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Effects of compressive uniaxial stress on the electronic structure of GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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We present a theoretical analysis of the effects of compressive uniaxial stress on the electronic structure of GaAs-$Ga_{1-x}Al_xAs$ quantum wells grown along the [001] axis. Strain interactions are incorporated by use of known deformation potentials of the bulk semiconductors, and, therefore, our analysis contains no adjustable parameters. We consider the cases where the external uniaxial stress **X** is parallel (**X** ∥ [001]) and perpendicular (**X** ∥ [100]) to the [001] growth axis of the quantum well. Our results indicate that, unlike the bulk case, the strain-induced energy shifts depend sensitively on whether the compressive stress is applied along the [001] or [100] axis. These differences are a direct consequence of the mixing of the bulk heavy-hole and light-hole states by the strain interactions and by the quantum-well potential. For **X** ∥ [100], the strain-induced energy shifts associated with the heavy- and light-hole quantum-well states are strong nonlinear functions of the magnitude of the applied compressive stress due to the admixing by the strain Hamiltonian of the corresponding bulk states. However, for **X** ∥ [001], a strong nonlinear behavior is only predicted for the light quantum-well states due to the mixing between the bulk light and spin split-off states. The strain-induced energy shifts are dependent on the GaAs quantum-well thickness. The results of our analysis are in excellent agreement with experimental measurements of strain-induced energy shifts in quantum wells.

Much information on the nature of an electronic state can be obtained by monitoring its response to an externally applied field (electric, magnetic, strain, etc.). In most cases, the field lowers the symmetry of the system, and the symmetry properties of the perturbed states are revealed by their response to the applied field. There is currently a great deal of interest in the study of the response of spatially confined electronic states in semiconductor quantum wells to the application of electric,[1] magnetic,[2] and strain[3] fields.

We present a theoretical study of the effects of an applied compressive stress on the electronic structure of GaAs-$Ga_{1-x}Al_xAs$ quantum wells grown along the [001] axis. We specifically consider the cases where the uniaxial stress **X** is applied in a direction *parallel* (**X** ∥ [001]) and *perpendicular* (**X** ∥ [100]) to the [001] growth axis of the quantum well which is chosen to coincide with the spin quantization axis. In contrast with bulk behavior, the strain-induced energy shifts depend sensitively on whether the external compressive stress is applied along the [001] or [100] axis. For a stress applied perpendicular to the quantum-well growth axis and to the spin quantization axis, the heavy and light quantum-well states are admixed by the strain Hamiltonian. Consequently, the transition energies associated with the heavy and light quantum-well states are strong nonlinear functions of the magnitude of the applied stress and exhibit a behavior which depends on the thickness of the GaAs quantum well. However, for a stress applied in a direction parallel to the quantum-well growth axis and to the spin quantization axis, only the transition energies associated with the light quantum-well states show a strong nonlinear behavior as a function of the applied stress, because the strain Hamiltonian does not admix the heavy and light states.

The electronic-structure calculations presented below are based on a $\mathbf{k}\cdot\mathbf{p}$ formalism adapted to treat semiconductor heterojunctions and superlattices.[4,5] A distinctive feature of the present $\mathbf{k}\cdot\mathbf{p}$ theory is the correct description of the superlattice point-group symmetry.[6] This is accomplished by explicitly including the difference in crystal potentials between the constituent semiconductors forming the superlattice. At a general $\mathbf{k}$ point, the bulk Bloch states in each semiconductor are expanded in terms of a single set of zone-center ($\mathbf{k}=\mathbf{0}$) basis functions which are energy eigenstates of a reference Hamiltonian. In the presence of stress, the bulk Hamiltonian acting on the cell-periodic part of a Bloch state in semiconductor i ($i=1,2$) is

$$H^{(i)}(\mathbf{k})=\frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2+V^{\mathrm{ref}}(\mathbf{x})+\Delta V^{(i)}(\mathbf{x})+H^{(i)}_{\mathrm{spin}}+H^{(i)}_{\mathrm{stress}}\ , \tag{1}$$

where the spin-orbit and stress interactions are described by $H^{(i)}_{\mathrm{spin}}$ and $H^{(i)}_{\mathrm{stress}}$, respectively. Explicit expressions for these operators in a zone-center representation can be found in Ref. 4. Spin-orbit and stress interactions are included in the description of the bulk Bloch states of the constituent semiconductors. The Hamiltonian describing the strain interactions, $H^{(i)}_{\mathrm{stress}}$, is written in terms of known deformation potentials of the bulk constituent semiconductors forming the quantum-well structure. The opera-

tor $\Delta V^{(i)}(\mathbf{x})$ is the difference between the pseudopotential of semiconductor i and that of the reference Hamiltonian,

$$\Delta V^{(i)}(\mathbf{x}) \equiv V^{(i)}(\mathbf{x}) - V^{\mathrm{ref}}(\mathbf{x}) \ , \tag{2a}$$

with

$$V^{\mathrm{ref}}(\mathbf{x}) \equiv \tfrac{1}{2}\left[V^{(1)}(\mathbf{x}) - V^{(2)}(\mathbf{x})\right] \ . \tag{2b}$$

The inclusion of $\Delta V^{(i)}(\mathbf{x})$ to second order in the energies and to first order in the wave functions in Lowdin perturbation theory affords a correct description of the superlattice point-group symmetry. As a result, energy-band crossings, mixings, and splittings are properly described within the confines of the present model.[6] Moreover, explicit consideration of the difference in the crystal potentials of the constituent semiconductors through the inclusion of the term $\Delta V^{(i)}(\mathbf{x})$ in the expression for the interface boundary conditions results in a mixing of the heavy, light, and spin split-off states throughout the superlattice Brillouin zone.

In the present $\mathbf{k}\cdot\mathbf{p}$ model, we explicitly include the zone-center basis states of the reference Hamiltonian belonging to the irreducible representations Γ_7, Γ_8, and Γ_6 of the T_d double group. An additional 46 zone-center states (including spin) are incorporated through Lowdin perturbation theory.[4,5] Momentum matrix elements are explicitly calculated from a pseudopotential plane-wave representation of the reference Hamiltonian and, therefore, the present model requires a minimum number of empirical parameters. These empirical parameters (energy band offsets, deformation potentials, elastic constants, spin-orbit splittings, etc.) are listed in Ref. 5 for GaAs and AlAs. We emphasize that the present analysis contains *no adjustable parameters* to describe the admixing of the bulk states by the strain interactions and by the quantum-well interfaces.

We now consider the effects of an applied compressive stress on the electronic structure of GaAs-$Ga_{1-x}Al_xAs$ quantum wells grown along the [001] axis. The present study is restricted to the alloy composition $x=0.30$, and we consider superlattices in which the $Ga_{1-x}Al_xAs$ layers are sufficiently thick so that the results for isolated GaAs quantum wells can be recovered. We analyze the strain-induced zone-center ($\mathbf{k}_{\parallel}=\mathbf{0}$) energy shifts of the heavy-hole to conduction (HH_1-C_1, HH_2-C_1) and light-hole to conduction (LH_2-C_1) transitions as a function of the orientation and magnitude of the applied compressive stress. Exciton binding energies are fairly invariant with respect to the magnitude of the applied stress[3] and consequently we neglect exciton effects in the analysis presented below. We consider, in turn, stress applied perpendicular ($\mathbf{X}\parallel[100]$) and parallel ($\mathbf{X}\parallel[001]$) to the [001] quantum-well growth axis. Strain interactions are included in the description of the bulk Bloch states of GaAs and

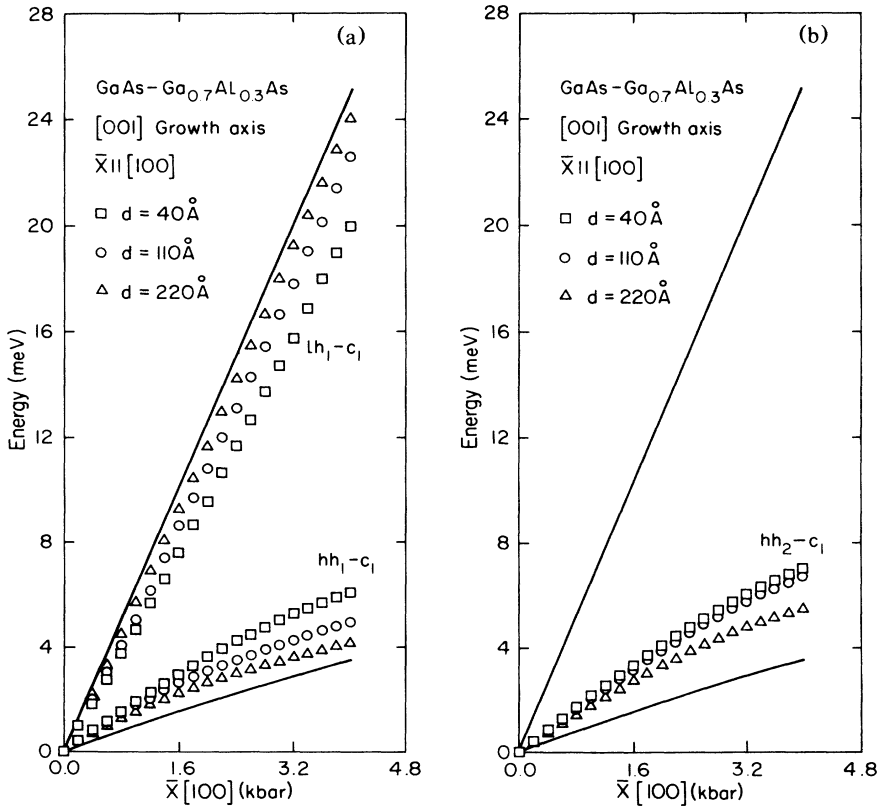

FIG. 1. Strain-induced transition-energy shifts for a compressive stress applied along the [100] axis of a GaAs-$Ga_{0.70}Al_{0.30}As$ quantum well grown along the [001] axis. (a) Transitions HH_1-C_1 and LH_1-C_1. (b) Transition HH_2-C_1. The strain-induced transitions in bulk GaAs are also indicated by the solid lines.

$Ga_{1-x}Al_xAs$ and therefore no adjustable parameters are required in the analysis whose results are presented below.

We quantize spin along the [001] quantum-well growth axis and denote its projection on the quantization axis by m_j. In the case of $\mathbf{X} \| [100]$, bulk light ($m_j = \pm \frac{1}{2}$) and heavy ($m_j = \pm \frac{3}{2}$) states are admixed by the bulk strain interactions. However, in the case of $\mathbf{X} \| [001]$, $|m_j|$ is a good quantum number for the bulk states, and bulk light ($m_j = \pm \frac{1}{2}$) and heavy ($m_j = \pm \frac{3}{2}$) states are not admixed by the bulk strain interactions, although they are admixed by the quantum-well potential.[6] These interactions result in strain-induced transition energy shifts which are nonlinear functions of the magnitude of the applied compressive stress. The nonlinear behavior is more pronounced when the corresponding bulk states are coupled by the bulk strain Hamiltonian.

Figure 1 indicates the zone-center ($\mathbf{k}_\parallel = \mathbf{0}$) strain-induced energy shifts for the transitions HH_1-C_1, HH_2-C_1, and LH_1-C_1 as a function of the magnitude of the compressive stress applied perpendicular to the [001] growth axis, $\mathbf{X} \| [100]$. We consider GaAs quantum wells of thicknesses equal to 40, 110, and 220 Å to compare with recent measurements of the strain-induced energy shifts in GaAs-$Ga_{0.70}Al_{0.30}As$ quantum wells.[3] The agreement between the results presented in Fig. 1 and the measurements reported in Ref. 3 is excellent and provides support to the theoretical formalism used herein. In fact, for applied compressive stresses up to 2 kbar (the range of pressure covered by the experimental study reported in Ref. 3), the discrepancy between the results afforded by our model and those reported in Ref. 3 is about 20% in the worst cases and generally less than 10% in most instances. The impressive agreement between the theoretical results presented here and available experimental measures is a truly remarkable achievement given that our theoretical analysis is *free of adjustable parameters* and, in this way, contrasts with the phenomenological model presented in Ref. 3. For comparison purposes, the zone-center strain-induced energy shifts for the HH-C and LH-C transitions in bulk GaAs are also shown in Fig. 1.

Inspection of Fig. 1 reveals that the strain-induced interactions between the heavy ($m_j = \pm \frac{3}{2}$) and light ($m_j = \pm \frac{1}{2}$) states result in zone-center energy shifts which are functions of the thickness of the quantum well. This result has its origin in the fact that the degree of admixture of light- and heavy-bulk states in the resulting quantum-well wave function depends on the quantum-well width. For thick quantum wells, the strain-induced zone-center energy shifts approach the bulk limit. For thin quantum wells, the pressure dependence of the zone-center energies deviate from the bulk behavior and can be traced in the interactions between the light and heavy states as these states are admixed by the external stress and by the quantum-well potential.

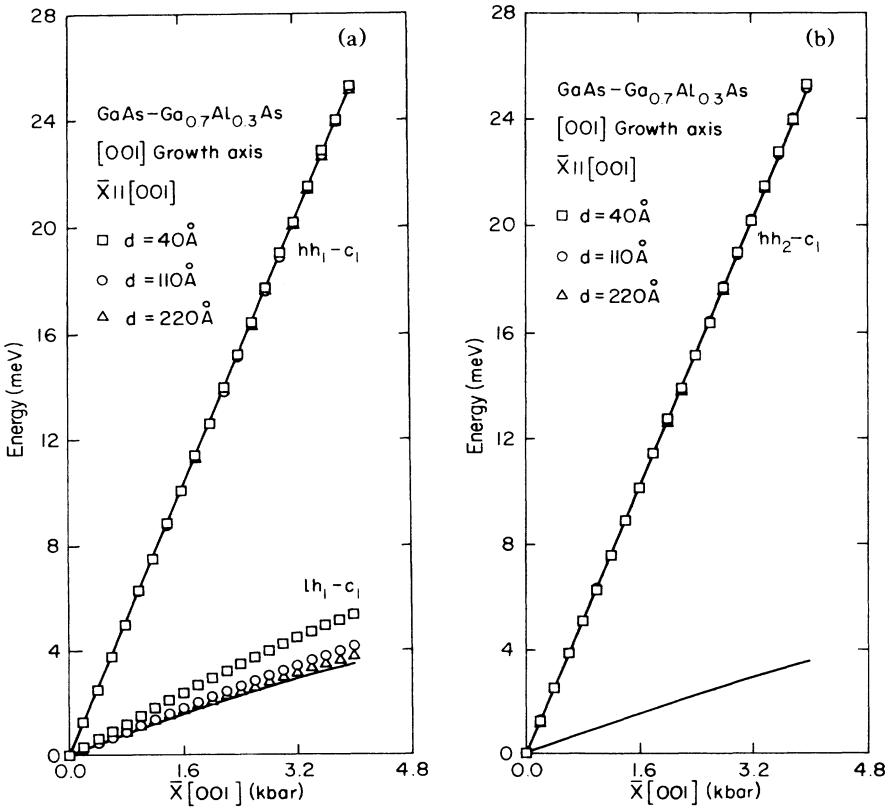

FIG. 2. Strain-induced transition energy shifts for a compressive stress applied along the [001] axis of a GaAs-$Ga_{0.70}Al_{0.30}As$ quantum well grown along the [001] axis. (a) Transitions HH_1-C_1 and LH_1-C_1. (b) Transition HH_2-C_1. The strain-induced transitions in bulk GaAs are also indicated by the solid lines.

Strain-induced energy shifts for the transition HH_2-C_1 are shown in Fig. 1(b). Comparison between Figs. 1(a) and 1(b) reveals that the strain-induced energy shifts are larger for the transition HH_2-C_1 than for the transition HH_1-C_1, indicating that the transitions to excited states deviate more from the bulk GaAs behavior. However, the thickness dependence of the strain-induced energy shifts is weaker for the HH_2-C_1 transitions than for the HH_1-C_1 transitions.

The results of our analysis on the zone-center ($\mathbf{k}_{\parallel}=\mathbf{0}$) strain-induced transition energy shifts for a compressive stress applied parallel to the quantum-well growth axis, $\mathbf{X}\parallel[001]$, are indicated in Fig. 2. Again, the zone-center strain-induced energy shifts for bulk GaAs are also shown for comparison. Inspection of Fig. 2 reveals that when the compressive stress is applied parallel to the quantum growth axis, the LH_1-C_1 transition energy shifts are thickness dependent and strongly nonlinear, whereas the HH_1-C_1 and HH_2-C_1 transitions are virtually independent on the quantum-well width and are very nearly linear functions of the magnitude of the applied stress. For a stress applied in a direction parallel to the spin quantization axis, the bulk strain Hamiltonian does not admix states with different values of $|m_j|$. The nonlinear behavior shown in Fig. 2 for the LH_1-C_1 transition results from the mixing by the strain Hamiltonian of the light-hole states $|j=\frac{3}{2}, m_j=\pm\frac{1}{2}\rangle$ and spin split-off states $|j=\frac{1}{2}, m_j=\pm\frac{1}{2}\rangle$. The slight nonlinearity revealed by Fig. 2 for the HH_1-C_1 and HH_2-C_1 transitions is the result of the mixing of the bulk heavy- and light-hole states by the quantum-well potential. This mixing is reproduced by our $\mathbf{k}\cdot\mathbf{p}$ model through the inclusion of the term $\Delta V^{(i)}(\mathbf{x})$ in the expression of the interface boundary conditions.

Comparison between Figs. 1 and 2 indicates that the strain-induced energy shifts are very different for the cases where the compressive stress is applied perpendicular ($\mathbf{X}\parallel[100]$) or parallel ($\mathbf{X}\parallel[001]$) to the quantum-well growth axis. These differences are a direct consequence of the mixing of the heavy- and light-hole states by the strain interactions. In the bulk, the distinction between the cases $\mathbf{X}\parallel[100]$ and $\mathbf{X}\parallel[001]$ is, of course, immaterial.

In summary, a realistic $\mathbf{k}\cdot\mathbf{p}$ model is used to analyze the effects of applied compressive stress on the electronic structure of GaAS-$Ga_{1-x}Al_xAs$ quantum wells. Strain interactions are embodied with our model through known deformation potentials of the bulk semiconductors and, therefore, our analysis is *free of adjustable parameters.* The strain-induced zone-center energy shifts are shown to exhibit very different behavior depending on the crystallographic axis along which the compressive stress is applied. In the case where the compressive stress is applied along a direction *perpendicular* to the [001] growth axis ($\mathbf{X}\parallel[100]$), the strain-induced energy shifts involving both the heavy- and light-hole quantum-well states are nonlinear functions of the magnitude of the applied compressive stress. Moreover, this behavior depends sensitively on the thickness of the GaAs quantum well and results from the strain-induced mixing between the heavy-, light-, and spin split-off-hole states which make up the quantum-well wave function. In the case where the compressive stress is applied along a direction *parallel* to the [001] growth axis ($\mathbf{X}\parallel[001]$), only the strain-induced energy shifts involving the light-hole quantum-well states are strong nonlinear functions of the magnitude of the applied compressive stress. Again, this behavior depends on the width of the GaAs quantum wells and results from the strain-induced mixing between the light- and spin split-off-hole states. Our calculations show a weak nonlinear behavior for the transitions involving the heavy-hole states. This nonlinearity results from the mixing of the heavy- and light-states by the quantum-well potential. The results of our parameter-free analysis are in excellent agreement with measurements of strain-induced energy shifts in GaAs-$Ga_{0.70}Al_{0.30}As$ quantum wells.[3]

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[1]R. T. Collins, K. v. Klitzing, and K. Ploog, Phys. Rev. B 33, 4378 (1986).

[2]L. L. Chang, in *Proceedings of the NATO Advanced Study Institute on Molecular Beam Epitaxy and Heterostructures,* edited by L. L. Chang and K. Ploog (Nijhoff, The Netherlands, 1985), p. 461.

[3]C. Jagannath, E. S. Koteles, J. Lee, Y. J. Chen, B. S. Elman, and J. Y. Chi, Phys. Rev. B 34, 7027 (1986).

[4]D. L. Smith and C. Mailhiot, Phys. Rev. B 33, 8345 (1986).

[5]C. Mailhiot and D. L. Smith, Phys. Rev. B 33, 8360 (1986).

[6]C. Mailhiot and D. L. Smith, Phys. Rev. B 35, 1242 (1987).