Effect of band structure on Stark shifts in GaAs quantum wells

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We have carried out a pseudopotential calculation of Stark effect on electron states in GaAs-$Ga_{1-x}Al_xAs$ quantum-well structures. We find that in isolated wells the band-structure effect due to field-induced mixing of bulk Γ and X states is negligible in electric fields $(0–5)\times10^5$ V/cm. However, in double-barrier structures normally used to study resonant tunneling the effect of Γ-X mixing drastically reduces the magnitude of critical field, at which quadratic Stark effect and the particle-in-a-box model collapse, to around 2×10^5 V/cm. We predict that this critical field is also a sensitive measure of the interface quality.

The effect of an external electric field upon electron states (the so-called Stark effect) in quantum-well structures and its many manifestations have received a great deal of attention in the literature.[1–12] Of particular interest are the magnitude of the field-induced changes in the energy levels and localization of the wave function associated with the Stark resonance lying at the bottom of the conduction band. This is because in GaAs and in alloys of GaAs and AlAs the conduction band exhibits well-known secondary minima located at the Brillouin-zone boundary (i.e., at the X and L points) and separated by only a few tenths of an eV from the principal Γ valley. In calculations of Stark shifts reported in the literature, the microscopic crystal potential is replaced by a steplike potential representing the conduction-band offset between the GaAs well and the barrier material. The electron wave function is reduced to a nodeless envelope of the true solution of the Schrödinger equation. That is equivalent to assuming that the wave function is made up of bulk Bloch states derived from the bottom of the Γ minimum. This is the familiar particle-in-a-box or effective-mass model[13] which can be solved analytically and within which the effect of an external electric field can also be accounted for with rigor. The effect of a weak electric field gives the quadratic Stark behavior, which can be explained by second-order perturbation theory.[10] However, this model is questionable in narrow wells exposed to high fields. In our pseudopotential calculations,[14] the band structures of GaAs and $Ga_{1-x}Al_xAs$ are fully accounted for. Accordingly, in this study we set out to investigate the applicability of the above-mentioned approximations. In particular, we wish to establish whether the inclusion of the full band structure alters the magnitude of the applied field at which the simple quadratic behavior breaks down.

The band diagram for a GaAs quantum-well structure along the [001] direction, exposed to an external field, is shown in Fig. 1. The band offsets seen by both Γ and X electrons are indicated, as well as the effect of the field upon the wave function [Fig. 1(b)]. Since we want to investigate the effect of an external field, it is convenient to assume that there are no free charges in the structure. The field which acts perpendicular to the interfaces is then a simple linear function of the coordinate.

In order to create a workable computational model, we proceed as follows. We first carry out a full-scale pseudopotential superlattice calculation for GaAs-$Ga_{1-x}Al_xAs$. We have described such calculations in some detail in our previous publications. The solutions $\varphi(n,k)$ of the *superlattice* problem $H\varphi(n,k)=E(n,k)\varphi(n,k)$ in the absence of the field are then used to construct the wave functions ψ of the Stark Hamiltonian, i.e.,

$$\psi=\sum_{n,k} B(n,k)\varphi(n,k) , \tag{1}$$

which satisfy the Schrödinger equation $[H+V-E]\psi=0$. V represents the external field. n and k are the superlattice band and reduced (one-dimensional) wave vector, respectively. The values of k in the expansion in (1) are unambiguously determined by the choice of superlattice period. The solution is obtained numerically in the same manner as for the superlattice with $V=0$. The width of the barrier layer is chosen to be as large as is necessary to achieve a stable ground state.

We can first of all show that when the input into our numerical calculation is equivalent to that used in analytical[11] calculations, the same result is obtained. This is achieved simply by removing the X-related superlattice states from the expansion in (1). We find differences of order 1%, i.e., within the numerical error. The shift is quadratic over the full range of the field $[(1–5)\times10^5$ V/cm] we employed. It shows that at least as far as the states derived from the Γ valley are concerned, the field has been allowed to act over a sufficiently large length outside the well and that the effect of the artificial periodic boundary conditions imposed by our superlattice scheme is negligible.

We then turn on the full band-structure input in (1) and repeat the calculation. The results for several well widths are shown in Fig. 2. We also present a typical re-

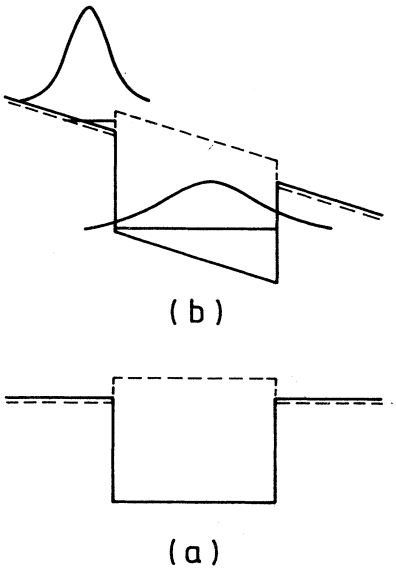

FIG. 1. (a) This figure shows the band offsets for electrons associated with the Γ and X valleys of the conduction band in GaAs-$Ga_{1-x}Al_xAs$ structures. (b) The effect of the applied field upon the potential and wave-function localization is shown schematically. (The X-valley offsets are shown with a dashed line.)

sult for the wave function in Fig. 3. Only the ground-state resonance derived from the well is reported here. The effect of the inclusion of the X-like states introduces deviations which are numerically insignificant and for any practical purposes may be ignored.

In order to demonstrate that no misrepresentation of the Stark shift took place as a result of the choice of a finite barrier width in the full calculation, we present in

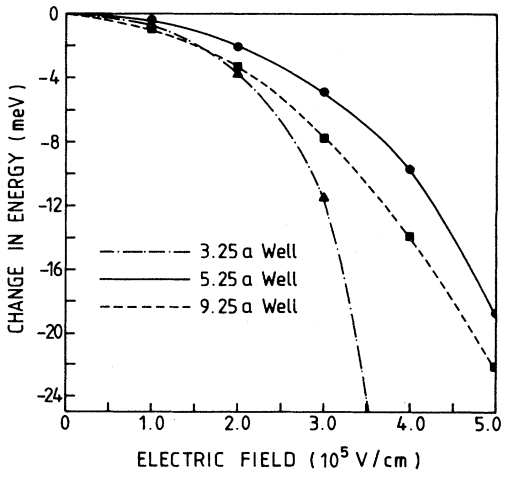

FIG. 2. The Stark shift in the ground-state energy of quantum wells of GaAs-$Ga_{0.62}Al_{0.38}As$ of widths $3.25a$, $5.25a$, and $9.25a$, where a is the lattice constant of bulk GaAs.

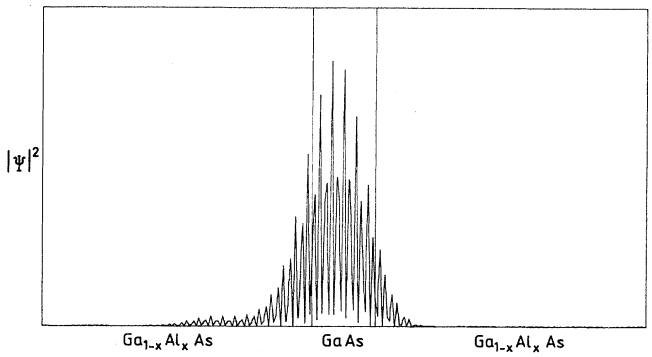

FIG. 3. The electron charge density associated with the Stark-shifted ground state at an external field of 4×10^5 V/cm. The position of the interfaces is indicated by vertical lines.

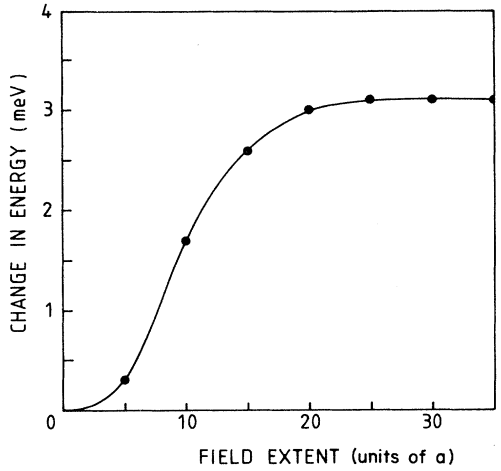

FIG. 4. The convergence of the Stark shift as a function of the superlattice period employed in the calculation. The well width is kept constant.

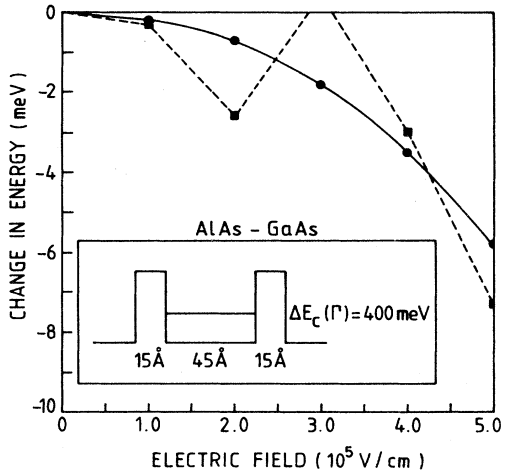

FIG. 5. Inset shows a sketch of the double-barrier structure of GaAs-AlAs studied by Sollner *et al.* (Ref. 18) and investigated in this calculation. The figure shows the Stark shift of the resonance derived from the well calculated without X states (circles connected with a solid line, only the central Γ valley included) and with the full band structure (squares; the interrupted line serves merely to guide the eye).

Fig. 4 the result of our convergence test. We have also verified that changing the boundary conditions at large distances from our well (e.g., by adding a well there) does not alter the Stark shift. We can therefore conclude that even strong external electric fields such as those reported in Fig. 2 are insufficient to induce a significant coupling between states of Γ and X character.

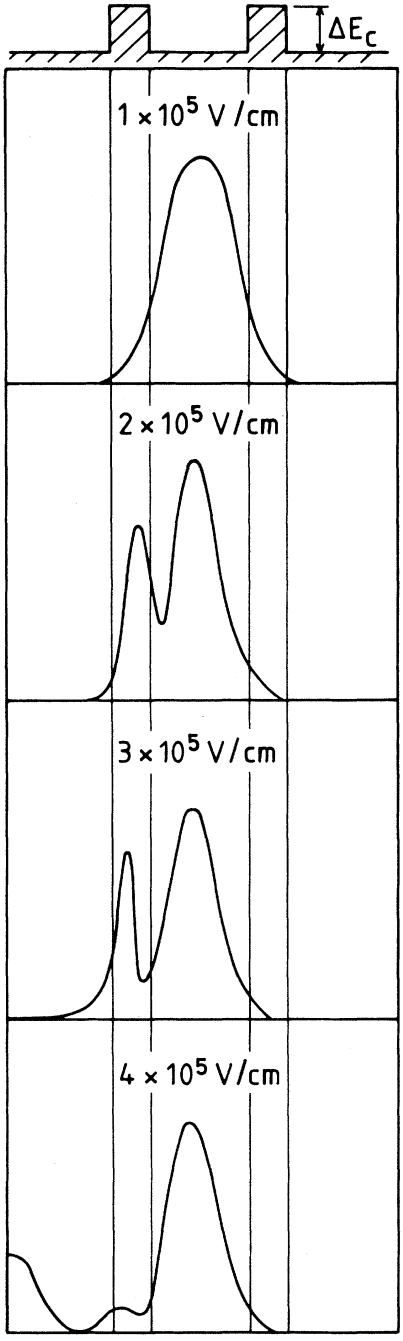

FIG. 6. A sketch of the charge-density distribution obtained for the Stark resonance of Fig. 5, as a function of the applied electric field.

The quadratic Stark shift δE of state $|0\rangle$ is, from second-order perturbation theory, $\delta E \simeq \sum_j |\langle 0|V|j\rangle|^2 / \Delta E(0,j)$. The mixing via V must be large enough to compete with the separation $\Delta E(0,j)$ of the higher-lying states $|j\rangle$ and the ground state whose Stark shift is being calculated. Since the lowest X states are localized in the barrier,[15] the overlap with the Γ-like level in the well is small. Although we have shown that there are higher-lying X-like levels whose wave functions extend significantly into the quantum well, their matrix elements with the Γ ground state are small. This implies that only first-order effects are likely to bring about significant changes in the Stark shift of the lowest level due to Γ-X coupling. Such effects occur when the field lowers the X states in the barrier far enough for them to become degenerate[16] with the Γ resonance level in the well and when the spatial separation of the two states is sufficiently small. Our result shows that this does not happen in the structures and fields considered above. However, it is also clear from our results that if the interface is not perfect, the magnitude of the breakdown field may be significantly lower than that obtained for the idealized structure considered here. This is because imperfections (e.g., impurities, interdiffusion of unwanted atomic species) at the interface introduce a coupling between states of Γ and X character, broaden the X resonances, and change their matrix elements with the Γ states. There are indications in spectroscopic data that such imperfections exist.[17]

The result in Fig. 2 shows an anomalous ordering of the Stark shift. At a very low field ($< 10^4$ V/cm), the magnitude of the Stark shift scales with the well width. This is because the dominant contribution comes from the matrix element between the lowest two confined levels. The narrowest well has only one confined state and the interaction with the Γ resonances is weaker than that between the two localized states characteristic of the other two wells. The matrix element increases with the wave-function overlap. Hence the widest well has the largest shift. However, as the field increases, the Γ state approaches the top of the barrier, the wave function leaks through the barrier and benefits from the deeper potential there. This happens more quickly in narrow wells and consequently their shift becomes larger in high fields.

The first-order effect of Γ-X coupling which we noted does not materialize in our single-well systems can be demonstrated in a double-barrier GaAs-AlAs structure shown in the inset of Fig. 5. Such structures are frequently used to study resonant tunneling processes.[18] A convergent solution for the Stark shift of the ground-state resonance derived from the well in the double-barrier structure is obtained in the manner described above. The result in Fig. 5 of our pseudopotential calculations shows that the quadratic Stark shift breaks down as a result of the inclusion of X-like states (i.e., the full band structure) into the expansion of the wave function in (1). This result can be understood in simple physical terms from a sketch of the wave function of the Stark resonance versus field (Fig. 6). As the field increases in strength, the charge is pushed into the barrier where the potential is repulsive. The Stark shift becomes negative. When the field is in-

creased further, the wave function penetrates the barrier and tunnels into the region of deeper potential in the GaAs. At this point the simple picture of a narrow resonance collapses and the energy given in Fig. 5 becomes meaningless. An analogous breakdown also occurs in the particle-in-a-box model and can be readily accounted for in the language of scattering theory.[11,19] The effect of the inclusion of the full band structure (i.e., of the secondary valley X states which are characterized by large effective mass and density of states) is simply to lower the critical-field strength at which the breakdown takes place.

ACKNOWLEDGMENTS

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