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Optical polarization properties of interband transitions in strained group-III-nitride alloy films on GaN substrates with nonpolar orientation

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The authors present results of a perturbation theory study of the combined effects of composition and anisotropic in-plane strain on the optical polarization properties of the three interband transitions in the vicinity of the fundamental energy gap of wurtzite group-III-nitride alloy films, pseudomorphically grown on GaN substrates with nonpolar orientation such as *M*-plane GaN($1\bar{1}00$). Valence band mixing induced by the anisotropic in-plane strain is shown to have a dramatic influence on the optical polarization properties. The results indicate that an increased efficiency of light emission in the visible spectral range can be achieved with compressively strained $In_xGa_{1-x}N$ active layers. While $Al_xGa_{1-x}N$ layers under tensile strain will exhibit a very poor light emission efficiency in the ultraviolet (UV) spectral range, efficient emission in the UV range can instead be achieved with $In_xAl_{1-x}N$ films. These results also hold for alloy films on *A*-plane GaN($11\bar{2}0$) substrates. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2965119]

It has been demonstrated that wurtzite group-III-nitride semiconductor heterostructures with *M*-plane [$1\bar{1}00$] and *A*-plane [$11\bar{2}0$] orientation (Fig. 1) are free from large pyro- and piezoelectric fields. The absence of these internal electric fields can lead to a significant improvement in the emission efficiency.[1] These nonpolar oriented films are mostly grown on *R*-plane ($1\bar{1}02$) sapphire, SiC($1\bar{1}00$), and γ-$LiAlO_2$(100) substrates. However, defects related to misfit as well as threading dislocations and stacking faults in such films, arising from the large lattice mismatch between the film and substrate, resulted in devices with poor emission efficiency. Defect-free *M*-plane nitride films have finally been grown on bulklike *M*-plane and *A*-plane GaN substrates, and subsequently light emitting diode[2,3] (LED) and laser[4,5] operation have been demonstrated using this type of films. LEDs and lasers fabricated from group-III-nitrides have an $Al_xGa_{1-x}N$ or $In_xGa_{1-x}N$ alloy film as the active region to obtain ultraviolet (UV) or visible emission, respectively. Alloying leads to a modification of the electronic band structure (EBS). Apart from a change in the energy gap, alloying can affect the optical polarization properties of the interband transitions in the vicinity of the fundamental energy gap and influence the performance of devices. For instance, an emission with a polarization direction lying in the film plane can propagate toward the surface and be efficiently extracted out of the LED, while an emission with polarization perpendicular to the film plane propagates inside the film and is easily reabsorbed.[6] For edge emitting lasers, the threshold current density for lasing in the preferred transverse electric (TE) mode is reduced if the emission polarization is predominantly along a direction lying in the film plane. Vertical-cavity surface-emitting lasers would also benefit from such a configuration. Thus, a strong in-plane polarization of the emission is desirable for efficient LED and laser operation.

Studies on *C*-plane $Al_xGa_{1-x}N$ LEDs have shown that the emission efficiency decreases with increasing Al concentration due to an enhanced out-of-plane (**z**) polarization of the lowest energy transition,[6,7] which makes light extraction difficult. Its origin has been attributed to the Al concentration dependence of the EBS parameter associated with the crystal-field splitting. With pseudomorphic growth of thin alloy films on nonpolar oriented substrates such as *M*-plane GaN, the variation of the EBS parameters with alloy composition will not be the only factor influencing the EBS. In addition, the EBS will be affected by the in-plane strain in the films, which would vary with alloy composition in a predictable manner. It is important to note that since the lattice constants are different along directions parallel and perpendicular to the ***c***-axis, which lies in the nonpolar oriented plane, the in-plane strain in these alloy films would be anisotropic. Such anisotropic strain can modify the EBS of group-III-nitrides significantly.[8,9] Here, we present the results of a perturbation theory study of the effect of anisotropic strain on the EBS of $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$, and $In_xAl_{1-x}N$ alloy films on *M*-plane GaN substrates. The emphasis lies on the determination of the optical polarization properties of the three interband transitions in the vicinity of the fundamental energy gap and conclusions drawn from them for the feasi-

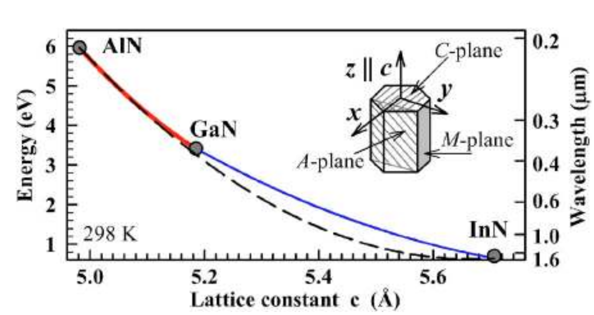

FIG. 1. (Color online) Unstrained excitonic energy gap of $Al_xGa_{1-x}N$ (thick line), $In_xGa_{1-x}N$ (thin line), and $In_xAl_{1-x}N$ (dashed line) alloys as a function of lattice constant *c*. The inset is a schematic of the wurtzite unit cell showing the choice of coordinates.

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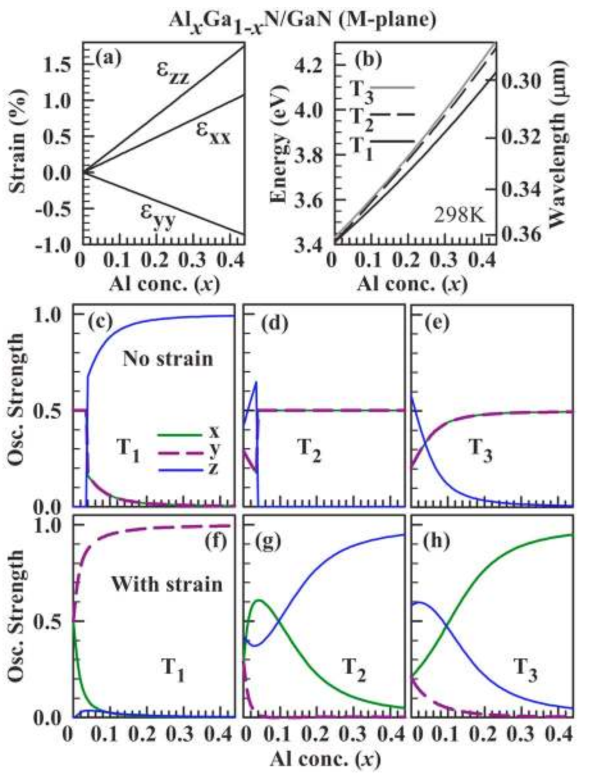

FIG. 2. (Color online) (a) Variation of the strain components ε_{xx}, ε_{yy}, and ε_{zz} of an $Al_xGa_{1-x}N$ film pseudomorphically grown on an *M*-plane GaN substrate as a function of the Al concentration *x*. (b) Energy of the three interband excitonic transitions T_1, T_2, and T_3 in the strained films in the vicinity of the fundamental energy gap. Relative oscillator strengths of (c) T_1, (d) T_2, and (e) T_3 in the absence of strain for light linearly polarized along **x**, **y**, and **z**. Their relative oscillator strengths under strain are shown in (f)–(h).

bility of using such strained alloy films for light emission applications.

Figure 1 shows the excitonic energy gap of unstrained ternary wurtzite group-III-nitride alloys as a function of the lattice constant *c*. The trend is similar with respect to the other lattice constant *a* of the wurtzite crystal structure. The inset shows the wurtzite unit cell and the choice of coordinates. To calculate the influence of strain on the EBS, we have used the Bir–Pikus Hamiltonian.[8,10] At the Γ point (crystal momentum $\mathbf{k}=0$), the conduction band (CB) of wurtzite group-III-nitrides is composed of atomic *s* orbitals with wavefunctions of $|S\rangle$ symmetry, while the three uppermost valence bands (VBs) are formed out of *p* orbitals with wavefunctions being a combination of $|X\rangle$, $|Y\rangle$, and $|Z\rangle$ symmetries. A transition involving an $|S\rangle$-like CB state and an $|X\rangle$-like, $|Y\rangle$-like, or $|Z\rangle$-like VB state requires **x**, **y**, or **z** polarized light, respectively. Due to the anisotropic strain, the VBs get mixed, and consequently the polarization properties of the three interband transitions in the vicinity of the fundamental energy gap are modified. We adopt a nomenclature[8] wherein the strain-modified excitonic transitions are labeled T_1, T_2, and T_3 in order of increasing energy. Their polarization properties are determined by the relative oscillator strength components $f_{i\beta}$, with $i=1,2,3$ and $\beta=\mathbf{x},\mathbf{y},\mathbf{z}$ representing the three transitions and their polarization components, respectively.

Reference 11 lists the material parameter values of AlN, GaN, and InN used in our calculations. The CB deformation potential α for AlN and InN was derived from the listed values[12] of the hydrostatic deformation potential a_1 and the

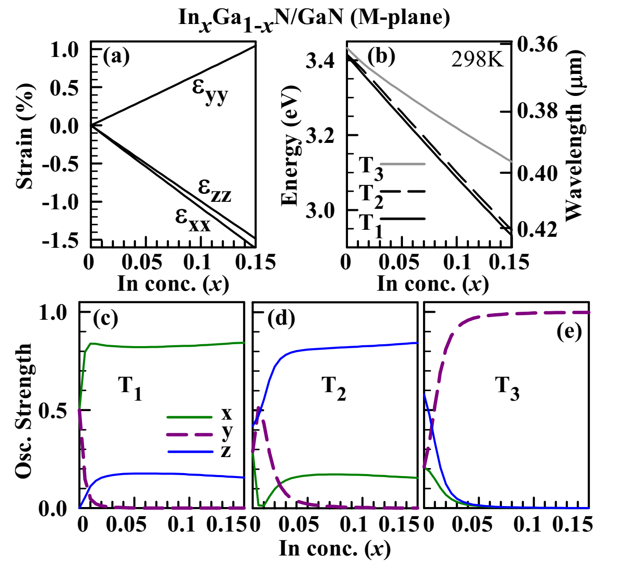

FIG. 3. (Color online) (a) Variation of the strain components ε_{xx}, ε_{yy}, and ε_{zz} of an $In_xGa_{1-x}N$ film pseudomorphically grown on an *M*-plane GaN substrate as a function of the In concentration *x*. (b) Energy of the three interband excitonic transitions T_1, T_2, and T_3 in the strained films in the vicinity of the fundamental energy gap. Relative oscillator strengths of (c) T_1, (d) T_2, and (e) T_3 under strain for light linearly polarized along **x**, **y**, and **z**.

VB deformation potential D_1, using $\alpha=a_1+D_1$. Other relevant deformation potentials were obtained under the quasicubic approximation.[10] The parameters for the alloys were obtained through linear interpolation. For the energy gaps of the unstrained alloys, an additional bowing parameter of 0.7 eV for $Al_xGa_{1-x}N$, 1.4 eV for $In_xGa_{1-x}N$, and 6.0 eV for $In_xAl_{1-x}N$ was taken into account.[12,13] The alloy composition range was limited to values for which the reported critical film thickness[14,15] for pseudomorphic growth is at least 10 nm in order to enable quantum well growth. The values of the matrix elements $|\langle S|p_x|X\rangle|^2$, $|\langle S|p_y|Y\rangle|^2$, and $|\langle S|p_z|Z\rangle|^2$ in these materials are nearly equal under the quasicubic approximation,[16] leading to the sum rules $\Sigma_{i=1}^{3} f_{i,\beta}=1$ and $\Sigma_{\beta=x}^{z} f_{i,\beta}=1$ for the alloys.

Figure 2(a) shows that the strain experienced by an $Al_xGa_{1-x}N$ alloy film on an *M*-plane GaN substrate is tensile and anisotropic in the plane of the film, since its components ε_{xx} along **x** and ε_{zz} along **z** are different. The strain-modified transition energies in Fig. 2(b) show that the lowest energy transition T_1 falls in the UV spectral range. Figures 2(c)–2(e) show the variation of $f_{i\beta}$ with Al concentration, assuming that the alloy film remains unstrained. In the absence of any strain, we see that $f_{ix}=f_{iy}$, which is expected from the Bir–Pikus Hamiltonian for wurtzite crystal symmetry. At the same time, T_1 is predominantly **z** polarized for $x_{Al}>0.05$. This result suggests that the emission can be easily collected along **y**, leading to high-efficiency LEDs and lasers. This is in agreement with a simplistic deduction from the experimental results on *C*-plane devices,[17,18] which indicated that *M*-plane $Al_xGa_{1-x}N$-based LEDs and lasers would emit light efficiently. However, once the expected in-plane tensile strain in the film is taken into account, the polarization properties are significantly modified through VB mixing as shown in Figs. 2(f)–2(h). With strain, T_1 becomes predominantly **y** polarized. This will hinder light extraction along **y** in a LED and is also detrimental for TE-mode lasing. Thus, strained $Al_xGa_{1-x}N$ films on *M*-plane GaN substrates will not result in efficient UV light emitters.

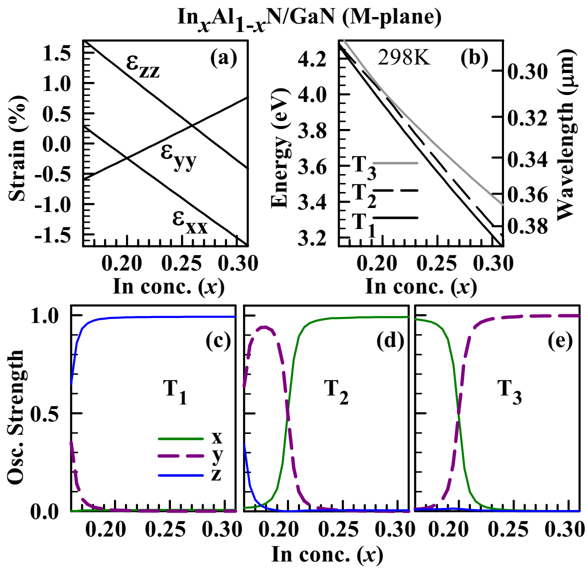

FIG. 4. (Color online) (a) Variation of the strain components ε_{xx}, ε_{yy}, and ε_{zz} of an $In_xAl_{1-x}N$ film pseudomorphically grown on an *M*-plane GaN substrate as a function of the In concentration *x*. (b) Energy of the three interband excitonic transitions T_1, T_2, and T_3 in the strained films in the vicinity of the fundamental energy gap. Relative oscillator strengths of (c) T_1, (d) T_2, and (e) T_3 under strain for light linearly polarized along **x**, **y**, and **z**.

Figure 3(a) shows that the strain experienced by an $In_xGa_{1-x}N$ alloy film on an *M*-plane GaN substrate is compressive and anisotropic in the plane of the film. The strain-modified transition energies are shown in Fig. 3(b). In this case, the T_1 transition falls into the blue spectral range. Figures 3(c)–3(e) show the variation of $f_{i\beta}$ with In concentration, taking into account the effect of the strain in the film. This is again very different from the unstrained situation (not shown here), where we obtain $f_{1x}=f_{1y}=0.5$ and $f_{1z}=0$ for all x_{In}. We find that with strain-induced VB mixing there is an increase of about 70% in the **x** polarization component of T_1 for $x_{In}>0.01$, together with a small **z** polarization component. Since emission with **x** polarization can be easily collected along **y**, the utilization of such strained films will result in LEDs with higher efficiencies. In addition, TE-mode lasing with a higher efficiency can be achieved with this material, if the cavity is defined along **z** as compared to when the cavity is defined along **x**. This explains very well the recent experimental results of Okamoto *et al.*[4]

Finally, Fig. 4(a) depicts the case of $In_xAl_{1-x}N$ alloy films on an *M*-plane GaN substrate, where the in-plane strain experienced by the film is highly anisotropic and can be both tensile or compressive depending on the In concentration. The strain-modified transition energy plots in Fig. 4(b) show that the T_1 transition spans a similar UV range as $Al_xGa_{1-x}N$. Figures 4(c)–4(e) show the variation of $f_{i\beta}$ with In concentration, taking into account the strain in the film. Note that when $\varepsilon_{xx}=\varepsilon_{yy}$ at $x_{In}\approx 0.2$ the wurtzite symmetry is restored and consequently we again obtain $f_{ix}=f_{iy}$. Here, T_1 acquires a large **z** polarization component for $x_{In}>0.17$, and therefore the emission can be easily collected along **y**. Thus, from a consideration of oscillator strengths, LEDs and lasers fabricated using such a film will be more efficient light emitters as compared to strained $Al_xGa_{1-x}N$ films on an *M*-plane GaN substrate.

In conclusion, we have shown that the oscillator strengths of interband transitions in group-III-nitride ternary alloy films, pseudomorphically grown on *M*-plane GaN substrates, are strongly modified by anisotropic in-plane strain. They favor the use of $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ films as active layers for efficient light emission in LEDs and lasers, while $Al_xGa_{1-x}N$ films are likely to exhibit very poor light emission efficiency. The symmetry of the Bir-Pikus Hamiltonian is such that the results for *A*-plane films are identical to the ones obtained for *M*-plane films, when **x** and **y** are interchanged everywhere.[19] Thus, the above conclusions also hold or pseudomorphic growth on *A*-plane GaN substrates.

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