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SPIN–ORBIT-COUPLING, ELECTRIC-FIELD AND FREE-CARRIER-SCREENING EFFECTS ON VALENCE BAND STRUCTURE OF STRAINED COUPLED QUANTUM WELLS

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We have calculated the structure of the valence bands and its dependence on the electric field and the density of free carriers in a lattice mismatched single and double quantum well. Our calculation is based on simultaneous solving of the effective mass equation for the envelope functions and Poisson's equation. The 6×6 Luttinger–Kohn Hamiltonian is diagonalized into two 3×3 blocks by a unitary transformation. We have shown how including the coupling between spin–orbit split-off band and light- and heavy-hole bands influences the shape of the valence bands. Further it has been found that at high densities of the free carriers and at non-zero electric field, the free-carrier screening affects the valence band structure and wave functions. This effect is considerably pronounced in double quantum well because of large spreading of the quantum states. The studying of the above effects is useful for band-structure engineering.

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Semiconductor heterostructures made of lattice-mismatched materials are interesting from fundamental point of view and also because of their applications in device technology. This interest is caused by the fact that the strain induced by lattice mismatch modifies considerably optical and electronic properties of the structure.

A few years ago it was found [1] that coupling between the heavy-hole band, light-hole bands, and the spin–orbit split-off bands cannot be neglected even in a material with a relatively large spin–orbit split-off energy. The reason is that strain enhances intersubband interaction. The strained quantum well or multiple quantum well are semiconductor structures which are often utilized in the construction of semiconductor lasers. In the so-called field-effect quantum-well lasers electrons and holes are injected laterally by p- and n-junctions. In the lasing mode effects of the free-carrier screening at the applied gate field must be taken into account. This necessity was pointed out in Refs. [2, 3] but the strained structure was

not considered in those papers. The quantum well for a quantum laser is usually not simple; very often one uses the so-called separately confined quantum well or multiple quantum well (MQW). Differences between the band structure in a single quantum well (SQW) and MQW can be demonstrated by differences between SQW and a double quantum well (DQW, two wells separated by a thin barrier).

In the present paper we have calculated the valence band structure of strained SQW and DQW under an electric field applied perpendicular to the interface between different materials. The coupling of hole bands with the spin–orbit split-off band and the influence of free-carrier screening on the valence band structure have been taken into account.

For our calculation we have used the 6×6 Luttinger–Kohn Hamiltonian [4] in the basis $|\frac{3}{2},-\frac{3}{2}\rangle$, $|\frac{3}{2},-\frac{1}{2}\rangle$, $|\frac{1}{2},-\frac{1}{2}\rangle$, $|\frac{1}{2},\frac{1}{2}\rangle$, $|\frac{3}{2},\frac{1}{2}\rangle$, $|\frac{3}{2},\frac{3}{2}\rangle$, and the 6×6 Bir–Pikus Hamiltonian [5] for strain. The total Hamiltonian for the strained structure can be transformed [6] by a unitary transformation into a block diagonal form with a new basis of the states which will be denoted as $|1\rangle$, $|2\rangle,\ldots,|6\rangle$

$$\hat{\bar{H}} = \hat{U}\left(\hat{H}+V(z)\right)\hat{U}^{+} = \begin{pmatrix} \hat{H}^{\mathrm{U}} & 0 \\ 0 & \hat{H}^{\mathrm{L}} \end{pmatrix}, \tag{1}$$

where the upper and lower blocks, $\hat{H}^{\mathrm{U}}$ and $\hat{H}^{\mathrm{L}}$, are both 3×3 matrices. $V(z)$ is a step-like function, and elements of the matrix are functions of k_x, k_y, k_z, Luttinger mass parameters, deformation potentials and components of the strain tensor. Material of the quantum well is under biaxial strain and the strain-tensor components are

$$\epsilon_{xx}=\epsilon_{yy}\equiv\epsilon=\Delta a/a_0, \quad \epsilon_{zz}=-(2C_{12}/C_{11})\epsilon, \quad \epsilon_{xy}=\epsilon_{yz}=\epsilon_{xz}=0. \tag{2}$$

C_{11} and C_{12} are elastic constants, Δa is the difference of lattice constants.

In the envelope function approximation, which we used, the hole wave function has the form

$$\Psi_m^{\mathrm{U,L}}(r)=\sum_{\nu} f_m^{\nu}(k_{\|},z)\exp(\mathrm{i}k_{\|}\cdot\rho)|\nu\rangle, \tag{3}$$

where f^{ν} is the envelope function, $k_{\|}$ is the in-plane wave vector, $\rho$is the in-plane vector, $|\nu\rangle$ is the transformed Bloch basis at the zone centre. When solving the Schrödinger equation, we had to solve two sets of three coupled differential equations for the components of the "envelope-function vector" f, i.e.,

$$\sum_{\nu'}\left[H_{\nu\nu'}^{\mathrm{U,L}}+V_{\nu}(z)\delta_{\nu\nu'}\right]f_m^{\nu'}(k_{\|},z)=E_m^{\mathrm{U,L}}(k_{\|})f_m^{\nu'}(k_{\|},z). \tag{4}$$

$V_{\nu}(z)$ ($\nu=1$, 2 or 5, 6) is a step-like potential for holes modified by the hydrostatic part of the strain, while for $\nu=3$, 4 it is the step-like potential for the spin–orbit band.

The coupled differential equations were solved using the variational method [7, 8]. Eigenfunctions of the system (4) are written through coefficients which depend on $k_{\|}$ and the wave functions of the decoupled system. The problem is then reduced to finding eigenvalues and eigenfunctions of an $(n_{\mathrm{h}}+m_{\mathrm{l}}+k_{\mathrm{so}})\times(n_{\mathrm{h}}+m_{\mathrm{l}}+k_{\mathrm{so}})$ matrix, n_{h}, m_{l}, and k_{so} being the total number of heavy, light, and spin–orbit states, respectively. This is done by the Jacobi method of diagonalization.

The effect of external electric field F on valence band structure was calculated by including the term $-eFz$ into $V_v(z)$. The presence of the charged carriers causes the screening potential V_P which is the solution of the Poisson equation

$$(d^2/dz^2)V_P(z) = -(e/\varepsilon_0\varepsilon_r)\,[p(z) - n(z)]\,, \tag{5}$$

ε_0 (ε_r) is dielectric permittivity of the vacuum (material), $p(z)$ ($n(z)$) is the charge density of holes (electrons). Schrödinger and Poisson equations are solved self-consistently.

Calculations were performed for the semiconductor structure consisting of $In_{1-x}Ga_xAs$ wells and InP barriers. The thickness of the well L_W was 60 Å, while that of the barrier between the wells, L_B, was 30 Å. The lattice constant of the well material depends on the Ga mole fraction, thus this value determines the strain. We have constricted to the value $x = 0.27$, then the well material is compressed. This case is of interest for laser construction, since in compression the highest valence band has lower effective mass than in tension. The physical parameters depend on x and their values were taken from Ref. [9].

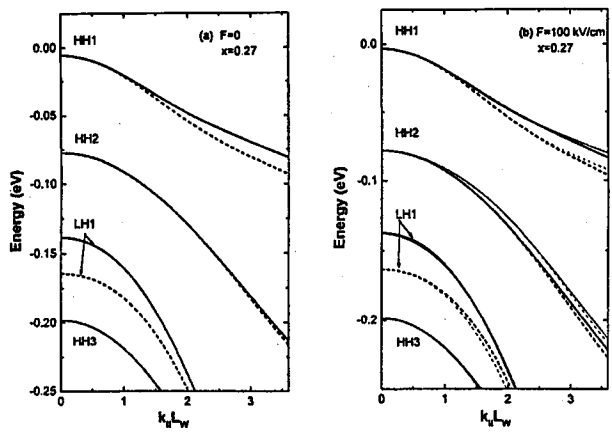

Fig. 1. Valence band structures of 60 Å $In_{1-x}Ga_xAs$/InP QW ($x = 0.27$) without applied electric field (a) and with electric field $F = 100$ kV/cm (b). Solid (dashed) lines represent calculations with (without) SO coupling, thinner lines in (b) are results obtained with H^L.

The results of the calculation of the valence band structure of the quantum well with (solid lines) and without (dashed lines) the spin–orbit (SO) coupling are shown in Figs. 1a (without field) and 1b (with applied electric field). At $k_\parallel = 0$ the SO coupling affects the energy of the light hole. For $k_\parallel \neq 0$ both light-hole and heavy-hole energies are changed by SO coupling. The picture is similar when the electric field is applied. Because of the asymmetry of the problem, results of calculations with H^U and H^L differ. For DQW (Fig. 2a) all energies are doubly degenerate at $k_\parallel = 0$ and for $k_\parallel \neq 0$ the degeneracy is lifted due to intersubband interaction. At applied electric field (Fig. 2b) energies are shifted and due to the breaking of the inversion symmetry H^U and H^L give different dispersion laws.

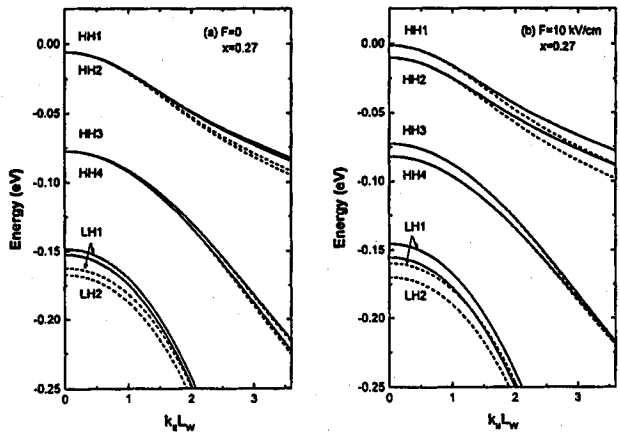

Fig. 2. The result of valence-band-structure calculation for DQW with 60 Å $In_{1-x}Ga_xAs$ ($x = 0.27$) wells and 30 Å thin InP barrier with electric field $F = 0$ (a) and $F = 10$ kV/cm (b). Solid (dashed) lines are results with (without) SO coupling. Only calculations with H^U are presented.

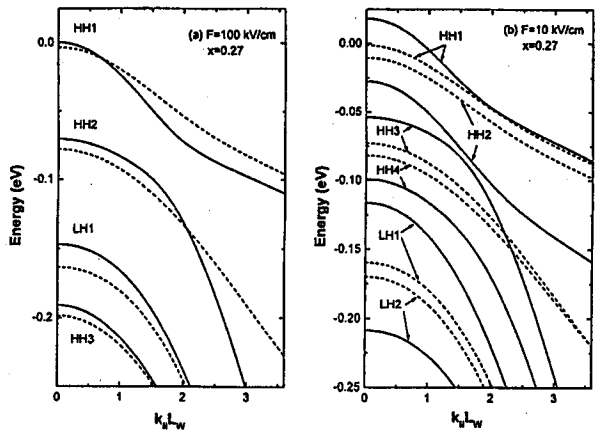

Fig. 3. (a) Valence-band structures of $In_{1-x}Ga_xAs$ ($x = 0.27$) QW of width of 60 Å with applied electric field $F = 100$ kV/cm with (solid lines) and without (dashed lines) free-carrier screening. (b) The same for DQW and $F = 10$ kV/cm. The electron and hole concentrations are equal, $N = P = 3 \times 10^{18}$ cm^{-3}.

In Fig. 3a the influence of injected charges on the valence band structure of the quantum well is shown. The electron and hole density injected is 3×10^{18} cm^{-3}. While for zero-electric field the inclusion of screening potential of charges has no considerable effect (not shown), applied gate field causes remarkable changes in the band structure due to carrier screening. The effect is even stronger for DQW (Fig. 3b). This is probably caused by space separation of electrons and holes and

by inducing internal electric field between those charges. A detailed description of this problem will be the subject of future study.

It was found that spin–orbit coupling affects all subband energies at finite $k_{\|}$, the effect being the strongest for the light-hole band. The variations of subband energy with $k_{\|}$ are smaller than those obtained with SO coupling, which causes changes in the density of states and also in laser gain. Further, the carrier-screening effect is remarkable, especially in the applied electric field.

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