Spatial dependence of the strain-induced coupling in highly strained quantum wells

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The strain-induced modifications of the orbital components of the valence-band wave functions in strained GaAs quantum wells grown on GaP substrates and strained InAs quantum wells grown on GaAs substrates are studied. The relative weight of the orbital components is analyzed by comparing the piezoreflectance and the derivative of the reflectance spectra. Depending on the localization of the wave function the strain-induced changes are very different. [S0163-1829(96)01847-4]

Heterostructures of materials that have different lattice parameters have internal strains that influence strongly their properties.¹ Most of the studies are related to systems where the magnitude of the built-in strain is small. A very interesting and less studied situation is the case of the heterostructures where the strain produces modifications of the energies that are equivalent to the spin-orbit (SO) splitting. In those systems the valence-band wave function may be strongly modified. In this paper the strain-induced changes of the valence-band wave functions are analyzed. Two cases will be considered here: one where the hole wave functions are localized in the strained material of the heterostructure, and another where the hole wave function has a strong amplitude in the unstrained region of the heterostructure. The first case corresponds to strained GaAs quantum wells (QW's) grown on GaP substrates. Due to the band alignment the hole wave functions are localized in the strained GaAs QW's. Moreover, GaP and AlAs have very similar electronic structure and also both materials have similar band alignment with GaAs. The main difference between the QW's of GaAs grown on GaP or on AlAs is the strain present in the GaAs layers when they are grown on GaP. Therefore the effect of the strain can be distinguished from the effect of confinement. The second case corresponds to strained InAs QW's grown on GaAs substrates. In this system due to the small thickness of the InAs QW (1 ML) and to the band alignment the wave functions of the holes penetrate in the GaAs unstrained barriers. Despite the higher value of the strain to which are submitted the InAs layers as compared with the preceding case, due to the delocalization of the wave function the strain-induced modifications of the wave function are very different.

In bulk material, the wave functions of the valence bands at the Γ point have $\{p_x, p_y, p_z\}$ components, being $\{x, y, z\}$: $\{[100], [010], [001]\}$. Heavy-hole (hh) wave functions have only p_x and p_y components, whereas light-hole (lh) and SO wave functions also have a p_z component. The effect that an external applied stress has on those states has been discussed by several authors.^{2,3} The nonhydrostatic component of the applied stress is normally not very high. On the contrary the

built-in strain present on strained heterostructures may have strong nonhydrostatic components. Let us consider the case of strained heterostructures oriented along the $[001]$ direction. An in-plane strain in the (001) plane couples the lh and SO states. If the tetragonal component of the uniaxial strain produces changes in the energy levels that are of the same order as the SO splitting, strong modifications of the orbital components of the lh and SO wave functions may appear. In particular, for a highly compressed material the lh state loses the p_z component, which is transferred to the SO state. Therefore, the orbital components of lh-like states may be very different from the equivalent states of the unstrained heterostructures. A method to analyze the orbital components of the electronic states is to compare the piezoreflectance and the derivative of the reflectance spectra. In a piezoreflectance experiment a very small sinusoidal in-plane strain is applied to the sample. The main effect of this modulated strain is to modify the energy of the transitions. The magnitude recorded is the normalized change of the reflectance due to the modulation of the transition energies. Therefore the piezoreflectance spectra and the derivative of the reflectance are very similar; the difference is that in the piezoreflectance spectra a modulating factor affects each optical transition. This piezomodulating factor is proportional to the modification of the energy of the transition due to the applied in-plane strain; its value depends on the type of transition observed. A $[001]$ in-plane strain does not produce the same effect on a state with p_x and p_y components as in a state that has also a p_z component. For example, in a $[001]$ -oriented GaAs/Al_xGa_{1-x}As QW a $\{001\}$ in-plane strain produces a modification of the energy of the transition of about 2.7 times higher for a lh-like transition than for a hh-like transition and an equivalent enhancement of the lh-like transition in the piezoreflectance spectra has been observed when compared with the derivative of the reflectance.⁴

Despite the large lattice mismatch between GaAs and GaP (3.7%) strained GaAs QW's can be grown pseudomorphically on GaP substrates for GaAs QW thicknesses up to 5–6 ML. The band alignment between GaAs and GaP is not well known. We have determined it by studying the optical properties of several strained GaAs quantum wells. Three strained GaAs quantum wells were grown on GaP substrates.

FIG. 1. Experimental (full points) and theoretical (lines) energies of the hh-like and lh-like transitions in strained GaAs QW's grown on GaP substrates as a function of the GaAs QW thickness.

The QW's were separated by 200 ML of GaP and the thickness of the QW's was varied between 2 and 6 ML. In Fig. 1 we present the experimental energy position of the two transitions observed in the piezoreflectance spectra related to the GaAs QW's as a function of the QW thickness. Also in Fig. 1 the calculated energy position is presented. The theoretical study can be done with simple envelope function models including the spin-orbit band, or with more sophisticated tight-binding Hamiltonians. Because the tight-binding Hamiltonians describe the electronic band structure in the full Brillouin zone of the bulk crystal and take into account all the couplings between the different bands we decided to use the tight-binding approach. The calculation was made by using a nearest-neighbor empirical tight-binding (ETB) Hamiltonian model with sp^3s^* orbital basis,⁵ including spin-orbit splitting.⁶ The ETB parameters of Priester *et al.*,⁷ were used for GaP, which is not strained, and the TB parameters of GaAs are given in Table I. Those values give a better description of the deformation potentials than the values of Ref. 7. The strain modifies the interatomic distances and bond angles. In an ETB model this results in modifications of the angular dependence of the structure factors⁸ and of the nondiagonal Hamiltonian parameters, which are usually evaluated by a scaling formula of the type⁹ $H_{\alpha\beta}(d) = H_{\alpha\beta}(d_0)(d/d_0)^{-\nu}$, where α, β are atomic orbitals, and d_0 and d are the unstrained and strained interatomic distances, respectively. The value of ν depends on the atomic orbitals α, β . The values of ν_{sp} and ν_{sp^*} are taken from Ref. 7, whereas $\nu_{ss} = 4.4$ and $\nu_{pp} = 2.596$ have been fitted to reproduce the experimental hydrostatic deformation potential of the conduction-band minimum and fundamental transition of GaAs.¹⁰ The calculations were performed by using the surface Green-function matching method,¹¹ and the only parameter adjustable is the valence-band offset (VBO) between GaAs and GaP. The results of Fig. 1 correspond to a VBO of 0.4 eV, where we have used the following energy reference: $E_V(\text{GaP}) = 0$ eV and $E_V(\text{GaAs}) = 0.4$ eV at the Γ point. The two transitions observed are attributed to transitions between

FIG. 2. (a) Spatial distribution of the total LDOS for the first lh-like valence band state of a GaAs QW of 6 ML. (b) Spatial distribution of the ratio between the p_z and p_x components for the same state.

the first and second confined states of the valence band and the first confined state of the electron with a strong s component, respectively. In the figure they are labeled according to the nature of the bulk valence band states from where they

TABLE I. Empirical matrix elements of the sp^3s^* Hamiltonian, in eV, including the spin-orbit splitting λ [a denotes anion, c denotes cation]. C_{11} and C_{12} are given in units of 10^{10} N m⁻².

	InAs	GaAs
$E(s,a)$	-9.5381	-8.3431
$E(p,a)$	0.7733	0.9252
$E(s^*,a)$	7.2730	7.4249
$E(s,c)$	-2.7219	-2.6569
$E(p,c)$	3.5834	3.5523
$E(s^*,c)$	6.6095	6.6235
$V(s,s)$	-5.6052	-6.4513
$V(x,x)$	1.8398	1.9546
$V(x,y)$	4.3977	5.0178
$V(sa,pc)$	3.0205	4.4607
$V(sc,pa)$	5.3894	5.7413
$V(s^*a,pc)$	3.2191	4.3083
$V(s^*c,pa)$	3.7234	4.6473
λ_a	0.1385	0.1338
λ_c	0.1290	0.0553
C_{11}	8.33	11.81
C_{12}	4.53	5.32

FIG. 3. Derivatives of the piezoreflectance and of the derivative of the reflectance spectra of a strained GaAs QW of 6 ML. The transitions are labeled according to the nature of the valence-band states. The spectra have been normalized in such a way that the transition corresponding to the hh has the same intensity in all of them.

originate. The experimental value of the VBO obtained can be compared with the theoretical estimation of the midgap energy model 0.31 eV (Ref. 12) or the model-solid theory 0.56 eV.¹³

A very interesting result is the relative weight of the orbital components of the wave function of the second confined state of the valence band. This state comes from the lh band. The wave function of this level is localized in the strained GaAs layers. As a result of this localization the relative weight of the orbital components changes strongly as

FIG. 4. Piezoreflectance and derivative of the reflectance spectra of a strained InAs QW grown on GaAs substrates. The QW related transitions are labeled according to their character. The spectra have been normalized in such a way that the transition corresponding to the hh has the same intensity in all of them.

FIG. 5. (a) Spatial distribution of the total LDOS for the first lh-like valence-band state of a InAs QW of 1 ML. (b) Spatial distribution of the ratio between the p_z and p_x components for the same state.

compared with the same state in GaAs/AlAs QW's. For example, in Fig. 2 we present the spatial dependence of the local density of states (LDOS), which is proportional to the squared amplitude of the wave function, for a GaAs QW of 6 ML. In that figure we present the spatial dependence of the total LDOS of the lh wave function. As can be observed most of the lh wave function is localized in the strained GaAs region. Also in that figure the spatial dependence of the relative contribution of the p_z and p_x components is presented. As can be observed this ratio decreases strongly in the strained region due to the coupling between lh and SO states induced by the strain. On the contrary in the unstrained GaAs/AlAs system the p_z component has a weight higher than the p_x and p_y component. Due to the negligible value of the p_z component and due to the similar localization of the first confined (hh-like) and second confined (lh-like) valence-band states, we expect that for light polarized in the growth plane the transition between those states and the first confined state of the conduction band with strong s component should have a similar intensity. Moreover, because both valence-band states have nearly identical orbital components both transitions should have very similar piezomodulation factors. These two facts can be observed in Fig. 3 where we present the derivative of the piezoreflectance spectra and the second derivative of the reflectance spectra of the 6-ML sample. The derivatives are presented to enhance the transition coming from the QW. As can be observed both transitions have similar intensity and the ratio between the piezomodulation factors of the lh and hh transitions is 1.2, where

the theoretical value for this ratio is 1.23. This calculated ratio was obtained from the transition energies that result when the whole structure is submitted to an in-plane compression and extension of 0.1%. In that way the spatial distribution of the states and the different deformation potential of the binary compounds are taken into account. This behavior is completely different from that observed in unstrained GaAs/AlAs QW's. For the equivalent transitions and experimental setup to the one used here the hh-like transition has an intensity approximately 3 times greater than the lh-like transition, and the ratio between the piezomodulation factors is about 2.4–2.8. This difference is due to the coupling induced by the strain between the lh and SO states, and also to the localization of the wave function in the strained region. If the VBO between GaAs and GaP were so that the valence-band wave function were not localized in the strained region no such changes in the orbital component should be observed.

Due to the high lattice mismatch between GaAs and InAs (7.1%) only strained InAs QW's with a thickness of 1.5–1.7 ML can be grown pseudomorphically on GaAs substrates.^{14,15} In Fig. 4 we present the piezoreflectance and DR spectra of an InAs QW of 1 ML. We observe two transitions related to the InAs QW and another one related to the GaAs. From the position of the transitions a VBO of 0.05 eV is obtained, where we have used the following energy reference $E_V(\text{InAs})=0$ eV and $E_V(\text{GaAs})=0.05$ eV at the Γ point. The InAs QW related transition arises from the first (hh-like) and second (lh-like) states in the valence band with a concentration in the InAs layers and the first level of the conduction band with a concentration in the InAs layers, respectively. They are labeled in the figure according to their character. The TB parameters used here are given in Table I. With those parameters a good description of the valence band, conduction band, and deformation potential parameters

of InAs is obtained. This VBO is also again between the theoretical estimations of the midgap model 0 eV (Ref. 12) or the model-solid theory 0.23 eV.¹³ If we compare this system with the previous one a very different behavior is observed. In particular a clear enhancement of the lh transition is observed in the piezoreflectance spectrum. Such enhancement is observed for a system that has an in-plane strain much higher than the preceding one (the lattice mismatch between GaAs and InAs is 7% whereas the lattice mismatch between GaP and GaAs is 3.7%), but the localizations of the wave functions are completely different. In Fig. 5 we present the spatial dependence of the total LDOS of the lh wave function. As can be observed most of the lh wave function is localized in the unstrained region. Also in that figure the spatial dependence of the relative contribution of the p_z and p_x components is presented. As can be observed this ratio decreases in the strained region due to the coupling between lh and SO states induced by the strain. The calculated value of the ratio of the piezomodulated factors is 2.7, which compares with the experimental value of 2.5.

In conclusion we have analyzed the effect of the strain-induced coupling between the lh and SO states in highly strained materials. We have studied strained GaAs QW's grown on GaP substrates. In this system the hole wave functions are localized in the strained GaAs region. The strain produces a strong reduction of the weight of the p_z orbital components in the lh-like levels. Such reduction of the p_z component of the lh level is not so important in the case of strained InAs QW grown on GaAs substrates due to the fact that the wave functions are not so strongly localized in the strained region.

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