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Strain dependence of effective masses in tetrahedral semiconductors

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The complete first-order strain dependences of the conduction- and valence-band effective masses of germanium and zinc-blende semiconductors at $\vec{k} = 0$ is calculated using third-order perturbation theory and the Pikus-Bir Hamiltonian. These dependences are expressed analytically in relatively few matrix elements and self-energies using a model band structure consisting of the spin-orbit-split $\Gamma_{25'}$ upper valence bands and the $\Gamma_{2'}$, Γ_{15}, $\Gamma_{12'}$, and Γ_1 conduction bands. These matrix elements and self-energies are evaluated from pseudopotential theory. While a two-band model consisting of the $\Gamma_{25'}$ valence and $\Gamma_{2'}$ conduction bands is adequate to describe the electron and the light-hole effective masses, more terms involving also the Γ_{15}, $\Gamma_{12'}$, and the Γ_1 conduction bands are required to interpret the dependence of these masses on strain. Our results account for the strain dependence of conduction masses observed in GaAs. They also indicate that the anomalous strain dependence of the cyclotron hole masses observed for Ge by Hensel and Suzuki are not due to a strain-dependent spin-orbit interaction, as suggested by these authors, but to orbital terms involving the higher conduction bands.

I. INTRODUCTION

The $\vec{k}\cdot\vec{p}$ perturbation theory has proved to be very useful for interpreting effective masses in tetrahedrally bonded semiconductors.[1-3] For example, the isotropic effective mass m_c^* of the lowest conduction-band minimum at the center of the Brillouin zone ($\Gamma_{2'}$ and Γ_1, for crystals of diamond and zinc-blende symmetry, respectively) can be expressed as

$$\frac{m_e}{m_c^*} \cong 1 + \frac{2P^2}{3m_e}\left(\frac{2}{E_0} + \frac{1}{E_0+\Delta_0}\right), \tag{1}$$

where P is the momentum matrix element between the Γ_1 ($\Gamma_{2'}$) conduction-band minimum and the Γ_{15} ($\Gamma_{25'}$) valence states, and E_0 and Δ_0 are the direct energy gap and upper-valence-band spin-orbit splitting, respectively. With $P^2/m_e \cong 13$ eV, Eq. (1) describes well the lowest Γ conduction-band mass of Ge and a large number of III-V semiconductors.[2,3]

It is also tempting to use Eq. (1) to describe the dependence of the mass on hydrostatic pressure. A hydrostatic stress increases the gaps E_0 and $E_0+\Delta_0$. This increase, which amounts to 8% at 10 kbar in GaAs,[4,5] should produce a corresponding increase in m_c^* according to Eq. (1) if P^2 remains independent of stress. Actually, P is roughly inversely proportional to the lattice constant a_0.[6] Therefore, an increase in P^2 of ~1% is expected at 10 kbar. Experimentally, an increase of 6% in m_c^* is found at 10 kbar,[7] in agreement with the above considerations.

In the same spirit it is possible to use Eq. (1) to estimate the effect of pure shear stresses along [100] or [111] on m_c^*. This effect arises from the shear-induced splitting of the Γ_{15} ($\Gamma_{25'}$) p-like valence-band triplet into a singlet and a doublet. Under shear, the mass m_c^* becomes anisotropic with different components $m_{c\parallel}^*$ and $m_{c\perp}^*$, parallel and perpendicular, respectively, to the stress axis. These can be expressed as[6,8-12]

$$\frac{m_e}{m_{c\parallel}^*} = 1 + \frac{2P^2}{m_e(E_0-\delta E_0)} \cong 1 + \frac{2P^2}{m_eE_0}\left(1 + \frac{\delta E_0}{E_0}\right), \tag{2a}$$

$$\frac{m_e}{m_{c\perp}^*} = 1 + \frac{2P^2}{m_e(E_0+\frac{1}{2}\delta E_0)} = 1 + \frac{2P^2}{m_eE_0}\left(1 - \frac{\delta E_0}{2E_0}\right), \tag{2b}$$

where we have assumed for simplicity that $\Delta_0 \ll E_0$. In Eqs. (2), δE_0 is the stress-induced shift of the singlet state.

For a given uniaxial stress χ, δE_0 is roughly isotropic and independent of the stress direction in the III-V compounds. It is positive for a compressive stress.[13] Thus, upon compression, a decrease in the parallel-mass component would be expected, with a magnitude roughly independent of stress direction. This prediction is in total disagreement with experiment: while a small decrease in $m_{c\parallel}^*$ is observed in GaAs, for example, for a stress along [100],[14] a large *increase* is found for a [111] stress.[14,15] Related anomalies have also been observed for the dependence of the resistivity of n-GaAs on uniaxial stress.[16] Similar problems arise when trying to interpret the stress dependence of the Γ_{15} ($\Gamma_{25'}$) valence-band masses on the basis of $\vec{k}\cdot\vec{p}$ theory and the stress-induced splitting of the Γ_{15}^{v}-orbital triplet.[17] These difficulties led Hensel and Suzuki to introduce a dependence of the spin-orbit Hamiltonian on uniaxial stress to explain them.[17,18] Such a dependence is difficult to reconcile with rigid-ion models[17] and with the observed[19] nearly negligible dependence of Δ_0 on hydrostatic stress.

In this paper we present calculations which show that the splitting of the Γ_{15} ($\Gamma_{25'}$) valence band is not the only term which contributes significantly to the dependences of m_c^* and the valence band masses on uniaxial stress. In fact, the stress dependence of these masses can be viewed as resulting largely from third-order perturbation terms involving the $\vec{k}\cdot\vec{p}$ Hamiltonian twice and the stress Hamiltonian once. One such term gives the effect described by Eq. (2). The usual argument, that this term is the only one which needs to be considered in view of the small value of E_0, is shown not to hold: δE_0 has anomalously small values because of a fortuitous cancellation of kinetic and potential energy contributions. It is shown using the pseudopotential method that this cancellation does not take place for many other matrix elements of the stress Hamiltonian. Hence third-order perturbation terms involving also the Γ_{15} and the $\Gamma_{12'}$ conduction bands contribute significantly to the stress dependence of the effective mass and, in the case of a [111] stress, even reverse the predictions of Eq. (2). Thus agreement with the experimental results for m_c^* is restored.

These additional perturbation terms give also a substantial contribution to the dependence of the hole masses on stress. They largely eliminate the discrepancies with the two-band theory reported in Ref. 17 without having to invoke a stress dependence of the spin-orbit splitting. The additional perturbation terms should also yield a substantial contribution to the nonlinearities in the dependence of energy gaps on uniaxial stress which have been reported for Ge and GaAs.[20]

II. GENERAL THEORY

A. Strain Hamiltonian and effective mass

The general theory of strain effects around critical points in crystals has been given by Pikus and Bir,[11,21] who express the effect of a general strain $\underline{\epsilon}$ by the first-order $\vec{k}\cdot\vec{p}$-strain Hamiltonian

$$H\psi = (H_0 + H')\psi = E\psi \,, \tag{3a}$$

$$H_0 = p^2/2m_e + V(\vec{r}) \,, \tag{3b}$$

$$H' = \hbar\vec{k}\cdot\vec{p}/m_e - (\hbar/m_e)\epsilon_{ij}p_ik_j - (1/m_e)\epsilon_{ij}p_ip_j + \epsilon_{ij}V_{ij} \,, \tag{3c}$$

$$V_{ij} = \frac{\partial}{\partial\epsilon_{ij}} V[(\underline{1}+\underline{\epsilon})\cdot\vec{r}]\,\big|_{\underline{\epsilon}\to 0} \,, \tag{3d}$$

where $\underline{1}$ is the unit tensor, $\underline{\epsilon}$ is the strain tensor, and all other symbols have their usual meaning. In Eq. (3c), summation over repeated indices is implied (i, $j = x$, y, and z). For simplicity and for later use, we define hydrostatic, tetragonal, and trigonal (rhombohedral) shear strains ϵ_H, ϵ_T, and ϵ_R, as

$$\epsilon_H = \tfrac{1}{3}\mathrm{Tr}(\epsilon) = \tfrac{1}{3}\sqrt{3}\, e_1 \,, \tag{4a}$$

$$\epsilon_T = \epsilon_{zz} - \tfrac{1}{3}\mathrm{Tr}(\underline{\epsilon}) = \tfrac{1}{3}\sqrt{6}\, e_{3\alpha} , \tag{4b}$$

$$\epsilon_R = \epsilon_{xy} = e_{5xy} \,. \tag{4c}$$

The quantities ϵ_H, ϵ_T, and ϵ_R are related as shown to the quantities e_1, $e_{3\alpha}$, and e_{5xy} previously defined by Kane.[22] For a uniaxial stress χ along [001] ($\chi = \chi_T$) or [111] ($\chi = \chi_R$), the two cases that we consider here, we have

$$[001] \text{ or } [111]\text{:}\quad \epsilon_H = \tfrac{1}{3}(s_{11} + 2s_{12})\chi_{T,R} \,, \tag{5a}$$

$$[001]\text{:}\quad \epsilon_T = \tfrac{2}{3}(s_{11} - s_{12})\chi_T , \quad \epsilon_R = 0 \,, \tag{5b}$$

$$[111]\text{:}\quad \epsilon_R = \tfrac{1}{6}S_{44}\chi_R , \quad \epsilon_T = 0 \,. \tag{5c}$$

The strain dependence of band-effective masses is calculated from expansions of energy levels to first order in $\underline{\epsilon}$ and second order in $\vec{k}$. For a given level E_ν, the required third-order expansion is[23]

$$E_\nu(\vec{k}) = E_\nu(0) + \frac{\hbar^2k^2}{2m_e} + H'_{\nu\nu} - \sum_{\mu\neq\nu}\frac{|H'_{\mu\nu}|^2}{E_\mu - E_\nu} + \sum_{\mu\neq\nu}\frac{|H'_{\mu\nu}|^2(H'_{\mu\mu} - H'_{\nu\nu})}{(E_\mu - E_\nu)^2} + \sum_{\substack{\mu,\lambda\neq\nu\\ \mu\neq\lambda}}\frac{H'_{\nu\mu}H'_{\mu\lambda}H'_{\lambda\nu}}{(E_\mu - E_\nu)(E_\lambda - E_\nu)} \,. \tag{6}$$

The band-effective mass follows from

$$\left(\frac{m_e}{m_\nu^*}\right)_{ij} = \frac{1}{\hbar^2}\,\frac{\partial^2}{\partial k_i\partial k_j}E_\nu(\vec{k}) \,. \tag{7}$$

Quantitively, it is seen from Eq. (3c) that in the perturbation H' the first term is linear in $\vec{k}$, the second bilinear in $\vec{k}$ and $\underline{\epsilon}$, and the third and fourth are linear in $\underline{\epsilon}$. The energy expansion (6) can be separated into zero-order [first by order of appearance in Eq. (6)], first-order (third), second-order (second and fourth), third-order two-band (fifth), and third-order three-band (sixth) terms. Deformation potentials representing effects linear in strain (by definition at $\vec{k} = 0$) clearly come only from the first-order term in Eq. (6) and the two strain-linear terms in Eq. (3c). The band-effective mass (by definition at $\underline{\epsilon} = 0$) arises only from terms quadratic in $\vec{k}$ and thus in the tetrahedral semiconductors comes only from the second-order terms in Eq. (6), the second of which is evaluated only with the $\vec{k}$-linear term in Eq. (3c).[24,25]

Strain-linear corrections to the band-effective masses come from terms linear in the strain and simultaneously quadratic in $\vec{k}$. The usual such term, as indicated in Sec. I, is the third-order two-band term, which expresses the strain-linear correction in terms of the deformation potentials (i.e., expectation values of the strain Hamiltonian of the valence and conduction bands). The other two possibilities not considered so far in the literature are the third-order three-band and the second-order terms in Eq. (6). In the latter case, the required dependence is obtained by using the $\vec{k}$-linear and bilinear terms of Eq. (3c).

B. Model band structure

From Sec. II A it follows that deformation potentials, band-effective masses, and strain-linear corrections to the masses come from a relatively small number of nonvanishing matrix elements and expectation values. We consider henceforth only the states at $\vec{k} = 0$. For the tetrahedrally bonded semiconductors the most important $\vec{k} = 0$ states are the $\Gamma_{25'}$ valence band, and the $\Gamma_{2'}$, Γ_{12}, $\Gamma_{12'}$, and Γ_1 conduction-band levels, at energies 0, $\overline{E}_0$, $\overline{E}_0'$, $\overline{E}_0''$, and $\overline{E}_0'''$, respectively, in the absence of spin-orbit splitting. These states transform according to the coordinate representations $(X = yz, Y = zx, Z = yx)$, (xyz), (x, y, z), $[\alpha = xyz(x^2 + y^2 - 2z^2)$, $\beta = xyz(x^2 - y^2)]$, and 1, respectively.[26] Other states at $\vec{k} = 0$ are relatively far removed in energy and their influence is expected to be less.

We identify the following nonvanishing momentum matrix elements involving $\vec{k}$-linear perturbations:

$$\langle \Gamma_{25'}(Z) | p_z | \Gamma_{2'} \rangle = P\,, \tag{8a}$$

$$\langle \Gamma_{25'}(Z) | p_x | \Gamma_{15}(y) \rangle = Q\,, \tag{8b}$$

$$\langle \Gamma_{25'}(X) | p_x | \Gamma_{12'}(\alpha) \rangle = R\,, \tag{8c}$$

$$\langle \Gamma_{15}(z) | p_z | \Gamma_1 \rangle = T\,. \tag{8d}$$

These matrix elements and others to be defined later are summarized in Table I. The meaning of P, Q, R, and T is similar to those previously defined in atomic units by Cardona and Pollak,[27] except that our matrix elements P, Q, and T are a factor of 2 smaller, and R is a factor of $2\sqrt{2}$ smaller. Strain-linear perturbations depend on the type of stress applied and will be discussed below. The bilinear term is related trivially to the k-linear term for the high-symmetry stresses of interest.

The spin-orbit splitting of the valence band can be incorporated explicitly by using the linear combinations of the $\Gamma_{25'}$ wave functions that diagonalize the spin-orbit Hamiltonian. The states of interest and their energies, projected along the z axis in the (j, m_j) representation, are given in terms of the corresponding orbital functions X, Y, and Z, by[6]

$$(\tfrac{3}{2}, \tfrac{1}{2}):\ (X{\downarrow} + iY{\downarrow} - 2Z{\uparrow})/\sqrt{6} \text{ at } E = \tfrac{1}{3}\Delta_0\,, \tag{9a}$$

$$(\tfrac{3}{2}, -\tfrac{3}{2}):\ (X{\downarrow} - iY{\downarrow})/\sqrt{2} \text{ at } E = \tfrac{1}{3}\Delta_0\,, \tag{9b}$$

$$(\tfrac{1}{2}, \tfrac{1}{2}):\ (X{\downarrow} + iY{\downarrow} + Z{\uparrow})/\sqrt{3} \text{ at } E = -\tfrac{2}{3}\Delta_0\,. \tag{9c}$$

TABLE I. Definitions of interband matrix elements used to express effective masses and their linear strain dependences. The pseudopotential variables are defined in Sec. III. $\Gamma_{12'}(\alpha) = xyz(x^2 + y^2 - 2z^2)$; $\Gamma_{12'}(\beta) = xyz(x^2 - y^2)$.

Quantity	Definition	Pseudopotential expression
P	$\langle \Gamma_{25'}(Z) \| p_z \| \Gamma_{2'} \rangle$	$[\beta_{2'}\beta_{25'} + (2/\sqrt{3})\gamma_{2'}\gamma_{25'}]\hbar G_0$
Q	$\langle \Gamma_{25'}(X) \| p_y \| \Gamma_{15}(z) \rangle$	$\beta_{25'}\hbar G_0$
R	$\langle \Gamma_{25'}(X) \| p_x \| \Gamma_{12'}(\alpha) \rangle$	$(\sqrt{2}/\sqrt{3})\gamma_{25'}\hbar G_0$
T	$\langle \Gamma_{15'}(z) \| p_z \| \Gamma_1 \rangle$	$\hbar G_0$
c_T	$\langle \Gamma_{2'} \| H_{\epsilon T} \| \Gamma_{12}(\alpha) \rangle / \epsilon_T$	$4\sqrt{2}\gamma_{2'}\Omega + (1/\sqrt{2})\gamma_{2'}v_8' + \frac{8}{11}\sqrt{3}\,\beta_{2'}v_{11}'$
c_{R1}	$\langle \Gamma_{2'} \| H_{\epsilon R} \| \Gamma_{15}(\overline{z}) \rangle / \epsilon_R$	$\beta_{2'}[-4\sqrt{3}\,\Omega - \sqrt{3}v_8' + \pi\sqrt{3}\,\zeta(v_4^s + v_{12}^s)]$ $+ \gamma_{2'}[\frac{2}{3}\sqrt{2}v_3' - \frac{14}{11}\sqrt{2}v_{11}' + \frac{1}{2}\pi\zeta(v_3^s + 5v_{11}^s)]$
c_{R2}	$\langle \Gamma_{15}(\overline{x}) \| H_{\epsilon R} \| \Gamma_{12'}(\beta) \rangle / \epsilon_R$	$-\frac{4}{3}\sqrt{2}v_3' + \frac{4}{11}\sqrt{2}v_{11}' - \pi\sqrt{2}\,\zeta(v_3^s - v_{11}^s)$
c_{R3}	$\langle \Gamma_1 \| H_{\epsilon R} \| \Gamma_{25}(\overline{z}) \rangle / \epsilon_R$	$\beta_{25'}[-4\sqrt{3}\,\Omega - \sqrt{3}v_8' - \pi\sqrt{3}\,\zeta(v_4^s + v_{12}^s)]$ $+ \gamma_{25'}[-(2\sqrt{2}/\sqrt{3})v_3' + \frac{2}{11}\sqrt{6}v_{11}'$ $- (\pi\sqrt{3}/\sqrt{2})\zeta(v_3^s + 3v_{11}^s)]$

The quantity Δ_0 is the spin-orbit splitting of the valence band. The spin-orbit splitting of the Γ_{15} conduction band introduces only a correction to second order in Δ_0'/E_g, where Δ_0' is the spin-orbit splitting of the second conduction band and E_g is a relevant energy separation (e.g., to the $\Gamma_{2'}$ conduction band). For our purposes the Γ_{15} spin-orbit splitting is negligibly small and will be ignored.

C. Hydrostatic strain

For hydrostatic strain, the Pikus-Bir Hamiltonian, evaluated for $\vec{k} = k\hat{x}$ perpendicular to the quantization axis $\hat{z}$ of the spin-orbit-split valence bands, becomes

$$H_H' = (\hbar k/m_e)(1-\epsilon_H)p_x + H_{\epsilon H}' \,, \tag{10a}$$

where the k-linear and bilinear terms have the symmetry of p_x, and the strain-linear term

$$H_{\epsilon H}' = \epsilon_H[-(\vec{p}^2/m_e) + (V_{xx}+V_{yy}+V_{zz})] \tag{10b}$$

has the symmetry Γ_1 of the unperturbed lattice, and therefore, contributes only to self-energy terms. For the νth state ($\nu = \Gamma_{25'}, \Gamma_{2'}, \Gamma_{15}, \Gamma_{12'}$, and Γ_1), we write these as

$$3a_\nu \epsilon_H = \langle \Gamma_\nu | H_{\epsilon H}' | \Gamma_\nu \rangle \,. \tag{11}$$

These self-energies, and others to be defined later, are given in Table II. The Pikus-Bir deformation potential a is given by

$$a = a_{2'} - a_{25'} \,. \tag{12}$$

The complete set of nonvanishing matrix elements and self-energies for hydrostatic strain is summarized in Table III. Spin-orbit-split valence bands are assumed. For hydrostatic strain, the quantities P', Q', and R' are given by

$$P' = (\hbar/m_e)(1-\epsilon_H)P \,, \tag{13a}$$

$$Q' = (\hbar/m_e)(1-\epsilon_H)Q \,, \tag{13b}$$

$$R' = (\hbar/m_e)(1-\epsilon_H)R \,, \tag{13c}$$

$$T' = (\hbar/m_e)(1-\epsilon_H)T \,. \tag{13d}$$

From Table III and Eqs. (6), (7), and (11)–(13), we calculate

$$\frac{m_e}{m_c^*} = 1 + \frac{2P^2}{3m_e}\left\{ \frac{2}{E_0}\left[1-\epsilon_H\left(2+\frac{3a}{E_0}\right)\right] + \frac{1}{E_0+\Delta_0}\left[1-\epsilon_H\left(2+\frac{3a}{E_0+\Delta_0}\right)\right]\right\} \tag{14a}$$

$$\cong 1 + \frac{2P^2}{m_e\overline{E}_0}\left[1-\epsilon_H\left(2+\frac{3a}{\overline{E}_0}\right)\right], \tag{14b}$$

$$\left(\frac{m_e}{m^*_{3/2,1/2}}\right)_{\perp} = 1 - \frac{P^2}{3m_e(\overline{E}_0-\frac{1}{3}\Delta_0)}\left[1-\epsilon_H\left(2+3\,\frac{a_{2'}-a_{25'}}{\overline{E}_0-\frac{1}{3}\Delta_0}\right)\right] - \frac{5Q^2}{3m_e(\overline{E}_0'-\frac{1}{3}\Delta_0)}\left[1-\epsilon_H\left(2+3\,\frac{a_{15}-a_{25'}}{\overline{E}_0'-\frac{1}{3}\Delta_0}\right)\right] - \frac{4R^2}{3m_e(\overline{E}_0''-\frac{1}{3}\Delta_0)}\left[1-\epsilon_H\left(2+3\,\frac{a_{12'}-a_{25'}}{\overline{E}_0''-\frac{1}{3}\Delta_0}\right)\right]. \tag{14c}$$

The quantity $\overline{E}_0$ has the meaning

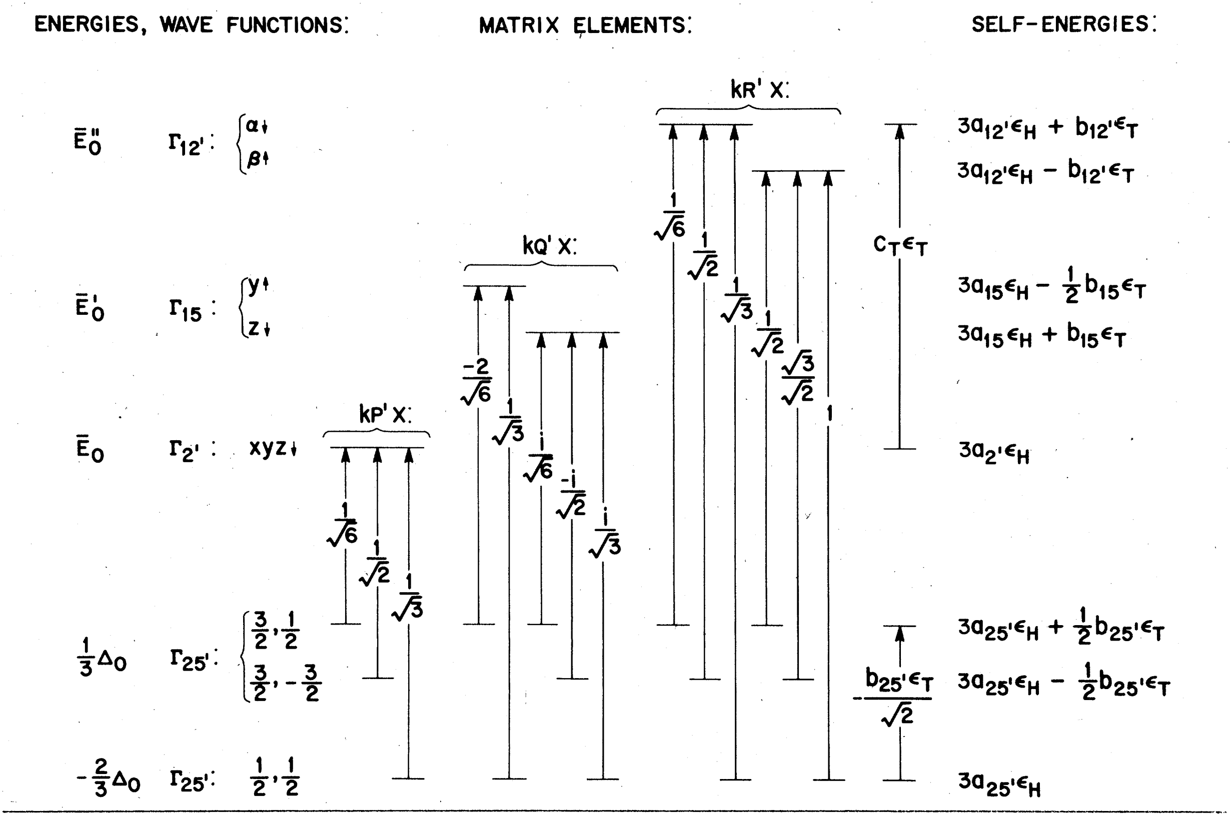
$$\overline{E}_0 = E_0 + \tfrac{1}{3}\Delta_0 \,. \tag{15}$$

Equation (14b) is the expansion of Eq. (14a) to

TABLE II. Definitions of self-energies used to express deformation potentials and linear strain dependences of effective masses. The pseudopotential variables are defined in Sec. III.

Quantity	Definition	Pseudopotential expression
$a_{25'}$	$\langle \Gamma_{25'}(Z) \| H_{\epsilon H} \| \Gamma_{25'}(Z)\rangle / 3\epsilon_H$	$-\frac{2}{3}\Omega(3\beta_{25'}^2 + 4\gamma_{25'}^2) - \beta_{25'}^2\bar{v}_8{}' + 2\sqrt{2}\,\beta_{25'}\gamma_{25'}(\bar{v}_3' - \bar{v}_{11}')$
$a_{2'}$	$\langle \Gamma_{2'} \| H_{\epsilon H} \| \Gamma_{2'}\rangle / 3\epsilon_H$	$-\frac{2}{3}\Omega(3\beta_{2'}^2 + 4\gamma_{2'}^2) + (3\beta_{2'}^2 + 4\gamma_{2'}^2)\bar{v}_8' + 2\sqrt{6}\,\beta_{2'}\gamma_{2'}(\bar{v}_3' + \bar{v}_{11}')$
a_{15}	$\langle \Gamma_{15}(z) \| H_{\epsilon H} \| \Gamma_{15}(z)\rangle / 3\epsilon_H$	$-2\Omega - \bar{v}_8'$
$a_{12'}$	$\langle \Gamma_{12'}(\alpha) \| H_{\epsilon H} \| \Gamma_{12'}(\alpha)\rangle / 3\epsilon_H$	$-\frac{8}{3}\Omega - 2\bar{v}_8'$
a_1	$\langle \Gamma_1 \| H_{\epsilon H} \| \Gamma_1\rangle / 3\epsilon_H$	$-2\Omega + 3\bar{v}_8'$
$b_{25'}$	$\langle \Gamma_{25'}(Z) \| H_{\epsilon T} \| \Gamma_{25'}(Z)\rangle / \epsilon_T$	$-8\gamma_{25'}^2\Omega + \frac{16}{11}\sqrt{2}\,\beta_{25'}\gamma_{25'}v_{11}' + \beta_{25'}^2 v_8'$
b_{15}	$\langle \Gamma_{15}(z) \| H_{\epsilon T} \| \Gamma_{15}(z)\rangle / \epsilon_T$	v_8'
$b_{12'}$	$\langle \Gamma_{12'}(\alpha) \| H_{\epsilon T} \| \Gamma_{12'}(\alpha)\rangle / \epsilon_T$	$-4\Omega + v_8'$
$d_{25'}$	$\langle \Gamma_{25'}(\overline{Z}) \| H_{\epsilon R} \| \Gamma_{25'}(\overline{Z})\rangle / \epsilon_R$	$-2\beta_{25'}^2[4\Omega - v_8' - \pi\zeta(v_4^s - v_{12}^s)]$ $+ 2\sqrt{2}\,\beta_{25'}\gamma_{25'}[\frac{4}{3}v_3' + \frac{12}{11}v_{11}' + \pi\zeta(v_3^s - v_{11}^s) + 4\gamma_{25'}^2 v_8']$
d_{15}	$\langle \Gamma_{15}(\overline{z}) \| H_{\epsilon R} \| \Gamma_{15}(\overline{z})\rangle / \epsilon_R$	$-2[4\Omega - v_8' + \pi\zeta(v_4^s - v_{12}^s)]$

TABLE III. Nonvanishing k-linear, ϵ-linear, and bilinear (ϵk) matrix elements for hydrostatic and tetragonal shear strains evaluated in a direction $\vec{k}=k\hat{x}$ perpendicular to the quantization axis $\hat{z}$ of the spin-orbit-split valence band and the axis of the [001] uniaxial stress. The quantities P', Q', and R' are defined in Eqs. (13) for hydrostatic strain and in Eqs. (20) for tetragonal shear strain.



first order in $\Delta_0/\bar{E}_0$. The term 2 in each postfactor of ϵ_H is a second-order contribution that comes from the cross term of k-linear and bilinear (in k and ϵ) terms in the Pikus-Bir Hamiltonian.

One can calculate similarly the masses for the $(\frac{3}{2}, -\frac{3}{2})$ band in the x direction; the resulting expression is identical in form to Eq. (14c) except that the prefactors 1, 5, and 4 of the P^2, Q^2, and R^2 terms must be replaced by 3, 3, and 12, respectively, owing to the different weighting factors in Table III. For the $(\frac{1}{2}, \frac{1}{2})$ band, the respective values are 2, 4, and 8, and the terms Δ_0 must be replaced by $(-2\Delta_0)$. Along the quantization direction z, where $\vec{k}=k\hat{z}$, the multiplying factors for the $(\frac{3}{2}, \frac{1}{2})$, $(\frac{3}{2}, -\frac{3}{2})$, and $(\frac{1}{2}, \frac{1}{2})$ bands are 4, 2, 16; 0, 6, 0; and 2, 4, 8, respectively, where for the $(\frac{1}{2}, \frac{1}{2})$ band Δ_0 must be replaced by $(-2\Delta_0)$. The $\Gamma_{2'}$ mass is isotropic.

For a pure hydrostatic stress, the quantization direction for the valence band is that of $\vec{k}$, and only the results for $\vec{k}\parallel\hat{z}$ have physical meaning. The perpendicular values given above and in Eq. (14c) are valid if the quantization direction $\hat{z}$ is determined by a directional perturbation, e.g., a uniaxial stress along $\hat{z}$. Corresponding coefficients for hydrostatic stress for $\vec{k}$ parallel to [111] are given at the end of Sec. II E.

D. Tetragonal strain

For a tetragonal shear strain resulting from a uniaxial stress along [001] the Pikus-Bir Hamiltonian, evaluated for $\vec{k}=k\hat{x}$, becomes

$$H' = (\hbar k/m_e)(1+\tfrac{1}{2}\epsilon_T)p_x + H'_{\epsilon T}, \tag{16a}$$

where the k-linear and bilinear terms have the symmetry of p_x, and the strain-linear term

$$H'_{\epsilon T} = \tfrac{1}{2}\epsilon_T[(1/m_e)(p_x^2+p_y^2-2p_z^2) - (V_{xx}+V_{yy}-2V_{zz})] \tag{16b}$$

has the symmetry Γ_{12}. Therefore, $H'_{\epsilon T}$ generates self-energy shifts of the $\Gamma_{25'}$, Γ_{15}, and $\Gamma_{12'}$ states, and couples $\Gamma_{2'}$ to $\Gamma_{12'}$. We define the nonvanishing self-energy terms $b_{25'}$, b_{15}, and $b_{12'}$ as

$$b_{25'}\epsilon_T = \langle\Gamma_{25'}(Z)|H'_{\epsilon T}|\Gamma_{25'}(Z)\rangle, \tag{17a}$$

$$b_{15}\epsilon_T = \langle\Gamma_{15}(z)|H'_{\epsilon T}|\Gamma_{15}(z)\rangle, \tag{17b}$$

$$b_{12'}\epsilon_T = \langle\Gamma_{12'}(\alpha)|H'_{\epsilon T}|\Gamma_{12'}(\alpha)\rangle. \tag{17c}$$

The self-energy terms for the $\Gamma_{25'}X, Y$ and $\Gamma_{15}x, y$ states are $-\frac{1}{2}$ times their z-symmetric counterparts. The self-energy for the $\Gamma_{12'}(\beta)$ state is the negative of that for $\Gamma_{12'}(\alpha)$. The Pikus-Bir deformation potential b has the value

$$b = \tfrac{1}{3} b_{25'} \,. \tag{18}$$

The $\Gamma_{2'} - \Gamma_{12'}$ coupling is defined by the coefficient c_T, where

$$c_T \epsilon_T = \langle \Gamma_{2'} \,|H'_{\epsilon T}|\, \Gamma_{12'}(\alpha)\rangle \,. \tag{19}$$

There is no coupling between $\Gamma_{2'}$ and $\Gamma_{12'}(\beta)$. The coupling between the $(\frac{3}{2}, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2})$ valence bands is given in terms of $b_{25'}$ as indicated in Table III; no change of valence-band representation occurs because the shear is parallel to the original quantization direction. In Table III, the quantities P', Q', and R' for the $\vec{k}$ direction perpendicular to the [001]-stress–quantization direction are given for tetragonal strain, from Eq. (16a), by

$$P' = (\hbar/m_e)(1 + \tfrac{1}{2}\epsilon_T)P \,, \tag{20a}$$

$$Q' = (\hbar/m_e)(1 + \tfrac{1}{2}\epsilon_T)Q \,, \tag{20b}$$

$$R' = (\hbar/m_e)(1 + \tfrac{1}{2}\epsilon_T)R \,. \tag{20c}$$

For the direction parallel to the [001]-stress–quantization axis the quantities $+\frac{1}{2}\epsilon_T$ in Eqs. (20) are replaced by $-\epsilon_T$.

From Table III and Eqs. (6), (7), and (16)–(20), the strain-dependent $\Gamma_{2'}$ conduction-band mass perpendicular to [001] becomes

$$\left(\frac{m_e}{m^*_c}\right)_\perp = 1 + \frac{2P^2}{3m_e}\left\{\frac{2}{E_0}\left[1 + \epsilon_T\left(1 - \frac{1}{4}\frac{b_{25'}}{E_0}\right)\right] + \frac{1}{E_0 + \Delta_0}\left[1 + \epsilon_T\left(1 - \frac{b_{25'}}{E_0}\right)\right]\right\} - \frac{4c_T\epsilon_T RP}{3m_e(\overline{E}''_0 - \overline{E}_0)}\left(\frac{2}{E_0} + \frac{1}{E_0 + \Delta_0}\right) \tag{21a}$$

$$\cong 1 + \frac{2P^2}{m_e\overline{E}_0}\left[1 + \epsilon_T\left(1 - \frac{b_{25'}}{2\overline{E}_0}\right)\right] - \frac{4RP\epsilon_T c_T}{m_e\overline{E}_0(\overline{E}''_0 - \overline{E}_0)} \,. \tag{21b}$$

Equation (21b) is the expansion of Eq. (21a) to first order in $\Delta_0/\overline{E}_0$. The cross term between k-linear and bilinear terms gives the term 1 in the postfactors of the ϵ_T terms. The two-band third-order terms, which are usually assumed to give the entire stress dependence of the conduction-band mass,[12] are those proportional to $b_{25'}$. For the direction $\vec{k} = k\hat{z}$ parallel to the stress/quantization axis the mass is given by replacing everywhere ϵ_T with $-2\epsilon_T$.

The valence-band masses can be evaluated similarly. We find that the $(\frac{3}{2}, \frac{1}{2})$ mass perpendicular to the [001]-stress–quantization direction is

$$\left(\frac{m_e}{m^*_{3/2,1/2}}\right)_\perp = 1 - \frac{P^2}{3m_eE_0}\left[1 + \epsilon_T\left(1 + \frac{b_{25'}}{2E_0}\right)\right] - \frac{5Q^2}{3m_e(\overline{E}'_0 - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_T\left(1 + \frac{5b_{25'} + 2b_{15}}{10(\overline{E}'_0 - \frac{1}{3}\Delta_0)}\right)\right] - \frac{4R^2}{3m_e(\overline{E}''_0 - \frac{1}{3}\Delta_0)} \times\left[1 + \epsilon_T\left(1 + \frac{b_{25'} + b_{12'}}{2(\overline{E}''_0 - \frac{1}{3}\Delta_0)}\right)\right] + \frac{2b_{25'}\epsilon_T}{3m_e\Delta_0}\left(\frac{P^2}{E_0} - \frac{Q^2}{\overline{E}'_0 - \frac{1}{3}\Delta_0} + \frac{4R^2}{\overline{E}''_0 - \frac{1}{3}\Delta_0} + \frac{c_T PR\,\Delta_0}{b_{25'}E_0(\overline{E}''_0 - \frac{1}{3}\Delta_0)}\right) . \tag{22}$$

The only strain-linear terms taken into account by Hensel and Suzuki[17] are those proportional to P^2, Q^2, and R^2 in the last row of Eq. (22). Because the strain lifts degeneracies, no simple change of coefficients will give expressions for the perpendicular masses for the $(\frac{3}{2}, -\frac{3}{2})$ and $(\frac{1}{2}, \frac{1}{2})$ valence bands as in the hydrostatic case, but they can be calculated easily from Table III and the above if needed. We give explicitly only the mass of the $(\frac{3}{2}, \frac{1}{2})$ band parallel to the [001]-stress–quantization axis, which is

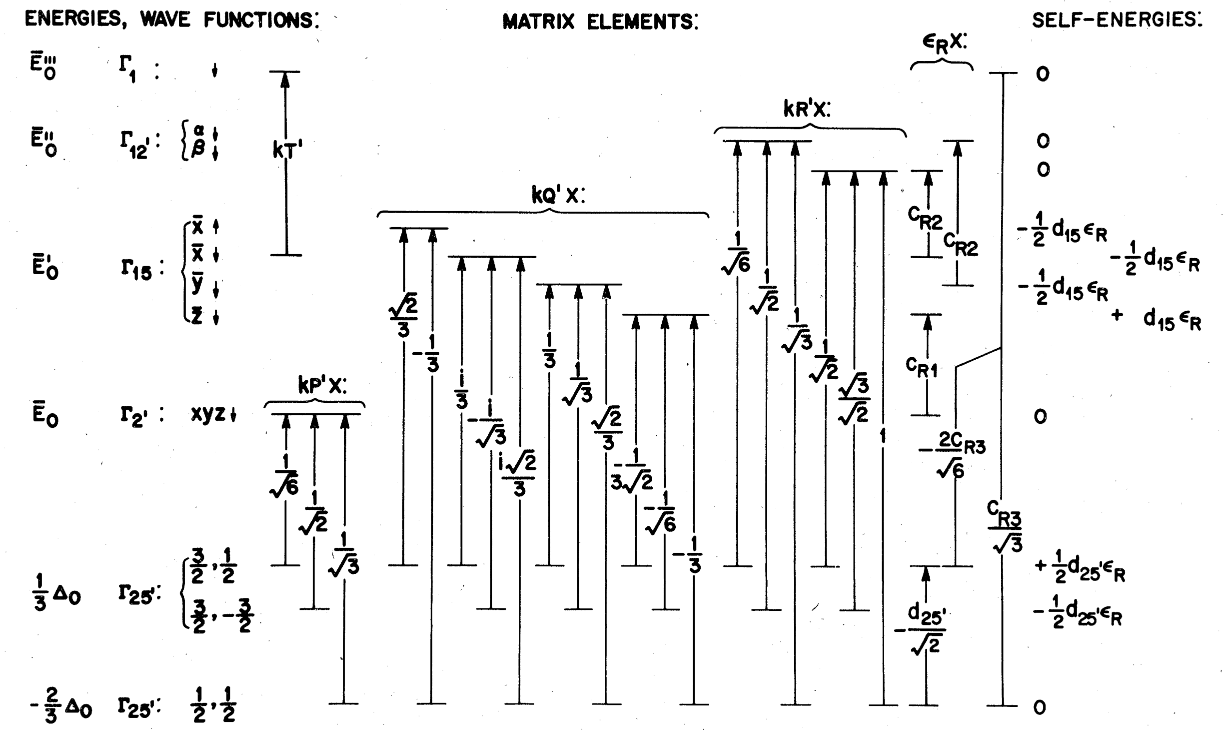
$$\left(\frac{m_e}{m^*_{3/2,1/2}}\right)_\parallel = 1 - \frac{4P^2}{3m_eE_0}\left[1 + \epsilon_T\left(-2 + \frac{b_{25'}}{2E_0}\right)\right] - \frac{2Q^2}{3m_e(\overline{E}'_0 - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_T\left(-2 + \frac{b_{25'} + b_{15}}{2(\overline{E}'_0 - \frac{1}{3}\Delta_0)}\right)\right] - \frac{16R^2}{3m_e(\overline{E}''_0 - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_T\left(-2 + \frac{b_{25'} - 2b_{12'}}{2(\overline{E}''_0 - \frac{1}{3}\Delta_0)}\right)\right] - \frac{4b_{25'}\epsilon_T}{3\Delta_0 m_e}\left(\frac{P^2}{E_0} - \frac{Q^2}{\overline{E}'_0 - \frac{1}{3}\Delta_0} + \frac{4R^2}{\overline{E}''_0 - \frac{1}{3}\Delta_0} + \frac{4c_T PR\,\Delta_0}{b_{25'}E_0(\overline{E}''_0 - \frac{1}{3}\Delta_0)}\right) . \tag{23}$$

To use Eqs. (21)–(23) with uniaxial stress, the hydrostatic correction terms from Eqs. (14) must be added because both components ϵ_H and ϵ_T are present.

E. Trigonal (rhombohedral) strain

For a trigonal shear strain resulting from a uniaxial stress in the [111] direction, it is more con-

TABLE IV. Nonvanishing k-linear, ϵ-linear, and bilinear (ϵk), matrix elements for $\vec{k}=k\hat{\bar{x}}$ for trigonal shear strain resulting from a uniaxial stress perpendicular to the quantization axis ($\hat{\bar{z}}=(\hat{x}+\hat{y}+\hat{z})/\sqrt{3}$) of the spin-orbit-split valence bands. The quantities P', Q', R', and T' are defined in Eqs. (26).



venient to rotate all wave functions and operators into directions parallel and perpendicular to the [111] axis.[6] The rotated momentum operators for example are the linear combinations

$$\bar{p}_x=(p_x-p_y)/\sqrt{2}\ , \tag{24a}$$

$$\bar{p}_y=(p_x+p_y-2p_z)/\sqrt{6}\ , \tag{24b}$$

$$\bar{p}_z=(p_x+p_y+p_z)/\sqrt{3}\ . \tag{24c}$$

If analogous linear combinations of all threefold-degenerate wave functions are formed similarly and the quantization axis for spin-orbit splitting is taken to be $\hat{\bar{z}}=(\hat{x}+\hat{y}+\hat{z})/\sqrt{3}$, then the previous formalism is unchanged except for different values of momentum matrix elements. In the rotated bases, the Pikus-Bir Hamiltonian evaluated for $\vec{k}=k\hat{\bar{x}}=k(\hat{x}-\hat{y})/\sqrt{2}$, perpendicular to the stress-quantization axis $\hat{\bar{z}}$ becomes

$$H'=(\hbar k/m_e)(1+\epsilon_R)\bar{p}_x+H'_{\epsilon R}\ . \tag{25}$$

The k-linear and bilinear terms have the symmetry of $\bar{p}_x$, and lead to the values of momentum matrix elements in the rotated system, with $\vec{k}$ perpendicular to the stress and quantization axis, as summarized in Table IV. Here the coefficients P', Q', and R' are given by

$$P'=(\hbar/m_e)(1+\epsilon_R)P\ , \tag{26a}$$

$$Q'=(\hbar/m_e)(1+\epsilon_R)Q\ , \tag{26b}$$

$$R'=(\hbar/m_e)(1+\epsilon_R)R\ , \tag{26c}$$

$$T'=(\hbar/m_e)(1+\epsilon_R)T\ , \tag{26d}$$

where P, Q, R, and T are defined in Table I. For $\vec{k}$ parallel to the [111]-stress-quantization axis, the quantities $+\epsilon_R$ in Eqs. (26) are replaced by $-2\epsilon_R$. The strain-linear term

$$H'_{\epsilon R}=-2\epsilon_R[(1/m_e)(p_xp_y+p_yp_z+p_zp_x)-(V_{xy}+V_{yz}+V_{zx})] \tag{27}$$

has the symmetry $\Gamma_{25'}(\bar{Z})$ and generates self-energy terms in $\Gamma_{25'}$ and Γ_{15}. It also couples Γ_{15} to $\Gamma_{2'}$ and $\Gamma_{12'}$, and $\Gamma_{25'}$ to Γ_1. The self-energy terms can be expressed by two coefficients $d_{25'}$ and d_{15} defined as

$$d_{25'}\epsilon_R=\langle\Gamma_{25'}(\bar{Z})|H'_{\epsilon R}|\,\Gamma_{25'}(\bar{Z})\rangle\ , \tag{28a}$$

$$d_{15}\epsilon_R=\langle\Gamma_{15}(\bar{z})|H'_{\epsilon R}|\,\Gamma_{15}(\bar{z})\rangle\ . \tag{28b}$$

The self-energy terms for the $\Gamma_{25'}\overline{X}, \overline{Y}$ and $\Gamma_{15}\overline{x}, \overline{y}$ states are $-1/2$ times their $\overline{z}$-symmetric counterparts in Eqs. (28). The Pikus-Bir deformation potential, d, is given by

$$d = d_{25'}/2\sqrt{3}\ . \tag{29}$$

The $\Gamma_{2'}$-Γ_{15}, Γ_{15}-$\Gamma_{12'}$, and $\Gamma_{25'}$-Γ_1 couplings are represented by the constants c_{R1}, c_{R2}, and c_{R3}, defined by

$$c_{R1}\epsilon_R = \langle \Gamma_{2'} | H'_{\epsilon R} | \Gamma_{15}(\overline{z}) \rangle\ , \tag{30a}$$

$$c_{R2}\epsilon_R = \langle \Gamma_{15}(\overline{x}) | H'_{\epsilon R} | \Gamma_{12'}(\beta) \rangle\ , \tag{30b}$$

$$c_{R3}\epsilon_R = \langle \Gamma_{25'}(\overline{z}) | H'_{\epsilon R} | \Gamma_1 \rangle\ . \tag{30c}$$

The coupling between $\Gamma_{15}(\overline{y})$ and $\Gamma_{12'}(\alpha)$ is also given by c_{R2}. The matrix elements of $H'_{\epsilon R}$ between $\Gamma_{15}(\overline{x})$ and $\Gamma_{12'}(\alpha)$, and between $\Gamma_{15}(\overline{y})$ and $\Gamma_{12'}(\beta)$, are zero. No coupling occurs between $\Gamma_{2'}$ and the states $\Gamma_{15}(\overline{x})$ and $\Gamma_{15}(\overline{y})$, nor between $\Gamma_{15}(\overline{z})$ and $\Gamma_{12'}$, nor between $\Gamma_{25'}(\overline{x})$ or $\Gamma_{25'}(\overline{y})$ and Γ_1. Nonvanishing terms are summarized in Table IV.

It is straightforward to evaluate the conduction-band mass from Eqs. (6) and (7) and Table IV. We find for the mass perpendicular to the [111]-stress–quantization axis that

$$\begin{aligned}\left(\frac{m_e}{m_c^*}\right)_{\perp} &= 1 + \frac{2P^2}{3m_e}\left\{\frac{2}{E_0}\left[1 + \epsilon_R\left(2 - \frac{1}{4}\frac{d_{25'}}{E_0}\right)\right] + \frac{1}{E_0+\Delta_0}\left[1 + \epsilon_R\left(2 - \frac{d_{25'}}{E_0+\Delta_0}\right)\right]\right\} \\ &\quad + \frac{4PQc_{R1}\epsilon_R}{3\sqrt{3}\,m_e(\overline{E}_0' - \overline{E}_0)}\left(\frac{2}{E_0} + \frac{1}{E_0+\Delta_0}\right) \qquad (31a)\\ &\cong 1 + \frac{2P^2}{m_e\overline{E}_0}\left[1 + \epsilon_R\left(2 - \frac{d_{25'}}{2\overline{E}_0}\right)\right] + \frac{4PQ\epsilon_R c_{R1}}{\sqrt{3}\,m_e\overline{E}_0(\overline{E}_0' - \overline{E}_0)}\ . \qquad (31b)\end{aligned}$$

Equation (31b) is the expansion of Eq. (31a) to first order in $\Delta_0/\overline{E}_0$. The expressions are identical in form to those obtained for tetragonal shear, except that the cross term between the k-linear and bilinear terms per unit strain is twice as large, and the sign of the three-band term is reversed. The two-band third-order terms are those proportional to $d_{25'}$. For the direction $\vec{k} = k\hat{z}$ parallel to the [111]-stress–quantization axis, the mass is given by replacing ϵ_R everywhere with $-2\epsilon_R$.

The $(\frac{3}{2}, \frac{1}{2})$ valence-band mass evaluated perpendicular to the [111]-stress–quantization axis is

$$\begin{aligned}\left(\frac{m_e}{m^*_{3/2,1/2}}\right)_{\perp} &= 1 - \frac{P^2}{3m_eE_0}\left[1 + \epsilon_R\left(2 + \frac{d_{25'}}{2E_0}\right)\right] - \frac{3Q^2}{3m_e(\overline{E}_0' - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_R\left(2 + \frac{3d_{25'} + 2d_{15}}{6(\overline{E}_0' - \frac{1}{3}\Delta_0)}\right)\right] \\ &\quad - \frac{4R^2}{3m_e(\overline{E}_0'' - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_R\left(2 + \frac{d_{25'}}{2(\overline{E}_0'' - \frac{1}{3}\Delta_0)}\right)\right] + \frac{2d_{25'}\epsilon_R}{3m_e\Delta_0}\left(\frac{P^2}{E_0} + \frac{Q^2}{\overline{E}_0' - \frac{1}{3}\Delta_0} + \frac{4R^2}{\overline{E}_0'' - \frac{1}{3}\Delta_0}\right) \\ &\quad - \frac{2\epsilon_R}{3\sqrt{3}\,m_e}\left(\frac{c_{R1}PQ}{E_0(\overline{E}_0' - \frac{1}{3}\Delta_0)} - \frac{\sqrt{2}\,c_{R2}QR}{(\overline{E}_0' - \frac{1}{3}\Delta_0)(\overline{E}_0'' - \frac{1}{3}\Delta_0)} + \frac{4c_{R3}TQ}{(\overline{E}_0' - \frac{1}{3}\Delta_0)(\overline{E}_0''' - \frac{1}{3}\Delta_0)}\right)\ .\end{aligned} \tag{32}$$

The parallel component can be calculated similarly and we find

$$\begin{aligned}\left(\frac{m_e}{m^*_{3/2,1/2}}\right)_{\parallel} &= 1 - \frac{4P^2}{3m_eE_0}\left[1 + \epsilon_R\left(-4 + \frac{d_{25'}}{2E_0}\right)\right] - \frac{6Q^2}{3m_e(\overline{E}_0' - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_R\left(-4 + \frac{3d_{25'} - 5d_{15}}{6(\overline{E}_0' - \frac{1}{3}\Delta_0)}\right)\right] \\ &\quad - \frac{8R^2}{3m_e(\overline{E}_0'' - \frac{1}{3}\Delta_0)}\left[1 + \epsilon_R\left(-4 + \frac{d_{25'}}{2(\overline{E}_0'' - \frac{1}{3}\Delta_0)}\right)\right] - \frac{4d_{25'}\epsilon_R}{3m_e\Delta_0}\left(\frac{P^2}{E_0} + \frac{Q^2}{\overline{E}_0' - \frac{1}{3}\Delta_0}\right) \\ &\quad + \frac{2\epsilon_R}{3\sqrt{3}\,m_e}\left(\frac{8c_{R1}PQ}{E_0(\overline{E}_0' - \frac{1}{3}\Delta_0)} - \frac{\sqrt{2}\,c_{R2}QR}{(\overline{E}_0' - \frac{1}{3}\Delta_0)(\overline{E}_0'' - \frac{1}{3}\Delta_0)} + \frac{8c_{R3}TQ}{(\overline{E}_0' - \frac{1}{3}\Delta_0)(\overline{E}_0'' - \frac{1}{3}\Delta_0)}\right)\ .\end{aligned} \tag{33}$$

The $(\frac{3}{2}, \frac{3}{2})$ and $(\frac{1}{2}, \frac{1}{2})$ masses can be calculated similarly if needed.

For a [111] uniaxial stress, the contribution from the hydrostatic component must be added. For the $\Gamma_{2'}$ band, this correction is identical to that given in Eqs. (14a) and (14b). The expressions differ from Eq. (14c) for the valence bands because the weighting factors of Table IV are different from those of Table III. It is straightforward to show that the weighting factors 1, 5, 4 of the P, Q, R terms in Eq. (14c) should be replaced by 1, 3, 4 and 4, 6, 8 for the $(\frac{3}{2}, \frac{1}{2})$ mass perpendicular $(\hat{\overline{x}})$ and parallel $(\hat{\overline{z}})$, respectively, to the [111]-stress–quantization axis. For the $(\frac{3}{2}, \frac{3}{2})$ and $(\frac{1}{2}, \frac{1}{2})$ bands the perpendicular values are 3, 5, 12 and 2, 4, 8, and the parallel values are 0, 2, 8 and 2, 4, 8, respectively.

III. PSEUDOPOTENTIAL EVALUATION

A. Stress-induced changes in lattice potential

We evaluate the expressions of the previous sections with a pseudopotential model previously used

TABLE V. Pseudopotentials of the unperturbed crystal.

Pseudopotential	Plane-wave representation
$V_3^s(\vec{r})$	$(v_3^s/\sqrt{2})[-(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})+(\bar{1}\bar{1}1)-(\bar{1}\bar{1}\bar{1})+(\bar{1}11)+(1\bar{1}1)+(11\bar{1})]$
$V_8^s(\vec{r})$	$v_8^s[-(220)+(2\bar{2}0)+(\bar{2}20)-(\bar{2}\bar{2}0)+\text{c.p.}]$[a]
$V_{11}^s(\vec{r})$	$(v_{11}^s/\sqrt{2})[-(311)-(31\bar{1})-(3\bar{1}1)+(3\bar{1}\bar{1})-(\bar{3}\bar{1}\bar{1})-(\bar{3}\bar{1}1)-(\bar{3}1\bar{1})+(\bar{3}11)+\text{c.p.}]$

[a] c.p. means cyclic permutation.

to evaluate deformation potentials in Ge.[6] We recall that these expressions are based on two approximations: (i) inversion symmetry, and (ii) a $\Gamma_{25'}$, $\Gamma_{2'}$, Γ_{15}, $\Gamma_{12'}$, and Γ_1 basis set, as discussed before. Here, we make the additional assumptions that these expressions can be evaluated using pseudopotential coefficients up to v_{12} [plane waves up to (222)] and wave functions using (111) and (200) plane waves.

The nonvanishing pseudopotentials $V_3^s(\vec{r})$, $V_8^s(\vec{r})$, and $V_{11}^s(\vec{r})$ are obtained from the standard definitions[28]

$$V(\vec{r})=\sum_G \left[V_G^s\cos(\vec{G}\cdot\vec{\tau})+iv_G^a\sin(\vec{G}\cdot\vec{\tau})\right]e^{-i\vec{G}\cdot\vec{r}}\,, \tag{34a}$$

$$v_G^s=\tfrac{1}{2}[v_1(\vec{G})+v_2(\vec{G})],\quad v_G^a=\tfrac{1}{2}[v_1(\vec{G})-v_2(\vec{G})]\,, \tag{34b}$$

$$v_1(\vec{G})=\frac{2}{V_0}\int d^3r\,V_1(\vec{r})e^{-i\vec{G}\cdot\vec{r}}\,, \tag{34c}$$

where $\vec{\tau}=(\frac{1}{8}a_0)(\hat{x}+\hat{y}+\hat{z})$, V_0 is the volume of the unit cell, a_0 is the lattice constant, and $V_1(\vec{r})$ is the potential of atom 1. The pseudopotentials are listed in Table V. The plane-wave notation is standard

$$(hk\bar{l})=e^{iG_0(hx+ky-lz)}\,, \tag{35a}$$

$$G_0=2\pi/a_0\,. \tag{35b}$$

In Table V and elsewhere, c.p. means cyclic permutation. Using Table V one can obtain explicit expressions for the strain-linear terms $H'_{\epsilon H}$, $H'_{\epsilon R}$, and $H'_{\epsilon T}$ in Eqs. (10b), (16b), and (27), by use of the definition, Eq. (3d).

We should point out that while the pseudopotential Hamiltonian yields correct energies it is not likely to yield correct values of matrix elements between *different* true states if pseudo-wave-functions are used.[29] Nevertheless, we are using such matrix elements only in the expressions for the effective masses (related to *energies)*. Hence the use of pseudo-wave-functions seems justified.

Because hydrostatic strain leaves the symmetry of the crystal unchanged, its only effect is to change the magnitudes of the form factors. These can be evaluated by considering their change with volume:[6]

$$H'_{\epsilon H}=3\epsilon_H\left[-\frac{1}{3}\frac{\vec{p}^2}{m_e}+\left(\frac{\bar{v}'_3}{v_3^s}\right)V_3^s(\vec{r}) + \left(\frac{\bar{v}'_8}{v_8^s}\right)V_8^s(\vec{r})+\left(\frac{\bar{v}'_{11}}{v_{11}^s}\right)V_{11}^s(\vec{r})\right]\,, \tag{36a}$$

$$\bar{v}'_j=-(\tfrac{1}{3}v'_j+v_j^s)=V\frac{dv_j^s}{dV}\,, \tag{36b}$$

$$v'_j=G\,\frac{dv_j^s}{dG}\,. \tag{36c}$$

Here, v'_j and $\bar{v}'_j$ are the logarithmic wave vector and volume derivatives of v_j^s, respectively. Thus $H'_{\epsilon H}$ is expressed in terms of the unperturbed crystal pseudopotentials given in Table V.

Tetragonal shear induces a change in $V(\vec{r})$ that transforms as Γ_{12}. Because the volume does not change, the form factors are invariant and the change in $V(\vec{r})$ arises from the expansion of the plane-wave terms themselves, in terms of the first-order changes in the wave vectors $\vec{G}_{hkl}$ under shear ("derivative" terms[6]). Under tetragonal shear the primitive lattice vectors become to first order in ϵ_T:

$$\vec{G}_{[\bar{1}11]}\to\vec{G}_{[\bar{1}11]}+\tfrac{1}{2}\epsilon_T G_0(-\hat{x}+\hat{y}-2\hat{z})\,, \tag{37a}$$

$$\vec{G}_{[1\bar{1}1]}\to\vec{G}_{[1\bar{1}1]}+\tfrac{1}{2}\epsilon_T G_0(\hat{x}-\hat{y}-2\hat{z})\,, \tag{37b}$$

$$\vec{G}_{[11\bar{1}]}\to\vec{G}_{[11\bar{1}]}+\tfrac{1}{2}\epsilon_T G_0(\hat{x}+\hat{y}+2\hat{z})\,. \tag{37c}$$

Changes in other reciprocal-lattice vectors can be calculated from appropriate linear combinations. Expanding the plane-wave parts of the pseudopotentials in Table V to first order in ϵ_T and using Eqs. (37) leads to the complete expression

$$H'_{\epsilon T}=\epsilon_T[(1/2m_e)(p_x^2+p_y^2-2p_z^2) + V_8^T(\vec{r})+V_{11}^T(\vec{r})]\,, \tag{38}$$

where $V_8^T(\vec{r})$ and $V_{11}^T(\vec{r})$ are given in Table VI. The $V_3^T(\vec{r})$ component vanishes because tetragonal shear does not change the length of the (111) reciprocal lattice vectors to first order.

Trigonal shear induces a $\Gamma_{25'}$ change in $V(\vec{r})$, where as for tetragonal shear the form factors remain invariant. The first-order changes in the plane waves due to changes in the wave vectors

TABLE VI. Stress-induced changes in pseudopotentials for tetragonal shear ([001]-stress–quantization axis).

Component	Plane-wave representation
$V_8^T(\vec{r})$	$-\frac{1}{4}v_8'[2(220)-2(2\bar{2}0)-2(\bar{2}20)+2(\bar{2}\bar{2}0)$
	$-(202)+(20\bar{2})+(\bar{2}02)-(\bar{2}0\bar{2})$
	$-(022)+(02\bar{2})+(0\bar{2}2)-(0\bar{2}\bar{2})]$
$V_{11}^T(\vec{r})$	$\frac{2}{11}\sqrt{2}v_{11}'[2(113)+2(1\bar{1}3)+2(\bar{1}13)-2(\bar{1}\bar{1}3)$
	$+2(\bar{1}\bar{1}\bar{3})+2(\bar{1}1\bar{3})+2(1\bar{1}\bar{3})-2(11\bar{3})$
	$-(311)-(31\bar{1})-(3\bar{1}1)+(3\bar{1}\bar{1})$
	$-(\bar{3}\bar{1}\bar{1})-(\bar{3}\bar{1}1)-(\bar{3}1\bar{1})+(\bar{3}11)$
	$-(131)-(13\bar{1})-(\bar{1}31)+(\bar{1}3\bar{1})$
	$-(\bar{1}\bar{3}\bar{1})-(\bar{1}\bar{3}1)-(1\bar{3}\bar{1})+(1\bar{3}1)]$

(derivative terms) can be calculated from

$$\vec{G}_{[\bar{1}11]} \rightarrow \vec{G}_{[\bar{1}11]} - 2\epsilon_R G_0 \hat{x} , \tag{39a}$$

$$\vec{G}_{[1\bar{1}1]} \rightarrow \vec{G}_{[1\bar{1}1]} - 2\epsilon_R G_0 \hat{y} , \tag{39b}$$

$$\vec{G}_{[11\bar{1}]} \rightarrow \vec{G}_{[11\bar{1}]} - 2\epsilon_R G_0 \hat{z} . \tag{39c}$$

But in addition there are "phonon" terms which come from the structure factors.[6] These express the effect of the relative shift of the two sublattices which occurs because the four (111) bonds are no longer equivalent under tetragonal shear.

The phonon terms can be calculated as follows.[6] Suppose a trigonal shear is applied to the crystal by, e.g., a uniaxial stress along [111]. The unit cell is therefore compressed along [111] and the [111] bond becomes inequivalent to the other three. The crystal strain along [111] is $2\epsilon_R$. Due to competition between bending and stretching, however, the relative change of length of the [111] bond is less than that of the relative change of length of the unit cell along [111]; we denote the *relative discrepancy* by ζ so that instead of the relative change $2\epsilon_R$ expected for a uniform deformation of the unit cell, the actual relative change of the bond length is $2\epsilon_R(1-\zeta)$. For group-IV and -III-V semiconductors $\zeta \simeq 0.6$.[30]

Now the Pikus-Bur Hamiltonian is obtained by applying the inverse transformation to the Hamiltonian to restore the deformed unit cell to its original dimensions. Along [111], this transformation changes all relative lengths again by $-2\epsilon_R$, in which case the new relative bond length is $1+2\epsilon_R(1-\zeta)-2\epsilon_R=1-2\epsilon_R\zeta$. Thus in Eq. (34a) the structure factor for trigonal shear along [111] becomes

$$\cos(\vec{G}\cdot\vec{\tau}) \rightarrow \cos[\vec{G}\cdot(1-2\epsilon_R\zeta)\vec{\tau}]$$

$$\simeq \cos(\vec{G}\cdot\vec{\tau}) + 2\epsilon_R\zeta(\vec{G}\cdot\vec{\tau})\sin(\vec{G}\cdot\vec{\tau}) . \tag{40}$$

The correction term also generates phonon contributions from the forbidden v_4^s and v_{12}^s pseudopotential terms.

The pseudopotentials for trigonal shear lead to the explicit perturbation Hamiltonian

TABLE VII. Stress-induced changes in pseudopotentials for trigonal shear ($[111]=\bar{z}$ stress–quantization axis). The superscripts d and p identify derivative (macroscopic strain) and phonon contributions, respectively. $1-\zeta$ represents the fraction of strain along $\bar{z}$ that appears across the bond parallel to the stress.

Component	Plane-wave representation
$V_3^{R,d}(\vec{r})$	$\frac{1}{3}\sqrt{2}v_3'[3(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})+(\bar{1}\bar{1}1)$
	$+3(\bar{1}\bar{1}\bar{1})+(\bar{1}11)+(1\bar{1}1)+(11\bar{1})]$
$V_3^{R,p}(\vec{r})$	$(\pi\zeta/2\sqrt{2})v_3^s[3(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})+(\bar{1}\bar{1}1)$
	$+3(\bar{1}\bar{1}\bar{1})+(\bar{1}11)+(1\bar{1}1)+(11\bar{1})]$
$V_4^{R,p}(\vec{r})$	$\pi\zeta v_4^s[(200)+(020)+(002)+(\bar{2}00)+(0\bar{2}0)+(00\bar{2})]$
$V_8^{R,d}(\vec{r})$	$v_8'[(220)+(2\bar{2}0)+(\bar{2}20)+(\bar{2}\bar{2}0)+\text{c.p.}]$[a]
$V_{11}^{R,d}(\vec{r})$	$\frac{1}{11}\sqrt{2}v_{11}'[7(311)-(31\bar{1})-(3\bar{1}1)+5(3\bar{1}\bar{1})+7(\bar{3}\bar{1}\bar{1})$
	$-(\bar{3}\bar{1}1)-(\bar{3}1\bar{1})+5(\bar{3}11)+\text{c.p.}]$
$V_{11}^{R,p}(\vec{r})$	$-(\pi\zeta/2\sqrt{2})v_{11}^s[5(311)-3(31\bar{1})-3(3\bar{1}1)-(3\bar{1}\bar{1})+5(\bar{3}\bar{1}\bar{1})$
	$-3(\bar{3}\bar{1}1)-3(\bar{3}1\bar{1})-(\bar{3}11)+\text{c.p.}]$
$V_{12}^{R,p}(\vec{r})$	$-\pi\zeta v_{12}^s[3(222)-(2\bar{2}\bar{2})-(\bar{2}2\bar{2})-(\bar{2}\bar{2}2)$
	$+3(\bar{2}\bar{2}\bar{2})-(\bar{2}22)-(2\bar{2}2)-(22\bar{2})]$

[a] c.p. means cyclic permutation.

TABLE VIII. Pseudopotential wave functions for evaluating hydrostatic pressure and tetragonal shear perturbations. For $\Gamma_{25'}$ and Γ_{15}, only the wave functions transforming as Z and z are shown. The coefficients $\beta_{25'}$, $\gamma_{25'}$, $\beta_{2'}$, and $\gamma_{2'}$ are defined in Eqs. (42).

State	Plane-wave representation
$\Gamma_{25'}(Z)$	$(\beta_{25'}/\sqrt{8})[(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})-(\bar{1}\bar{1}1)+(\bar{1}\bar{1}\bar{1})+(\bar{1}11)+(1\bar{1}1)-(11\bar{1})]$ $+(\gamma_{25'}/\sqrt{2})[(002)+(00\bar{2})]$
$\Gamma_{2'}$	$(\beta_{2'}/\sqrt{8})[(111)-(1\bar{1}\bar{1})-(\bar{1}1\bar{1})-(\bar{1}\bar{1}1)-(\bar{1}\bar{1}\bar{1})+(\bar{1}11)+(1\bar{1}1)+(11\bar{1})]$ $+(\gamma_{2'}/\sqrt{6})[(200)+(020)+(002)-(\bar{2}00)-(0\bar{2}0)-(00\bar{2})]$
$\Gamma_{15}(z)$	$(1/\sqrt{8})[(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})-(\bar{1}\bar{1}1)-(\bar{1}\bar{1}\bar{1})-(\bar{1}11)-(1\bar{1}1)+(11\bar{1})]$
$\Gamma_{12'}(\alpha)$	$(1/\sqrt{12})[(200)+(020)-2(002)-(\bar{2}00)-(0\bar{2}0)+2(00\bar{2})]$
$\Gamma_{12'}(\beta)$	$\frac{1}{2}[(200)-(020)-(\bar{2}00)+(0\bar{2}0)]$
Γ_1	$(1/\sqrt{8})[(111)-(1\bar{1}\bar{1})-(\bar{1}1\bar{1})-(\bar{1}\bar{1}1)+(\bar{1}\bar{1}\bar{1})-(\bar{1}11)-(1\bar{1}1)-(11\bar{1})]$

$$H_{\epsilon R}=\epsilon_R[-(2/m_e)(p_xp_y+p_yp_z+p_zp_x)+V_3^{R,d}(\vec{r})+V_3^{R,p}(\vec{r})+V_4^{R,p}(\vec{r})+V_8^{R,d}(\vec{r})+V_{11}^{R,d}(\vec{r})+V_{11}^{R,p}(\vec{r})+V_{12}^{R,p}(\vec{r})]\ , \tag{41}$$

where the superscripts d and p refer to derivative (macroscopic strain) and phonon terms, respectively. All are given explicitly in Table VII. We note that the $V^p(\vec{r})$ terms can also be used to calculate electron-phonon interaction constants, provided that the sign is changed and ξ is replaced by a factor of 4.[6]

B. Wave functions

The plane-wave representations for the $\Gamma_{25'}$, $\Gamma_{2'}$, Γ_{15}, $\Gamma_{12'}$, and Γ_1 states are standard[30] and are given in Table VIII. The projection coefficients $\beta_{25'}$, $\gamma_{25'}$, $\beta_{2'}$, and $\gamma_{2'}$ for the $\Gamma_{25'}$ and $\Gamma_{2'}$ wave functions are given by[6,31]

$$\gamma_{25'}/\beta_{25'}=-2\sqrt{2}\,(v_3^s-v_{11}^s)\{\Omega+v_8^s+[(\Omega+v_8^s)^2+8(v_3^s-v_{11}^s)^2]^{1/2}\}^{-1}\ , \tag{42a}$$

$$\gamma_{2'}/\beta_{2'}=-2\sqrt{6}\,(v_3^s+v_{11}^s)\{\Omega+v_8^s+[(\Omega+v_8^s)^2+24(v_3^s+v_{11}^s)^2]^{1/2}\}^{-1}\ , \tag{42b}$$

$$\beta^2+\gamma^2=1\ , \tag{42c}$$

$$\Omega=\hbar^2G_0^2/2m_e\ . \tag{42d}$$

For trigonal shear it is more convenient to use the linear combinations of the $\Gamma_{25'}$ and Γ_{15} wave functions corresponding to rotation into the $\bar{x}$, $\bar{y}$, $\bar{z}$ coordinate system, with $\bar{z}$ along the [111]-stress axis. The $\Gamma_{25'}(\bar{Z})$ and $\Gamma_{15}(\bar{z})$ wave functions are given in Table IX.

C. Matrix elements and expectation values

The matrix elements and expectation values of Tables I and II, calculated from the above perturbation Hamiltonians, are also given in terms of pseudopotential parameters in Tables I and II.

IV. RESULTS AND DISCUSSION

In this section, we evaluate explicitly for Ge the terms calculated in previous sections, using data[6,30,32-36] summarized in Table X. Although the stress-induced anisotropy of the $\Gamma_{2'}$ conduction-band mass is not easily accessible to measurement for this material ($\Gamma_{2'}$ is not the lowest conduction-band minimum) the stress-induced anisotropy of the upper valence-band $(\frac{3}{2}, \frac{1}{2})$ mass has been measured to high precision by Hensel and Suzuki.[17] This anisotropy is different from that predicted by two-band

TABLE IX. Pseudopotential wave functions for evaluating trigonal shear perturbations. Only the wave functions transforming as $\bar{Z}$ and $\bar{z}$ are given explicitly. The coefficients $\beta_{25'}$ and $\gamma_{25'}$ are defined in Eqs. (42).

State	Plane-wave representation
$\Gamma_{25'}(\bar{Z})$	$(\beta_{25'}/\sqrt{24})[3(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})+(\bar{1}\bar{1}1)+3(\bar{1}\bar{1}\bar{1})+(\bar{1}11)+(1\bar{1}1)+(11\bar{1})]$ $+(\gamma_{25'}/\sqrt{6})[(200)+(020)+(002)+(\bar{2}00)+(0\bar{2}0)+(00\bar{2})]$
$\Gamma_{15}(\bar{z})$	$(1/\sqrt{24})[3(111)+(1\bar{1}\bar{1})+(\bar{1}1\bar{1})+(\bar{1}\bar{1}1)-3(\bar{1}\bar{1}\bar{1})-(\bar{1}11)-(1\bar{1}1)-(11\bar{1})]$

TABLE X. Values of parameters for Ge, used to evaluate pseudopotential expressions derived in text.

Data	Calculated values
$a_0/a_B = 10.691$ [a]	$\Omega = 4.700$ eV
$v_3^s = -3.27$ eV [b]	$\beta_{25'} = 0.833$
$v_4^s = -1.77$ eV [c]	$\gamma_{25'} = 0.554$
$v_8^s = 0.44$ eV [b]	$\beta_{2'} = 0.845$
$v_{11}^s = 1.06$ eV [b]	$\gamma_{2'} = 0.534$
$v_{12}^s = 0.82$ eV [c]	$\bar{v}'_3 = 1.09$ eV
$v'_3 = 6.53$ eV [c]	$\bar{v}'_8 = -1.93$ eV
$v'_4 = 6.33$ eV [c]	$\bar{v}'_{11} = -1.51$ eV
$v'_8 = 4.49$ eV [c]	$\epsilon_H = -0.00149$ (10 kbar uniaxial; 10/3 kbar hydrostatic)
$v'_{11} = 1.36$ eV [c]	
$v'_{12} = 0.16$ eV [c]	$\epsilon_T = -0.00829$ (10 kbar uniaxial)
$\zeta = 0.66$ [d]	$\epsilon_R = -0.00248$ (10 kbar uniaxial)
$S_{11} = 9.78 \times 10^{-4}$ kbar^{-1} [e]	
$S_{12} = -2.66 \times 10^{-4}$ kbar^{-1} [e]	
$S_{44} = 14.90 \times 10^{-4}$ kbar^{-1} [e]	
$E_0 = 0.889$ eV [f]	
$\Delta_0 = 0.287$ eV [f]	
$\bar{E}'_0 = 3.235$ eV [f]	
$\bar{E}''_0 = 10.5$ eV [g]	
$\bar{E}'''_0 = 8.3$ eV [g]	

[a] Reference 32.
[b] Reference 33.
[c] Reference 6.
[d] Reference 30.
[e] Reference 34.
[f] Reference 35.
[g] Estimated value, equal to corresponding value for GaAs (Ref. 36).

terms alone. As we shall show, this difference can be explained in terms of matrix element effects, which is more reasonable than invoking stress-induced spin-orbit effects. The case of the conduction-band mass anisotropy is best illustrated by GaAs, and will be considered in detail in the following paper.

The calculated values of matrix elements, deformation potentials, and stress-induced changes in the $\Gamma_{2'}$ conduction- and $\Gamma_{25'}$ valence-band effective masses are summarized in Tables XI and XII and are compared to experimental values[17,20,37,38] where possible. The "experimental" values of the matrix elements P, Q, and R were calculated from the γ_1, γ_2, γ_3, and κ valence-band parameters[17] using the general expressions for these quantities in terms of F, G, H_1, and H_2[37] and assuming no contributions from higher bands. In general, the agreement is good; the maximum discrepancy, that for the shear deformation potential b, is 20%. While calculated strain-linear terms may not be so accurately determined due to cancellations between intrinsically large component terms (in c_{R2}, for example), we believe this establishes an approximate scale of uncertainty for the quantities calculated here, provided that they are determined primarily by interactions among the bands included in our model. We mention that the values for b and d differ somewhat from those cited in Ref. 6 due to the correction of minor errors[39] in Eq. (A.17) in Ref. 6, and the use of slightly different pseudopotential parameters.[33] The b deformation potentials of the valence and conduction bands are found to have opposite signs, while the d deformation potentials have the same sign, as indicated by piezoreflectance measurements on Ge by Sell and Kane.[40]

Calculated values of the $\Gamma_{2'}$ conduction-band mass and its strain-linear corrections, evaluated from the data of Table X, are given in Table XII.

TABLE XI. Values of matrix elements and self-energy terms for Ge, calculated from pseudopotential theory from data summarized in Table X.

Quantity	Calc. value	Expt. value
P	$1.05\hbar G_0$	$1.18\hbar G_0$ [a]
Q	$0.83\hbar G_0$	$0.69\hbar G_0$ [a]
R	$0.45\hbar G_0$	$0.47\hbar G_0$ [a]
T	$1.00\hbar G_0$	
c_T	17.36 eV	
c_{R1}	−33.40 eV	
c_{R2}	1.09 eV	
c_{R3}	−36.21 eV	
$a_{25'}$	−5.62 eV	
$a_{2'}$	−17.58 eV	
a_{15}	−7.47 eV	
$a_{12'}$	−8.67 eV	
a_1	−15.19 eV	
a	−11.96 eV	−10.6 ± 1.0 eV [b]; −11.4 ± 0.3 eV [c]
$b_{25'}$	−7.13 eV	−7.32 ± 0.45 eV [b]
b_{15}	4.49 eV	
$b_{12'}$	−14.31 eV	
b	−2.38 eV	−2.86 ± 0.15 eV [b]
$d_{25'}$	−20.20 eV	−18.3 ± 1.7 eV [b]
d_{15}	−17.88 eV	
d	−5.83 eV	−5.28 ± 0.50 eV [b]

[a] References 17 and 37.
[b] Reference 20.
[c] Reference 38.

The conduction-band mass is found to be $0.045m_e$, compared to an experimental value at 4 K of $(0.0380 \pm 0.0005)m_e$.[41] The agreement again is reasonably good, primarily because the conduction-band mass is determined mainly from interactions with the $\Gamma_{25'}$ valence bands. The main point of this paper can be appreciated from Table XII: the usually neglected bilinear and three-band terms describing the effect of stress on the kinetic energy and matrix elements are entirely comparable to the two-band terms, which describe strain-linear effects caused by changes in energy denominators. In fact, for [111] shear the three-band term is larger than the two-band term and is of opposite sign, so that the sum of the three types of strain-linear terms is essentially zero. This leaves only the hydrostatic term as the main contributor to the strain-induced mass change for [111] stress, a prediction which is well satisfied by piezoresistance measurements on n-type GaAs to be discussed in the next paper.

Results for the $(\frac{3}{2},\frac{1}{2})$ valence-band masses are given in Table XIII. In general, the calculated and experimental masses differ by about 20% and 30% for the parallel and perpendicular cases, respectively. The larger discrepancies observed here are not surprising in view of the fact that (especially for the perpendicular (xx and $\overline{xx}$) components) the masses are influenced significantly by interactions with higher bands which we have not considered. Nevertheless, for the parallel case the calculated strain-linear coefficients, summarized in the last column of Table XIII, are in remarkably good agreement with the experimental values. The small effective mass values for the parallel components indicate directly that interactions with the lower conduction bands are more significant for them than for the perpendicular components, and thus we expect the model to be better in this case.

The evidence for a spin-dependent deformation potential derives primarily from a difference in deformation potentials measured directly either (a) by optical or cyclotron-resonance determinations of the strain-induced splitting of the degenerate $(\frac{3}{2},\frac{1}{2})$ and $(\frac{3}{2},\frac{3}{2})$ sub-levels, or (b) the strain dependence of the $(\frac{3}{2},\frac{1}{2})$ mass. If one assumes, as done in Ref. 17, that the latter effect is given entirely by the "three-band" terms coupling the conduction bands to the $(\frac{3}{2},\frac{1}{2})$ and $(\frac{1}{2},\frac{1}{2})$ valence bands, then the two should be identical.[42] In fact, based upon this assumption, one finds that the deformation potential so calculated is about 20% lower than that obtained directly from the $(\frac{3}{2},\frac{1}{2})$, $(\frac{3}{2},\frac{3}{2})$ splitting. The difference has been attributed phenomenologically to spin-dependent terms of symmetry $l_i\sigma_j\epsilon_{ij}$, where $\vec{l}$ is the orbital-angular-momentum operator. Theoretical estimates show that this

TABLE XII. Calculated stress-induced changes in the conduction band mass $m_e/m_c^* = 22.42 = (0.045)^{-1}$ for Ge for 10-kbar uniaxial stresses.

Component		Bilinear	Two-band	Three-band	Subtotal	Total, shear plus hydrostatic
Hydrostatic		0.064	−1.145	0	−1.081	−1.08
tetragonal shear	∥	0.355	1.298	−0.555	1.098	0.02
	⊥	−0.178	−0.649	0.278	−0.549	−1.63
trigonal shear	∥	0.212	1.100	−1.439	−0.127	−1.21
	⊥	−0.106	−0.550	0.720	−0.064	−1.02

TABLE XIII. Values and calculated stress-induced changes in the $(\frac{3}{2},\frac{1}{2})$ valence-band mass of Ge at 10 kbar uniaxial stress, for components parallel and perpendicular to the stress-quantization axes as indicated. Experimental values (from Ref. 17) are shown in parentheses.

Stress-quantization axis	$(m_e/m_v^*)_{ii}$; $ii=$	Component	Bilinear	Two-band	Three-band HS	Three-band Rest	Subtotal	Total, shear plus hydrostatic
$[001]=z$	xx: -6.57 (-9.141 ± 0.003)	hydrostatic	-0.02	0.24	0	0	0.22	1.49
		shear	0.06	-0.16	1.42	-0.05	1.27	(1.08 ± 0.08)
	zz: -16.89 (-21.83 ± 0.19)	hydrostatic	-0.05	0.94	0	0	0.89	-2.39
		shear	-0.30	-0.51	-2.84	0.37	-3.28	(-2.4 ± 0.5)
$[111]=\bar{z}$	$\overline{xx}$: -5.19 (-7.692 ± 0.009)	hydrostatic	-0.02	0.24	0	0	0.22	1.65
		shear	0.03	-0.14	1.68	-0.14	1.43	(1.05 ± 0.07)
	$\overline{zz}$: -19.16 (-24.8 ± 0.2)	hydrostatic	-0.06	0.95	0	0	0.89	-2.09
		shear	-0.20	-0.42	-3.19	0.83	-2.98	(-1.7 ± 0.5)

term should actually be much smaller, probably not more than 10% of the value necessary to explain the discrepancy mentioned above.[17,19]

In Table XIII, we have divided all three-band terms into two groups: the first, labeled HS, consists of the three $(\Gamma_{2'},\Gamma_{15},\Gamma_{12'})-(\frac{3}{2},\frac{1}{2})-(\frac{1}{2},\frac{1}{2})$ terms considered by Hensel and Suzuki, while the contribution from the remaining three-band terms shown in Tables III and IV are grouped under the heading "rest." It can be seen clearly that the remaining three-band terms *cannot* be neglected with respect to the dominant three-band terms; for the parallel projections (calculated most accurately in our model, as discussed above) along [001], respectively, they comprise 15% and 35% of the total three-band contribution, entering in such a way as to simulate the observed apparently lower deformation potential. In fact, correcting the term $D_{u'}=2.81\pm0.20$ eV by all terms neglected by HS (bilinear, two-band, "rest," and hydrostatic), we find that the correct value should be ~4.3 eV, as compared with $D_{u'}\cong3.85\pm0.25$ eV. For the deformation potential $D_u=2.31\pm0.17$ eV, a similar calculation gives an improved value ~2.7 eV, as compared with $D_u=3.25\pm0.20$ eV. Thus agreement between theory and experiment is restored, without recourse to spin-dependent deformation potentials.

In fairness, however, we point out that the HS terms are nearly equal to the total result calculated for the perpendicular masses (see Table XIII) due to accidental cancellations. Thus a discrepancy with the more accurately measured perpendicular stress dependences remains. Because the perpendicular masses are large it is probable that other bands not included in the model may be responsible for the discrepancy. Thus the remaining differences should also be explainable without having to invoke a dependence of the spin-orbit splitting upon stress.

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[1] E. O. Kane, J. Phys. Chem. Solids 1, 82 (1956); 1, 249 (1956).

[2] H. Ehrenreich, J. Appl. Phys. Suppl. 32, 2155 (1961).

[3] M. Cardona, J. Phys. Chem. Solids 24, 1543 (1963).

[4] D. L. Camphausen, G. A. N. Connell, and W. Paul, Phys. Rev. Lett. 26, 184 (1971).

[5] B. Welber, M. Cardona, C. K. Kim, and S. Rodriguez, Phys. Rev. B 12, 5729 (1975).

[6] M. Cardona, in *Atomic Structure and Properties of Solids*, ed. by E. Burstein (Academic, New York, 1972), p. 514.

[7] W. M. DeMeis, Technical Report HP-15, Harvard University (unpublished); G. D. Pitt, J. Lees, R. A. Hoult, and R. A. Stradling, J. Phys. C 6, 3282 (1973).

[8] G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela 1, 1642 (1959) [Sov. Phys.-Solid State 1, 1502 (1959)].

[9] S. Zhukotynski and N. Saleh, Phys. Status Solidi B 38, 571 (1970).

[10] D. G. Seiler, D. L. Alsup, and R. Muthukrishnan, Solid State Commun. 10, 865 (1972); R. Mutukrishnan and D. G. Seiler, Phys. Status Solidi B 54, K83 (1972).

[11] G. L. Bir and G. E. Pikus, *Simmetriya i Deformatsionnie Effekty v Polyprovodnikakh* (Symmetry and Deformation Effects of Semiconductors) (Nauka, Moscow, 1972).

[12] A. K. Walton and S. F. Metcalfe, J. Phys. C 9, 3605 (1976).

[13] A. A. Gavini and M. Cardona, Phys. Rev. 177, 1351 (1969).

[14] G. Abstreiter, D. E. Aspnes, and M. Cardona (unpublished).

[15] V. N. Malinko, E. V. Pidlisnii, and G. G. Tsebulya, Ukr. Fiz. Zh. 16, 1041 (1972); 17, 2068 (1972).

[16] D. E. Aspnes and M. Cardona, following paper, Phys. Rev. B 17, 741 (1978).

[17] J. C. Hensel and K. Suzuki, Phys. Rev. B 9, 4219 (1974).

[18] K. Suzuki and J. C. Hensel, Phys. Rev. B 9, 4184 (1974).

[19] F. Cerdeira, J. S. de Witt, U. Rössler, and M. Cardona, Phys. Status Solidi B 41, 735 (1970).

[20] M. Chandrasekhar and F. H. Pollak, Phys. Rev. B 15, 2127 (1977).

[21] G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela 1, 1642 (1959) [Sov. Phys.-Solid State 1, 1502 (1959)].

[22] E. O. Kane, Phys. Rev. 178, 1368 (1969).

[23] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968).

[24] The k-linear term in the mass that arises from the absence of inversion symmetry in non-group-IV crystals is neglected here, since it is known to be negligibly small for our purposes (see Ref. 25).

[25] C. R. Pidgeon and S. H. Groves, Phys. Rev. 186, 824 (1969).

[26] We use the inversion-symmetric (O_7^h) representation because the antisymmetric potential has only a second-order effect on the strain-linear corrections to the band effective mass. Its neglect introduces only minor errors while greatly simplifying the resulting equations.

[27] M. Cardona and F. H. Pollak, Phys. Rev. 142, 530 (1966).

[28] M. L. Cohen and T. K. Bergstresser, Phys. Rev. 141, 789 (1966).

[29] B. J. Austin, V. Heine, and L. J. Sham, Phys. Rev. 127, 276 (1972).

[30] R. M. Martin, Phys. Rev. B 1, 4005 (1970).

[31] F. Bassani, in *Semiconductors and Semimetals*, edited by R.K. Willardson and A. C. Beer (Academic, New York, 1966), Vol. 1, p. 21.

[32] R. W. G. Wyckoff, *Crystal Structures* (Wiley-Interscience, New York, 1963), Vol. I.

[33] K. C. Pandey and J. C. Phillips, Phys. Rev. B 9, 1552 (1974).

[34] H. B. Huntington, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1962), Vol. 7, p. 273.

[35] D. E. Aspnes, Phys. Rev. B 12, 2297 (1975).

[36] D. E. Aspnes, C. G. Olson, and D. W. Lynch, Phys. Rev. B 12, 2527 (1975).

[37] P. Lawaetz, Phys. Rev. B 4, 3460 (1971).

[38] B. Welber, M. Cardona, Y.-F. Tsay, and B. Bendow, Phys. Rev. B 15, 875 (1977).

[39] Specifically, in Eq. (A.17) the factor of $\frac{1}{2}$ preceding the term $dv_8/d(\ln G)$ should be replaced by 1, and a missing term, $-2\gamma_{25'}^2 v_8$, should be added to the right-hand side.

[40] D. D. Sell and E. O. Kane, Phys. Rev. B 5, 417 (1972).

[41] R. Aggarwal, Phys. Rev. B 2, 446 (1970).

[42] These terms are "three-band" because the spin-orbit splitting is nonzero, and the $j=\frac{3}{2}$ and $j=\frac{1}{2}$ levels are nondegenerate. In the absence of spin-orbit splitting, they correspond to two-band terms.