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June 1987

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ENERGY SPECTRA OF SHALLOW DONORS AND ACCEPTORS IN GaAs-$Ga_{1-x}Al_xAs$ SUPERLATTICES

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ABSTRACT - The energy spectra of shallow donors and acceptors in GaAs-$Ga_{1-x}Al_xAs$ quantum-well structures have been calculated. The binding energies of the impurities were obtained within a variational calculation in the effective-mass approximation. Calculations were performed for various types of impurity as functions of the position of the impurity in a GaAs quantum well of infinite depth and for various slab thicknesses. The effect of the spatially dependent screening is modeled with a function of the form $\varepsilon^{-1}(r) = \varepsilon_0^{-1} + (1 - \varepsilon_0^{-1})\, e^{-r/a}$, with a screening parameter $\underline{a} \approx 1.1$ a.u. characteristic of bulk GaAs. Results are compared with Bastard's theory, which is based on a constant ε_0 screening, and it is found that spatially dependent screening effects can be quite important for all acceptors in GaAs quantum wells over a large range of slab thicknesses. Calculated results with improved statistics are in quantitative agreement with experimental data.

1. INTRODUCTION

Because of the potential device applications of heterostructures, the understanding of the nature of impurity states associated with quantum wells and supperlattices[1-10] is of considerable technical and scientific relevance. The study of these impurities was pioneered by Bastard[11], who evaluated the binding energy of the impurity state as a function of layer thickness and of the impurity position within the layer. This study was followed by several other calculations[11-15].

Photoluminescence spectra[16-19] of GaAs-$Ga_{1-x}Al_xAs$ heterostructures have revealed various impurity features which are much weaker than in bulk GaAs. They have been assigned variously to acceptors and donors.

We studied the effects of spatially dependent screening[20-23] on various impurities in GaAs quantum wells of infinite depth[24].

2. HYDROGENIC IMPURITIES IN A QUANTUM-WELL STRUCTURE

The Hamiltonian of a hydrogenic impurity in a single GaAs quantum well of infinite depth is, in the effective mass approximation,

$$H = -\frac{\nabla^2}{2\,m^*} - \frac{Z\quad e^2}{\varepsilon(r)\,[\rho^2 + (z - z_i)^2]^{1/2}} + V(z) \qquad (1)$$

where $\rho = (x^2+y^2)^{1/2}$, the $z = 0$ origin is chosen at the center of the well, z_i is the position of the impurity within the slab, $r = [\rho^2 + (z - z_i)^2]^{1/2}$ is the distance from the carrier to the impurity site, $V(z)$ is the potential-energy barrier which confines the electron (hole) within the well of thickness L,

$$V(z) = \begin{cases} +\infty\ , & |z| > L/2\ , \\ 0\ , & |z| < L/2\ , \end{cases} \qquad (2)$$

and Z is the net charge of the hydrogenic impurity (Z=1 for the simple neutral impurities and Z=2 for the singly ionized, double impurities). The carrier effective mass and the GaAs spatially dependent dielectric screening are given by m^* and $\varepsilon(r)$, respectively. The spatially dependent dielectric screening used here is that of Hermanson[20],

$$\varepsilon^{-1}(r) = \varepsilon_o^{-1} + (1 - \varepsilon_o^{-1})\exp(-r/a), \qquad (3)$$

where ε_o is the static dielectric constant and $\underline{a}$ is a screening parameter. Wang and Kittel[21] used this model dielectric function and chose $\underline{a}$ so that the Fourier transform of (3) fits the dielectric function of Walter and Cohen[22]: ε_o=11.47 and $\underline{a}$=1.09 a.u. for Si; ε_o=14.00 an $\underline{a}$=1.15 a.u. for Ge. In the case of GaAs the static dielectric constant[23] is ε_o=12.58, and we took $\underline{a}$=1.1 a.u. as the characteristic value for the screening parameter.

As an exact solution of the Schrödinger equation for the Hamiltonian (1) is not possible, we followed the variational approach

of Bastard[11], and taken a trial wave function

$$\psi(\rho,z) = \begin{cases} N \cos(\pi z/L) \exp\{-\lambda^{-1}[\rho^2+(z-z_i)^2]^{1/2}\}, & |z| < L/2 , \\ 0 \quad , & |z| > L/2 , \end{cases} \tag{4}$$

where λ is the variational parameter and N is a normalization factor. The trial impurity ground-state energy is minimized with respect to λ. All necessary integrals are performed analytically; only the minimization requires numerical handling.

The impurity binding energy is finally given by

$$E(L,z_i) = (\hbar^2\pi^2/2m^*L^2) - \zeta(L,z_i) , \tag{5}$$

where the first term corresponds to the energy of a free electron (hole) at the bottom (top) of the conduction (valence) band.

Results are presented in reduced atomic units (a.u.*), which correspond to a length unit of an effective Bohr radius $a_o^* = \hbar^2\varepsilon_o/m^*e^2$, and an energy unit of an effective Rydberg $R_o^* = m^*e^4/2\hbar^2\varepsilon_o^2$. For GaAs these units are $a_o^* \approx 22$ Å and $R_o^* \approx 26$ meV for acceptors (holes).

3. RESULTS AND DISCUSSION

Although the calculations have been carried out[24] for neutral donors and acceptors, and for singly ionized double donors and double acceptors, only the results for neutral acceptors are presented here.

The spatially dependent screening effects on the binding energies of simple neutral acceptors at the on-center position as a function of slab thickness is shown in Figure 1(a). There is a substantial increase in the acceptor binding energy with respect to the constant ε_o theory over a large range of thicknesses. Increases range from ~4 meV for L = 50 Å to ~2 meV for L = 350 Å. In Figure 1(b) we display the binding energies of neutral simple acceptors as functions of z_i, the impurity position, for L = 50 Å and 200 Å. The importance of the spatially

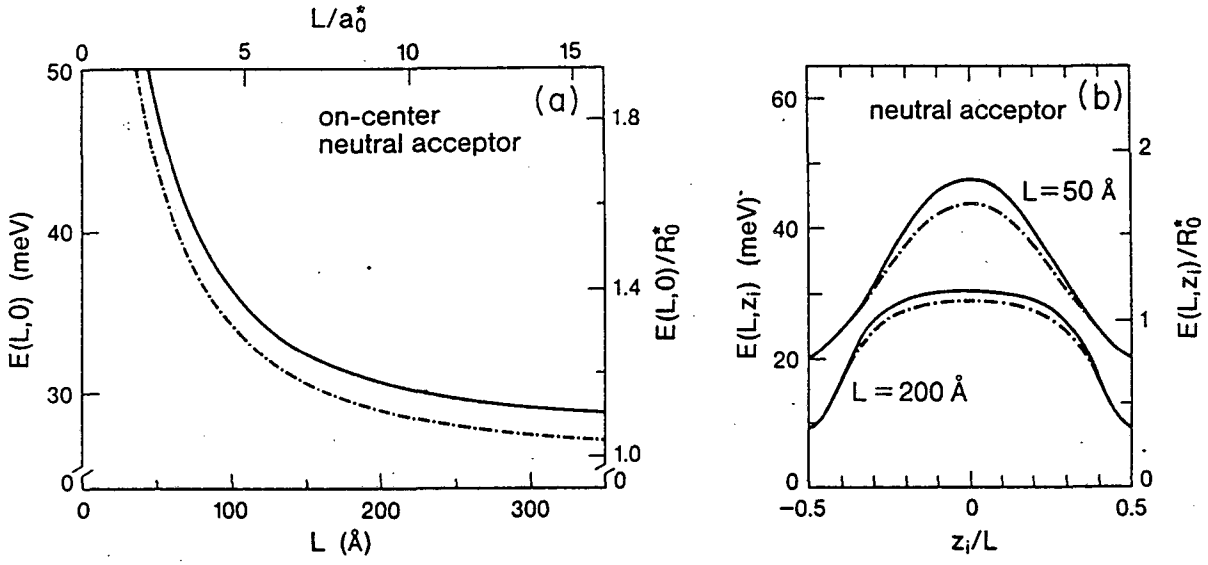

Figure 1.- Binding energy $E(L,z_i)$ for the ground state of a neutral acceptor as a function of: (a) the GaAs quantum-well thickness, L, with the impurity position at the center of the well; (b) the impurity position z_i within the quantum well for thicknesses L = 50 Å and L = 200 Å. The dash-dotted curve is for constant $\varepsilon = \varepsilon_0$; the solid curve is for a spatially dependent $\varepsilon = \varepsilon(r)$.

dependent screening effects diminishes as the impurity approaches the edge of the GaAs quantum well and the hole wave function increases its p-like character.

Comparison with the photoluminescence measurements of Miller et al.[17] are shown in Figure 2. The density of impurity states (shown in Figure 3 for various slab thicknesses) allows one to evaluate the energy of the center of gravity of the impurity band (dashed line in Figure 2) as well as the energies for which the integrated density of

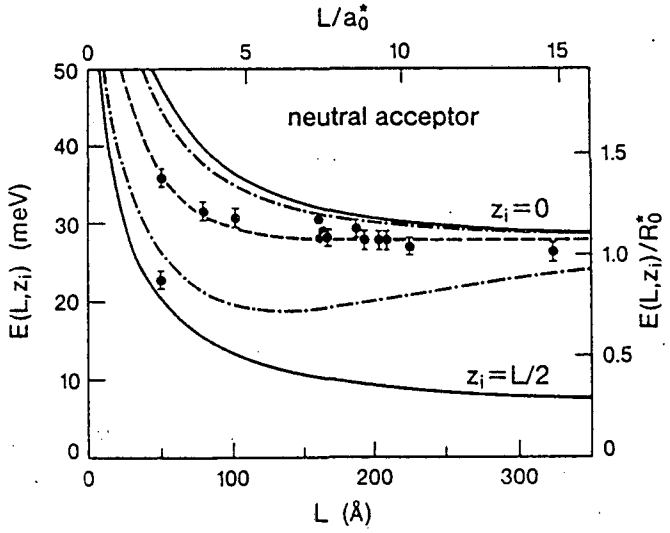

Figure 2.- Binding energy $E(L,z_i)$ versus quantum-well thickness, L, for a neutral acceptor at the center (z_i = 0) or at the boundary (z_i = L/2) of the well. Experimental results (⊙) are those of Miller et al. (Reference 17).

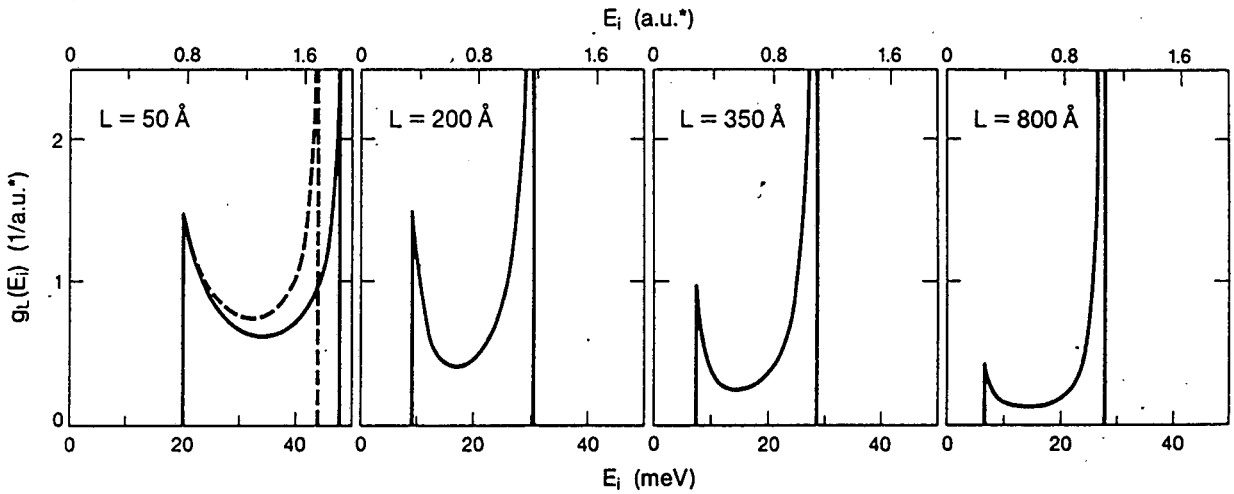

Figure 3.- Density of states $g_L(E_i)$ in reduced atomic units as a function of the neutral-acceptor binding energy $E_i = E(L,z_i)$ for various quantum-well thicknesses. Solid curves are obtained with a spatially dependent screening $\varepsilon = \varepsilon(r)$. Shown for comparison are also the results (dashed curve) calculated with a constant $\varepsilon = \varepsilon_0$ screening for L = 50 Å.

impurity states reaches the values 0.25 and 0.75 (dash-dotted curves in Figure 2). A clear picture of the relative strength of the two singularities, E_i^{min} and E_i^{max}, emerges. For L = 50 Å, the on-edge peak has considerable strength, in good agreement with the additional shoulder observed in photoluminescence data[17]. It is quite apparent from Figure 2 that there is very good agreement between the theoretical results for the center of gravity of the impurity band and the experimental measurements.

In conclusion we would like to point out that the experimentally measured energy levels (Figure 2), which have an error of ± 1 meV, seem to be scattered throughout the impurity band, and not necessarily concentrated at the top, the <u>on-center</u> location. If at all, they seem to follow the center of gravity of the band. Therefore this comparison seems to indicate a <u>random distribution of impurities</u> in the slab. Previous comparisons with experiment, assuming only an <u>on-center</u> location, should thus be viewed with caution.

4. ACKNOWLEDGMENTS.

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