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Band structure of semiconductor superlattices

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A theory of the band structure of semiconductor superlattices has been developed for both the direct-band-gap and indirect-band-gap barrier layers taking into account the multivalley and nonparabolic band structure of the materials forming the superlattice. For direct-band-gap barrier layers the nonparabolicity in the band structure may alter the electronic energy levels measured from the bottom of the potential wells by as much as 26%. On the other hand for indirect-band-gap barrier layers the alteration due to the nonparabolicity is about 14%. It is also found that even for indirect-band-gap barrier layers the band structure is mainly determined by the states corresponding to the direct-gap minimum. Energy levels calculated on the basis of the theory presented are also found to agree with those obtained in recent experiments with double-barrier heterostructures.

I. INTRODUCTION

The properties of semiconductor superlattices have been intensively studied in recent years with the hope of realizing negative differential conductivity.[1–3] It is also reported that superlattice structures with a period of 50–80 Å and having barrier layers with widths as small as 10 Å may be successfully fabricated with high consistency. The prediction that such structures would have minibands within the permitted band has also been confirmed indirectly by experiments.[3–5] The miniband parameters have been calculated[3] using simple square-well models for the potential distribution in the direction of the superlattice axis. For the solution of the Schrödinger equation, the effective mass of the electron was taken to be a suitable average of the electron effective mass in the two materials. The barrier potential was taken to be around 0.8 times the difference in the band gaps (direct for one material, indirect for the other). Reasonable agreement has been claimed between experiment and the results obtained from this simple theory.[3–5]

Considering a model potential distribution, it may be shown[6] that this simple theory is unlikely to give quantitatively good results, and a more exact theory is necessary for the interpretation of experimental results. The purpose of this paper is to develop an exact theory of the band structure of semiconductor superlattices, taking into account the full complexity of the band structure of the materials that form the superlattice.

II. STRUCTURE AND PROPERTIES OF MATERIALS

The pairs of materials chosen to form the alternate layers in a superlattice are characterized by almost identical lattice constants. This ensures a minimum amount of lattice deformations across the layer boundaries. The differences in the forbidden gaps of the pairs of materials are a few tenths of an electron volt. GaAs-$Ga_{1-x}Al_xAs$ seems to be the most favored pair,[3–5] while use of GaAs-$GaAs_{1-x}P_x$ has also been reported.[2]

The formation of the alternate barriers and wells at the conduction-band edge may be understood by considering a layer of the larger gap material flanked by two smaller gap material layers, both materials being *n* type. As the layers come into contact, a discontinuity in the conduction-band edge appears, equal to the difference in the chemical affinities of the materials. Electrons spill over from the middle layer on either side till the Fermi levels line up. In this process, the middle layer is left with virtually no conduction electrons, and may now be looked upon as insulating. The depletion zones created by the transfer of electrons extend from the two boundaries into the bulk of the middle layer. The potential profile will therefore be a rectangular barrier with a symmetrically sagging roof. The carrier concentration in the materials being of the order of 10^{16} cm^{-3}, the potential would decrease at the rate of about 2.7×10^{-4} eV/Å. Since the width of the barrier is not larger than 100 Å, the sag may be neglected in comparison with the barrier height. This condition will always be assumed to be satisfied in the superlattices considered.

The potential well region is formed by the GaAs layers, as the conduction-band minimum for this material is lower than that of its mixed compounds (i.e., GaAlAs, GaAsP) used in the superlattice structure.

The conduction band of GaAs has the lowest minimum at the Γ-point and secondary minima separated from this by more than 0.4 eV.[7] We may hence assume that the electrons will occupy only the Γ-point minimum up to room temperature, and since the E-k relation for this minimum is isotropic, we may also assume that the electrons will be characterized by an isotropic effective mass. We should note that we shall be concerned with

electron energies significantly higher than that corresponding to the minima. The effective mass should therefore be considered to be a function of energy, and in our analysis we shall assume that the functional relation is given by the simplified Kane relation

$$\hbar^2 k^2/2m^* = E(1 + E/E_G), \tag{1}$$

where E is the total kinetic energy of the electron measured from the band edge, and k is the magnitude of the wave vector.

The position of the conduction-band minimum in the mixed compounds forming the barrier layers depends on the ionic replacement fraction x. We may obtain[8] the relative position of the different minima for a particular value of x by interpolation between the values corresponding to GaAs and AlAs in the case of $Ga_{1-x}Al_xAs$, and to GaAs and GaP in the case of $GaAs_{1-x}P_x$. The interpolation curves are shown in Fig. 1. It may be seen that depending on the value of x, the lowest minimum will be either a Γ-point minimum or an X-point minimum. If the value of x is less than 0.37 for $Ga_{1-x}Al_xAs$ and less than 0.53 for $GaAs_{1-x}P_x$, the lowest conduction-band minimum for the mixed compound is also a Γ-point minimum. The Γ-point minimum is separated from other minima by more than 5 kT at room temperature for x less than 0.25 for $Ga_{1-x}Al_xAs$, and 0.36 for $GaAs_{1-x}P_x$. For x up to these values, we may hence consider the effective mass of the electron to be isotropic, as in the potential wells. We may also use Eq. (1) to include the effects of nonparabolicity. However, when the value of x is larger, the Γ-point minimum and the X-point minima are at comparable heights. We then have to consider possible states of the electron, when travelling through the barrier layer, corresponding to both these minima, and the a tual band energies may be obtained only by a diagonalization process. The problem is complicated by the fact that the E-k relation for the minimum away from the zone center is of the form

$$E = \tfrac{1}{2}\hbar^2(\vec{k} - \vec{k}_l)\cdot \overleftrightarrow{M} \cdot (\vec{k} - \vec{k}_l), \tag{2}$$

where $\vec{k}_l$ gives the position of the minimum in k space, and $\overleftrightarrow{M}$ is the effective-mass tensor. Usually there are also a number of symmetrically located minima at the same level. The nonparabolic E-k relation for this minimum is not yet well known. We shall, however, use the following relation to evaluate the effects of nonparabolicity for the elliptic bands

$$\hbar^2 k^2/2m^* = (E - E_0)[1 + (E - E_0)/E_G], \tag{3}$$

where E_0 is the energy at the minimum; E_G is the energy gap between the conduction band and the valence band at $\vec{k} = \vec{k}_l$. The above relation, although not rigorously derived, has been used in the literature for transport calculations in indirect-gap materials like Ge.[9]

For large values of x nearing unity, the indirect minimum has the lowest position and is separated from the Γ-point minimum by more than 0.7 eV in $Ga_{1-x}Al_xAs$. For this composition, it may appear that we should consider only the states corresponding to the indirect minima. It will however be shown that due to the smaller value of effective mass for the Γ-point minimum, states corresponding to the latter play an equally important role in determining the band structure even for such high values of x.

We may hence conclude that for obtaining accurately the band structure of semiconductor super-

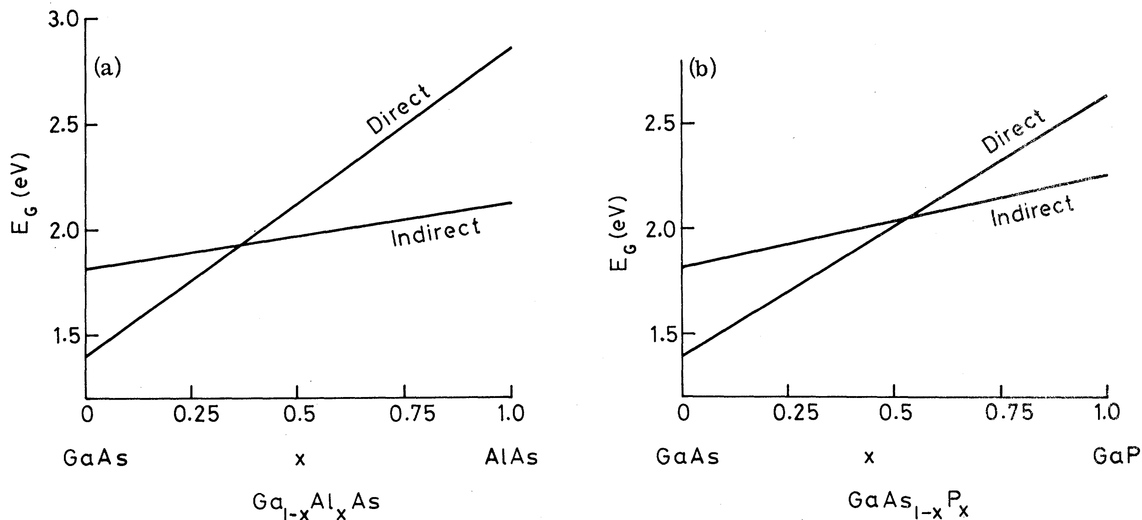

FIG. 1. Interpolation curves for (a) $Ga_{1-x}Al_xAs$ and (b) $GaAs_{1-x}P_x$.

lattices, we may consider the electron characterized by an isotropic effective mass in the potential well region, but in the barrier region it may have different kinds of states characterized by either an isotropic effective mass or a tensorial anisotropic effective mass. Our theory should take into account all these possible states. However, before presenting this theory, we discuss in Sec. III the nature of the bands that may be obtained for the lower values of x for which we may assume, as discussed above, an isotropic effective mass in the barrier layer.

III. BAND CALCULATIONS FOR DIRECT GAP IN BARRIER LAYER

We assume that the width of the potential wells is a and that of the barrier layers is b, as shown in Fig. 2. The difference in the conduction-band edges results in a barrier of height V_1. In earlier analyses, V_1 was taken to be 0.8 times the difference in the band gap of the two materials. However, recent work by Dingle *et al.*[5] indicates that a more appropriate value of the factor is 0.88, and this value has been used in our analysis. The value of a for the experimental structures varies between 40 and 100 Å, and that for b ranges between 10 and 100 Å. For the calculation of the band structure, we shall assume that the interfaces between the layers are sharply defined and devoid of any surface effects, so that the potential distribution may be considered to be an array of square wells. To obtain the band structures, we have to solve the Schrödinger equation for the atomic potentials having the one-dimensional periodicity of the superlattice structure. We shall, however, make three simplifying assumptions: (i) The effect of the atomic potentials is only to modify the effective-mass value of the electron corresponding to the E-k relation of the particular material.[10] (ii) The electron mean free path is much larger than the superlattice period, so that the collision effects may be neglected. (iii) The total length of the structure is long enough for neglecting the boundary effects.

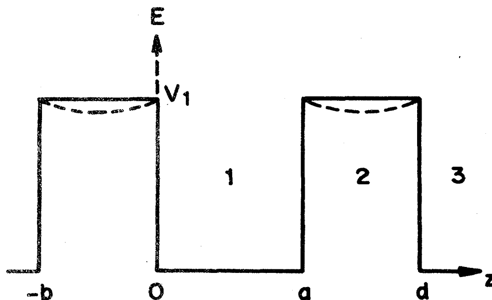

FIG. 2. Potential profile for the superlattice structure. The dashed lines indicate schematically the small sag expected in the barrier layer.

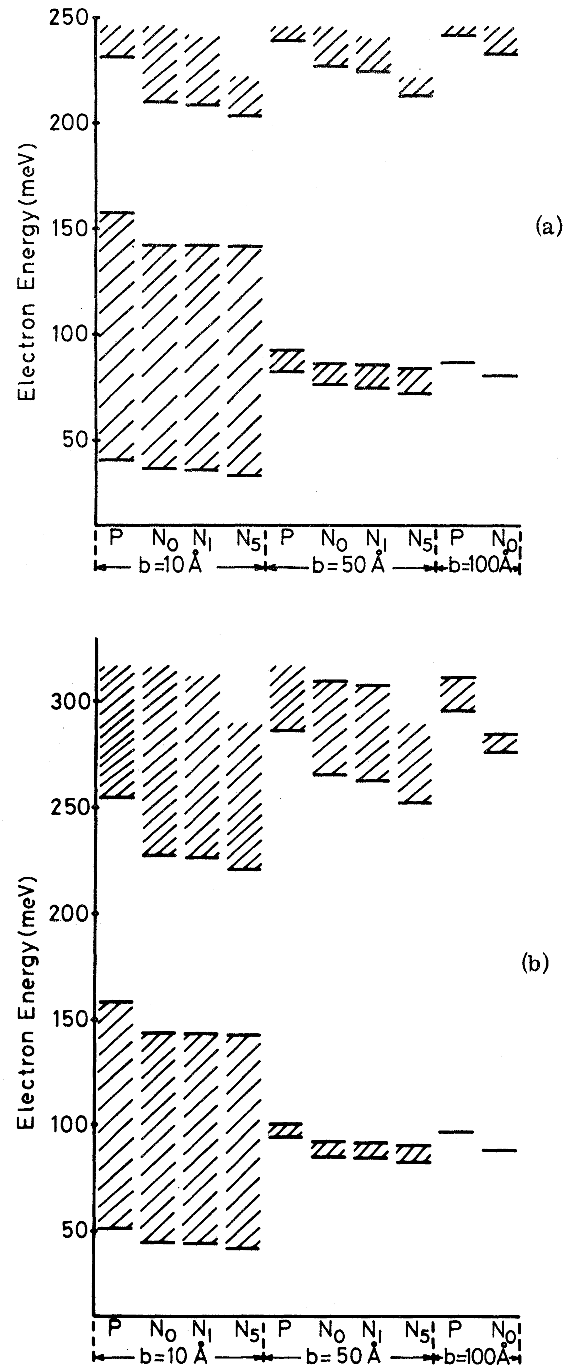

FIG. 3. Energy levels up to the barrier for superlattices with $a = 50$ Å, and b as indicated. (a) $Ga_{0.8}Al_{0.2}As$, (b) $GaAs_{0.7}P_{0.3}$. The P columns are for parabolic bands; N_0, N_1, and N_5 are for nonparabolic bands with $E_t = 0$, kT, and $5kT$ at room temperature.

Let us consider an electron with energy E_1 and wave vector $\vec{k}$ having the components k_x, k_y, k_1 in region 1 (see Fig. 2). Let the same electron,

when it enters region 2, have energy E'_T and wave vector $\vec{k}'$ with the components k'_x, k'_y, k_2. Since energy is conserved in the transition, $E'_T = E_T$. We also note that the wave function at the boundary between two adjacent layers should be continuous. Since this continuity is to be ensured for all values of x and y for a fixed value of z (e.g., $z=0$), it also follows that the x and y components of the wave vector should also be conserved, i.e., $k'_x = k_x$, $k'_y = k_y$. Using the energy-conservation condition and a parabolic E-k relation for the two materials, we then obtain

$$(\hbar^2/2m_1^*)(k_t^2+k_1^2) = (\hbar^2/2m_2^*)(k_t^2+k_2^2) + V_1, \qquad (4)$$

where $k_t^2 = k_x^2 + k_y^2$, m_1^* is the electron effective mass in the potential well, and m_2^* is the electron effective mass in the barrier layer. Since

$$k_1 = (2m_1^* E/\hbar^2)^{1/2}, \qquad (5)$$

we obtain from Eq. (4)

$$k_2 = \{(2m_2^*/\hbar^2)[E - V_1 + E_t(1 - m_1^*/m_2^*)]\}^{1/2}, \qquad (6)$$

where E is the energy corresponding to the z component of the wave vector in the potential well region, and $E_t = \hbar^2 k_t^2/2m_1^*$ is the transverse energy in the GaAs layer. We find from the above relation that k_2 is imaginary if $E < [V_1 - E_t(1 - m_1^*/m_2^*)]$, and its magnitude depends on E as well as on E_t, since $m_1^* \neq m_2^*$. The latter dependence will have the effect of broadening the bands, since E_t will vary from electron to electron even if E is the same. The magnitude of this broadening will be discussed later. For the present, we calculate only the band structure, assuming

$$E_t(1 - m_1^*/m_2^*) \ll V_1.$$

The wave functions for the two regions may be written as

$$\psi_1(z) = Ae^{ik_1 z} + Be^{-ik_1 z},$$
$$\psi_2(z) = Ce^{k_{2i} z} + De^{-k_{2i} z},$$
$$\psi_3(z) = \psi_1(z-d)e^{ikd},$$

where

$$k_{2i} = [(2m_2^*/\hbar^2)(V_1 - E)]^{1/2}, \quad \text{for } 0 < E < V_1.$$

Using the conditions of continuity of the wave function and its derivative at $z=0$ and $z=b$, we get the familiar dispersion relation

$$[(k_{2i}^2 - k_1^2)/2k_1k_{2i}]\sinh(k_{2i}b)\sin(k_1a) + \cosh(k_{2i}b)\cos(k_1a) = \cos(kd) \qquad (7)$$

In Fig. 3 we have shown the band structure for $a = 50$ Å, and $b = 10$, 50, and 100 Å, using for m_1^* the effective-mass value of GaAs, and for m_2^* the effective-mass values for $Ga_{0.8}Al_{0.2}As$ and $GaAs_{0.7}P_{0.3}$. The barrier heights were taken to be 0.88×0.28 eV and 0.88×0.36 eV, respectively.

The effect of nonparabolicity may be included straightaway into the dispersion relation by putting

$$k_1 = [(2m_1^*/\hbar^2)E(1 + E_T/E_{G1})]^{1/2} \qquad (8)$$

and

$$k_{2i} = \{(2m_2^*/\hbar^2)(V_1 - E)[1 - (V_1 - E_T)/E_{G2}]\}^{1/2}, \qquad (9)$$

which follow from Eqs. (1) and (3). We show in Fig. 3 the modification in the bands resulting from the nonparabolicity. E_{G1} was taken to be 1.4 eV, and E_{G2} was taken as 1.68 eV for $Ga_{0.8}Al_{0.2}As$, and 1.76 eV for $GaAs_{0.7}P_{0.3}$, respectively. E_T was taken to be equal to E.[11] The nonparabolicity may change the parameters by as much as 15% for the low values of x considered in the examples. However, the change would be larger and will be more significant for higher values of x when the barrier heights become larger, (see Fig. 5), results for which are presented later.

In order to assess the magnitude of band broadening (mentioned earlier), we have also calculated the band parameters for $GaAs_{0.7}P_{0.3}$ and $Ga_{0.8}Al_{0.2}As$ corresponding to $a = 50$ Å and $b = 10$, 50 and 100 Å, taking $E_t = \hbar^2 k_t^2/2m_1^*$ to be equal to kT and $5kT$ at 300 °K. We find that the parameters change by about 1.3% for $E_t = kT$ and by about 7% for $E_t = 5kT$. Since most of the electrons are contained in the energy interval $(0-2)kT$ of the conduction-band edges. we may conclude that the band broadening for the particular case considered here will be of the order of 3%. The results are shown in Fig. 3.

IV. BAND CALCULATIONS FOR INDIRECT GAP IN BARRIER LAYER

In order to keep our derivation general, we assume that the crystallographic axes of $Ga_{1-x}Al_xAs$ layers are oriented in an arbitrary direction with respect to the superlattice axis, which we have chosen as the z axis (Fig. 4). As noted earlier, there are a number of equivalent minima corresponding to the indirect-band gap located in the directions of symmetry. We first consider one of these minima, the E-k relation for which is given by Eq. (2). The wave vector of the electron in $Ga_{1-x}Al_xAs$, k_2, for a state corresponding to the minimum may be obtained by applying the conditions of conservation of total energy and of conservation of the transverse components of the wave vector. We thus obtain

$$\frac{\hbar^2(k_x^2+k_y^2)}{2m_1^*}+E=\frac{\hbar^2(k_x-k_{x0})^2}{2m_{xx}}+\frac{\hbar^2(k_y-k_{y0})^2}{2m_{yy}}+\frac{\hbar^2(k_2-k_{z0})^2}{2m_{zz}}+\frac{\hbar^2(k_x-k_{x0})(k_y-k_{y0})}{m_{xy}}+\frac{\hbar^2(k_y-k_{y0})(k_2-k_{z0})}{m_{yz}}$$
$$+\frac{\hbar^2(k_2-k_{z0})(k_x-k_{x0})}{m_{xz}}+V_2, \tag{10}$$

where V_2 is the potential barrier between the Γ-point conduction-band edge of GaAs and the $\langle 100\rangle$ conduction-band edge of $Ga_{1-x}Al_xAs$; k_{x0}, k_{y0}, k_{z0} are the components of $\vec{k}_i$, the wave vector giving the location of the minimum; m_{xx}, m_{xy}, etc. are the components of the effective-mass tensor. We should note here that since k_x and k_y in the barrier layer are the same as in the potential well region, the terms $(k_x-k_{x0})^2$ and $(k_y-k_{y0})^2$ will be large and the corresponding energies will also be large. For these energies, the effects of nonparabolicity would be important, and we should use the exact dispersion relation between E and k_x, k_y to obtain precise results. However, as our interest at this stage is only to deduce the general shape of superlattice band structure for indirect-gap barrier layers, we start by assuming that the parabolic relation remains valid.

Equation (10) gives complex values of k_2, which may be written as

$$k_2=k_{2r}\pm ik_{2i}\ , \tag{11}$$

where

$$k_{2r}=k_{z0}+m_{zz}\left(\frac{k_{x0}-k_x}{m_{xz}}+\frac{k_{y0}-k_y}{m_{yz}}\right), \tag{12}$$

and

$$k_{2i}=[(2m_{zz}/\hbar^2)(V_2'-E)]^{1/2}, \tag{13}$$

where

$$V_2^1=V_2+\frac{\hbar^2k_x^2}{2}\left(\frac{1}{m_{xx}}-\frac{1}{m_1^*}-\frac{m_{zz}}{m_{xz}^2}\right)+\frac{\hbar^2k_y^2}{2}\left(\frac{1}{m_{yy}}-\frac{1}{m_1^*}-\frac{m_{zz}}{m_{yz}^2}\right)+\frac{\hbar^2k_{x0}^2}{2}\left(\frac{1}{m_{xx}}-\frac{m_{zz}}{m_{xz}^2}\right)+\frac{\hbar^2k_{y0}^2}{2}\left(\frac{1-}{m_{yy}}-\frac{m_{zz}}{m_{yz}^2}\right)$$
$$+\hbar^2(k_x-k_{x0})(k_y-k_{y0})\left(\frac{1}{m_{xy}}-\frac{m_{zz}}{m_{xz}m_{yz}}\right)-\hbar^2k_xk_{x0}\left(\frac{1}{m_{xx}}-\frac{m_{zz}}{m_{xz}^2}\right)-\hbar^2k_yk_{y0}\left(\frac{1}{m_{yy}}-\frac{m_{zz}}{m_{yz}^2}\right). \tag{14}$$

We find from Eq. (14) that the x and y components of the wave vector, as in the earlier case, changes effectively the barrier potential and would cause broadening of the minibands. The effect is expected to be larger in this case as $1/m_1^*$ may differ by larger amounts from $1/m_{xx}$, $1/m_{yy}$, etc. We also note that the effects of location of the minimum away from the zone center is an enhancement of the barrier potential. The magnitude of this enhancement depends on the direction of $\vec{k}_i$ with respect to that of the superlattice. In fact, we should point out that the effective barrier height for the different equivalent minima may be very much different as their orientations are different.

In order to obtain the E-k relation for the superlattice related to the indirect minima under consideration, we use Eq. (11) to construct the electron-wave function in the barrier layer,

$$\psi_2(z)=Ce^{(ik_{2r}-k_{2i})z}+De^{(ik_{2r}+k_{2i})z}. \tag{15}$$

$\psi_1(z)$ and $\psi_3(z)$ remain unchanged from Sec. III. Matching the derivatives and values of the wave

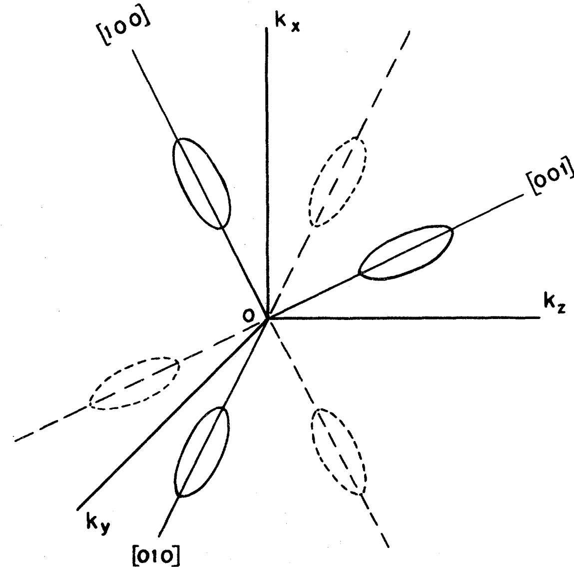

FIG. 4. Orientation of the ellipsoidal constant energy surfaces in the indirect-gap barrier layer. The k_z axis denotes the superlattice direction.

functions at the boundaries $z=0$ and $z=b$, we get

$$\frac{k_{2r}^2+k_{2i}^2-k_1^2}{2k_1k_{2i}}\sinh(k_{2i}b)\sin(k_1a)+\cosh(k_{2i}b)\cos(k_1a)=\cos(k_{2r}b-kd). \qquad (16)$$

The E-k relation for the superlattice for states corresponding to the minimum away from the zone center may in general be worked out from Eq. (16), together with Eqs. (12), (13), and (14). However, we discuss only the detailed nature of the bands that are obtained when the $\langle 100\rangle$ direction of $Ga_{1-x}Al_xAs$ coincides with the z direction, as this is likely to apply to practical structures. For this orientation, we have to consider separately two sets of energy ellipsoids—the two ellipsoids lying along the k_z axis, and the four along the k_x and k_y axes.

For the k_z ellipsoids, Eqs. (12), (13), and (14) gives

$$k_{2r}=k_{z0} \qquad (17)$$

and

$$k_{2i}=[(2m_l/\hbar^2)(V_2-E)]^{1/2}, \qquad (18)$$

where m_l is the longitudinal effective mass of an electron in the ellipsoids. In obtaining (18), the terms involving k_x and k_y in Eq. (14) have been dropped, as their band-broadening effects have been discussed in detail earlier.

For the k_x and k_y ellipsoids, Eqs. (12), (13), and (14) give

$$k_{2r}=0 \qquad (19)$$

and

$$k_{2i}=[(2m_t/\hbar^2)(V_2'-E)]^{1/2}, \qquad (20)$$

where

$$V_2'=V_2+\hbar^2k_{\mu 0}^2/2m_l, \quad \mu=x,y, \qquad (21)$$

and m_t is the transverse effective mass of an electron in the ellipsoids. Due to Eq. (19), the E-k relation for the k_x and k_y ellipsoids reduces from Eq. (16) to the form of Eq. (7), with k_{2i} being characterized by the electron effective mass m_t, and an enhanced barrier V_2'. The additional term $\hbar^2k_{x0}^2/2m_l$ or $\hbar^2k_{y0}^2/2m_l$ in Eq. (21) effectively increases the barrier V_2. A precise estimate of this enhancement, however, is not possible because, as has been pointed out earlier, the nonparabolicity effects in the k_x and k_y terms in Eq. (10) have not been taken into account. An order-of-magnitude estimate can only be made, and this indicates that electrons in the k_x and k_y ellipsoids are characterized by a barrier even larger than that arising from the difference in the direct gaps, and by a mass greater than the zone-center mass but less than the longitudinal mass. As a result, bands arising due to these ellipsoids would be narrow and would probably lie in the region between the bands arising from the direct-gap barrier and from the k_z ellipsoids.

To obtain the band structure arising due to the k_z ellipsoids, Eqs. (17) and (18) may be put in Eq. (16). It is then evident that the E-k relation would be critically dependent on the value of $k_{z0}b$, and we may expect significant changes in the superlattice bands with little change in the thickness of the barrier layers. However, when b is large, i.e., when the barrier layer contains a large number of lattice points in the direction of the superlattice axis, we may apply the cyclic boundary condition

$$\psi_2(z)=\psi_2(z+b).$$

The E-k relation then becomes

$$\frac{k_{z0}^2+k_{2i}^2-k_1^2}{2k_1k_{2i}}\sinh(k_{2i}b)\sin(k_1a)+\cosh(k_{2i}b)\cos(k_1a)=\cos(kd). \qquad (22)$$

In this relation k_{2i} is given by Eq. (18), and it is readily seen that the barrier height V_2 is determined only by the indirect-band gap. Since this gap is much smaller than the direct gap for large values of x in $Ga_{1-x}Al_xAs$, one might expect that this minimum will predominantly determine the superlattice E-k relation. However, this expectation is not fulfilled, mainly because the term k_{z0}^2 in the first term on the L.H.S. is much larger than either k_1^2 or k_{2i}^2 and would cause the bands to become extremely narrow, on the assumption that k_{z0} for $Ga_{1-x}Al_xAs$ lies at the zone edge.[12] To bring out this point, we present in Fig. 5 the band structures arising from a $Ga_{1-x}Al_xAs$ barrier layer with $x=0.5$ and 0.7, both for the direct gap in accordance with Sec. III and for the indirect gap using Eq. (22). For this latter case, k_{z0} has been assumed equal to $2\pi/d_1$, where $d_1=5.653$ Å is the lattice constant of the materials. We have also presented in Fig. 5 the energy levels obtained for the direct gap neglecting the effects of nonparabolicity. It is seen that the nonparabolicity alters the results by about 26%, which should be considered significant when comparing theoretical results with experiments.

V. DISCUSSIONS AND CONCLUSIONS

We have developed in this paper a complete theory of the superlattice minibands considering the nonparabolic E-k relation and also the multipole minima in the E-k space for the material forming the barrier layers. We find that the miniband parameters calculated by using the nonparabolic relation differ in some cases by large amounts from those obtained with the constant effective-mass approximation. The agreement reported earlier be-

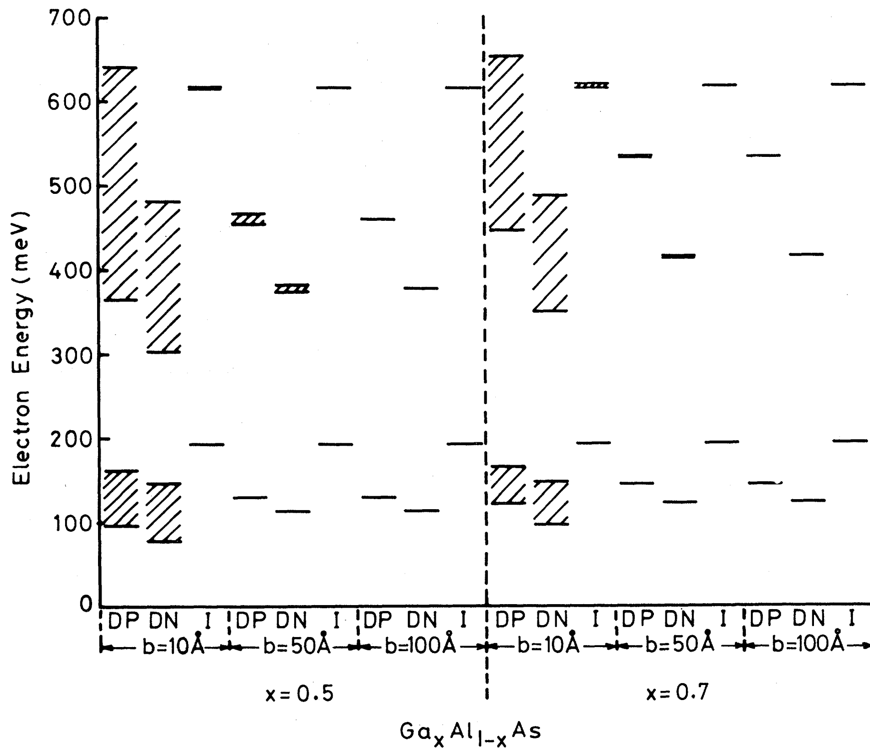

FIG. 5. Energy levels for $Ga_{1-x}Al_xAs$ superlattices with $x=0.5$ and 0.7, $a=50$ Å, and b as indicated. The I columns are for the indirect gap, the DN and DP columns for the direct gap, assuming nonparabolic and parabolic bands, respectively.

tween experiment and theory based on this approximation therefore requires further examination. We also find that for compositions of the barrier layer for which the band gap corresponding to the Γ-point minimum is larger than that corresponding to the X-point minima, the miniband energies have two possible sets of values arising from the two kinds of minima. The bands arising from the Γ-point minimum are in fact lower in position as well as wider, although the corresponding barrier potential is higher. We also find from the calculations made for barrier widths of 10, 50, and 100 Å that for the compositions used in the experiments, minibands may be obtained only for barrier layers having a thickness of about 10 Å, and these minibands will originate from the states corresponding to the Γ-point minimum. The states corresponding to the X-point minima give rise to bands of negligible widths even for a barrier thickness of 10 Å. It has also been shown that for all the cases considered, the bands or the energy levels may be broadened as a result of the conservation of transverse momentum, but for lattice temperatures near the room temperatures, the broadening would not be significant.

Experimental results proving definitely the formation of discrete levels in a structure analogous to the superlattice structures has recently been reported by Chang *et al.*[4] and by Dingle *et al.*[5] It is of interest to compare our calculated results with those of these experiments. In the experiment of Dingle *et al.*, the absorption spectra were measured for a single-well heterostructure made with GaAs and $Ga_{0.8}Al_{0.2}As$. The energy levels obtained from the analysis of the experimental data were found to agree with theoretical calculations apparently based on an energy-independent effec-

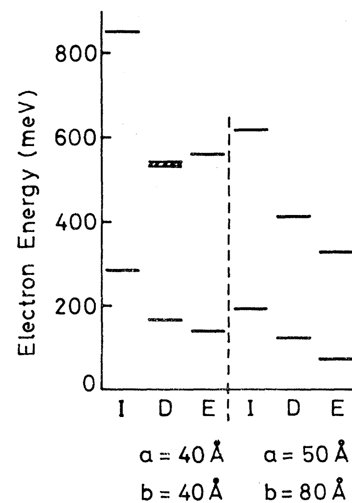

FIG. 6. Energy levels for superlattice structure with values of a and b as used in the experiment of Ref. 4. D—Theoretical values for direct gap, I—theoretical values for indirect gap, E—experimental values.

tive mass corresponding to GaAs. We find from calculations,[13] using the nonparabolic dispersion relation and the effective masses corresponding to GaAs and $Ga_{0.8}Al_{0.2}As$ as required by expressions (7)–(9), that the theoretical values decrease from those of Dingle by small amounts, the maximum difference being about 12 meV. The agreement observed by Dingle *et al.* between their theoretical values and experimental results therefore remain unaffected, even when we include the effects of all the complexities discussed in this paper.

The results obtained by Chang *et al.* from the resonant tunneling experiment are shown in Fig. 6, along with our calculated values for the experimental superlattice parameters.[13] We find on comparison that the experimental results agree fairly well with those obtained for the Γ-point minimum, including the effects of nonparabolicity. It may, however, be noted that according to our theory, discrete levels arising from the X-point minima and positioned at intermediate heights between those observed experimentally are also expected. The probability of resonant tunneling through these states may, however, be lower, and a more sensitive method of detection may be required to observe the effect of these states.

In conclusion, we would like to point out that according to the present calculations (see Figs. 3 and 5), there is a greater possibility of obtaining superlattice minibands and the associated negative differential mobility if the structures are made with $Ga_{1-x}Al_xAs$ with $x < 0.25$ or $GaAs_{1-x}P_x$ with $x < 0.36$. For higher values of x, as is evident from these calculations, discrete levels are likely to be obtained rather than minibands.

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[11] Note that E_T, the total energy, may be quite different from E, the energy corresponding to k_z. The variation of E_T would cause broadening of the bands through the effects of nonparabolicity, in addition to that arising from the variation of the effective barrier height mentioned earlier. However, as the average difference between E_T and E is of the order of kT for nondegenerate materials and of the order of the Fermi level for degenerate materials, the broadening through nonparabolicity may be considered negligible at ordinary temperatures and for not-too-high ($< 10^{18}$ cm^{-3}) electron concentrations.

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