The anisotropy of the in–plane dispersion relations of the hole subbands of GaAs–GaAlAs quantum well

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Abstract

The in–plane dispersion relations of the valence subbands of $GaAs-Ga_{0.7}Al_{0.3}As$ quantum well are calculated within the envelope function approximation. The anisotropy related with the difference between the Luttinger parameters γ_2 and γ_3 is taken into account consistently. The anisotropy proved to be considerable for the ground valence subbands of heavy and light holes and the great values of $k_\perp$. The cross sections of the constant-energy surfaces of the valence subbands by the k_xk_y plane are built. The envelope wave functions of the valence subbands as the mixture of the hole states distinguished in m_J at $k_\perp$=0 are found. The change of the percental contribution of the hole states different in m_J to the resultant state with $k_\perp$ varying is investigated.

Introduction

The in-plane dispersion relations and the Landau levels attached to the valence subbands of semiconductor heterostructures have recently been extensively studied in connection with magneto–optical experiments [1–11]. The great significance of the determination the $\mathbf{k}_\perp$–dependences of the eigenvalues $\varepsilon_n(\mathbf{k}_\perp)$ is primarily due to the fact that the transport and optical properties of the superlattices depend on the in–plane effective mass. This mass is determined from cyclotron resonance experiments with the magnetic field parallel to the superlattice axis. For instance, in case of a weak coupling between the wells, the galvanomagnetic phenomena occur practically in the layer plane.

For the theoretical calculations of the dispersion relations the envelope function approximation has often been used [4,12,13]. This approximate scheme has proved efficient, relatively reliable as compared with more sophisticated approaches [14–16]. The problem of valence subbands in heterostructures has been extensively discussed by Altarelli et al. [3,5,6]. Ando [4] has reported complete calculations of hole levels in p–type doped $GaAs-Ga_{1-x}Al_xAs$ heterostructures neglecting however the difference between the γ parameters of $GaAs$ and $Ga_{1-x}Al_xAs$. Calculations of hole subbands in modulation-doped heterojunctions have also been reported [7,8]. The in-plane dispersion relations using the axial approximation for the γ parameters have been described by Bastard et al. [9].

Hamiltonian and the basic wave functions

In the present paper, we shall only consider systems with large spin-orbit interactions. This is true for $GaAs-Ga_{1-x}Al_xAs$. For semiconductors with spin-orbit splitting much larger than the hole confinement energies, the split-off states may be ignored. We show in Fig.1 the valence band edge profile of $GaAs-Ga_{1-x}Al_xAs$ quantum well. Throughout the paper, the z axis is taken to be along the growth direction of the quantum well.

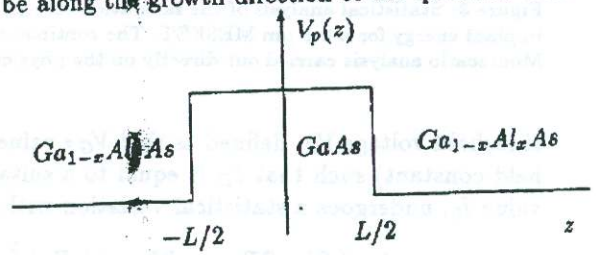

Fig. 1. Valence band edge profile of quantum well

Neglecting the inversion-asymmetry splitting, the valence band Hamiltonian takes the form

$$\mathcal{H}_{\Gamma_8}=\begin{bmatrix} \mathcal{H}_{hh} & c & b & 0 \\ c^* & \mathcal{H}_{lh} & 0 & -b \\ b^* & 0 & \mathcal{H}_{lh} & c \\ 0 & -b^* & c^* & \mathcal{H}_{hh} \end{bmatrix} \begin{matrix} 3/2 \\ -1/2 \\ 1/2 \\ -3/2 \end{matrix} \qquad (1)$$

first derived by Luttinger [17] for bulk materials. In (1) there are

$$\mathcal{H}_{hh}(\mathbf{k}_\perp,z)=-\tfrac{1}{2m_0}p_z(\gamma_1-2\gamma_2)p_z+V_p(z)-\\ -\tfrac{\hbar^2k_\perp^2}{2m_0}(\gamma_1+\gamma_2)\,, \qquad (2)$$

$$\mathcal{H}_{lh}(\mathbf{k}_\perp,z)=-\tfrac{1}{2m_0}p_z(\gamma_1+2\gamma_2)p_z+V_p(z)-\\ -\tfrac{\hbar^2k_\perp^2}{2m_0}(\gamma_1-\gamma_2)\,, \qquad (3)$$

$$c(\mathbf{k}_\perp,z)=\tfrac{\hbar^2}{2m_0}\sqrt{3}\,[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y]\,, \qquad (4)$$

$$b(\mathbf{k}_\perp,z)=\tfrac{\hbar}{2m_0}\sqrt{3}\,(k_x-ik_y)(\gamma_3p_z+p_z\gamma_3)\,. \qquad (5)$$

In (2)-(5) the γ parameters are position-dependent and products of the form γp_z have been symmetrised,

$p_z = -i\hbar\partial/\partial z$, $\mathbf{k}_\perp=(k_x,k_y)$ is bidimensional wave vector. $V_p(z)$ is the algebraic energy shift of the Γ_8 edge in the $Ga_{1-x}Al_xAs$ with respect to $GaAs$, which is a constant, $V_p(z)=0$ for z inside the well and $V_p(z)<0$ outside, m_0 is the free electron mass. On the right of (1) m_J-value (the z projection of the total angular momentum of the hole) is indicated. The off-diagonal terms in (1) vanish at $\mathbf{k}_\perp=0$. If they were always negligible, the valence levels would remain heavy hole-like ($m_J=\pm\frac{3}{2}$) or light hole-like ($m_J=\pm\frac{1}{2}$) at $\mathbf{k}_\perp\neq 0$ and the valence problems would always decouple into two independent Ben Daniel-Duke problems [18]. Although in the following we shall discuss heavy hole or light hole dispersion relations, the notion of heavy hole character (as well as of light hole one) at finite $k_\perp$ of a given subband has little physical meaning, for the $b-$ and $c-$ terms very effectively mix the $k_\perp=0$ eigenstates.

We write the envelope function of an approximate scheme as [9]

$$\vec{\psi}_{\mathbf{k}_\perp}=\begin{bmatrix}\sum_m \alpha_m^+(\mathbf{k}_\perp)\xi_m(z)\\ \sum_n \beta_n^-(\mathbf{k}_\perp)\varphi_n(z)\\ \sum_n \beta_n^+(\mathbf{k}_\perp)\varphi_n(z)\\ \sum_m \alpha_m^-(\mathbf{k}_\perp)\xi_m(z)\end{bmatrix}\frac{1}{\sqrt{S}}\exp(i\mathbf{k}_\perp\cdot\mathbf{r}_\perp), \qquad (6)$$

where the summations over n and m have been restricted to the bound states of the wells at $\mathbf{k}_\perp=0$, $\alpha_m^+(\mathbf{k}_\perp),\beta_n^-(\mathbf{k}_\perp),\beta_n^+(\mathbf{k}_\perp),\alpha_m^-(\mathbf{k}_\perp)$ are the unknown complex coefficients, S is the layer area in the xy plane, $\mathbf{r}_\perp=(x,y)$ is bidimensional position vector and $\xi_m(z),\varphi_n(z)$ are the heavy hole and light hole eigenfunctions at $\mathbf{k}_\perp=0$, respectively, which can be found by solving the equations

$$\mathcal{H}_{hh}(\mathbf{k}_\perp=0)\xi_m(z)=HH_m^0\xi_m(z),$$
$$\mathcal{H}_{lh}(\mathbf{k}_\perp=0)\varphi_n(z)=LH_n^0\varphi_n(z), \qquad (7)$$

where HH_m^0 and LH_n^0 are the heavy hole and light hole eigenenergies at $\mathbf{k}_\perp=0$, respectively, m and n denote the numbers of the relevant bound states of the well.

Note that another eigenfunction expansions of the envelope wave functions (EWF) have also been used. Sanders et al. [19] expanded EWF into a sum of Gaussian-type orbitals of the form $\exp(-\beta z^2)$ and $z\exp(-\beta z^2)$, fifteen Gaussian orbitals of each type had been used.

The valence barrier height V_p has been taken equal to -150meV (about 40 percent of the total bandgap difference between $GaAs$ and $Ga_{0.7}Al_{0.3}As$) [9]. For simplicity, the γ parameters in the barrier material $Ga_{1-x}Al_xAs$ are assumed to be the same as those in $GaAs$ well. This approximation is good as long as the penitration of quantum-well-state wave functions into the barrier is sufficiently small. For the Luttinger parameters of $GaAs$ we adopt values of γ_1=6.85, γ_2=2.1, γ_3=2.9 [20]. There are six bound states of the heavy (four) and light (two) holes for the well width L=10nm.

For L=15nm there are nine bound states. The eigenenergies of these states are obtained by solving the equation [21]

$$\sqrt{\frac{|\varepsilon_n|}{\varepsilon_\infty}}=n-\frac{2}{\pi}\arcsin\sqrt{\frac{\varepsilon_n}{V_p}}, \qquad (8)$$

where $n=1,2,3...$; ε_n denotes the eigenvalue of the heavy (HH_n^0) or light (LH_n^0) hole for a given n, $\varepsilon_\infty=\pi^2\hbar^2/(2m_{hhz}L^2)$ for heavy and $\varepsilon_\infty=\pi^2\hbar^2/(2m_{lhz}L^2)$ for light hole ($m_{hhz}=m_0/(\gamma_1-2\gamma_2)$ and $m_{lhz}=m_0/(\gamma_1+2\gamma_2)$ denote the effective masses of the heavy and light holes, respectively, for the z motion). The number of bound states of the quantum well $N=1+Int\left(\sqrt{|V_p|/\varepsilon_\infty}\right)$, where $Int(x)$ denotes the integer part of x.

The in-plane dispersion relations of the hole subbands

Substituting the expansion (6) for the envelope functions into the Schrödinger equation

$$\mathcal{H}_{\Gamma_8}\vec{\psi}_{\mathbf{k}_\perp}=E\vec{\psi}_{\mathbf{k}_\perp} \qquad (9)$$

the problem reduces to finding the envelope- function expansion coefficients and the corresponding eigenvalue E by solving the system of the four equations.

Then, the $\mathcal{H}_{\Gamma_8}$ eigenvalues are obtained via a numerical diagonalization of $2(n+m)\times 2(n+m)$ Hermitian matrix by the Jacobi method [10,11] for every value of $\mathbf{k}_\perp=(k_\perp\cos\theta,k_\perp\sin\theta)$, where θ denotes an angle between the vector $\mathbf{k}_\perp$ and the x axis. Flat band conditions lead to twofold degeneracy of $(n+m)$ eigenenergies (Kramers degeneracy). The components of $2(n+m)$ orthonormal eigenvectors of the $2(n+m)\times 2(n+m)$ Hermitian matrix mentioned above represent the envelope- function expansion coefficients $\alpha_m^+(\mathbf{k}_\perp)$, $\beta_n^-(\mathbf{k}_\perp)$, $\beta_n^+(\mathbf{k}_\perp)$, $\alpha_m^-(\mathbf{k}_\perp)$ for the given $\mathbf{k}_\perp$ and $(n+m)$ twofold eigenenergies. This procedure may have difficulties in heterostructures whose γ parameters are markedly different (e.g., $HgTe-CdTe$) since the probability current conservation conditions are not the same at $\mathbf{k}_\perp\neq 0$ as at $\mathbf{k}_\perp=0$, and since the wave function (6) may not have enough flexibility to accommodate these changes. A better way is to look for a variational solution of (1) using different forms of $\vec{\psi}_{\mathbf{k}_\perp}$ within each kind of layer and to enforce the probability current conservation at the interfaces [3,5]. Using the axial approximation [9] for γ's, that amounts to replace γ_2 and γ_3 in (4) by their arithmetic average $(2\gamma_2+3\gamma_3)/5$, one can then obtain the isotropic in-plane dispersion relations.

We show in Fig.2 the calculated in-plane dispersion relations of the valence subbands of $GaAs-Ga_{0.7}Al_{0.3}As$ quantum well of thickness L=15nm. The dashed lines are the subband dispersions obtained in the axial approximation. As seen from Fig. 2, the anisotropy is clearly visible for the ground heavy (HH_1) and light (LH_1) hole subbands. Note that $k_\perp$-value is in units of $\pi\times 10^6 cm^{-1}$=$0.028(2\pi/a_0)$,

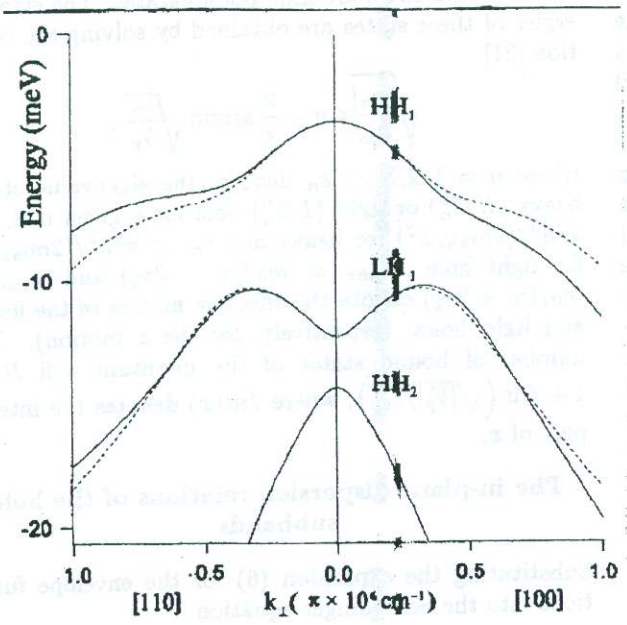

Fig. 2. In-plane dispersion relations of the valence subbands.

where a_0 denotes the $GaAs$ lattice constant.
As can be seen from Fig.2, the first light hole subband LH_1 displays a camel-back shape (it was first pointed out by Altarelly [5]), i.e., has negative zone center effective mass. Other subbands may also become camel-back shaped depending on the parameters which are input in the calculations.
We present in Fig.3 the constant energy contours of the HH_1 subband, $HH_1' = -10.5meV$, $HH_1'' = -12.85meV$ and $HH_1''' = -14.7meV$, in the $k_x k_y$ plane for L=10nm. The dashed lines correspond to the axial approximation. It is seen that the anisotropy increases with the hole energy increasing. For the direction making an angle 24.27° with the k_x (or k_y) axis, the anisotropic dispersion relations are found to coincide with the isotropic those for all subbands.

The hole envelope wave functions

Substitution of the calculated for a given $\mathbf{k}_\perp$ value envelope- function expansion coefficients $\alpha_m^+(\mathbf{k}_\perp)$, $\beta_n^-(\mathbf{k}_\perp)$, $\beta_n^+(\mathbf{k}_\perp)$, $\alpha_m^-(\mathbf{k}_\perp)$, which are the components of some eigenvector corresponding to, for example, HH_1 eigenvalue, into the expansion (6) yields the column vector $\vec{\psi}_{hh1}$ for this $\mathbf{k}_\perp$ value and the chosen eigenenergy HH_1. As already mentioned, the state whose envelope function is $\vec{\psi}_{hh1}$ must be in fact the mixture in which the coefficients $\alpha_m^+(\mathbf{k}_\perp)$, $\beta_n^-(\mathbf{k}_\perp)$, $\beta_n^+(\mathbf{k}_\perp)$, $\alpha_m^-(\mathbf{k}_\perp)$ determine the contributions of the hole bound- state eigenfunctions $\xi_m(z)$, $\varphi_n(z)$ to the envelope- function components of different m_J.
It is instructive to examine the hole envelope wave functions (see Fig.4 and 5). At the zone center all $2(n+m)$ envelope functions are pure heavy- or light- hole states while at a point slightly removed from $\mathbf{k}_\perp$=0 strong mixing of heavy- and light-hole components is evident. The degree of mixing is determined

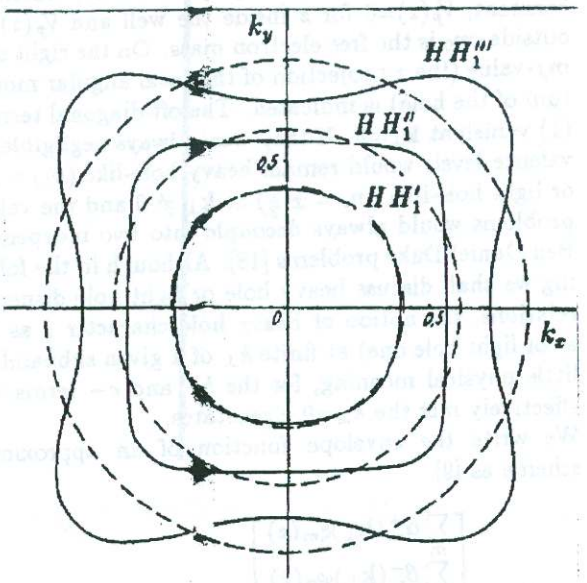

Fig. 3. The constant energy contours of the HH_1 subband.

by the proximity of adjacent states and depends on the numerical values of the expansion coefficients.

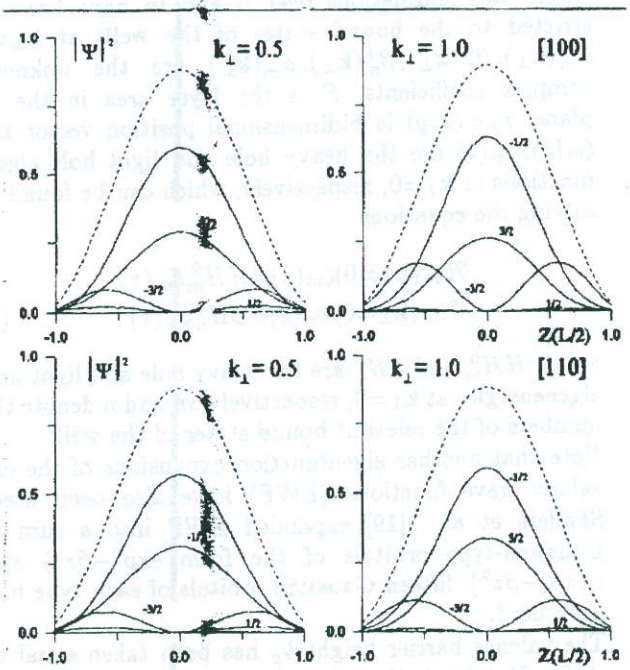

Fig. 4. The normalized probability density $|\psi|^2$ as a function of z for HH_1 valence-subband state.

In Fig.4 for two various directions the normalized probability density $|\vec{\psi}_{h1}|^2$ (proportional to the charge density) as a function of z is shown for a 15nm $GaAs - Ga_{0.7}Al_{0.3}As$ quantum well at $k_\perp$=0.5 and 1.0 (in units of $\pi \times 10^6 cm^{-1}$). The various envelope-function components are labeled by the m_J values in the figure.

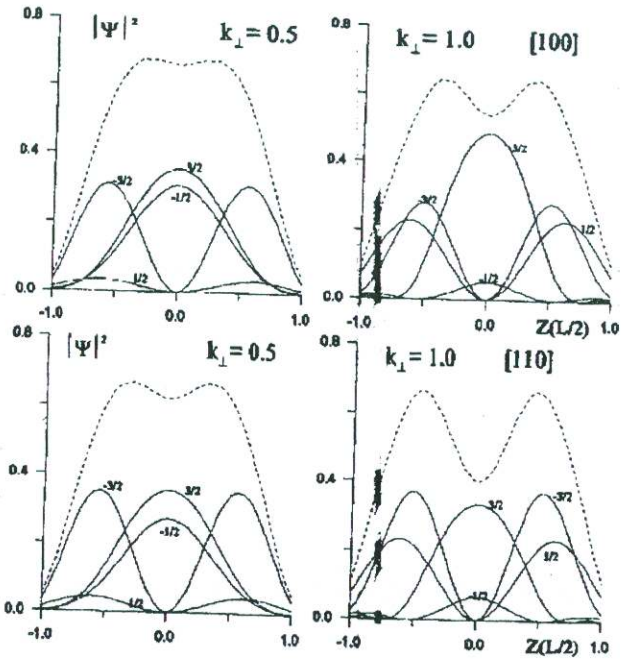

Fig. 5. The normalized probability density $|\psi|^2$ as a function of z for LH_1 valence-subband state.

The anisotropy is considerable for the LH_1 envelope function at $k_\perp$=1.0 (see Fig.5). The dashed lines in Fig.4 and 5 correspond to the total-over-m_J probability density as a function of z.

Conclusion

In summary, we have carried out a systematic study of the valence-band states of $GaAs - Ga_{1-x}Al_xAs$ quantum wells. First of all, the in-plane dispersion relations of the valence subbands are highly nonparabolic and in particular some valence subbands have negative zone center effective masses. According to our calculations, the anisotropy related with the difference between the Luttinger parameters γ_2 and γ_3 should be taken into account. We find also that the electronic valence-band structure is very complicated due to strong mixing of the heavy- and light-hole states away from $k_\perp$=0 in any direction.

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