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## Polarization effects due to thickness fluctuations in nonpolar InGaN/GaN quantum wells

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We have employed continuum elasticity theory and an eight band  $\mathbf{k} \cdot \mathbf{p}$  model to study the influence of thickness fluctuations in  $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$  quantum wells grown along the  $[1\bar{1}\bar{2}0]$  direction in GaN. Such fluctuations are the origin of polarization potentials that may spatially separate electrons and holes in the vicinity of a thickness fluctuation and therefore reduce the efficiency of light emitters. Our calculations reveal that even shallow fluctuations of one or two monolayers can induce a significant spatial separation of electrons and holes, in particular, if the lateral extent of such a fluctuation is large. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4818752>]

$\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$  quantum wells (QWs) form an excellent materials system for light emitting diodes, since high-efficiency emission can be obtained over a wide frequency range from infrared to ultra-violet.<sup>1</sup> Crystallizing in the thermodynamically stable wurtzite phase, InGaN films grown on GaN along the  $c$  axis<sup>2</sup> experience a combination of intrinsic spontaneous polarization and strain-induced piezoelectric polarization.<sup>3</sup> The resulting fields lead to a spatial separation of electron and hole states and thus to a reduction of the emission efficiency of such devices.<sup>4,5</sup> To avoid this problem, growth along nonpolar orientations has been proposed.<sup>6,7</sup> Nonpolar QWs, in which the  $c$  axis lies in the plane of the wells, should not exhibit any polarization fields. Pseudomorphic strain inside the QW still shifts valence and conduction bands, but no separation of electron and hole states should occur.

Realistic device structure, however, will exhibit fluctuations in the thickness of InGaN/GaN QWs. These introduce steps in the QW boundary that effectively contain interfaces (at least partially) oriented along the  $[0001]$  direction. The presence of such interfaces allows the manifestation of strain-induced and spontaneous polarization charges, and hence the formation of electric fields. The potential presence of such lateral fields in strained semiconductor heterostructures was recognized some time ago,<sup>8</sup> but to our knowledge the issue has not been investigated at all in the context of nitrides, in which polarization fields tend to be a lot stronger than in conventional III-Vs. While the fluctuation-induced fields are mainly oriented within the plane of the QW, as opposed to the perpendicular direction in case of polar QWs, they may still lead to a local spatial separation of electrons and holes. Thickness fluctuations could, therefore, in principle, lead to a reduction of the emission efficiency even in nonpolar QWs, and it is important to assess the magnitude of such effects.

Here, we report a theoretical investigation of the influence of thickness fluctuations on the electronic properties of nonpolar ( $a$ -plane) InGaN/GaN QWs. We introduce a

thickness fluctuation of variable depth and lateral extent in an otherwise homogeneous QW, with a typical composition of  $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$ , embedded in a GaN matrix. The model system is an 8-nm thick quantum well with fluctuations that range from 1 to 6 nm in lateral extent and 0.25 to 3 nm in depth (see Fig. 1). Periodic boundary conditions are assumed, allowing use of a plane-wave-based methodology as implemented in the Sphinx code.<sup>9</sup> The supercell has dimensions of 80 nm along  $[1\bar{1}\bar{2}0]$  ( $x$ ) and 20 nm along the  $[0001]$  direction ( $z$ ), and 0.5 nm perpendicular to the plane of Fig. 1, i.e., along the  $[1\bar{1}00]$  direction ( $y$ ).

The electronic properties of the system are computed using an eight-band  $\mathbf{k} \cdot \mathbf{p}$  model<sup>10</sup> and are significantly influenced by strain and polarization potentials, which are computed via a plane-wave-based second-order continuum elasticity model.<sup>11</sup> The parameters for the elastic and piezoelectric properties were taken from Ref. 12, and the bulk band parameters to obtain the electronic properties were taken from Ref. 13. Parameters for InGaN alloys are obtained by linear interpolation between InN and GaN. These models provide a continuum description of the system on an equidistant grid, and obviously do not describe atomistic effects, which could, in principle, be important for an accurate, quantitative description of thickness fluctuations caused by single atomic layers. Nevertheless, the well-established eight-band  $\mathbf{k} \cdot \mathbf{p}$  approach is particularly well suited to describing the influence of additional potentials, such as the polarization that arises from thickness fluctuations, on the localization of electrons and holes in a quantitative and computationally straightforward manner. The approach has been successfully applied to a wide range of III-N nanostructures and device structures.<sup>14–17</sup> We have also previously evaluated the validity and reliability of the employed model by comparing with atomistic tight-binding models<sup>18</sup> and consider this formalism fully capable of providing a qualitatively reliable picture of the effects to be studied in the present work.

The case of an ideal strained InGaN well in a strain-free GaN matrix, i.e., at the bulk GaN lattice parameters, can be treated analytically. The diagonal strain components along the in-plane  $y = [1\bar{1}00]$  and  $z = [0001]$  directions can then be calculated as

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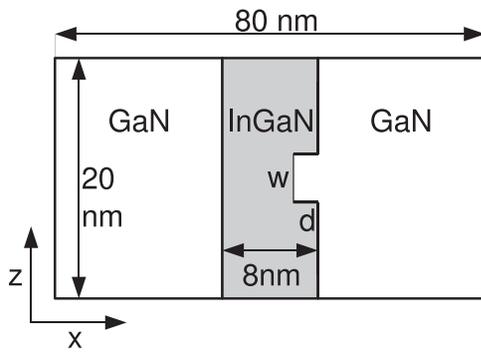


FIG. 1. Model quantum well with thickness fluctuation that is the subject of the present study.  $d$  is the depth and  $w$  is the lateral extent of the considered fluctuation. The growth direction is  $x = [11\bar{2}0]$ , and the fluctuation creates interfaces oriented along the  $z = [0001]$  direction.

$$\begin{aligned}\varepsilon_{yy} &= a(\text{GaN})/a(\text{In}_{0.2}\text{Ga}_{0.8}\text{N}) - 1 = -0.0218, \\ \varepsilon_{zz} &= c(\text{GaN})/c(\text{In}_{0.2}\text{Ga}_{0.8}\text{N}) - 1 = -0.0196.\end{aligned}\quad (1)$$

The  $\varepsilon_{xx}$  strain component can be derived as

$$\varepsilon_{xx} = -\frac{C_{12}}{C_{11}}\varepsilon_{yy} - \frac{C_{13}}{C_{11}}\varepsilon_{zz} = 0.0142, \quad (2)$$

and all off-diagonal strain components are zero. Starting from this idealized case, we systematically study the influence of thickness fluctuations of different depths and lateral extents.

For the case of a thickness fluctuation with  $w = 3$  nm, the diagonal strain components are shown in Fig. 2 for fluctuation depths of 0.25, 0.5, 1.0, and 2.0 nm along the  $x$ -axis through the center of the fluctuation. Small peaks in the absolute values of  $\varepsilon_{xx}$  and  $\varepsilon_{zz}$  are observed at the interface between InGaN and GaN in the area of the fluctuation, due to a buildup of strains occurring around the edges of the fluctuation close to this point.

The off-diagonal strain component  $\varepsilon_{xz}$  (which gives rise to a large part of the polarization potential) is plotted in Fig. 3, for fluctuations with  $d = 0.5$  nm (left) and  $d = 1.0$  nm

(right), with  $w = 3$  nm. We observe that the off-diagonal strain components are quite large in the vicinity of the step edges.

The strains induce piezoelectric polarization, which along with a minor contribution from spontaneous polarization ( $< 1$  meV in all cases) gives rise to a polarization potential  $V_p$ .<sup>11</sup> This potential takes the effect of dielectric screening into account, and directly enters the calculation of the electronic properties as an additional potential term in the  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian. Figure 4 shows that for shallow fluctuations of 0.25- and 0.5-nm depth, these potentials can already reach absolute values of approx. 20 meV, whereas the deeper fluctuations easily induce potentials of more than 50 meV.

We note that the piezoelectric constant  $e_{15}$  of InN and GaN has been controversially discussed not only for its absolute value but also for its sign.<sup>19,20</sup> We have therefore evaluated the influence of this parameter on the polarization potentials and the resulting charge carrier separation. Our tests indicate that using the (negative) values for  $e_{15} = e_{31}$  from Refs. 19 and 20 results in some differences compared to the results obtained with the values cited in Ref. 12. However, since the main differences in the polarization potential arise in close vicinity to the edges of the fluctuation, the quantitative effects on overall carrier localization are small. We therefore consistently use the piezoelectric constants from Ref. 12 within this work.

We have calculated the electron and hole ground states using the eight band  $\mathbf{k} \cdot \mathbf{p}$  model<sup>11</sup> taking the above computed strains and polarization potentials into account. To estimate the effect of the spatial separation of electron and hole states on the recombination rate, we calculate the electron-hole overlap as

$$M = \int_{\Omega} \rho_e(\mathbf{r})\rho_h(\mathbf{r})d\mathbf{r}, \quad (3)$$

where  $\rho_e(\mathbf{r})$  and  $\rho_h(\mathbf{r})$  are the electron and hole charge densities and  $\Omega$  is the unit cell.

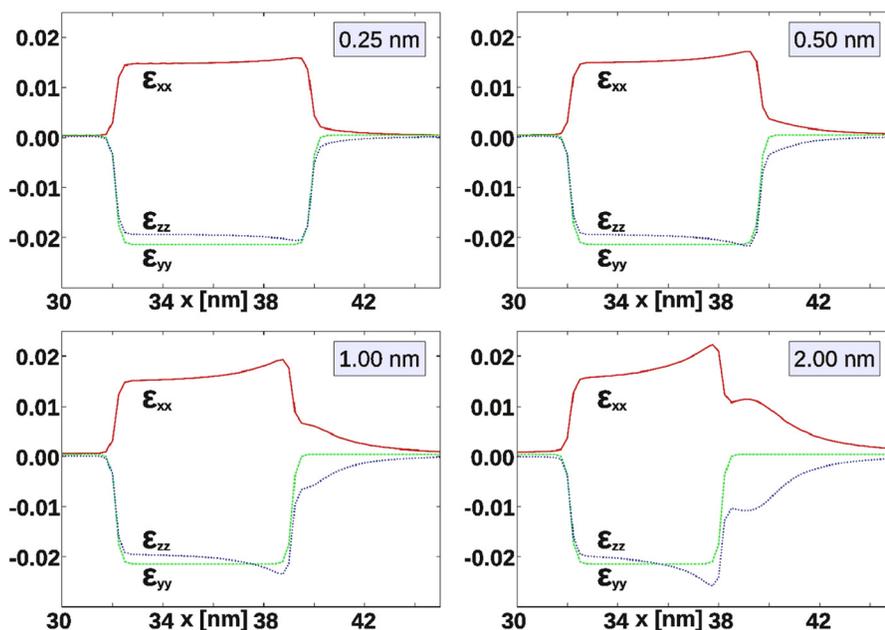


FIG. 2. Diagonal strain components for an 8-nm InGaN QW with a thickness fluctuation of depths 0.25, 0.5, 1, or 2 nm, plotted along the  $x = [11\bar{2}0]$  direction through the center of the fluctuation (which has a lateral extent of 3 nm). The red solid line depicts  $\varepsilon_{xx}$ , the dashed green one is  $\varepsilon_{yy}$ , and the dotted blue one depicts  $\varepsilon_{zz}$ .

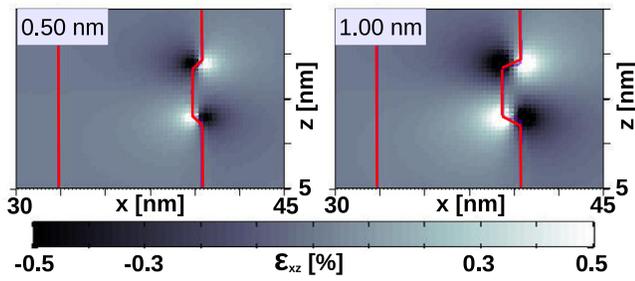


FIG. 3. Off-diagonal strain component  $\epsilon_{xz}$  for a quantum well with a thickness fluctuation with  $d = 0.5$  nm (left) and  $d = 1$  nm (right) with a lateral extent of  $w = 3$  nm. The solid red lines indicate the quantum well.

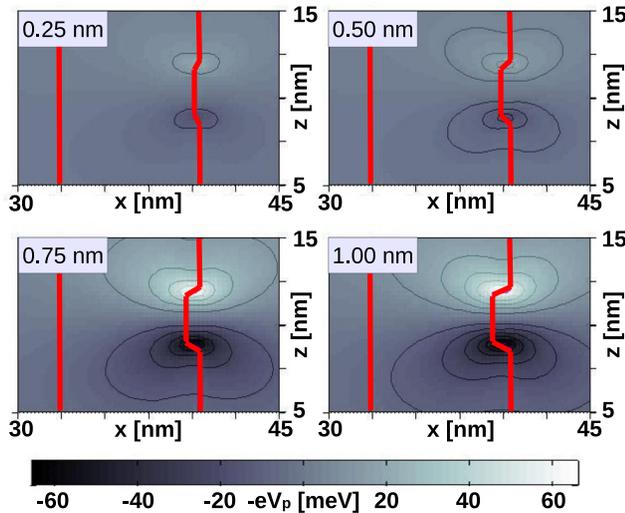


FIG. 4. Energy surface of the polarization potential  $-eV_p$  (in meV) in an 8-nm InGaN QW (marked as a solid red line) with a thickness fluctuation of depths 0.25, 0.5, 0.75, or 1 nm (top left to bottom right). The fluctuation has a lateral extent of 3 nm. The spacing between the single contour lines in the plot is 10 meV.

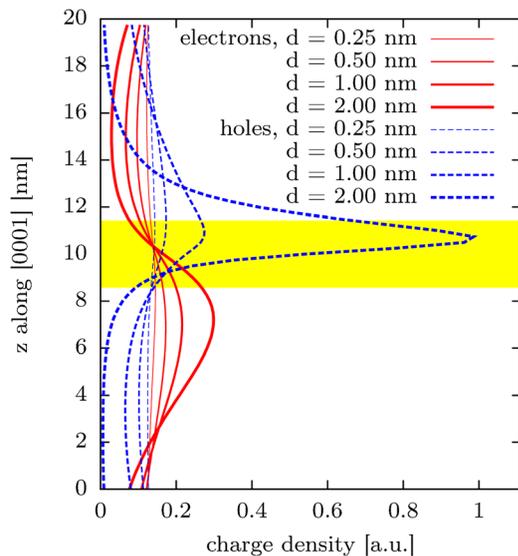


FIG. 5. Electron (red solid) and hole (blue dashed) charge densities for fluctuation depths of 0.25, 0.5, 1, and 2 nm depth in a thickness fluctuation of 3 nm lateral extent, integrated over  $x$  and plotted along the  $z = [0001]$  direction. Thicker lines indicate deeper fluctuations. The position of the fluctuation is marked yellow. Deeper fluctuations result in stronger localization.

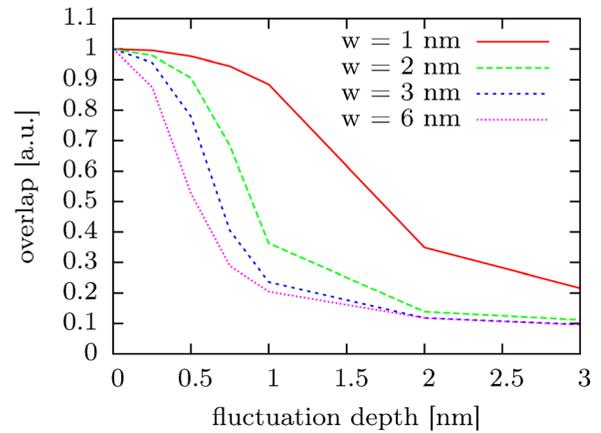


FIG. 6. Electron-hole overlap [Eq. (3)] as a function of the fluctuation depth for fluctuations with a lateral extent of 1, 2, 3, and 6 nm.

The electron and hole ground-state charge densities, integrated over all  $x$ -values, are shown in Fig. 5. The localization effect arising from the polarization potential is stronger for the holes than for the electrons. The larger the depth of the thickness fluctuation, the greater the localization of both electrons and holes.

For shallow fluctuations (0.25 and 0.5 nm) with small lateral extents, the electron-hole overlap is almost as large as the overlap for the ideal quantum well, i.e., electrons and holes experience only minor effects of spatial separation due to the polarization potentials. Figure 6 shows the electron-hole overlap as a function of the fluctuation depth for fluctuations of varying lateral extent, i.e., 1, 2, 3, and 6 nm wide. For the larger fluctuations (more than 0.5 nm depth), the polarization significantly reduces the electron-hole overlap. A notable reduction is also observed for shallower fluctuations when the lateral extent is large. Indeed, for a given depth of the fluctuation, the reduction is more significant when the lateral extent of the fluctuation is larger.

The GaN interlayer distance along the  $[11\bar{2}0]$ -direction is  $a/2 = 0.16$  nm. In carefully performed molecular beam epitaxy (MBE) or metalorganic chemical vapor deposition (MOCVD) growth, one expects that thickness fluctuations should not exceed one or two atomic steps. Figure 6 shows, however, that even modest fluctuations could give rise to sizeable reductions in overlap (and hence recombination efficiency) particularly for larger separations between the steps. In addition, growth on semipolar orientations<sup>21</sup> may produce additional tendencies for step formation at QW interfaces, triggering the effects described here.

In summary, we have conducted simulations for thickness fluctuations in a nonpolar InGaN QW based on an eight-band  $\mathbf{k} \cdot \mathbf{p}$  formalism in combination with continuum elasticity theory. The results show that thickness fluctuations on the order of a few atomic steps give rise to in-plane polarization fields capable of causing a significant electron-hole separation, and hence a reduction of recombination efficiency. Maintaining smooth, abrupt interfaces is therefore particularly important for nonpolar or semipolar nitride QWs.

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