Influence of piezoelectric fields on Rydberg energies in (Ga,In)As-GaAs single quantum wells embedded in *p-i-n* structures

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We have performed a variational calculation of the heavy-hole exciton for (Ga,In)As-GaAs strained-layer quantum wells embedded in *p-i-n* structures. The calculation has been made for sample growth along both the (001) and (111) directions. We show that the influence of the piezoelectric field may sometimes lead to strong orientation-dependent properties. In particular, when piezoelectric fields are present, the radiative lifetimes of heavy-hole excitons are strongly dependent on the thickness of the (Ga,In)As layer.

I. INTRODUCTION

There is great interest in the knowledge of the Rydberg energies of semiconductor quantum wells grown away from the standard (001) direction, and its piezoelectric-field dependence. First, we can invoke basic physical reasons such as: how long does the electron-hole pair remain bound? Second, we research the technological aspects. The threshold current for (111)-grown GaAs-(Ga,Al)As-based lasers is expected to be lower than for equivalent (001) lasers.[1] Combining this property, which is inherent to the geometry, with built-in strain effects by using (Ga,In)As strained layers might further lower this threshold current. Zinc-blende semiconductor compounds are submitted to strong internal piezoelectric fields if grown *with* the strain away from the (001) direction.[2] This was noticed by Smith and Mailhot who studied the effect for several superlattice combinations.[3] The extent of the influence of the piezoelectric fields on device performance is not yet known, since the physics is still at an early stage. The purpose of the present paper is to offer a comparison between the exciton binding energies and exciton radiative lifetimes of (001)- and (111)-grown (Ga,In)As-GaAs quantum wells, a combination of III-V compounds with strong technological potential for optoelectronics applications.

II. BASIC EQUATIONS AND METHOD

The resolution of the long-range Coulomb interaction in anisotropic physical systems where translational symmetry has been artifically broken, as in quantum wells, was initiated by Bastard a few years ago.[4] In his work, he focused on (001)-grown quantum wells and used the variational theorem to solve such a problem. In order to quantify the strengths of the approximations, and in order to obtain the numerical solutions, one can use trial functions which have degrees of sophistication.[5,6] Then, it becomes possible to show concretely the physical impact of the different variational parameters introduced in the different trial functions. Sophiscated calculations were made *a posteriori*, with more complete descriptions of the exciton wave functions, taking into account mass mismatch including contributions of states away from zone center, and dielectric-constant differences showed that the simple variational calculation weakly underestimated the Rydberg energies,[7–9] but was in turn an extremely good approximation. Besides this, since it can be easily extended to any potential line shapes, we have used it in this work.

In this spirit, we resolve the second-order differential equation of Ref. 4 where the eigenvector is written in cylindrical coordinates as

$$\Psi_{\rm exc}(z_e,z_h,\rho)=\chi_e(z_e)\chi_h(z_h)\Phi(\rho)\ , \tag{1}$$

where χ_e and χ_h are the standard envelope functions for electrons and heavy holes, respectively, obtained by solving a one-dimensional potential problem. As usual, the excitonic trial function is taken as $\Phi(\rho)=2/\lambda\exp(-\rho/\lambda)$, where λ is the variational parameter.

Before continuing, we wish to point out that using such a trial function has a wide range of applicability. It is no longer valid in the case of wide wells, when the energy splitting between the light holes and heavy holes becomes too small with respect to the Rydberg energy. An adapted version of the variational method was proposed by Deleporte *et al.*[10] and Peter *et al.*[11] for solving the problem of marginal potentials. Thus, we limited the calculation to well widths smaller than 150 Å and to indium compositions larger than 2%. The strain-induced splitting between the light holes (heavy holes) is larger than 9.4 meV (11 MeV), giving rise to valence (heavy hole) and conduction step values larger than 8 meV (6.2 meV) and 16 meV (12.3 meV), respectively. The electron–light-hole gap is marginally type II,[12] and the corresponding exciton problem cannot be treated by using the method developed here, but requires one to adapt the treatment of Refs. 10 and 11.

The resolution of the mathematical problem has been intentionally complicated as follows: instead of working in the context of flat barriers, we have biased the structures to reconcile the abstract calculation with a potential application. Moreover, embedded structures with built-

in piezoelectric fields in *p-i-n* structures eliminate residual mobile charges which are susceptible to screening the piezoelectric field.[3] A typical value of 1.5×10^4 V/cm (0.15 mV/Å) was taken from the device physics and used in the calculation. It corresponds to the *p-i-n* field in a 1-μm-thick undoped GaAs layer sandwiched between two *p*- and *n*-type degenerated GaAs layers.

III. RESULTS AND DISCUSSION

A. Envelope functions

The sketches of the conduction and valence potential profiles are different for (001)- and (111)-grown samples.[13] This is not surprising, and it results in cubic symmetry of the zinc-blende lattice. The deviation from spherical symmetry leads to anisotropic valence-band splitting. Figure 1 displays the evolution of this splitting with indium composition for both (001) and (111) built-in biaxial strains.

Figure 2 illustrates the electron and heavy-hole envelope functions for a 10-nm-wide $Ga_{0.92}In_{0.08}As$ well for the (001) and (111) orientations. The piezoelectric field (one order of magnitude larger than the *p-i-n* field for 10% indium) when taken opposite to the *p-i-n* field causes more signifincant changes than in the other case. This situation can be obtained by growth on a (111)*B* *n*-doped GaAs substrate: the InGaAs lattice is larger than the GaAs one, thus the polarization vector points from the cation to the anion *B* face.[14]

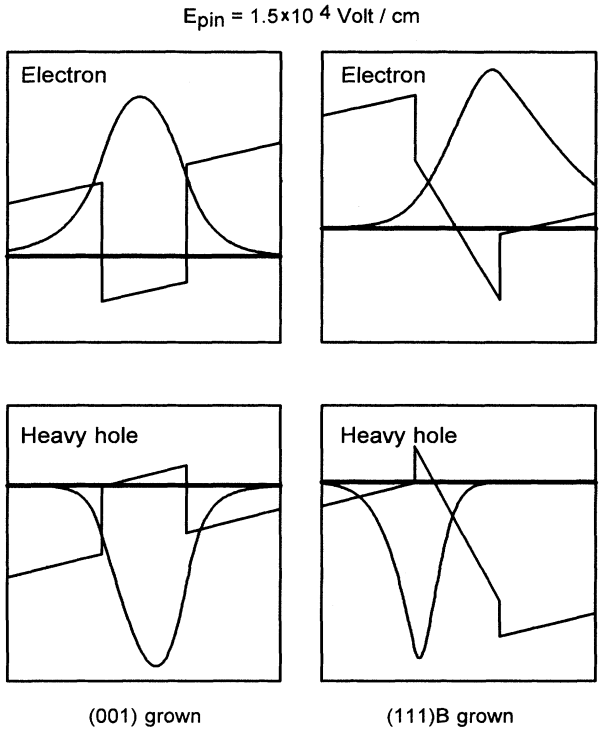

FIG. 2. Sketch of band line ups and envelope functions for two growth orientations.

B. Rydberg energies and oscillator strength

Figure 3 represents a plot of the (001) Rydberg energy at various indium compositions and for well widths smaller than 15 nm. This behavior is rather standard. Working at a constant well width, the Rydberg energy increases with increasing indium content: the deeper the

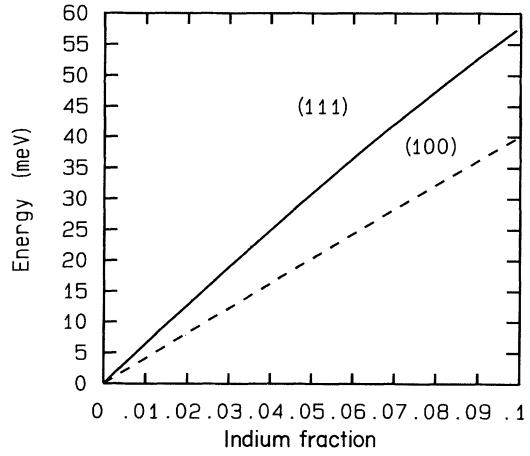

FIG. 1. Valence-band splitting for (Ga,In)As layers pseudomorphically grown onto GaAs substrate. Full line for (111) growth, dashed line for (001) growth.

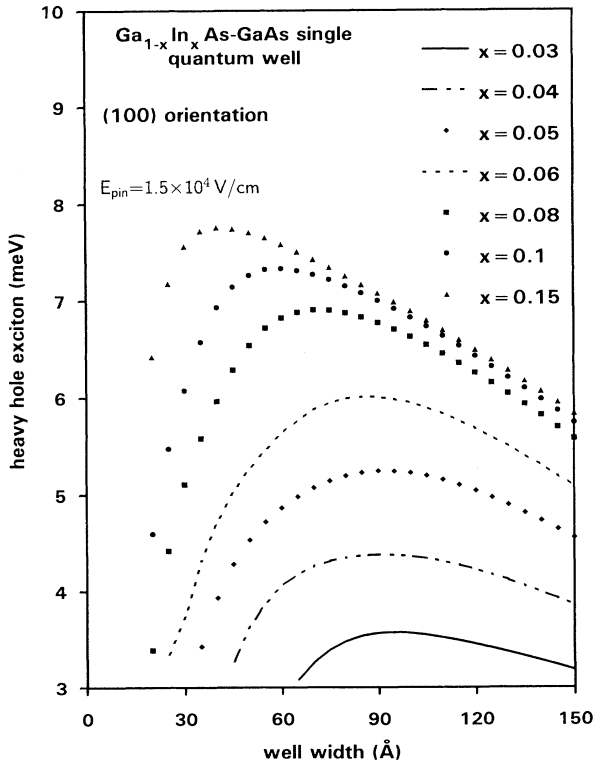

FIG. 3. Heavy-hole Rydberg energies for (Ga,In)As-GaAs (001)-grown single quantum wells embedded in a *p-i-n* structure.

confining potentials, the stronger the Rydberg energy. At a given indium composition, the Rydberg energy exhibits a maximum for a well-thickness value which results from balancing contributions of in-plane and on-axis effects with the Coulomb attraction. The situation is somewhat different for the (111) calculation and is reported in Fig. 4. We first notice that the Rydberg energy decreases when the indium content increases. This is in contrast with the (001) case and can be interpreted on a basis of arguments linked to envelope functions. For shallow potential steps, when the *p-i-n* field and the piezoelectric field have comparable (but opposite) values, the average electron coordinate $\langle z_e \rangle$ is much more sensitive to well-width effects than the heavy-hole one $\langle z_h \rangle$, essentially because the heavy-hole mass is particularly heavy, ~ 1 in the (111) direction. For higher indium content, the piezoelectric field dominates and leads to a spatial separation of the carriers, increasing λ. For thin wells, the situation is much more complicated to discuss. A general trend is observed: When the confined level is in the triangular part of the well, its envelope functions are much more sensitive to well-width modification than when the confined energy lies above this energy region when it "sees" wells which can be considered as essentially rectangular.

If Rydberg values are calculated in a ratio of 2, in Fig. 4, the situation is much more dramatic for oscillator strengths $|\Psi(0)|^2$, as shown in Fig. 5. For an indium content of 10%, this quantity scales almost four decades. This will have strong implications at the scale of radiative lifetimes $[\tau_{\text{rad}} \sim |\Psi(0)|^{-2}]$. A series of quantum wells

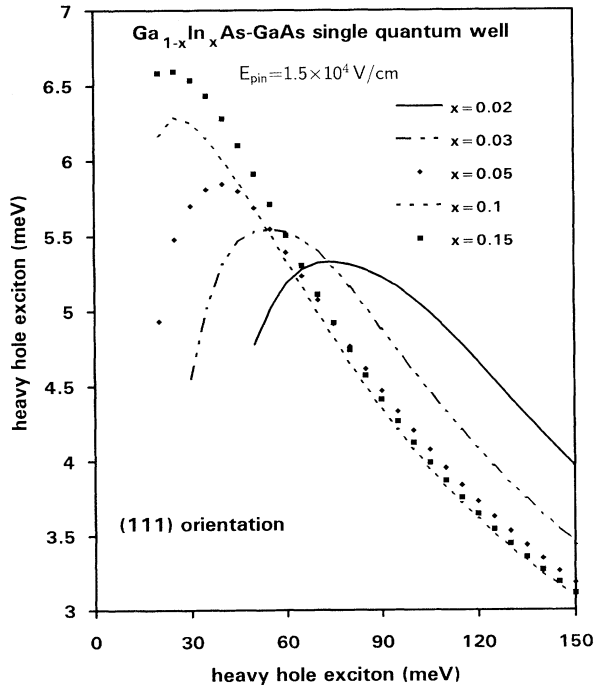

FIG. 4. Heavy-hole Rydberg energies for (Ga,In)As-GaAs (111)-grown single quantum wells embedded in a *p-i-n* structure. The piezoelectric field is opposite to the *p-i-n* field.

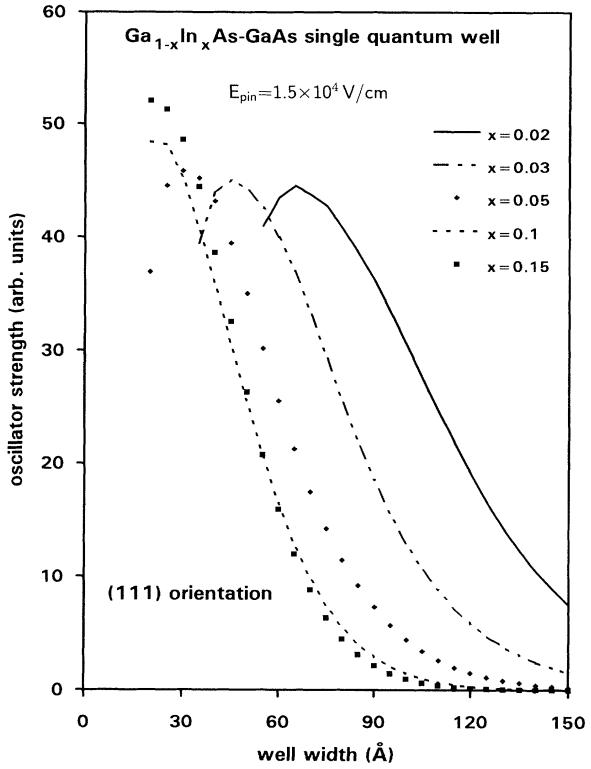

FIG. 5. Plot of the oscillator strength corresponding with the heavy-hole exciton energies of Fig. 4.

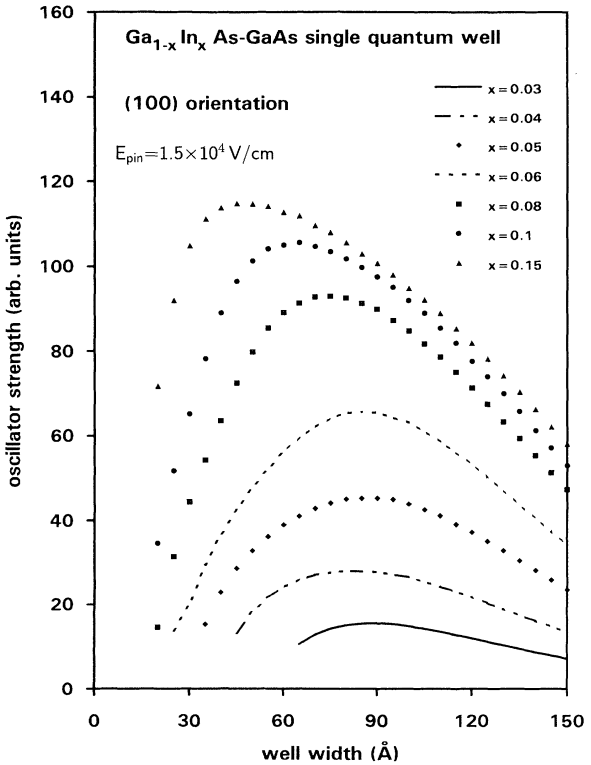

FIG. 6. Plot of the oscillator strength corresponding with the heavy-hole exciton energies of Fig. 3. Data reported here and in Fig. 5 are given at the same scale.

grown with identical indium content but various thicknesses will exhibit strongly different radiative lifetimes. Figure 6 is the analog of Fig. 5, and shows that the effect is not so dramatic for the (001) sample without a piezoelectric field opposite to the *p-i-n* field. Therefore, we understand why the piezoelectric field can be easily screened by photoinjection in (111)-grown 10-nm-thick $Ga_{0.92}In_{0.08}As$-GaAs,[15] or 25-nm-thick $Ga_{0.945}In_{0.055}As$-$Ga_{0.85}Al_{0.15}As$[16] single quantum wells while the effect is not observed for (001)-grown samples.

IV. CONCLUSION

We have calculated the exciton binding energy in (Ga,In)As-GaAs single quantum wells along the (001) and (111) directions embedded in *p-i-n* structures. The main influence of the built-in piezoelectric field is to produce a spatial separation of the electron-hole pair, making it possible to change the exciton radiative lifetime over more than three decades for (111)-grown strained-layer quantum wells.

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