation potentials and the band parameters of Ref. 16 we use the $\mathbf{k}\cdot\mathbf{p}$ approach to determine the energies of the three highest valence bands at the Γ point. For ideal (unrelaxed) strain conditions, we find no polarization switching for semipolar InGaN alloys grown on $(11\bar{2}2)$ GaN substrates. Polarization switching can occur, however, when we assume the strain to be partially relaxed.

Our first-principles calculations are performed using the plane-wave projector augmented wave method as implemented in the VASP code.[18] We use the Heyd–Scuseria–Ernzerhof (HSE06)[19,20] hybrid exchange-correlation functional with a screening parameter $\mu=0.2$ and a mixing parameter of $\alpha=0.25$ (HSE06). In previous work we showed that HSE06 gives accurate lattice parameters and band gaps in good agreement with experiment for the group-III nitrides.[17] The semicore *d* electrons of Ga and In are treated as valence electrons. A $6\times6\times4$ Γ-point centered *k*-point sampling and a plane-wave cutoff of 600 eV are used to ensure an accurate relaxation of the internal displacement parameter *u*.

The energies of the three highest valence bands at the Γ point (E_1 to E_3) can be obtained by the $\mathbf{k}\cdot\mathbf{p}$ theory by diagonalizing a strained 6×6 Hamiltonian of wurtzite symmetry.[21] Including strain components along the three directions in the normal coordinate system [see Fig. 1(a)] ε_{xx}, ε_{yy}, and ε_{zz} and shear strain (only ε_{xz} for simplicity) gives

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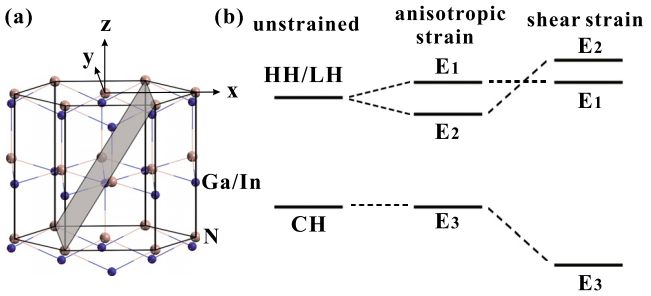

FIG. 1. (Color online) (a) The normal coordinate system of the wurtzite GaN crystal. The $(11\bar{2}2)$ plane is shown in gray. (b) Schematic illustration of strain effects on the band structure in $(11\bar{2}2)$ semipolar InGaN. In an unstrained alloy, the heavy hole (HH) and light hole (LH) bands are doubly degenerate. Anisotropic strain in the c plane causes the bands to split. Under shear strain, the E_2 band goes up and may switch order with the E_1 band.

$$E_1 = \Delta_{cr} + (D_1 + D_3)\varepsilon_{zz} + (D_2 + D_4)(\varepsilon_{xx} + \varepsilon_{yy}) - D_5(\varepsilon_{xx} - \varepsilon_{yy}),$$

$$E_{2,3} = \tfrac{1}{2}\Delta_{cr} + D_1\varepsilon_{zz} + D_2(\varepsilon_{xx} + \varepsilon_{yy}) + \tfrac{1}{2}[D_3\varepsilon_{zz} + D_4(\varepsilon_{xx} + \varepsilon_{yy}) + D_5(\varepsilon_{xx} - \varepsilon_{yy})] \pm \tfrac{1}{2}\delta,$$

$$\delta = \sqrt{[\Delta_{cr} + D_3\varepsilon_{zz} + D_4(\varepsilon_{xx} + \varepsilon_{yy}) + D_5(\varepsilon_{xx} - \varepsilon_{yy})]^2 + 8D_6^2\varepsilon_{xz}^2},$$

$$\Delta E_{12} = \tfrac{1}{2}[\Delta_{cr} + D_3\varepsilon_{zz} + D_4(\varepsilon_{xx} + \varepsilon_{yy})] - \tfrac{3}{2}D_5(\varepsilon_{xx} - \varepsilon_{yy}) - \tfrac{1}{2}\delta, \quad (1)$$

where Δ_{cr} is the crystal-field splitting and the spin-orbit splitting has been omitted. The eigenstate pertaining to E_1 has p_y character, and the other two have mixed p_x and p_z character.[21] ΔE_{12} gives the energy separation between the topmost two bands at the Γ point. As can be seen from Eq. (1), anisotropic strain (D_5) and shear strain (D_6) have opposite effects because D_5 is negative.[17] This is shown schematically in Fig. 1(b). A switch in the band ordering may occur if the shear strain and/or the deformation potential D_6 are large enough.

If only shear strain is present the equations simplify to

$$E_1 = \Delta_{cr},$$

$$E_{2,3} = \frac{\Delta_{cr}}{2} \pm \frac{\sqrt{\Delta_{cr}^2 + 8D_6^2\varepsilon_{xz}^2}}{2}. \quad (2)$$

Figure 2(a) shows the energies E_1 to E_3 as calculated in HSE06 for wurtzite GaN under shear strain. A similar plot is obtained for InN (not shown). As predicted by the $\mathbf{k}\cdot\mathbf{p}$ approach, the energy of one of the doubly degenerate valence bands remains constant under strain, while the other one increases. Concomitantly, the original crystal-field split-off band (CH) goes down in energy. We then fit the energy separation between E_2 and E_3 (ΔE_{23}) shown in Fig. 2(b) to the expression above to obtain the deformation potential D_6. At the experimental lattice parameters,[17] we obtain $D_6 = -3.95$ eV for GaN and $D_6 = -3.02$ eV for InN. These values are consistent with the general trend of our deformation potential set for the group-III nitrides[17] in the sense that the magnitude of the deformation potentials is larger for GaN than for InN. Our D_6 value for GaN is smaller in magnitude than that reported by Vurgaftman and Meyer,[22] which was obtained from other deformation potentials by means of the quasicubic approximation and not from direct measurements or calculations. For InN, our deformation potential is considerably smaller in magnitude than the value of $D_6 = -8.8$ eV proposed by Ueda *et al.*,[11] which was deduced indirectly from the dependence of the polarization on indium composition.

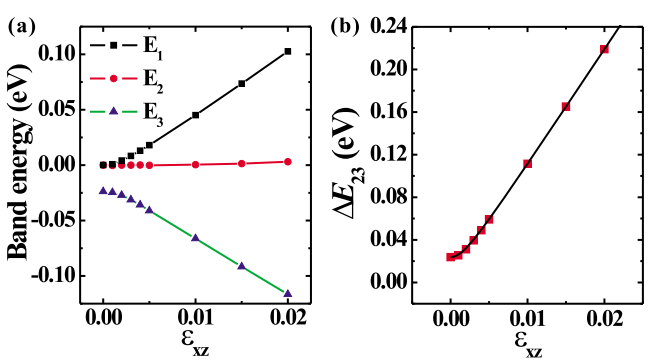

FIG. 2. (Color online) (a) Energies of the topmost three valence bands of GaN under shear strain ε_{xz}. The valence-band maximum at zero shear strain is taken as energy zero. (b) Energy separation ΔE_{23} between valence bands E_2 and E_3.

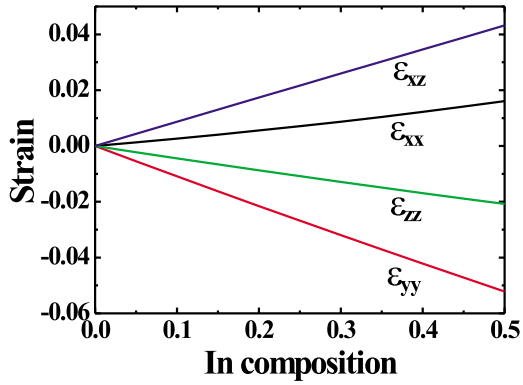

FIG. 3. (Color online) Strain components in $(11\bar{2}2)$ semipolar InGaN grown on GaN as a function of In composition: x, y, and z refer to the usual c-plane coordinate system.

Before we can investigate the effect of strain on the band structure the strain conditions in the alloy have to be determined. The lattice parameters follow from Vegard's law which simply averages over all local distortions: $a_{\mathrm{InGaN}} = a_{\mathrm{InN}} * x + a_{\mathrm{GaN}} * (1-x)$. The lattice mismatch to the GaN substrate induces composition-dependent compressive in-plane strain. If the InGaN layer thickness is below the critical value for misfit-dislocation formation, the lattice mismatch is accommodated by straining the layer elastically. The strain components in and out of the c plane, which are needed for the $\mathbf{k}\cdot\mathbf{p}$ approach, can be determined from the lattice mismatch in the semipolar plane.[23] Using the elastic constants of Wright[24] we obtain the strain components for $(11\bar{2}2)$ semipolar QWs in terms of the normal c-plane coordinate system as shown in Fig. 3. We observe that these pseudomorphic strain conditions lead to anisotropic strain in the c-plane ($\varepsilon_{xx} - \varepsilon_{yy} \neq 0$), and a large shear-strain component ε_{xz}.

To evaluate Eq. (1) for a given indium composition we linearly interpolate the deformation potentials of GaN and InN. In Fig. 4(a) we show the transition energies between the three valence bands and the conduction band, assuming that the $(11\bar{2}2)$ InGaN layer is pseudomorphically grown on a GaN substrate. Under these conditions, the two highest valence bands do not cross over and the band ordering does not switch with increasing In concentration. The value of ΔE_{12}

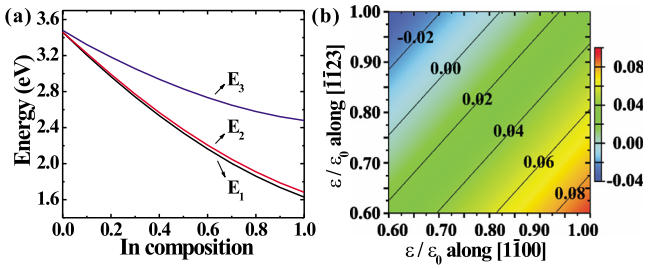

FIG. 4. (Color online) (a) Calculated transition energies between the conduction band and the topmost three valence bands of a $(11\bar{2}2)$ semipolar InGaN alloy at the lattice parameters of GaN as a function of In composition. (b) Contour plot of the energy separation between the topmost two valence bands for $In_{0.3}Ga_{0.7}N$ as a function of strain components along the $[1\bar{1}00]$ and $[\bar{1}\bar{1}23]$ directions, expressed relative to their coherent value obtained from the lattice mismatch.

and the In concentration at which polarization switching occurs also depend on the degree of quantum confinement and on the spin-orbit splitting. Both are not included in our current model but they do not change our qualitative results.

Due to the large lattice mismatch between InN and GaN (11%), strains in alloys with high In content will be large and may be partially relaxed by forming structural defects (such as dislocations and stacking faults). According to Fig. 3, the magnitude of the strain component along the y direction is larger than along the x and z directions. It is thus conceivable that the strain component in the y direction would be partially relaxed in an InGaN layer grown on GaN. In Fig. 4(b) we plot ΔE_{12} for an $In_{0.3}Ga_{0.7}N$ alloy as a function of the strain components along the $[1\bar{1}00]$ (y) and $[\bar{1}\bar{1}23]$ (projection of c axis on $(11\bar{2}2)$ plane) directions, expressed relative to their coherent value obtained from the lattice mismatch $[\epsilon_0=(a_{\text{substrate}}-a_{\text{alloy}})/a_{\text{alloy}}]$. We find that ΔE_{12} becomes negative if the strain relaxation along $[1\bar{1}00]$ is larger than that along $[\bar{1}\bar{1}23]$. We conclude that partial strain relaxation may play a role in polarization switching of semipolar InGaN grown on GaN substrates.

Partial strain relaxation has indeed recently been observed in semipolar InGaN samples.[25] The strain component along $[\bar{1}\bar{1}23]$ was found to experience a higher degree of relaxation through the formation of high-density dislocations facilitated by the existence of glide planes (c plane) and the presence of shear strain. This relaxation pattern differs from the one that we predict to promote polarization switching (Fig. 4).

In conclusion, we have studied strain effects on the valence-band structure of $(11\bar{2}2)$ semipolar InGaN/GaN QWs. We have quantified the shear-strain deformation potential D_6 in wurtzite GaN and InN using first-principles HSE06 calculations. Using the $\mathbf{k}\cdot\mathbf{p}$ approach and our consistent set of deformation potentials we find that pseudomorphic strain conditions do not lead to polarization switching with increasing In concentration. A reduction in the strain component along the y direction could lead to a band-ordering switch at In compositions around 0.3 but such a relaxation pattern is not supported by experimental observations.[25] We suggest that details of the band structure away from the zone center, along with band-filling effects, may play a role in the observed polarization switching.

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