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BINDING ENERGIES OF p-TYPE ACCEPTOR STATES IN $GaAs/Ga_{1-x}Al_xAs$ QUANTUM WELLS

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Abstract: Binding energies of p-type shallow acceptor states in $GaAs/Ga_{1-x}Al_xAs$ quantum wells are calculated. The complex valence band structure has been taken into account in a four band effective mass theory. The acceptor envelope function is expanded in valence envelope functions in the two-dimensional k-space.

1. Theory and results

In this paper we develop an effective mass theory to describe excited shallow acceptor states in $GaAs/Ga_{1-x}Al_xAs$ quantum wells. The acceptor Hamiltonian contains a kinetic part which is given by the Luttinger-Kohn Hamiltonian [1], a square well potential due to the valence band discontinuity, and the Coulomb potentials of the impurity charge and of all its image charges.

We expand the acceptor envelope function in the basis of valence envelope functions [2], and obtain

$$F^s(\rho,\theta,z) = \sum_n \int d\mathbf{k}\, G_n(\mathbf{k}) v^s_{n\mathbf{k}}(z) e^{i\mathbf{k}\cdot\boldsymbol{\rho}}, \tag{1}$$

where $\boldsymbol{\rho} = (\rho,\theta)$ is the in-plane coordinate and $\mathbf{k} = (k,\alpha)$ is the Bloch vector of the subbands. The acceptor envelope function of Eq. (1) satisfies by construction the current conserving boundary conditions. In expansion (1), n runs over all the discrete subbands in the quantum well.

In our calculations we neglect the in-plane anisotropy of the subbands. Thus the acceptor Hamiltonian is invariant for rotations around the growth axis (z-axis) and the eigenstates have a definite z-component of angular momentum, which we call m. Because of time-reversal symmetry each eigenstate of angular momentum m is degenerate with a state of opposite m. For on-center acceptors, parity with respect to inversion is another good quantum number. By axial symmetry $G_n(\mathbf{k}) = e^{im\alpha} g_n(k)$: the radial function $g_n(k)$ is expanded in a variational basis of hydrogenic wavefunctions. The evaluation of the

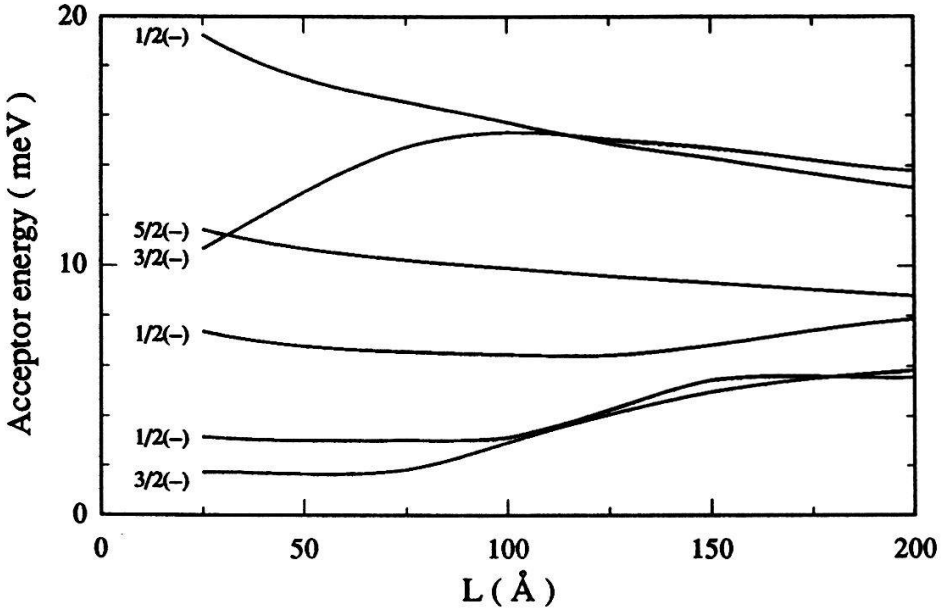

Figure 1 - Energy levels of p-type states for on-center acceptors in GaAs/$Ga_{0.6}Al_{0.4}As$ quantum wells as a function of the well width. The acceptor energies are given as binding energies with respect to the first heavy hole subband. The symmetry of the states is indicated by the absolute value of the angular momentum m and the parity with respect to inversion.

Coulomb potential between acceptor states is considerably simplified by the fact that the valence envelope functions are analytically known [2].

This method is particularly suited to find binding energies of excited states, which are extended in r-space; it is less suited to find the binding energy of the ground state, due to the neglect of the subband continuum. In Fig. 1, we present binding energies for excited acceptor states, which in the limit of wide wells go over into the bulk $2P_{3/2}[\Gamma_8]$, $2P_{5/2}[\Gamma_7 + \Gamma_8]$, and $3P_{3/2}[\Gamma_8]$ states. All these states have negative parity with respect to inversion. Comparison of the results of the present theory with far infrared absorption experiments [3] will be presented elsewhere.

2. References

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