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Optical studies of strain effects in quantum wells grown on (311) and (100) GaAs substrates

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Pseudomorphic InGaAs/GaAs quantum wells (QW's) grown on vicinal substrates show a blueshift of the photoluminescence (PL) emissions with respect to (100) (nominal) ones. This effect has been discussed in the literature and it is associated with an inhomogeneous distribution of stresses in narrow quantum wells. In order to study the shift of the PL emissions at large substrate misorientation angles, we have made PL measurements on three InGaAs/GaAs QW's (30 Å wide), grown on (311)*A*, (311)*B*, and (100) substrates. We have done theoretical calculations considering the effect of strain on the conduction and valence bands of the QW's, where a single fitting parameter accounts for the inhomogeneous distribution of strain. Our model agrees with previously obtained results and reproduces the experimental PL blueshifts observed for the studied samples, showing that in relatively wider quantum wells the inhomogeneous distribution of strain and indium segregation play a less important role than in narrow ones. In (100) and (311)*A* GaAs/AlGaAs samples subjected to an external hydrostatic pressure, our model shows, for both samples, that the blueshift of the QW PL emissions increases with pressure, in good agreement with experimental results, emphasizing the strong relation between strain and blueshift regardless of the growth direction.

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I. INTRODUCTION

Pseudomorphic quantum wells (QW's) have acquired importance due to the possibilities for band-structure engineering and applications, since strained layers show features such as the lifting of the light- and heavy-hole bands degeneracy and the decreasing of the highest valence-band effective mass.[1]

There are different methods to include the effect of strain on the QW conduction and valence bands, using the biaxial approximation.[1–3] In this approximation, the stress caused by the lattice mismatch between the barriers and quantum well creates a strain pattern whose components are the same in the QW plane ($\epsilon_{xx}=\epsilon_{yy}$) and different along the growth direction (ϵ_{zz}), with no shearing components. Furthermore, it is considered that stress has no influence on the barriers.[4] This approach leads to a good agreement with experimental results for (100) pseudomorphic samples.

For samples grown on non-(100) substrates the effect of stress is, in general, much more complex. The lowering in the symmetry of the system[5,6] and the presence of polarization fields[1,7] can substantially affect the strain field associated with the stress. In addition, vicinal InGaAs/GaAs samples present an inhomogeneous strain distribution in the QW plane, where some regions are subjected to a hydrostatic stress and others subjected to a biaxial stress. In this case, the biaxial approximation is no longer accurate.[3] These authors show that the signature of this inhomogeneous distribution of strain is a shift to higher energies (blueshift) of the photoluminescence (PL) peaks from narrow vicinal QW's with respect to (100) ones.

The aim of this paper is to study the effect of strain in the PL emissions of samples grown on (311) and (100) substrates, with a built-in strain (pseudomorphic InGaAs/GaAs samples) or subjected to an externally induced strain (lattice-matched GaAs/AlGaAs QW's subjected to hydrostatic pressure).

A theoretical model discussed in the Sec. II was used to obtain the expected shifts of the PL emissions, giving a background for interpreting the experimental results presented in Secs. III and IV. In Sec. V we summarize this work.

II. THEORY

We have performed theoretical calculations concerning the conduction- and valence-band bound states, at $\mathbf{k}_{\parallel}=0$ (where $\mathbf{k}_{\parallel}$ is the projection of the wave vector in the QW plane), for a single quantum well, considering strain and different degrees of substrate misorientation [non-(100) orientation] from [100] towards the [111] direction. The description of the model follows.

The three nominal directions are defined by the z axis along the [100] direction, the y axis along [011] direction, and the x axis along $[01\overline{1}]$ direction. To introduce the non-nominal directions we have defined x' along the $[01\overline{1}]$ direction, y' along the $[(-2/a),1,1]$ direction, and z' along the $[1,(1/a),(1/a)]$ direction, where $a=\sqrt{2}/\tan\theta$ and θ is the angle between the growth direction z' and the z direction, ranging from θ close to zero (nominal [100] direction), to θ equal to 54.7° ([111] direction).

With these definitions we have the transformation

$$\begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & \sin(\theta) \\ 0 & -\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ k_{z'} \end{pmatrix}. \tag{1}$$

The normal strain components $\epsilon_{x'x'}, \epsilon_{y'y'}$, and $\epsilon_{z'z'}$ related to the tension and compression along each specific direction and the shearing strain components $\epsilon_{x'y'}, \epsilon_{y'z'}$, and $\epsilon_{z'x'}$ are written in the basis $(\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}})$ by the transformation[8]

$$\begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{xy} \\ \epsilon_{yz} \\ \epsilon_{zx} \end{pmatrix} = T \begin{pmatrix} \epsilon_{x'x'} \\ \epsilon_{y'y'} \\ \epsilon_{z'z'} \\ \epsilon_{x'y'} \\ \epsilon_{y'z'} \\ \epsilon_{z'x'} \end{pmatrix}, \tag{2}$$

where

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos^2(\theta) & \sin^2(\theta) & 0 & 2\sin(\theta)\cos(\theta) & 0 \\ 0 & \sin^2(\theta) & \cos^2(\theta) & 0 & -2\sin(\theta)\cos(\theta) & 0 \\ 0 & 0 & 0 & \cos(\theta) & 0 & \sin(\theta) \\ 0 & -\sin(\theta)\cos(\theta) & \sin(\theta)\cos(\theta) & 0 & \cos^2(\theta)-\sin^2(\theta) & 0 \\ 0 & 0 & 0 & -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix}. \tag{3}$$

In summary, rewriting the given wave vector and the strain components (along the x', y', z' directions) in the basis $(\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}})$, the valence- and conduction-band Hamiltonians for the misoriented quantum well are obtained.

To solve the valence-band Hamiltonian and find the hole bound states, we have used the model proposed by Chao and Chuang,[2] which uses the complete Luttinger-Kohn Hamiltonian including deformation effects.

The conduction-band Hamiltonian including strain is given by

$$H_c = \frac{\hbar^2}{2m^*}(k_x^2+k_y^2+k_z^2) + \frac{2a_h}{3}(\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}), \tag{4}$$

where a_h is the hydrostatic deformation potential for the barriers or QW.[9]

In pseudomorphic quantum wells the cubic symmetry of GaAs is broken, leading to a complex distribution of strain, expected to be even more complex in non-(100) quantum wells.[5,6] In addition, quantum wells grown on misoriented substrates could also present intense polarization fields, able to produce a significative modification in the strain values.[7] To the best of our knowledge it does not exist an exact and well-defined way to consider these phenomena in the calculations. In order to deal with these systems we will introduce some approximations, as described below.

Pseudomorphic QW's are subjected to stress due to the difference in the lattice parameter between the barriers and the QW. The usual approach for (100) structures is to consider a biaxial strain inside the quantum well, i.e.,

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a_0 - a_m}{a_m} \tag{5}$$

and

$$\epsilon_{zz} = \frac{-2C_{12}}{C_{11}}\epsilon_{xx}, \tag{6}$$

where a_0 and a_m are, respectively, the lattice constants of the barriers and the QW, and C_{11} and C_{12} are the stiffness constants for the QW material.[2] In our model, we will also assume a biaxial strain in non-(100) pseudomorphic quantum wells.

It is already known that vicinal samples show a blueshift of the PL emissions with respect to the nominal ones.[3] This qualitative behavior is supported by our model if we suppose that the strain transformation [Eq. (2)] does not lead to any shearing components $(\epsilon_{yz}=0)$. This approximation leads to a blueshift that increases with the misorientation angle as pointed out by López *et al.*,[10] and it is a possible indication that the observed blueshift is related to the existence of only normal strain components in the QW plane.

These authors also show that an inhomogeneous strain distribution along the QW interfaces is of great importance in determining the experimental blueshift observed in narrow InGaAs/GaAs samples. In other words, there are regions of QW interfaces where the strain is biaxial and other regions where the strain is hydrostatic, and these strain changes are associated to the tangent of the misorientation angle.

To introduce this effect in our theoretical model, we defined an analogous parameter (Ξ) responsible for a biaxial to

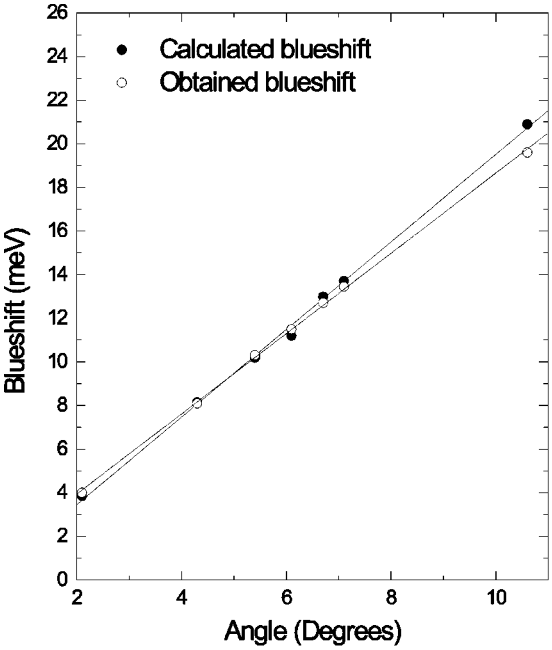

FIG. 1. Comparison between the calculated blueshift (solid circles) (Ref. 3) and the obtained by our model (open circles) as a function of the misorientation angle for a 5-ML-wide $In_{0.35}Ga_{0.65}As/GaAs$ QW. The electronic effective mass was obtained by a linear interpolation between InAs ($m_c^* = 0.028 m_0$) and GaAs ($m_c^* = 0.067 m_0$) effective mass. The parameter Ξ was set to 1, indicating an inhomogeneous distribution of strain in the QW.

hydrostatic conversion of strain, modifying the strain component along the growth direction ($\epsilon_{z'z'}$) to a new value given by

$$\varepsilon_{z'z'} = \chi(\epsilon_{z'z'} - \epsilon_{x'x'}) + \epsilon_{x'x'}, \tag{7}$$

where

$$\chi = 1 - \Xi \tan\theta. \tag{8}$$

In Eq. (7), $\chi = 1$ corresponds to a pure biaxial strain.

In order to test our model, we set our parameter (Ξ) to a correct value to obtain the total blueshift expected by the theoretical model proposed by Porto and Sanchez-Dehesa,[3] for a 5-ML-wide $In_{0.35}Ga_{0.65}As/GaAs$ QW with the tilt angle equal to 4.3° and in the absence of indium segregation. With the same value of Ξ, our model shows a reasonable agreement with the calculated blueshifts obtained by the authors for vicinal angles ranging from zero to 10.6° (Fig. 1). The deformation potentials, lattice, and stiffness constants were obtained according to Van de Walle[11] and the alloy parameters were calculated by linear interpolation. The band offset was determined considering a biaxial compression,[3] where the hydrostatic contribution is taken into account only by the changes in the strain components due to the parameter Ξ.

Therefore, the results obtained here agrees with the fact that in narrow QW's the experimental blueshifts can only be obtained by considering an inhomogeneous distribution of strain along the quantum well interfaces.[3] In addition, these authors show that as the quantum well becomes relatively wider, the contribution of the inhomogeneous distribution of the strain to the blueshift becomes minor.

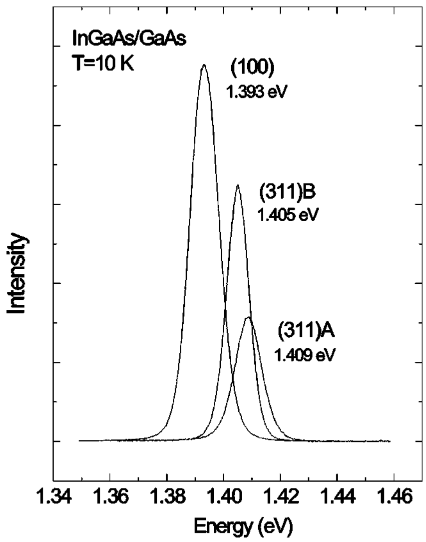

FIG. 2. PL spectra for the studied samples. The temperature of the experiment was 10 K.

Our theoretical model shows that for a given misorientation angle and indium content the blueshift of the PL emissions as a function of the well width presents a maximum. For a fixed well width, our calculations demonstrate that as the indium content increases, the blueshift also increases. These facts are in close agreement with previous obtained results.[3,10]

In order to simulate the effect of the hydrostatic pressure on GaAs/AlGaAs samples, we supposed that the hydrostatic stress causes a hydrostatic strain field along all the structure, not only inside the QW as admited for the InGaAs/GaAs samples.[4] We defined $\epsilon_{x'x'} = \epsilon_{y'y'} = \epsilon_{z'z'}$, where $\epsilon_{x'x'} = -P/3B$. In this equation, B is the GaAs bulk modulus [755 kbar (Ref. 12)] and P is the applied external hydrostatic pressure.[11]

For the QW grown on (100) substrate, θ is close to zero degrees; for the QW grown on (311) substrate, $\theta = 25.24°$. We supposed that $B(\mathrm{GaAs}) = B(\mathrm{AlGaAs})$, and we used the same strain values ($\epsilon_{x'x'}, \epsilon_{y'y'}, \epsilon_{z'z'}$) for the $(311)A$ and (100) samples, as the hydrostatic strain is an invariant under the transformation[8] expressed by the Eq. (2).

III. PSEUDOMORPHIC InGaAs/GaAs QW's GROWN ON (311) AND (100) SUBSTRATES.

The growth sequence of the epitaxial layers on the $(311)A$, $(311)B$, and (100) substrates was (i) a 1-μm undoped GaAs buffer layer, (ii) a 30-Å undoped $In_{0.2}Ga_{0.8}As$ quantum well, and (iii) a 500-Å undoped GaAs cap layer.

In the PL experiments, the samples scattered light was analyzed by a Jobin-Ivon T-64000 spectrometer operating in single mode connected to a charge-coupled device (CCD) camera. The excitation light was produced by an Ar laser emitting at 514.5 nm. Figure 2 shows the obtained spectra

TABLE I. Comparison between the experimental and theoretical blueshifts for the $In_{0.2}Ga_{0.8}As$ QW. The parameter Ξ was set to zero, indicating that the distribution of strain in the QW is mainly homogeneous.

Blueshift ($In_{0.2}Ga_{0.8}As$ QW)		
Theoretical	Experimental	
(311) orientation	(311)B sample	(311)A sample
13 meV	12 meV	15 meV

for the three samples, and clearly evidences a blueshift of the (311)A and (311)B PL emission energies with respect to the energy of the (100) sample.

The theoretical blueshift obtained by our model is shown in Table I, together with the experimental data, revealing a good agreement with the experimental results. It is worth mentioning that the calculations considered a homogeneous distribution of strain [$\chi = 1$, corresponding to a biaxial strain in Eq. (7)] and the absence of indium segregation.

During epitaxial growth, indium atoms have the tendency to segregate from underlying layers to the top, exchanging their positions with galium atoms of the top layer.[13] In addition, the distribution of strain in vicinal QW's is expected to be inhomogeneous; i.e., there are regions where strain is mainly hydrostatic and regions where it is mainly biaxial. These effects are very important in narrow vicinal InGaAs/GaAs QW's, being less important as the QW becomes relatively wider.[10] For the 5 ML InGaAs/GaAs QW discussed in the previous section, the experimental blueshift can be explained only if one considers indium segregation and an inhomogeneous distribution of strain.[3] In contrast, our theoretical result for the $In_{0.2}Ga_{0.8}As$ QW (30 Å wide) discussed in this section clearly shows that segregation effects and a nonhomogeneous distribution of strain play a less important role in our (311) structure. This is consistent with the fact that relatively wider QW's are less affected by these effects, as the segregation and the changes in the strain distribution play a less important role as the distance from the QW interfaces become bigger.

Previous results[10] show that the heavy-hole exciton binding energies vary slightly with the vicinal angle, for angles ranging from 0 to 6°. To the best of our knowledge, there is no further evidence of the relation between the exciton binding energy and the tilt angle for angles greater than 6°. However, the good agreement between our theoretical model and experience suggests that the heavy-hole exciton binding energies are almost the same for the (311)A, (311)B, and (100) InGaAs/GaAs samples studied.

A theoretical simulation considering an idealized $In_{0.2}Ga_{0.8}As$ *without strain* reveals a *redshift* (a shift to lower energies) of the (311) PL emissions with respect to the (100) ones. This hypothetical behavior reinforces the results shown in this section, where the blueshift of the PL emissions is closely related to the presence of mechanical deformations. In addition, our calculations show that the effect of the biaxial strain occurs mainly on the valence band of the (311) InGaAs/GaAs structure.

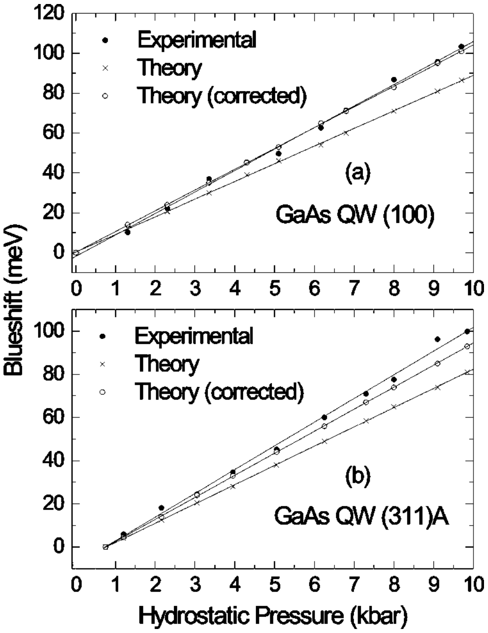

FIG. 3. Dependence of the blueshift with pressure for the GaAs/AlGaAs QW's (300 K). The solid circles correspond to the experimental data, in both samples (Ref. 14). The theoretical curves (crosses) indicate the obtained blueshift for each sample considering that the hydrostatic pressure produces a hydrostatic strain; the corrected theoretical curve [open circles, (100) sample] indicates the blueshift considering an additional nonhydrostatic strain field, adjusted to reobtain the (100) experimental data. Using the same nonhydrostatic parameter used for the (100) sample, the blueshift is still lower than the observed for the (311)A sample [open circles, (311)A sample]. The lines are a guide for the eyes. The only difference between two correspondent simulations for the samples is the angle θ [close to zero for (100) QW and 25.24° for the (311)A sample).

IV. STUDIES OF GaAs/AlGaAs QUANTUM WELLS GROWN ON (311) A AND (100) SUBSTRATES UNDER HYDROSTATIC PRESSURE

Photoluminescence under hydrostatic pressure was used to characterize the (311)A- and (100)-oriented GaAs/$Al_{0.35}Ga_{0.65}As$ 50-Å QW structures at room temperature. For details about the samples and the experimental setup, see Freire *et al.*[14]

Figures 3(a) and 3(b) shows the dependence on pressure of the PL peak energies from the (100) and (311)A QW layers. An increase (blueshift) of the emission energy as the pressure increases is observed for both samples. These experimental results clearly show that the blueshift of the QW PL emissions is closely related to an internal strain pattern acting on the sample caused by the external hydrostatic pressure.

We have used our theoretical model to simulate the effect of the pressure on the emission energies of the QW's, as discussed in Sec. II. The electronic effective mass in the barriers was obtained by $m_c^* = (0.067 + 0.083x)m_0$,[12] where x stands for the percentage of aluminum. The potential discontinuity at the interfaces for conduction and valence bands was assumed to be equal to 60% and 40%, respectively, of the difference in the energy gap of the two materials.[15] In this model, the band offset does not change with the hydrostatic pressure.[2] The results for the samples are shown in Fig. 3 (curves with crosses). In both samples, the hydrostatic approximation gives a smaller blueshift than the experimentally observed.

The growth of quantum wells breaks the cubic symmetry of GaAs, as discussed before. In addition, deformation components may arise due to the anisotropy of the sample [e.g., due to the difference in elastic constants between the barrier and the QW (Ref. 11)]. As a consequence, a hydrostatic stress field can lead to a nonhydrostatic strain field. To the best of our knowledge, we did not find quantitative information about the influence of these effects in similar samples.

In order to get a qualitative picture of this phenomenon, we tryed to fit the experimental data by adjusting the $\epsilon_{z'z'}$ value. In this way, this strain component is supposed to account for all of the nonhydrostatic distribution of strain. With the inclusion of this parameter of nonhydrostaticity, we have obtained a good agreement with the experimental data for the (100) sample, as can be seen in Fig. 3 [graphic (a), open circles, for $\epsilon_{z'z'} = 1.4\epsilon_{x'x'}$].

Using the same $\epsilon_{z'z'}$ fitted value for the (100) sample, we obtained the curve for the (311)*A* sample [graphic (b), open circles], also shown in Fig. 3. As the pressure increases, we note that the agreement with the experimental data becomes worse. This is consistent with the fact that QW's grown along the (311) direction have a still lower symmetry than the (100) ones, responsible for additional nonhydrostatic strain components. In addition, this structure is believed to have a complex array of microfacets along all the sample,[16] which can substantially interfere on the distribution of strain in the QW plane.

Notzel *et al.*[17] evidence the presence of this corrugated pattern inside the (311)*A* QW, responsible for a *redshift* of the PL emissions observed for (311)*A* samples with respect to the nominal ones. For a given pressure, our experimental data for the (311)*A* sample (Fig. 4) also show this redshift. Our simulations predict the occurrence of a redshift but lower than the experimentally observed. We claim that this difference is another evidence of an additional confinement potential taking place inside the (311)*A* quantum well,[18] caused by the corrugated pattern.

It is worth mentioning that although hydrostatic pressure modifies the energy of both the valence- and conduction-band edges, our theoretical calculations show that this effect is more pronounced on the conduction-band edge.

V. SUMMARY AND CONCLUSIONS

We developed a theoretical model that considers the QW conduction and valence bands including the effect of stress. The inhomogeneous distribution of strain was included in the simulations by an adjustable parameter responsible for the biaxial to hydrostatic conversion of strain, leading to a good agreement with previous results obtained for a narrow (5-ML-wide) InGaAs/GaAs QW, not considering indium segregation effects.[3]

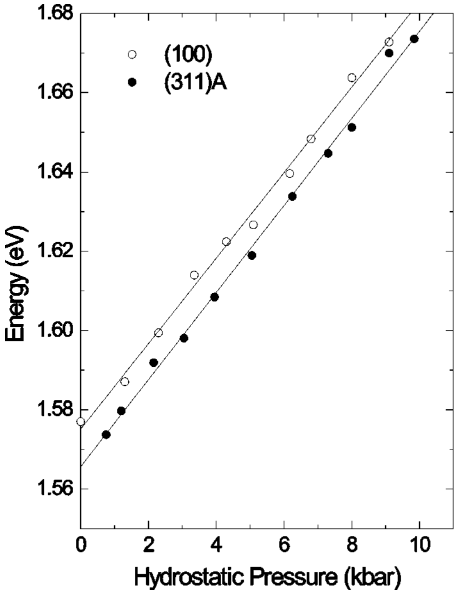

FIG. 4. The PL peak energy versus pressure for the (100) and (311)*A* GaAs QW's. For a given pressure, the (311)*A* PL emission energies are shifted to lower energies with respect to the (100) sample (redshift). The lines are a guide for the eyes.

In order to study the shift of the QW PL emissions for large misorientation angles and relatively wider QW's, we have made PL experiments in three $In_{0.2}Ga_{0.8}As$/GaAs QW's (30 Å wide) grown on (311)*A*, (311)*B*, and (100) substrates. There is a blueshift of the (311)*A* and (311)*B* PL emission energies with respect to the energy of the (100) sample.

The calculations have shown very good agreement with the experimental blueshift, considering only a homogeneous distribution of strain inside the (311)*A* and (311)*B* QW's. It is reasonable to accept that phenomena occurring next to the interfaces, like an inhomogeneous distribution of strain and indium segregation, will play a less significant role in the QW PL emissions as the QW becomes wider. The accordance between our theoretical and experimental results in the approximation used is qualitatively supported by previous results,[3] where relatively wider QW's account for a less important inhomogeneous strain effect.

The role of strain in the PL emissions was also studied in (100)- and (311)*A*-oriented GaAs/AlGaAs samples. In this case, the deformations are created by a hydrostatic pressure produced by a liquid piston-cylinder optical cell. Now the strain in the sample is not created by a mismatch of materials but by an *external* agent. As the pressure increases, the experimental data show a blueshift of the PL energies with respect to the zero (atmospheric) pressure, for both samples. As a consequence, the effects of deformations can be highlighted in order to show the qualitative influence of strain on the PL blueshift, regardless of the growth direction.

The theoretical model explains very well the observed blueshift in the experiments, emphasizing the role of nonhydrostatic strain produced by a hydrostatic stress. Our results corroborate the fact that the nonhydrostatic distribution of strain is more pronounced in the (311)*A* GaAs/AlGaAs QW, being a qualitative observation of the complicated pattern of strain distribution in (311) samples with no specific regard to the mechanisms that rule this distribution.

Note that we have discussed two different kinds of blueshift. In pseudomorphic InGaAs/GaAs QW's it is associated to a difference in PL energies between two QW's induced by the misorientation angle; in GaAs/AlGaAs samples the blueshift is associated with a difference in PL energies of the same QW, induced by the hydrostatic pressure. However, at the same pressure, we can see from Fig. 4 that there is a *redshift* of the (311)*A* GaAs/AlGaAs QW PL emission with respect to the (100). A hypothetical simulation of the InGaAs/GaAs samples studied here indicates that in the absence of strain there will also occur a *redshift* of the PL emissions of the high-index pseudomorphic QW in instead of a blueshift. As a consequence, our results confirm the strict relation between the strain and the blueshift in pseudomorphic samples.

Furthermore, the obtained experimental results under hydrostatic pressure corroborate the fact that the blueshift is closely related to the existence of only normal strain components in the QW, giving an additional support for considering zero the shearing strain ($\epsilon_{yz}=0$) in the transformation expressed by Eq. (2).

The results also indicate that the blueshift for the (311) InGaAs/GaAs samples is mainly due to the effect of the biaxial strain on the valence band and the blueshift for the GaAs/AlGaAs samples is mainly due to the action of hydrostatic strain on the conduction band. So our results emphasize that (normal) strain leads to a blueshift, but its influence on the conduction and valence bands depends on its nature.

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