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Interaction phenomena between deep levels and minibands in semiconductor superlattices

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Calculations of the electronic states are presented for a new superstructure. This consists of a conventional heterojunction superlattice interleaved with a periodic array of deep centers located in the barrier layers. By appropriate choice of the quantum-well thickness and of the location of the deep center within the barrier, strong mixing between the defect and superlattice states takes place. Enhancement of the miniband widths by several orders of magnitude and the creation of new "hidden" Bloch states within the band gap of the superlattice are found.

In recent years, intense research on superstructures such as heterojunction and doping superlattices (SL's), variable-gap semiconductors, and selectively doped interfaces has revealed a surprising variety of new phenomena.[1] In this communication we present calculations showing that deep levels introduced in the barriers of tight-binding SL's can have intriguing effects on the SL states. Figure 1 summarizes the main findings of the present study.

Let us consider the periodic structure whose conduction band is sketched in Fig. 1(a). We examine the introduction of a sheet of defects in the center of the barriers corresponding to a deep center lying in energy between the two original bands. Such deep levels could be obtained also by the deposition of sheets of shallow impurities at high surface concentration as shown by Hjalmarson.[2] Figure 1(b) shows the enhanced width of the bands in the resulting structure and the creation of one extra band due to the states introduced by the defects. This enhancement is maximized when [Fig. 1(c)] the energy level of the defect is matched to the ground state of the corresponding isolated quantum well.[3] In this context it is interesting to note that strong resonances in the current-voltage characteristic of certain multiple-quantum-well structures are observed when the applied voltage is such that the bottom of the first subband of the quantum wells is lined up with deep levels in the barrier layers.[4]

In an actually grown structure with weak coupling between wells (tight-binding SL) the states of the SL easily become localized. This occurs when the combined energy-level broadening due to intralayer thickness fluctuations and collisions is greater than the miniband widths.[5] Therefore we can have the interesting fact that the periodic introduction of a highly localized state in a periodic heterostructure causes a delocalization in the resulting states with consequent dramatic change in the electronic properties.

We shall also consider another variable: the position of the layer in the barrier. Figure 1(d) shows the case of energy matching of Fig. 1(c), but with the defect layer displaced significantly from the central position in the barrier. The ground-state miniband of Fig. 1(c) splits into two bands considerably narrower and shifted. This shift can be such that, as shown, a new SL band is formed lying in energy below the bottom of the quantum wells. This means that the resulting SL band gap can be made smaller than that of the bulk of both materials.

The band-structure calculation of heterojunction SL's is often performed via a Kane-type formalism based on the solution of an effective Hamiltonian as studied in detail by Bastard.[6] The results obtained with this technique

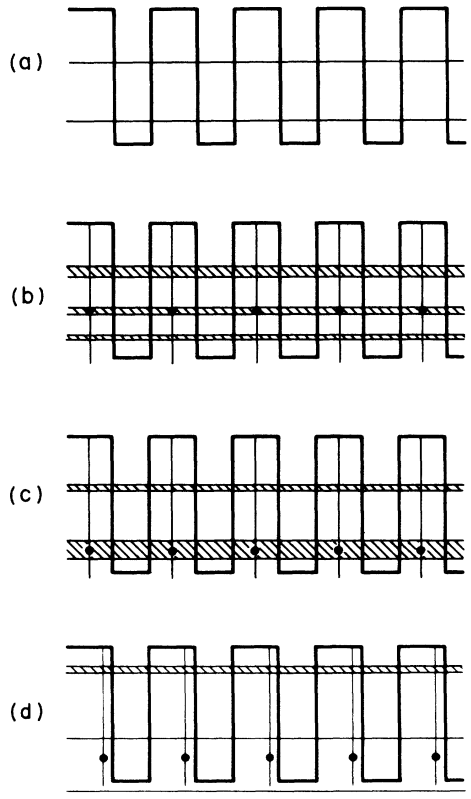

FIG. 1. Energy-band diagrams of multiple-quantum-well structure (a) without defects and (b)–(d) after their introduction. In (b) the defect sheets, shown as vertical lines, are in the middle of the barriers and their energy level, shown as a dot, is intermediate between the two original bands. In (c) the defects level is lined up with the ground level of the wells. In (d) with energies still matched, the defects are displaced from the central position. New quantum states, hidden below the bottom of the quantum wells, are found.

have been shown to be in excellent agreement with linear combination of atomic orbitals calculations.[6] We shall study our problem within the same formalism by using a model potential to describe the defect. Since the qualitative results of the calculations are not influenced by the details of the potential chosen (we have verified that only its symmetry and weight, i.e., its integral, are important) we shall use a δ function. This model is adequate for several types of deep centers as suggested by photoionization cross-section measurements[7] and allows us to express our results with a compact analytical formula.

Each δ in the barriers introduces one state whose energy level is controlled by the parameter P, the weight of the δ function.[8] The calculated relation between the Bloch wave number k and the energy E (referred to the bottom of the wells) is

$$\cos(ka)=\cos(k_1w)\cos(k_2b)-\frac{(k_1/m_1^*)^2+(k_2/m_2^*)^2}{2(k_1/m_1^*)(k_2/m_2^*)}\sin(k_1w)\sin(k_2b)+\frac{m_2^*P}{\hbar^2k_2}\left\{\cos(k_1w)\sin(k_2b)+\frac{\sin(k_1w)}{(k_1/m_1^*)(k_2/m_2^*)}\left[\left(\frac{k_2}{m_2^*}\right)^2\cos\left(k_2\frac{b+2s}{2}\right)\cos\left(k_2\frac{b-2s}{2}\right)-\left(\frac{k_1}{m_1^*}\right)^2\sin\left(k_2\frac{b+2s}{2}\right)\sin\left(k_2\frac{b-2s}{2}\right)\right]\right\}, \quad (1)$$

where m_1^*,w and m_2^*,b are effective masses and thicknesses relative to the well and barrier layers, respectively. s is the displacement of the defect from the center of the barrier, $a=w+b$ is the SL period. The wave numbers in the wells and barriers, k_1 and k_2, are given by

$$k_1=\frac{\sqrt{2m_1^*E}}{\hbar},\quad k_2=\frac{\sqrt{2m_2^*(E-\Delta E_c)}}{\hbar}.$$

In the case of no impurity ($P=0$) we find the results of Bastard.[6]

As an example we consider a $GaAs/Ga_{0.7}Al_{0.3}As$ periodic structure with $w=80$ Å and $b=100$ Å.[9] The first two bands of the unperturbed periodic structure are shown in the reciprocal space in the extended-zone scheme by the dashed curves in Fig. 2. The first band is centered at $E_0=42.5$ meV (which is the first energy level of the corresponding isolated quantum well[3]) and its width is $\Delta E_0=4.4\times10^{-2}$ meV. The second band is characterized by $E_1=165.6$ meV and $\Delta E_1=1.1$ meV.

Referring to this periodic structure, we consider now the case of defects centered in the barriers with energy levels matched to those of the isolated wells[3] [sketched in Fig. 1(c)]. Our model gives for the first two bands of the new structure the results shown by the thick solid curves in Fig. 2. We obtain $\Delta E_0=9.1$ meV, $\Delta E_1=2.4$ meV. The first band of the resulting structure is more than 200 times wider than without deep levels. The broadening depends on the SL parameters: the effect is larger for narrower starting bands (keeping $w=80$ Å, for $b=140$ Å, for instance, brings ΔE_0 down to 2.1×10^{-3} meV, and the miniband is broadened about 10^3 times). This broadening is maximum with the defect layer centered in the barrier. In this case, in fact, the overlapping between the defect and SL eigenstates is maximum. It is worth mentioning here that using the well width as a parameter, the energy levels of the well and of an available deep center can be very effectively matched.

Another noticeable aspect is that there is no energy gap at π/a in the dispersion relation. The periodic introduction of the defects (matched in energy and centered in the barriers) compensates the effect of the periodic SL potential and closes the gap. It is easy to show that *any* symmetric potential centered in the barriers can give the same result provided it has the proper weight. For what concerns the second band, it is approximately doubled in width and is shifted toward higher energies.

We consider now the effect of a displacement s of the defect from the central position in the barrier. In Fig. 2 the thin solid curve refers to the case of energy matching but with $s=10$ Å. The gap reopens at π/a (again this is a property of any symmetric potential). The first band narrows considerably ($\Delta E_0=1.9$ meV) and shifts toward lower energies.

This suggests that we are able to control the band gap of the SL by the introduction of defects. Figure 3 shows how far we can go in this direction. In this figure we plot the width of the first band as a function of defect displacement s for a 80-Å well SL for two barrier thicknesses in the above $GaAs/Ga_{0.7}Al_{0.3}As$ material system. The top curve (dashed area) refers to the 100-Å barrier case considered up to now, with bandwidth expanded 10 times for better reading. For $s\gtrsim37$ Å the first band is in a region of negative energies; we have introduced a miniband below the bottom of the quantum well [Fig. 1(d)]. The same figure shows that in that limit for the present structure the first band is so narrow that no band conduction is possible in a realistic (grown) structure due to fluctuations and collisions. But we can consider a different structure with thinner barrier layers where this is possible. The lower curve of Fig. 3 (dotted area) shows the results of the calculations for the top and bottom of the first band as a function of s relative to a 40-Å barrier structure in the same system.

The actual realization of these structures is not very demanding for modern growth techniques like state-of-the-art molecular-beam epitaxy (MBE). The key point is the availability of a well controllable deep center that can be introduced with sufficiently high surface concentration. The pioneering MBE work of Malik *et al.*[10] demonstrated the introduction of ultrathin ($\lesssim$ few tens of Å) doping sheets of known surface density and thickness (planar doping). More recently, Schubert, Cunningham, and Tsang,[11] have grown δ-doped *n-i-p-i* SL's consisting of single atomic planes of shallow dopants via the "impurity-growth mode." Their experiments show that

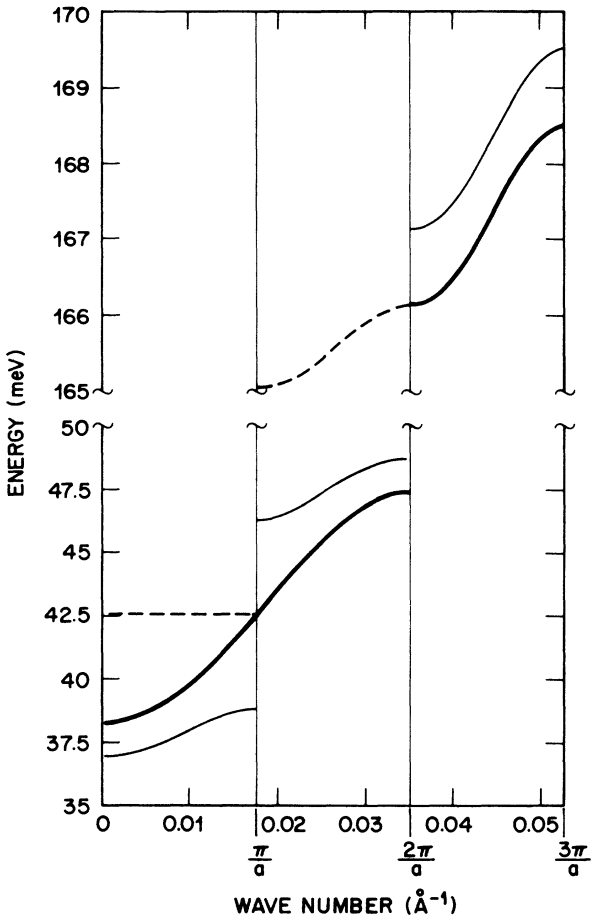

FIG. 2. Energy dispersion relation in the extended zone scheme for a 80-Å well, 100-Å barrier GaAs/$Ga_{0.7}Al_{0.3}As$ superlattice: dashed line, without defects; thick solid line, with defects centered in the barriers and energy matched to the ground state in the wells; thin solid line, with defects displaced 10 Å from the center and energies matched.

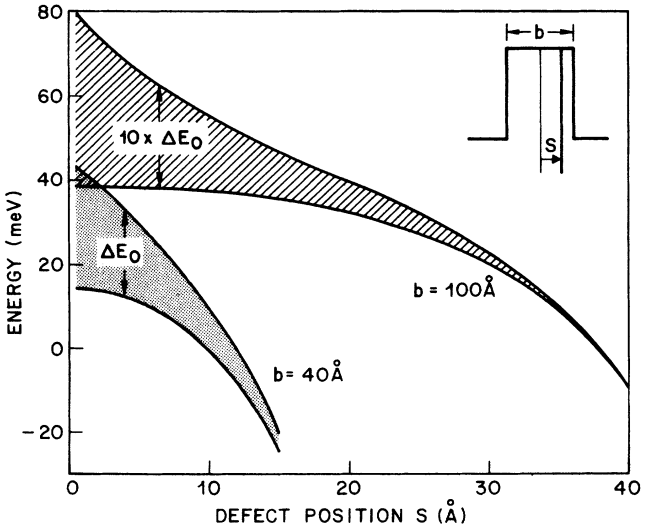

FIG. 3. Ground-state miniband width as a function of defect displacement for a 80-Å well GaAs/$Ga_{0.7}Al_{0.3}As$ superlattice. Two barrier thicknesses are examined with energy matching of the defect with the ground level of the well. The lower curve (barrier thickness $b = 40$ Å, dotted area) gives the top and bottom of the first miniband. The upper curve ($b = 100$ Å, dashed area) gives the bottom and expands the width 10 times for easier reading.

by proper control of the growth temperature the impurities were confined to single monolayers without degrading the crystallinity of the material (as shown by the superlattice formation). Of course this technique is not limited to dopants and can also be extended to impurities capable of introducing deep levels. Moreover, as discussed above, the latter could also be created using shallow dopants by the mechanism proposed by Hjalmarson.[2] This author showed that the energy levels of impurity pairs and clusters evolve to successively deeper levels as the spatial separation of the impurity atoms (e.g., Si in GaAs) decreases. Thus deposition of a dopant in a planar profile at sufficiently high densities may lead to the creation of sheets of deep levels.[2]

In conclusion, we have shown that new degrees of freedom in the design of SL can be achieved by introducing deep center sheets. This deep-level engineering gives control on the position of the energy bands and their width.

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[8]See, e.g., I. I. Goldman and V. D. Krivchenkov, *Problems in Quantum Mechanics* (Pergamon, New York, 1961), Chap. 1. This is derived in the case of an infinitely wide barrier. It is nevertheless an excellent approximation in the limit of relatively thick barriers and deep levels we are investigating.

[9]We assumed the following material parameters: $\Delta E_c = 271$ meV, $m^* = 0.096 m_0$ in the $Ga_{0.7}Al_{0.3}As$ barrier layer, and $m^* = 0.067 m_0$ in the GaAs well layer.

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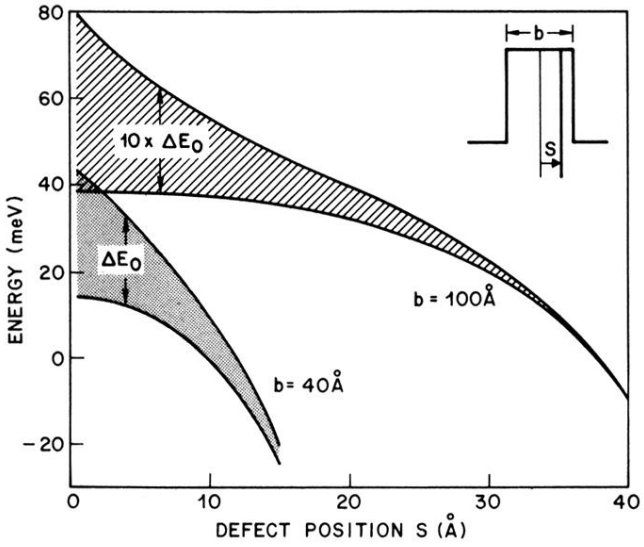

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