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Effect of deformation on the conduction band of III-V semiconductors

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We develop a theory describing the effect of mechanical deformation on the conduction-band eigenstates in the vicinity of the Γ point in the III-V semiconductors. In this theory all strain-induced effects are interpreted in terms of the admixture of *s*- and *p*-like states used to describe the conduction band for zero deformation. Unlike previous work, the results can be applied regardless of the relative size of the band gap E_g and spin-orbit splitting Δ. A previously neglected term in the part of the Hamiltonian describing the effect of deformation is found to produce substantial contributions for sufficiently large energies above the band edge. Both of these aspects are particularly important when the narrow-gap materials like InSb are considered. Our theory is also the first to predict the magnitude of the splitting of the conduction-band degeneracy for deformations of certain symmetry.

I. INTRODUCTION

The electronic-transport properties of a crystalline solid are determined to a great extent by the electron states in the vicinity of a band extremum. The theoretical study of such eigenstates is ideally suited to the $\vec{k}\cdot\vec{p}$ band-structure method. The local conduction-band minimum at the Γ point in the III-V semiconductors has been thoroughly studied in this way over the past 20 years. The results of these studies have led to the successful interpretation of many of the characteristics of *n*-type III-V compounds.

The effect of crystal deformation on these eigenstates has been much less well understood. Using the framework of the $\vec{k}\cdot\vec{p}$ method, we show that an intuitive understanding of the effect of mechanical strain can be achieved. This stems from the fact that the 8×8 deformation potential matrix in the combined conduction- and valence-band manifold, for all elastic strains, can be treated as a perturbation in the two-dimensional space of conduction band states at a given point in the Brillouin zone. Consequently, one can obtain analytic results for the deformed conduction band which do not impose any restrictions on the relative size of E_g and Δ as is the case in previous work. Furthermore, it is also possible to include the effect of *k*-dependent strain terms in the deformation-potential matrix. These *k*-dependent strain terms come from the modification of the $\vec{k}\cdot\vec{p}$ operator in the stressed material. We find that this effect increases in size with depth into the band.

II. Γ-POINT CONDUCTION-BAND MINIMUM IN THE III-V SEMICONDUCTORS

The Hamiltonian for a single electron moving in a periodic potential V is

$$H = H_0 + (\hbar/4m^2c^2)(\vec{\nabla} V \times \vec{p})\cdot\hat{\sigma} \ , \tag{1}$$

$$H_0 = \vec{p}\,^2/2m + V \ . \tag{2}$$

The second term on the right-hand side of (1) is the spin-orbit interaction. The potential V exhibits the spatial symmetry of the space group T_d^2.

The eigenstates of (1) are determined using the $\vec{k}\cdot\vec{p}$ band-structure method.[1-4] The wave function ψ is expressed, according to Bloch's theorem

$$\psi = e^{i\vec{k}\cdot\vec{r}}\, U_{\vec{k}}(\vec{r}) \ , \tag{3}$$

where $U_{\vec{k}}(\vec{r})$ is periodic with a period equal to the unit cell. Substitution of (3) in (1) gives the following equation for $U_{\vec{k}}$:

$$(H_0 + W_0)U_{\vec{k}} = E'_{\vec{k}} U_{\vec{k}} \ , \tag{4}$$

where

$$W_0 = (\hbar/m)\vec{k}\cdot\vec{p} + (\hbar/4m^2c^2)\big((\vec{\nabla} V \times \vec{p}) + (\vec{\nabla} V \times h\vec{k})\big)\cdot\hat{\sigma} \tag{5}$$

$$E'_{\vec{k}} = E_{\vec{k}} - \hbar^2\vec{k}\,^2/2m \ . \tag{6}$$

The $(\hbar/m)\vec{k}\cdot\vec{p}$ term in (5) is obviously the origin of the method's name. The second term in (5) arises from the spin-orbit interaction; the $\vec{k}$-dependent part of this term is normally neglected compared to the $\vec{k}$-independent part because the spin-orbit interaction occurs mainly near the atomic sites where the crystal momentum $\hbar\vec{k}$ is much smaller than the atomic momentum $\vec{p}$.

The solutions of (4) have been considered by Kane[1] using low-order perturbation theory to treat W_0. The set of basis functions for this calculation are the conduction- and valence-band states at Γ. They are denoted $S\uparrow, S\downarrow$ (for the conduction band), and $X\uparrow, X\downarrow, Y\uparrow, Y\downarrow, Z\uparrow, Z\downarrow$ (for the valence band). S transforms according to Γ_1 and X, Y, Z according to Γ_4 in the single point group T_d. These designations indicate the correspondence between these states and pure atomic states under the 24 operations in T_d. Although we are interested in the conduction-band minimum, the Γ-point valence-band states are included in the basis because of the large $\vec{k}\cdot\vec{p}$ matrix elements between the s- and p-like states, compared to their energy separation. One is thus faced with an 8×8 eigenvalue problem. For $\vec{k}$ lying along the z axis, the conduction-band energy[1] is given by

$$E_c'(E_c'+E_g)(E_c'+E_g+\Delta)-P^2k^2(E_c'+E_g+\tfrac{2}{3}\Delta)=0\ , \tag{7}$$

$$P=-(i\hbar/m)\langle S|p_z|Z\rangle\ , \tag{8}$$

$$\Delta=(3\hbar i/4m^2c^2)\langle X|(\vec{\nabla}V\times\vec{p})_z|Y\rangle\ . \tag{9}$$

Δ is the spin-orbit splitting of the valence band and E_g is the Γ-point band gap. The eigenfunctions of the conduction band are doubly degenerate and given by

$$\begin{aligned}\Phi_\alpha&=a_c[iS\downarrow]+b_c[(X-iY)\uparrow/\sqrt{2}]+c_c[Z\downarrow]\ ,\\ \Phi_\beta&=a_c[iS\uparrow]+b_c[-(X+iY)\downarrow/\sqrt{2}]+c_c[Z\uparrow]\ ,\end{aligned} \tag{10}$$

where

$$\begin{aligned}a_c&=Pk(E_c'+E_g+\tfrac{2}{3}\Delta)/N\ ,\\ b_c&=\frac{\sqrt{2}}{3}\Delta E_c'/N\ ,\\ c_c&=E_c'(E_c'+E_g+\tfrac{2}{3}\Delta)/N\ ,\end{aligned} \tag{11}$$

and N is chosen such that

$$a_c^2+b_c^2+c_c^2=1\ .$$

For $\vec{k}$ not lying along the z axis, the energy is still given by (7) but the eigenfunctions are no longer given by (10). However, (10) can be used to give the eigenfunctions if we replace $S, X, Y, Z, \uparrow, \downarrow$ by primed quantities given by

$$\begin{aligned}&\begin{bmatrix}\uparrow'\\ \downarrow'\end{bmatrix}=\begin{bmatrix}e^{-i\Phi/2}\cos\tfrac{1}{2}\Theta & e^{i\Phi/2}\sin\tfrac{1}{2}\Theta\\ -e^{-i\Phi/2}\sin\tfrac{1}{2}\Theta & e^{i\Phi/2}\cos\tfrac{1}{2}\Theta\end{bmatrix}\begin{bmatrix}\uparrow\\ \downarrow\end{bmatrix}\ ,\\ &\begin{bmatrix}X'\\ Y'\\ Z'\end{bmatrix}=\begin{bmatrix}\cos\Theta\cos\Phi & \cos\Theta\sin\Phi & -\sin\Theta\\ -\sin\Phi & \cos\Phi & 0\\ \sin\Theta\cos\Phi & \sin\Theta\sin\Phi & \cos\Theta\end{bmatrix}\begin{bmatrix}X\\ Y\\ Z\end{bmatrix}\ ,\\ &S'=S\ ,\end{aligned} \tag{12}$$

where Θ and Φ are the polar angles of the wave vector $\vec{k}$. The transformation given by (12) is identical to the transformation of the corresponding basis functions of the full rotation group under a change of coordinate system specified by the Euler angles $(\Phi, \Theta, 0)$. The effect of this change of coordinates is of course to make $\vec{k}$ and the z axis coincident.

The eigenvalues [Eq. (7)] and eigenfunctions [Eqs. (10) and (12)] have been used with marked success in explaining the electronic properties of n-type III-V semiconductors. This success undoubtedly stems from the exact treatment of the $\vec{k}\cdot\vec{p}$ interaction between the conduction and valence states at Γ. The valence-band structure originating from (4) has not enjoyed a comparable success; higher-order perturbation theory is, in fact, necessary in order to adequately characterize the valence band.

III. EFFECT OF DEFORMATION ON THE CRYSTAL HAMILTONIAN

For crystal deformations falling within the linear elastic limit of the material, the changes in band structure can be readily treated using low-order perturbation theory. The applicability of perturbation theory hinges upon an equivalence of the boundary conditions in the perturbed and unperturbed problems. The role of boundary conditions, in the effective mass method, is served by the periodicity of $U_{\vec{k}}$ in (3). Clearly crystal deformation produces a change in the unit cell size, and so perturbation theory cannot be directly applied to (4). However, the solutions of (4) in the deformed material could be formally expressed as a function of the undeformed coordinates ($\vec{r}$), rather than deformed coordinates ($\vec{r}'$), as there exists a one to one correspondence between $\vec{r}$ and $\vec{r}'$:

$$x_i'=\sum_j(\delta_{ij}+\epsilon_{ij})x_i\ . \tag{13}$$

The ϵ_{ij}'s are the components of the strain tensor $\hat{\epsilon}$. To proceed further mathematically the pseudo-Hamiltonian in (4) in the deformed problem must be expressed in terms of the undeformed coordinates using (13). This procedure introduces additional terms into the pseudo-Hamiltonian which now takes the form[5]

$$(H_0+W_0+D)\ , \tag{14}$$

where

$$D=\sum_{ij}D^{ij}\epsilon_{ij}\ , \tag{15}$$

$$D^{ij}=\frac{\hbar^2}{m}\frac{\partial^2}{\partial x_i\partial x_j}+V_{ij}-\frac{\hbar}{m}p_ik_j\ , \tag{16}$$

$$V_{ij}(\vec{r})=\left.\frac{\partial V((1+\hat{\epsilon})\vec{r})}{\partial\epsilon_{ij}}\right|_{\hat{\epsilon}\to 0}\ . \tag{17}$$

The effect of the crystal deformation is obviously contained in operator D in the pseudo-Hamiltonian. The three contributions to D, as given by (16), arise from the kinetic energy operator, the crystalline potential itself, and the $\vec{k}\cdot\vec{p}$ operator, respectively. The effect of the last term in (16) on the conduction-band structure has been omitted in all previous work. Such an omission appears unjustified when one recalls that it is in fact the size of the momentum matrix elements between the conduction- and valence-band states at Γ which is responsible for the nonparabolic nature of the conduction band as given by (7).

The matrix representation of D in the s-p manifold can be calculated on symmetry grounds alone. A quantitative determination requires the evaluation of several unknown matrix elements called deformation potentials. Such a matrix representation need only be calculated in a spinless basis, as we have excluded any strain-spin coupling. The D matrix in the S, X, Y, Z manifold takes the form

$$D = \left[\begin{array}{cccc} S & X & Y & Z \\ C_1\epsilon & C_2\epsilon_{yz} - iP\Sigma_{xi}k_i & C_2\epsilon_{xz} - iP\Sigma\epsilon_{yi}k_i & C_2\epsilon_{xy} - iP\Sigma\epsilon_{zi}k_i \\ C_2\epsilon_{yz} + iP\Sigma\epsilon_{xi}k_i & -a\epsilon + b(3\epsilon_{xx} - \epsilon) & n\epsilon_{xy} & n\epsilon_{xz} \\ C_2\epsilon_{xz} + iP\Sigma\epsilon_{yi}ki & n\epsilon_{xy} & -a\epsilon + b(3\epsilon_{yy} - \epsilon) & n\epsilon_{yz} \\ C_2\epsilon_{xy} + iP\Sigma\epsilon_{zi}k_i & n\epsilon_{xz} & n\epsilon_{yz} & -a\epsilon + b(3\epsilon_{zz} - \epsilon) \end{array}\right] , \qquad (18)$$

where $\epsilon = \mathrm{Tr}\hat{\epsilon}$.

C_1, C_2, a, b, and n are deformation potentials which clearly will determine the shift and splitting of the conduction- and valence-band states at Γ produced by the crystal deformation. These effects have already been extensively studied.[6-9] Terms in (18) involving the matrix element P defined in (8) arise exclusively from the third term in D as given by Eq. (16).

IV. SHIFT IN CONDUCTION-BAND ENERGY DUE TO CRYSTAL DEFORMATION

The use of mechanical deformation as a tool in studying the electronic eigenstates is a potentially very powerful one. The main reason for this is the relative ease with which the initial spatial symmetry can be experimentally altered. Not surprisingly the maximum information can be extracted in the case of anisotropic strains. However, on a practical level, large anisotropic strains are more difficult to produce than hydrostatic ones. Consequently, in most experiments in the III-V semiconductors involving anisotropic deformation, the components of the strain tensor seldom exceed 3×10^{-3}. Such a value could be expected in InSb for uniaxial compressions of the order of 2 kbar.

The change in energy of the conduction- and valence-band states at Γ is given by products of the deformation potentials and components of the strain tensor; such a dependence can be written symbolically $C^*\epsilon^*$, where C^* represents the appropriate deformation potential or combination of same, and ϵ^* represents components of the strain tensor. The shift of energy of the states close to the Γ point will be governed by a similar expression. In the group-IV and -III-V materials, one typically finds $C^* \lesssim 7$ eV. For the size of crystal strains discussed above, one obtains a value of $C^*\epsilon^* \leqslant 0.02$ eV. This is less than 10% of the conduction-valence-band Γ-point energy gap in all III-V semiconductors (InSb has the smallest gap, $E_g \simeq 0.20$ eV at $T = 300$ K). For $\vec{k} \neq 0$, the ratio of the strain-induced energy shift and the conduction–valence-band energy separation will be even smaller.

Under the conditions cited above, the shift in energy of the conduction band produced by crystal strain can be calculated by treating the deformation operator D only within the twofold manifold of states given by (10) and (12). From (10) and (18) we have

$$\begin{aligned} \langle \Phi'_\alpha | D | \Phi'_\alpha \rangle = {} & a_c^2 \langle S' | \hat{D} | S' \rangle \\ & + \tfrac{1}{2} b_c^2 [\langle X' | D | X' \rangle + \langle Y' | D | Y' \rangle] \\ & + c_c^2 \langle Z' | D | Z' \rangle + 2 a_c b_c \mathrm{Im} \langle S' | D | Z' \rangle \ ; \end{aligned} \qquad (19)$$

$$\because S' = S, \quad \therefore \langle S' | D | S' \rangle = C_1\epsilon \ .$$

From (12), we get

$$\begin{aligned} \langle X' | D | X' \rangle = {} & (\cos\Theta \cos\Phi)^2 \langle X | D | X \rangle + (\cos\Theta \sin\Phi)^2 \langle Y | D | Y \rangle + \sin^2\Theta \langle Z | D | Z \rangle \\ & + 2\cos^2\Theta \cos\Phi \sin\Phi \langle X | D | Y \rangle - 2\cos\Theta \sin\Theta \cos\Phi \langle x | D | Z \rangle - 2\cos\Theta \sin\Theta \sin\Phi \langle Y | D | Z \rangle \ , \end{aligned} \qquad (20)$$

$$\langle Y' | D | Y' \rangle = \sin^2\Phi \langle X | D | X \rangle + \cos^2\Phi \langle Y | D | Y \rangle - 2\sin\Phi \cos\Phi \langle X | D | Y \rangle \ , \qquad (21)$$

$$\begin{aligned} \langle Z' | D | Z' \rangle = {} & \sin^2\Theta \cos^2\Phi \langle X | D | X \rangle + \sin^2\Theta \sin^2\Phi \langle Y | D | Y \rangle + \cos^2\Theta \langle Z | D | Z \rangle \\ & + 2\sin^2\Theta \cos\Phi \sin\Phi \langle X | D | Y \rangle + 2\sin\Theta \cos\Theta \cos\Phi \langle X | D | X \rangle + 2\sin\Theta \cos\Theta \sin\Phi \langle Y | D | Z \rangle \ , \end{aligned} \qquad (22)$$

$$\langle S'|D|Z'\rangle = \sin\Theta\cos\Phi\langle S|D|X\rangle + \sin\Theta\sin\Phi\langle S|D|Y\rangle + \cos\Theta\langle S|D|Z\rangle \ , \tag{23}$$

$$\therefore \operatorname{Im}\langle S'|D|Z'\rangle = -Pk\sum_{ij}\frac{k_i k_j}{k^2}\epsilon_{ij} \ . \tag{24}$$

After some algebra we find

$$\begin{aligned}\langle\Phi'_\alpha|D|\Phi'_\alpha\rangle = {} & a_c^2 C_1\epsilon + \tfrac{1}{2}b_c^2\sum_i\langle i|D|i\rangle \\ & + \tfrac{1}{2}(2c_c^2 - b_c^2)\sum_i\langle i|D|i\rangle\frac{k_i^2}{k^2} \\ & + (2c_c^2 - b_c^2)\sum_{i>j}\langle i|D|j\rangle\frac{k_i k_j}{k^2} \\ & - 2a_c c_c\sum_{ij}\frac{k_i k_j}{k^2}\epsilon_{ij} \ ,\end{aligned} \tag{25}$$

where $|i\rangle$ represents $|X\rangle, |Y\rangle$, or $|Z\rangle$. But

$$\langle i|D|i\rangle = -(a+b)\epsilon + 3b\epsilon_{ii} \ , \quad \langle i|D|j\rangle = n\epsilon_{ij} \ , \tag{26}$$

$$\therefore \tfrac{1}{2}b_c^2\sum_i\langle i|D|i\rangle = \tfrac{1}{2}b_c^2(-3a\epsilon) \ , \tag{27}$$

$$\therefore \sum_i\langle i|D|i\rangle\frac{k_i^2}{k^2} = -(a+b)\epsilon + 3b\sum_i\frac{k_i^2}{k^2}\epsilon_{ii} \ , \tag{28}$$

$$\sum_{i>j}\langle i|D|j\rangle\frac{k_i k_j}{k^2} = \sum_{i>j} n\epsilon_{ij}\frac{k_i k_j}{k^2} \ , \tag{29}$$

$$\begin{aligned}\therefore \langle\Phi'_\alpha|D|\Phi'_\alpha\rangle = {} & a_c^2 C_1\epsilon + \tfrac{1}{2}b_c^2(-3a\epsilon) \\ & + \tfrac{1}{2}(2c_c^2 - b_c^2)(-a\epsilon) + \tfrac{1}{2}b(2c_c^2 - b_c^2) \\ & \times\left(3\sum\frac{k_i^2\epsilon_{ii}}{k_2^2} - \epsilon\right) + n(2c_c^2 - b_c^2) \\ & \times\sum_{i>j}\epsilon_{ij}\frac{k_i k_j}{k^2} - 2a_c c_c Pk\sum_{ij}\frac{k_i k_j}{k^2}\epsilon_{ij} \ .\end{aligned} \tag{30}$$

Now

$$\begin{aligned} a_c^2 C_1\epsilon + \tfrac{1}{2}b_c^2(-3a\epsilon) + \tfrac{1}{2}(2c_c^2 - b_c^2)(-a\epsilon) & = a_c^2 C_1\epsilon - a\epsilon(b_c^2 + c_c^2) \\ & = a_c^2 C_1\epsilon - a\epsilon(1 - a_c^2)(\because a_c^2 + b_c^2 + c_c^2 = 1) \\ & = C_1\epsilon - (1 - a_c^2)c\epsilon \ ,\end{aligned} \tag{31}$$

where $c = a + C_1$ is the hydrostatic deformation potential of the band gap E_g;

$$\begin{aligned}\therefore \langle\Phi'_\alpha|D|\Phi'_\alpha\rangle = {} & C_1\epsilon - (1 - a_c^2)c\epsilon + \tfrac{1}{2}b(2c_c^2 - b_c^2) \\ & \times\left(\sum_i\frac{3\epsilon_{ii}k_i^2}{k^2} - \epsilon\right) + n(2c_c^2 - b_c^2) \\ & \times\sum_{i>j}\frac{\epsilon_{ij}k_i k_j}{k^2} - 2a_c c_c Pk\sum_{ij}\frac{\epsilon_{ij}k_i k_j}{k^2} \ .\end{aligned} \tag{32}$$

It is easily shown that

$$\langle\Phi'_\alpha|D|\Phi'_\alpha\rangle = \langle\Phi'_\beta|D|\Phi'_\beta\rangle \ . \tag{33}$$

Now

$$\langle\Phi'_\alpha|D|\Phi'_\beta\rangle = \tfrac{1}{2}a_c b_c(2i\operatorname{Re}\langle S'|D|X'\rangle - 2\operatorname{Re}\langle S'|D|Y'\rangle) \ , \tag{34}$$

$$\begin{aligned}\operatorname{Re}\langle S'|D|X'\rangle = {} & \cos\Theta\cos\Phi C_2\epsilon_{yz} \\ & + \cos\Theta\sin\Phi C_2\epsilon_{xz} - \sin\Theta\epsilon_{xy} \ ,\end{aligned} \tag{35}$$

$$\operatorname{Re}\langle S'|D|Y'\rangle = -\sin\Phi C_2\epsilon_{yz} + \cos\Phi\epsilon_{xz} \ , \tag{36}$$

$$\begin{aligned}|\langle\Phi'_\alpha|D|\Phi'_\beta\rangle|^2 = 2a_c^2 b_c^2 C_2^2\Bigg[& \epsilon_{xy}^2 + \epsilon_{yz}^2 + \epsilon_{xz}^2 \\ & - \left(\epsilon_{xy}\frac{k_z}{k} + \epsilon_{xz}\frac{k_y}{k} + \epsilon_{yz}\frac{k_x}{k}\right)^2\Bigg] \ .\end{aligned} \tag{37}$$

The eigenvalues of this (2×2) eigenvalue problem are given by

$$\begin{aligned}\Delta E^{\pm}(\hat{\epsilon}) = {} & |\langle\Phi'_\alpha|D|\Phi'_\alpha\rangle| \pm |\langle\Phi'_\alpha|D|\Phi'_\beta\rangle| \\ = {} & C_1\epsilon - c\epsilon(1 - a_c^2) + \tfrac{1}{2}b(2c_c^2 - b_c^2)\left(3\sum_i\frac{\epsilon_{ii}k_i^2}{k^2} - \epsilon\right) + n(2c_c^2 - b_c^2)\sum_{i>j}\frac{\epsilon_{ij}k_i k_j}{k^2} - 2a_c c_c Pk\sum_i\frac{\epsilon_{ii}k_i^2}{k^2} \\ & - 4a_c c_c Pk\sum_{i>j}\frac{\epsilon_{ij}k_i k_j}{k^2} \pm 2^{1/2}a_c b_c C_2\left(\epsilon_{xy}^2 + \epsilon_{yz}^2 + \epsilon_{xz}^2 - \frac{1}{k^2}(\epsilon_{xz}k_x + \epsilon_{xz}k_y + \epsilon_{xy}k_z)^2\right)^{1/2} \ .\end{aligned} \tag{38}$$

The first term of (38) represents a uniform k-independent shift of the conduction band with deformation. At the Γ point all the remaining terms in (38) are zero and thus $C_1\epsilon$ is the total shift of the Γ-point energy. The last term in (38) predicts a splitting of the conduction-band degeneracy for strains of sufficiently low symmetry.

The k dependence of the energy shift of the conduction band is given by the factors $(1-a_c^2)$, $(2c_c^2-b_c^2)$, and $4a_c c_c$ appearing in (38). These quantities are plotted in Figs. 1, 2, and 3, respectively, in the range $0<k<0.03$ a.u. The spherical surface $k=0.03$ encloses approximately 6×10^{18} states/cm^3. Four curves for each factor are drawn, corresponding to $P^2=0.44$, $E_g=0.00767$, and $\Delta = 0$, 0.0077, 0.031, and ∞ a.u. The $\Delta=0.031$ curves correspond to InSb. The strong k dependence of all these curves is a measure of the increasing admixture, with depth into the band, of the p-like states in the undeformed conduction-band eigenstates. For reasonable values of the deformation potentials ($\lesssim 5$ eV), use of Figs. 1–3 shows that the terms involving P in (38) will be non-negligible for $k \gtrsim 0.015$ a.u. A Fermi wave vector of this value corresponds to a carrier concentration of approximately 0.8×10^{18} cm^{-3}.

Note from Figs. 1–3 that $1-a_c^2$ is not very sensitive, and $4a_c c_c$ only slightly so, to the value of the spin-orbit splitting. However, the value of $2c_c^2 - b_c^2$ can change by up to 100% as Δ goes from 0 to ∞.

V. COMPARISON WITH PREVIOUS CALCULATIONS

The effect of deformation on the conduction band of the III-V semiconductors was first considered by Bir and Pikus.[10] In that work the $\vec{k}\cdot\vec{p}$, spin orbit, and deformation-dependent interactions are considered simultaneously, thereby requiring the solution of a complex eightfold eigenvalue problem. In Sec. IV we showed that such an approach is unnecessary for rapid convergence of the solution at least for deformations in the linear elastic region. Bir and Pikus were able to obtain analytical expressions only in the limits $E_g \gg \Delta$ and E_g

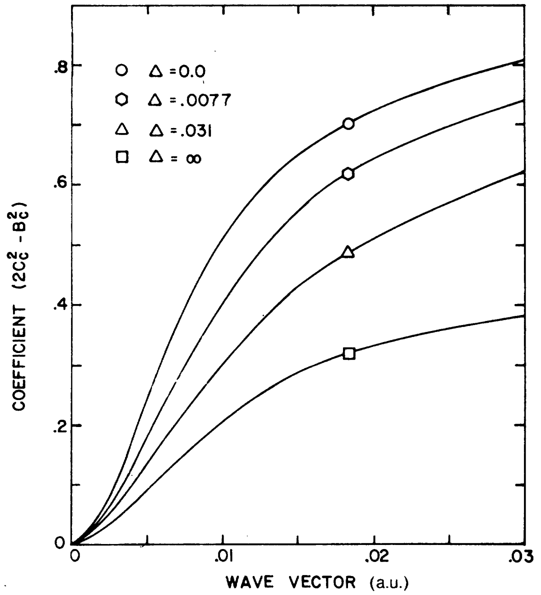

FIG. 2. Deformed conduction-band coefficient $(2c_c^2-b_c^2)$ vs wave vector for $P^2=0.44$, $E_g=0.0077$ a.u.

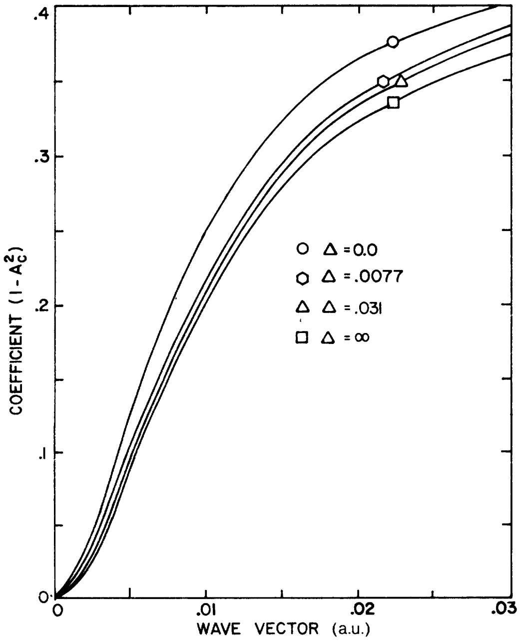

FIG. 1. Deformed conduction-band coefficient $(1-a_c^2)$ vs wave vector for $P^2=0.44$, $E_g=0.0077$ a.u.

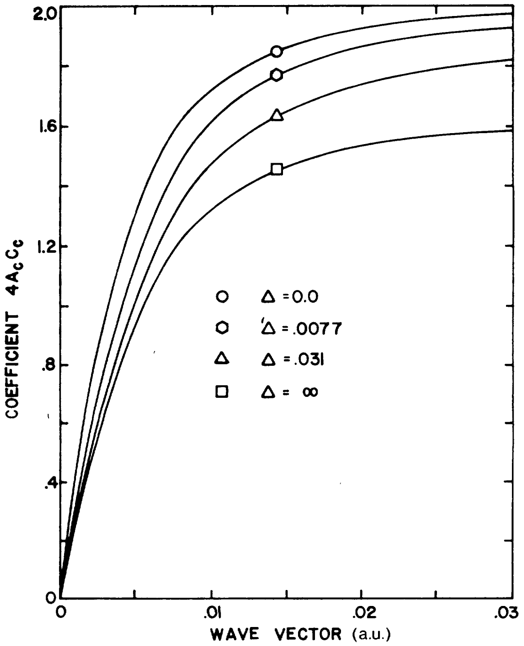

FIG. 3. Deformed conduction-band coefficient $(4a_c c_c)$ vs wave vector for $P^2=0.44$, $E_g=0.0077$ a.u.

$\ll \Delta$. Their results are presented below:

$$E_g \ll \Delta \ ,$$

$$\Delta E(\hat{\epsilon}) = C_1\epsilon + \frac{E}{E_g + 2E}\left[-c\epsilon + \frac{b}{2}\left(3\sum\frac{\epsilon_{ii}k_i^2}{k^2} - \epsilon\right) + n\sum_{i>j}\frac{k_i k_j \epsilon_{ij}}{k^2}\right] \ ; \tag{39}$$

$$E_g \gg \Delta \ ,$$

$$E(\hat{\epsilon}) = C_1\epsilon + \frac{2E}{E_g + 2E}\left[-c\epsilon + \frac{b}{2}\left(3\sum\frac{\epsilon_{ii}k_i^2}{k^2} - \epsilon\right) + n\sum_{i>j}\frac{k_i k_j \epsilon_{ij}}{k^2}\right] \ . \tag{40}$$

Note in (39) and (40) the absence of any terms involving P; this is to be expected since such terms arise only from the normally neglected portion of the deformation operator D. The lack of any splitting of the conduction-band degeneracy in (39) and (40) is a consequence of various algebraic approximations which allowed the solution of the (8×8) eigenvalue problem. It is possible to compare the other terms in our result (38) with the Bir and Pikus results (39) and (40). In the limit $E_g \ll \Delta$, and for $E < E_g + \Delta$, we have from (7) and (11):

$$\begin{aligned}
&a_c = Pk\cdot\tfrac{2}{3}\cdot\Delta/N \ , \\
&b_c = \frac{\sqrt{2}}{3}\cdot\Delta\cdot E/N \ , \\
&c_c = \tfrac{2}{3}\cdot\Delta\cdot E/N \ , \\
&E(E+E_g) = \tfrac{2}{3}P^2k^2 \ , \\
&\therefore N^2 = \Delta^2\cdot\tfrac{4}{3}E\cdot(E_g + 2E) \ , \\
&a_c^2 = (E_g + E)/(E_g + 2E) \ , \\
&(1 - a_c^2) = E/(E_g + 2E) \ ;
\end{aligned} \tag{41}$$

$$(2c_c^2 - b_c^2) = \frac{\frac{8}{9}\Delta^2E^2 - \frac{2}{9}\Delta^2E^2}{\frac{2}{3}\Delta^2(E_g + 2E)E} = \frac{E}{E_g + 2E} \ . \tag{42}$$

For $E_g \gg \Delta$, an exactly similar analysis yields

$$(1 - a_c^2) = E/(E_g + 2E) \ , \tag{43}$$

$$(2c_c^2 - b_c^2) = 2E(E_g + 2E) \ . \tag{44}$$

Substitution of (41)–(44) into (38) shows that the comparable terms in the Bir and Pikus results (39) and (40) and our own work (38) are identical in the limits $E_g \ll \Delta$ and $E_g \gg \Delta$. Thus the curves for $\Delta = 0$ and $\Delta = \infty$ in Figs. 1 and 2 also accurately present the Bir and Pikus results. It should be noted, however, that considerable error can be made from indiscriminate application of their work. For example, in InSb where $E_g = 0.21$ eV and $\Delta = 0.9$ eV, one might be tempted to use the Bir and Pikus result derived for $E_g \ll \Delta$. From Fig. 2 it is apparent that an error of up to 50% or more could be made in the terms involving b and n in the deformed conduction-band dispersion relation. The resulting substantial error in the energy shift would be in addition to the one caused by the omission of the terms involving matrix element P.

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