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Electronic structure of GaAs-$Ga_{1-x}Al_xAs$ quantum well and sawtooth superlattices

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We report pseudopotential calculations concerning the electronic structure of GaAs-$Ga_{1-x}Al_xAs$ sawtooth (100) superlattice of period 140 Å. We present energy levels and electron charge densities of the confined states and compare them with our results for the usual quantum-well structure. In both systems we find new resonances and confined states with large amplitudes at interfaces. Our results also shed fresh light upon the microscopic origin of the confinement effect.

Very recently, Capasso *et al.*[1] drew attention to some interesting applications of graded-gap structures such as sawtooth superlattices of $Ga_{1-x}Al_xAs$. Although the quantum-well systems have been frequently studied by a number of techniques, no quantitative predictions are available for graded structures. In this Rapid Communication, we report for the first time the electronic structure of a (100) sawtooth superlattice of $Ga_{1-x}Al_xAs$, $0 \leq x \leq 0.3$, of period 140 Å. We have also computed the electronic structure of a conventional quantum-well GaAs-$Ga_{0.8}Al_{0.2}As$ superlattice of the same period and we compare the results with those for the sawtooth structure. These calculations reveal the existence of several new confined states peculiar to these systems. They also shed fresh light on the microscopic origin of the confinement effect.

With the exception of ultrathin layers (e.g., 20 Å) the electronic properties of semiconductor superlattices have been described in terms of a variety of matching techniques which exploit the rectangular well character of these structures (e.g., Ando, Fowler, and Stern[2]) and ignore the rapidly varying microscopic potential. Our method of calculation is based on the self-consistent pseudopotential approach which has been successfully used to model point and line defects in semiconductors and which is free of the constraints familiar from the envelope function or complex band-structure methods.[3] Our Hamiltonian is $H = H_0 + V$ where H_0 represents bulk GaAs. We expand the superlattice solution ψ in terms of the eigenfunctions $\phi_{n,\vec{k}}$ of H_0 (n is band index and $\vec{k}$ is the wave vector). We have $H_0\phi_{n,\vec{k}} = E_{n,\vec{k}}\phi_{n,\vec{k}}$. The potential V is the difference between the self-consistent atomic potential of the atoms of $Ga_{1-x}Al_xAs$ and GaAs at the relevant sites. We assume that the difference between the lattice constants of GaAs and GaAlAs can, as a first approximation, be ignored. We also use the virtual crystal approximation to represent the alloy potential. We use nonlocal pseudopotentials with spin-orbit coupling, adjusted to reproduce the electronic structure of bulk $Ga_{1-x}Al_xAs$ for all x. The Schrödinger equation to be solved is

$$(H_0 - E + V)\psi = 0 \quad , \tag{1}$$

where $\psi = \sum_{n,i} A_{n,\vec{k}_i}\phi_{n,\vec{k}_i}$. Since V is a periodic potential, the superlattice period determines unambiguously the values of $\vec{k}_i$ in the expansion for ψ. Substituting for ψ in (1), multiplying from the left by $\phi^*_{n',\vec{k}_j}$ and integrating over all space gives linear equations for coefficients $A_{n,\vec{k}_i}$ of the form

$$A_{n',\vec{k}_j}(E_{n',\vec{k}_j} - E) + \sum_{n,i} A_{n,\vec{k}_i}\langle\phi_{n',\vec{k}_j}|V|\phi_{n,\vec{k}_i}\rangle = 0 \quad . \tag{2}$$

The secular equation is solved numerically in a self-consistent fashion by direct diagonalization. Manipulations exploiting the symmetry properties of Bloch functions can be used to optimize the computational procedure.[3,4] It transpires that the convergence properties of this method are such that systems of period 0–200 Å with arbitrary structures and doping profiles can be studied. A detailed report concerning our results and the more technical aspects of our calculations will be given elsewhere.[5] Here we intend to concentrate on some of the novel physical properties of GaAlAs superlattices which were brought to light by our calculations.

A summary of the energy levels and the corresponding charge densities of the sawtooth superlattice states, obtained at the center of the Brillouin zone, are presented in Figs. 1 and 2, respectively. We also compare our results with a similar calculation of ours on GaAs-$Ga_{0.8}Al_{0.2}As$ (100) superlattice of the same period [i.e., 70+70 (Å)].

Let us first focus on the conduction-band states. The lowest state strongly resembles state 1′ of the quantum-well structure. However, the peak is shifted towards the GaAs end and there is a tail into the graded part which gives rise to 1-meV dispersion, with a minimum away from the zone center. State 1′ is practically dispersionless. An analogous relationship is found for other states although the degree and character of dispersion does vary substantially depending on the nature of the state in question. States 2 and 3 still retain the main features of 2′ and 3′. All these states are derived mainly from the Γ valley states appearing in the expansion for ψ in (1). However, at least $\frac{1}{3}$–$\frac{1}{2}$ of the bulk Brillouin-zone volume is needed in order to provide an adequate description of the charge densities associated with these states. States 4–6 and 4′–6′ are dominated by contributions from the higher-lying X minima. Again, the sawtooth states retain the character of the corresponding quantum-well states.

The existence of states 1′ and 2′, which lie inside the confining barriers in the effective-mass model, has been predicted before. The existence of state 3′ can be easily understood on intuitive grounds, too. Above the confining barrier, a carrier experiences an inverted (repulsive) well. This forces the wave function out of the GaAs layers and into the confining material.[6] In the sawtooth structure, the process is blurred by the continuity of grading but remains

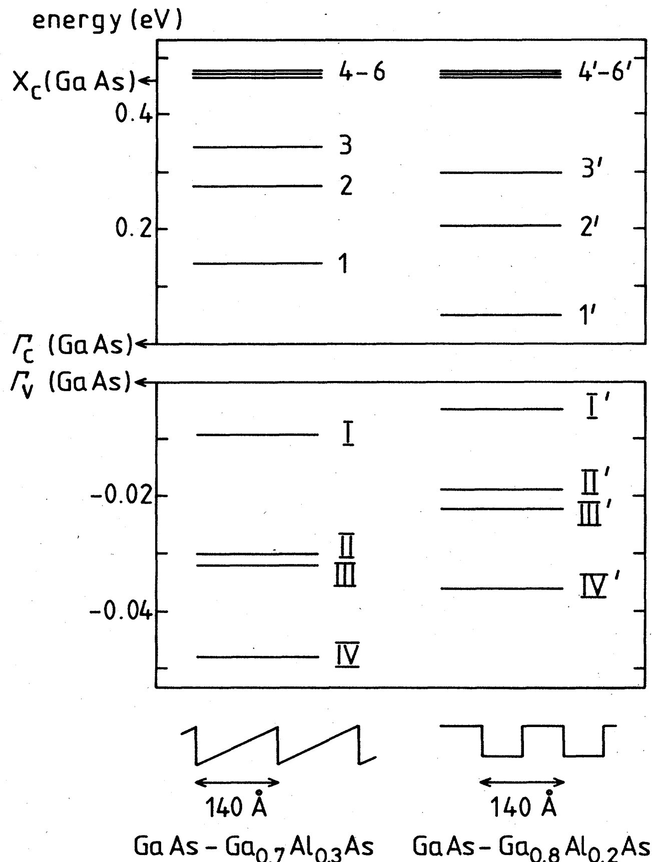

FIG. 1. The superlattice states, at the center of the Brillouin zone, obtained in the present calculation. On the left, states 1–6 and I–IV of the sawtooth $GaAs\text{-}Ga_{1-x}Al_xAs$ structure. On the right, states 1′–6′ and I′–IV′ of the quantum-well structure $GaAs\text{–}Ga_{0.8}Al_{0.2}As$. In both cases, the superlattice period is ~140 Å, along the ⟨100⟩ direction. The conduction-band states are measured in eV from the conduction-band edge of GaAs at Γ_c. The valence-band states are measured in eV from the valence band of GaAs at Γ_V.

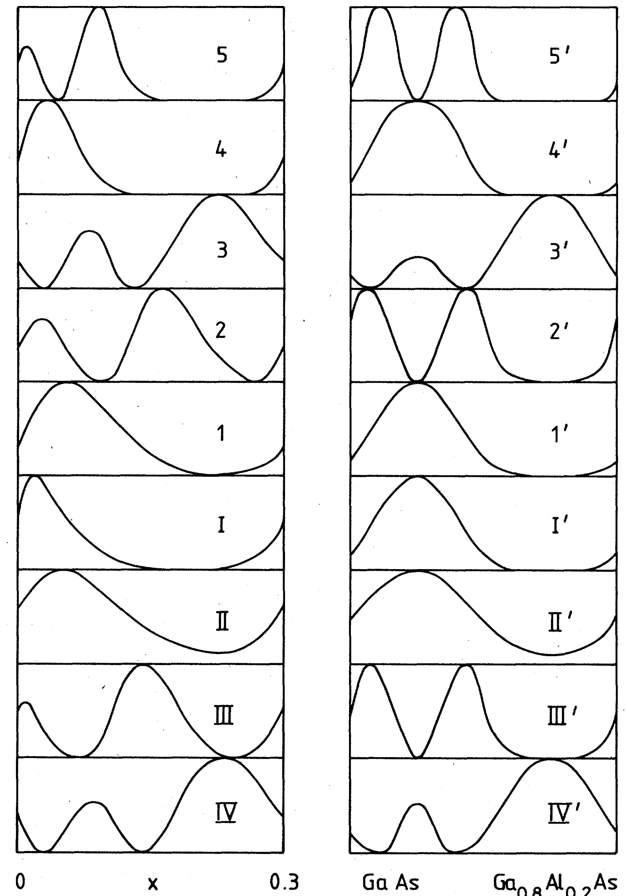

FIG. 2. A summary of the electron charge densities, at the center of the Brillouin zone, associated with the sawtooth and quantum-well superlattice states reported in Fig. 1. $|\psi|^2$ averaged over the interface plane is plotted along the superlattice axis in the ⟨100⟩ direction. The peak of $|\psi|^2$ is set to 1 to facilitate presentation.

essentially the same. Note that the sequence of confined X-like states resembles the sequence of Γ-like states, both in the sawtooth and quantum-well systems. To the best of our knowledge, quantitative predictions of the positions and charge densities of these states have not been reported in the literature. The quantum states above the barrier are sufficiently localized to alter the overall picture of the density of states. The existence of these states may help in understanding the real space-charge transfer and hot-electron transport phenomena in superlattice structures.

The above comparison can be readily extended to describe the states near the valence-band edge. As in the conduction band, there are the familiar confined states and localized resonances of broadly similar character in both systems.

Our calculations indicate that the short-wavelength component of potential V plays a significant part in the formation of the superlattice states. Indeed, our tests show that the long-wavelength part of V does not have an important role in determining the confined states with respect to the bulk GaAs band structure. When the values of $V(\vec{k})$, $\vec{k}\to 0$ are drastically altered and the calculation repeated, the results are not substantially affected. However, the magnitude of the band offsets which is in principle an observable quantity, and which is a key parameter in most of the popular computational schemes, does depend on $V(0)$. $V(\vec{k})$, $\vec{k}\to 0$ may account for $\approx$0–100 meV of the offset value in GaAs-GaAlAs systems and may reflect the degree of charge transfer depending on sample preparation and other material factors.

It might be worth pointing out that even the short-range terms determining the physical properties of the superlattice states are not identical to those that control the band offsets. If we neglect $V(0)$, the offsets can be computed from (1) simply by replacing all GaAs atoms with those of GaAlAs, i.e., by turning GaAs into GaAlAs and setting $V(0)=0$. The eigenvalue problem in (1) leads to setting up and diagonalizing a matrix of elements of V between the Bloch functions belonging to H_0 (GaAs). Hence, having ignored the difference in lattice constants, the only functions $\phi_{n,\vec{k}}$ that have nonzero off-diagonal matrix elements are those associated with different band index n and identical values of $\vec{k}$. On the other hand, for wide enough wells (e.g., ~200 Å), convergence tests show that, for example,

the confined states at the bottom of the conduction band are adequately described by $\phi_{n,\vec{k}}$ in (1) belonging to the lowest conduction band of GaAs. In fact, our tests concerning the structures of Figs. 1 and 2 show that it is possible to obtain—in a given range of energies—a set of nearly identical energy levels by solving Eq. (2) with potentials V whose short-ranged components have been altered to produce different band offsets. Similarly, two different potentials constructed so as to give the same offsets may yield different levels. Wave functions are particularly sensitive to changes in $V(\vec{k})$ at certain large values of the wave vector. This means that the physical processes underlying the confinement effect may not be unambiguously linked to an effective mass model Hamiltonian. It would not be surprising if direct observations of offsets did not agree with the values obtained by fitting the observed transition energies between confined levels via the envelope function effective-mass theory. The significance of short-range interactions in quantum-well superlattices has been anticipated on phenomenological grounds by Shu and Kroemer.[7] However, ours is the first calculation showing that such processes occur in GaAs-GaAlAs systems. In fact, we have performed pseudopotential calculations on other systems, e.g., InAs-GaSb superlattices. There we also find a rich variety of states in the relevant range of energies. Some of these states are localized in the confining layers and at interfaces.[8]

In conclusion, our calculations have revealed a number of new confined states in sawtooth and quantum-well superlattices. We show that although there are clear systematic differences between these two structures, both can be described in qualitatively identical terms. In particular, we show that some of these states are localized in the confining barriers or at interfaces. Our results also provide fresh insight into the microscopic processes underlying the formation of confined states. Our convergence tests indicate that the rapidly varying part of the potential plays an important role in confinement effects. In our calculations, the wave functions of superlattice states appear as linear combinations of GaAs Bloch functions defined on a unique grid of points in the wave-vector space. Although the largest coefficients are, as expected, derived from the lowest (highest) sampling points of the corresponding band, these contributions are themselves insufficient to provide a realistic description of the wave function along the full length of superlattice period. At least $\frac{1}{3}-\frac{1}{2}$ of the bulk Brillouin-zone volume is required to accomplish such a description of the sawtooth superlattice considered here. Finally, our results concerning other systems (e.g., GaSb-InAs superlattice) indicate that the above mentioned effects are commonly occurring in semiconductor superlattices.

[1]F. Capasso, S. Luryi, W. T. Tsang, C. G. Bethea, and B. F. Levine, Phys. Rev. Lett. **51**, 2318 (1983).
[2]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[3]M. Jaros, *Deep Levels in Semiconductors* (Hilger, London, 1982).
[4]M. J. Kirton and P. W. Banks, J. Phys. C **17**, 2475 (1984).
[5]K. B. Wong, M. A. Gell, and M. Jaros, J. Phys. C (to be published).
[6]M. Jaros and K. B. Wong, J. Phys. C **17**, L765 (1984).
[7]Q. G. Zhu and H. Kroemer, Phys. Rev. B **27**, 3519 (1983).
[8]M. A. Gell, K. B. Wong, and M. Jaros, J. Phys. C (to be published).