Stress Effects on Excitons Bound to Axially Symmetric Defects in Semiconductors*

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The effect of uniaxial stress on exciton states which possess an axis of symmetry is calculated for various directions of the applied stress. The specific example of a ⟨111⟩ symmetry axis is treated in detail. This example corresponds to the physical system of an exciton bound to an associated Cd-O pair in GaP. The model considers exchange splitting (j-j coupling) of the exciton and the effects of anisotropy in the stress splitting of the hole states.

I. INTRODUCTION

UNIAXIAL stress has become an important tool in the study of electronic states in solids.[1–4] Deformation potentials have been determined for the conduction and valence bands of the more common semiconductors[4–6] and the effect of strains on states bound to point defects and on exciton states in many materials have been studied both theoretically and experimentally.[7–9]

In this paper, we calculate the effect of an externally applied uniaxial stress on exciton states bound to a defect which possesses an axis of symmetry. An example of such a center with a ⟨111⟩ symmetry axis is the associated Cd-O pair in GaP.[10,11] We shall carry out our calculations for this symmetry although for the most part in an approximation for which the conclusions are independent of the orientation of the built-in symmetry axis. In this complex, the Cd and O occupy adjacent Ga and P sites, respectively, so that the symmetry axis of the pair and hence of the perturbing potential lies along a ⟨111⟩ crystallographic direction. The effect of this potential is to lift the degeneracy of the $P_{3/2}$-like valence band states so that the $j=\frac{3}{2}$, $m=\pm\frac{3}{2}$ states lie lower in hole energy than do the $m=\pm\frac{1}{2}$ states. The exchange interaction or j-j coupling of the $S_{1/2}$-like electron with the hole further splits the resulting exciton states according to their component M of total angular momentum along the symmetry axis. Several simplifying assumptions which we make in this treatment deserve special comment.

Since we treat the strain effects and the exchange interaction phenomenologically without delving quantitatively into their origins, the deformation potential constant D_u and the j-j coupling energy Δ are assumed to be experimentally determined parameters. In Secs. I–IV, the former is taken as stress isotropic so that the splitting of the valence band is independent of the crystallographic orientation of the stress axis.

The symmetry group of the unstrained electron and hole states is taken to be the complete rotation group plus the inversion rather than the crystallographic group T_d. We justify this approximation on the basis of the following two arguments. If we employ the eigenfunctions of angular momentum, $|j,m\rangle$, as our unperturbed basis states we find that even though the crystal potential can, in principle, mix states of different angular momenta, the mixing is small. A simple argument can be made to show this. The expansion of the T_d crystal potential in spherical harmonics Y_l^m contains, aside from the spherical Y_0^0 term, no terms lower than $l=3$. Hence, this potential can mix the $S_{1/2}$ and $P_{3/2}$ ($l=0$ and 1, respectively) electron and hole states only with states which transform as D, F, ... states ($l\geq 2$), all of which lie much higher in energy and hence mix with negligibly small coefficients. The inversion operation is included since the envelope

* Preliminary results of this investigation are presented in Bull. Am. Phys. Soc. **13**, 453 (1968).

[1] For a review of the role of piezoresistance in the study of semiconductor band structure prior to 1960, see R. W. Keyes, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1960), Vol. 11, p. 149.

[2] A theoretical development of stress effects on holes in semiconductors is given by G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela **1**, 154 (1959); **1**, 1642 (1959); G. L. Bir and G. E. Pikus, *ibid.* **2**, 2287 (1960); G. E. Pikus and G. L. Bir, *ibid.* **3**, 1001 (1961) [English transls.: Soviet Phys.—Solid State **1**, 136 (1959); **1**, 1502 (1959); **2**, 2039 (1960); **3**, 730 (1961)].

[3] For stress studies of donor states (in Si), see R. L. Aggarwal and A. K. Ramdas, in *Proceedings of the International Conference on the Physics of Semiconductors, Paris* (Dunod Cie, Paris, 1965); Phys. Rev. **137**, A602 (1965).

[4] For studies of spin resonance using stress (in Si), see J. C. Hensel and G. Feher, Phys. Rev. **129**, 1041 (1963); H. Hasegawa, *ibid.* **129**, 1029 (1963).

[5] For Ge, see J. J. Hall, Phys. Rev. **128**, 68 (1962); for Ge and Si, I. Balslev, *ibid.* **143**, 636 (1966); I. Balslev and P. Lawaetz, Phys. Letters **19**, 6 (1965).

[6] For GaP, see I. Balslev, J. Phys. Soc. Japan Suppl. **21**, 101 (1966).

[7] P. J. Price, Phys. Rev. **124**, 713 (1961).

[8] For a study of donors in Si, see D. K. Wilson and G. Feher, Phys. Rev. **124**, 1068 (1961).

[9] In II–VI compounds, see D. G. Thomas, J. Appl. Phys. **32**, Suppl. 2298 (1961); T. Koda and D. W. Langer, Phys. Rev. Letters **20**, 50 (1968); O. Akimoto and H. Hasegawa, *ibid.* **20**, 916 (1968).

[10] T. N. Morgan, B. Welber, and R. N. Bhargava, Phys. Rev. **166**, 751 (1968).

[11] C. H. Henry, P. J. Dean, and J. D. Cuthbert, Phys. Rev. **166**, 754 (1968).

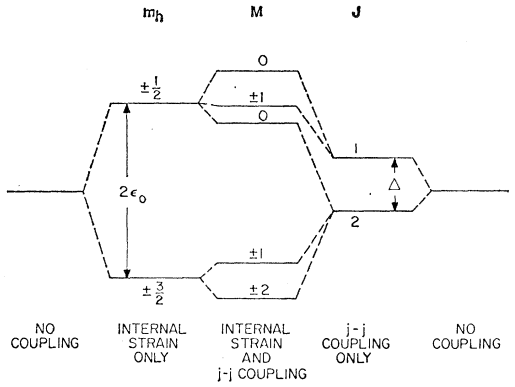


FIG. 1. Exciton energies in the presence of internal strain and j-j coupling. The figure is drawn for $y\equiv\Delta/2\epsilon_0=0.3$.

functions of the shallow effective-mass states are invariant under inversion (as is the band structure) and the deep states of interest (e.g., an electron bound to the O donor) are highly localized in a spherically symmetric core potential. Finally, we show in Appendix A that the conclusions of this paper are not altered if we exclude the inversion from our group operations. The most significant weakness of these approximations appears to be their inability to include the anisotropy of the stress-induced splitting, although for the $\langle100\rangle$, $\langle111\rangle$, and $\langle110\rangle$ stress axes which we discuss in detail, only the last suffers from this limitation. Consequently, in Sec. V, we extend the analysis of the $\langle110\rangle$ stress to include the effects of anisotropy.

II. NO EXTERNAL STRESS

A. Symmetry

A pair of impurities located on adjacent lattice sites destroys the equality of the four $\langle111\rangle$ directions and reduces the crystal symmetry group from T_d to C_{3v}.[12] In the above approximations, this is equivalent to the introduction of a unique direction into an otherwise spherically isotropic problem, and the symmetry group is $C_{\infty v}$. We choose this particular $\langle111\rangle$ direction as the direction of the z axis. We shall make the further approximation that the potential produced by the impurities resembles a uniaxial shear and is therefore invariant under inversion of the coordinates—in particular, $z\rightarrow-z$. Thus, the effective symmetry is $D_{\infty h}$. We show in Appendix A that our conclusions are independent of this latter assumption.

The distortion of the lattice by the pair of impurities partially lifts the degeneracy of the hole or electron states. In the example which we shall discuss, the impurities Cd on a Ga site and O on a P site in GaP have been found to produce an effect equivalent to an internal uniaxial tension (coupled perhaps with a hydrostatic pressure) which can be recognized by the splitting which it causes in the $P_{3/2}$ valence band. The energy of a hole in the band with quantum number $|m|=\frac{3}{2}$ is lowered relative to the $|m|=\frac{1}{2}$ band. A hole in equilibrium at low temperature thus occupies the lower $|m|=\frac{3}{2}$ band. In the conduction band, the energy levels of an $S_{1/2}$ electron are not split although they may be shifted as a result of a change in the band gap. The energy levels of a hole bound to the impurity complex reflect the valence band structure. We define the energy of the ground state of the hole, $|\frac{3}{2},\pm\frac{3}{2}\rangle$, to be $-\epsilon_0$ relative to the mean hole energy. The first excited state of the hole is then $|\frac{3}{2},\pm\frac{1}{2}\rangle$ and its energy is $+\epsilon_0$. The magnitude of the energy difference $2\epsilon_0$ between the two branches depends upon the strengths of the impurity potentials and the local distortion of the lattice (see Fig. 1). We shall not be concerned with the detailed nature of the distortion which generates this splitting. For the purposes of this work, it is sufficient to know that it has axial symmetry and produces the splitting $2\epsilon_0$, which we assume can be determined experimentally.

B. Exciton States

An $S_{1/2}$ electron and a $P_{3/2}$ hole in an isotropic potential are coupled through their Coulomb fields to produce either a fivefold degenerate state with total angular momentum $J=2$ or a threefold degenerate state with $J=1$.[13] As the hole and electron have opposite charge, the $J=2$ state lies lower in energy than the $J=1$ state. This is in contrast to the case of two electrons of like charge in an atom where the $J=1$ state lies lower. Relative to the mean energy the $J=2$ states have energy equal to $-\frac{3}{8}\Delta$, while the $J=1$ states have energy equal to $\frac{5}{8}\Delta$, where the exchange energy Δ can be determined experimentally.

If there is an axial internal strain, we do not expect J to be a good quantum number of the complete problem. In the case under consideration, however, the z axis is an axis of symmetry, so that the z component of angular momentum $|M|$ remains a good quantum number but the states with different $|M|$ are no longer degenerate. To determine the splitting of these states by the strain, we begin with the j-j coupling matrix $\mathbf{T}_j$ based on states of definite $m\equiv j_z$ for both the electron and the hole. This matrix can be obtained by transforming the diagonal matrix $\mathbf{T}_j^0$ from the basis consisting of the states $|J,M\rangle$ of definite total angular momentum J and z component M. In this latter representation,

$$(\mathbf{T}_j^0)_{\mu\nu}=\delta_{\mu\nu}(t_j)_\nu\Delta, \tag{1}$$

where

$$(t_j)_\nu=\tfrac{5}{8},\quad \nu=1-3,\quad (J=1)$$
$$(t_j)_\nu=-\tfrac{3}{8},\quad \nu=4-8,\quad (J=2).$$

[12] We use the symmetry notation of G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (MIT Press, Cambridge, Mass., 1965).

[13] For the theory of exchange interaction (j-j coupling), see E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1951).

The states $|m,m'\rangle$ of definite j_z for both electron and hole (written in that order) are related to the above states by the following transformation:

$$\begin{aligned}
|\tfrac{1}{2},\tfrac{3}{2}\rangle &= |2,2\rangle,\\
|\tfrac{1}{2},\tfrac{1}{2}\rangle &= \tfrac{1}{2}(\sqrt{3}|2,1\rangle-|1,1\rangle),\\
|\tfrac{1}{2},-\tfrac{1}{2}\rangle &= (|2,0\rangle-|1,0\rangle)/\sqrt{2},\\
|\tfrac{1}{2},-\tfrac{3}{2}\rangle &= \tfrac{1}{2}(|2,-1\rangle-\sqrt{3}|1,-1\rangle),\\
|-\tfrac{1}{2},\tfrac{3}{2}\rangle &= \tfrac{1}{2}(|2,1\rangle+\sqrt{3}|1,1\rangle),\\
|-\tfrac{1}{2},\tfrac{1}{2}\rangle &= (|2,0\rangle+|1,0\rangle)/\sqrt{2},\\
|-\tfrac{1}{2},-\tfrac{1}{2}\rangle &= \tfrac{1}{2}(\sqrt{3}|2,-1\rangle+|1,-1\rangle),\\
|-\tfrac{1}{2},-\tfrac{3}{2}\rangle &= |2,-2\rangle.
\end{aligned} \tag{2}$$

In this new representation, $\mathbf{T}_j$ becomes

$$\mathbf{T}_j=\tfrac{1}{2}\Delta\begin{pmatrix}
-\frac{3}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & -\frac{1}{4} & 0 & 0 & -\frac{1}{2}\sqrt{3} & 0 & 0 & 0\\
0 & 0 & \frac{1}{4} & 0 & 0 & -1 & 0 & 0\\
0 & 0 & 0 & \frac{3}{4} & 0 & 0 & -\frac{1}{2}\sqrt{3} & 0\\
0 & -\frac{1}{2}\sqrt{3} & 0 & 0 & \frac{3}{4} & 0 & 0 & 0\\
0 & 0 & -1 & 0 & 0 & \frac{1}{4} & 0 & 0\\
0 & 0 & 0 & -\frac{1}{2}\sqrt{3} & 0 & 0 & -\frac{1}{4} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3}{4}
\end{pmatrix}. \tag{3}$$

The internal strain matrix $\mathbf{T}_i$, which is diagonal in this representation, is given by

$$(\mathbf{T}_i)_{\mu\nu}=\epsilon_0(t_i)_\nu\delta_{\mu\nu}, \tag{4}$$

where

$$\begin{aligned}
(t_i)_\nu &= 1, \quad \text{for } |m'|=\tfrac{1}{2}, \quad \nu=2,3,6,7\\
(t_i)_\nu &= -1, \quad \text{for } |m'|=\tfrac{3}{2}, \quad \nu=1,4,5,8.
\end{aligned}$$

The complete interaction is described by the sum of $\mathbf{T}_i$ and $\mathbf{T}_j$. Since no more than two states are coupled together, the solution is easily obtained. The energies and nature of the wave functions are given in Table I and indicated schematically in Fig. 1. The solution could also have been accomplished by diagonalizing the sum of $\mathbf{T}_i+\mathbf{T}_j$ in the $|J,M\rangle$ representation.

III. EFFECT OF EXTERNALLY APPLIED STRESS

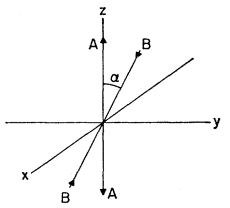
A. Symmetry

When an external uniaxial stress is applied to the crystal, the symmetry of the system is, in general,

TABLE I. Description of exciton states with internal strain.

States	Degeneracy	$\lvert m_j\rvert$	Energy	Limit for $\epsilon_0\gg\Delta$	Limit as $\epsilon_0\to 0$	(J)
I	2	2	$-\epsilon_0-\frac{3}{8}\Delta$	$-\epsilon_0-\frac{3}{8}\Delta$	$-\frac{3}{8}\Delta$	(2)
II	2	1	$\frac{1}{8}\Delta-(\epsilon_0^2-\frac{1}{2}\epsilon_0\Delta+\frac{1}{4}\Delta^2)^{1/2}$	$-\epsilon_0+\frac{3}{8}\Delta$	$-\frac{3}{8}\Delta$	(2)
III	2	1	$\frac{1}{8}\Delta+(\epsilon_0^2-\frac{1}{2}\epsilon_0\Delta+\frac{1}{4}\Delta^2)^{1/2}$	$\epsilon_0-\frac{1}{8}\Delta$	$\frac{5}{8}\Delta$	(1)
IVs	1	0	$\epsilon_0+\frac{5}{8}\Delta$	$\epsilon_0+\frac{5}{8}\Delta$	$\frac{5}{8}\Delta$	(1)
IVa	1	0	$\epsilon_0-\frac{3}{8}\Delta$	$\epsilon_0-\frac{3}{8}\Delta$	$-\frac{3}{8}\Delta$	(2)

FIG. 2. Coordinate axes showing the two stresses. A-A indicates the direction of the internal stress (tension). B-B indicates the direction of the external stress (compression).



greatly reduced. If the external stress lies in the x-z plane at an angle $\alpha\neq 0$ to the z axis (see Fig. 2), the symmetry group is C_{2h}.[12] This group contains the elements E (identity), C_2 (rotation about the y axis), σ_h (reflection in the x-z plane, $y\leftrightarrow -y$), and I (the inversion). Since holes and electrons have half-integral spin, we must use the double group which is the direct product $C_{2h}\times(E,R)$, $(R^2=E)$. The characters of the eight irreducible representations of this Abelian group are given in Table 15 of Ref. 12. The pairs of representations (Γ_3^+, Γ_4^+) and (Γ_3^-, Γ_4^-) are degenerate by time reversal (Kramer's degeneracy). The electron states belong to the former and the hole states to the latter pair of representations. They are described by the basis functions

$$e_+=(e^{1/2}+ie^{-1/2})/\sqrt{2}, \quad (\Gamma_3^+) \tag{5a}$$

$$e_-=(e^{1/2}-ie^{-1/2})/\sqrt{2}, \quad (\Gamma_4^+) \tag{5b}$$

for electrons, and

$$h_{1+}=(h^{1/2}+ih^{-1/2})/\sqrt{2}, \quad (\Gamma_3^-) \tag{6a}$$

$$h_{1-}=(h^{1/2}-ih^{-1/2})/\sqrt{2}, \quad (\Gamma_4^-) \tag{6b}$$

$$h_{3+}=(h^{3/2}-ih^{-3/2})/\sqrt{2}, \quad (\Gamma_3^-) \tag{6c}$$

$$h_{3-}=(h^{3/2}+ih^{-3/2})/\sqrt{2}, \quad (\Gamma_4^-) \tag{6d}$$

for holes, where the function $h^{1/2}$ is the hole wave function with $m=\frac{1}{2}$, etc. Only functions belonging to the same representation can be mixed by the external stress. This greatly simplifies the problem of solving for the hole states and their energies. A discussion of the behavior of these functions under the symmetry operations can be found in Appendix A. We shall use primes to label matrices based on these functions.

B. Hole States

A (small) compression along the z axis ($\alpha=0$) raises the energy of the $|m|=\frac{3}{2}$ hole states by an amount proportional to the strain S produced by the stress T, while the $|m|=\frac{1}{2}$ hole states are lowered by the same amount. We are not concerned with the effect of the hydrostatic part $\frac{1}{3}T$ of the stress. When this part is omitted, the hole energies are[14]

$$E'=-\epsilon_0+D_u(\tfrac{2}{3}S), \quad |m|=\tfrac{3}{2} \tag{7a}$$

$$E=\epsilon_0-D_u(\tfrac{2}{3}S), \quad |m|=\tfrac{1}{2}. \tag{7b}$$

[14] W. H. Kleiner and L. M. Roth, Phys. Rev. Letters **2**, 334 (1959).

The energy change per unit stress $B=D_uS/T$ may be determined by experiment and is assumed here to be isotropic.

To find the energies when a stress is applied in some other direction z' in the x-z plane at an angle α to the z axis, we resolve each of the states h^m into its components $h^{m'}$, which are quantized along the z' direction and hence exhibit a simple dependence on the stress.[15] Using the basis $h_i \equiv h^m$, $m=\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$ for $i=1-4$, these relations are, in matrix notation,

$$h(z)=\mathbf{H}_\alpha h(z'), \tag{8a}$$

with

$$\mathbf{H}_\alpha=\begin{bmatrix} \cos^3\beta & \sqrt{3}\cos^2\beta\sin\beta & \sqrt{3}\cos\beta\sin^2\beta & \sin^3\beta \\ -\sqrt{3}\cos^2\beta\sin\beta & \cos\beta(1-3\sin^2\beta) & \sin\beta(3\cos^2\beta-1) & \sqrt{3}\sin^2\beta\cos\beta \\ \sqrt{3}\cos\beta\sin^2\beta & -\sin\beta(3\cos^2\beta-1) & \cos\beta(1-3\sin^2\beta) & \sqrt{3}\sin\beta\cos^2\beta \\ -\sin^3\beta & \sqrt{3}\cos\beta\sin^2\beta & -\sqrt{3}\cos^2\beta\sin\beta & \cos^3\beta \end{bmatrix}, \tag{8b}$$

and

$$\beta=\tfrac{1}{2}\alpha.$$

The external strain matrix $\mathbf{T}_{ex}$ in the $h^{m'}(z')$ representation is the same as Eq. (4) with ϵ_0 replaced by $-D_u(\frac{2}{3}S)$,

$$(\mathbf{T}_{ex})_{\mu\nu}=-D_u(\tfrac{2}{3}S)(t_i)_\nu\delta_{\mu\nu}. \tag{9}$$

When we transform back to the representation based on the symmetrical functions of Eq. (6), this matrix becomes

$$\mathbf{T}_{ex}'=D_u\begin{array}{c} \begin{matrix} h_{1+} & h_{3+} & h_{1-} & h_{3-} \end{matrix} \\ \begin{bmatrix} -p & -q & 0 & 0 \\ -q^* & +p & 0 & 0 \\ 0 & 0 & -p & -q^* \\ 0 & 0 & -q & +p \end{bmatrix} \end{array}(\tfrac{2}{3}S), \tag{10}$$

where

$$p=\tfrac{1}{4}(1+3\cos 2\alpha)\equiv P_2(\cos\alpha), \tag{11a}$$

$$q=r+ik=\tfrac{1}{2}\sqrt{3}[\sin 2\alpha+\tfrac{1}{2}i(1-\cos 2\alpha)], \tag{11b}$$

and

$$p^2+|q|^2=1.$$

The strain is seen to mix only the functions within each representation. The matrix $\mathbf{T}_i$ representing the internal strain is still diagonal in this representation:

$$\mathbf{T}_i'=\epsilon_0\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{12}$$

The eigenvalues and eigenfunctions of the total strain matrix

$$\mathbf{T}_s'=\mathbf{T}_i'+\mathbf{T}_{ex}'$$

are the hole energies and wave functions when the system is subject to both strains. The solutions are two degenerate pairs of functions whose energies are

$$E'=-\epsilon(S), \tag{13a}$$

and

$$E''=+\epsilon(S), \tag{13b}$$

with

$$\epsilon(S)=(x^2-2px+1)^{1/2}\epsilon_0, \tag{13c}$$

and

$$x=2D_uS/3\epsilon_0. \tag{13d}$$

The corresponding wave functions are

$$h_+'=(\gamma h_{1+}+h_{3+})/N, \quad (E') \quad (\Gamma_3^-) \tag{14a}$$

$$h_+''=(h_{1+}-\gamma^* h_{3+})/N, \quad (E'') \quad (\Gamma_3^-) \tag{14b}$$

$$h_-'=(\gamma^* h_{1-}+h_{3-})/N, \quad (E') \quad (\Gamma_4^-) \tag{14c}$$

$$h_-''=(h_{1-}-\gamma h_{3-})/N, \quad (E'') \quad (\Gamma_4^-). \tag{14d}$$

Here,

$$\gamma=\rho+i\mu=\frac{qx}{1-px+\epsilon(S)/\epsilon_0} \tag{14e}$$

[see (11b)], and

$$N^2=1+|\gamma|^2. \tag{14f}$$

In Fig. 3, these energies are plotted versus strain energy for the stress directions ⟨100⟩, ⟨111⟩, and ⟨110⟩. The labels (a)–(e) in this figure are used to identify the corresponding cases in subsequent figures.

C. Exciton States

The $S_{1/2}$ wave functions belong to the Γ_3^+ and Γ_4^+ representations of the C_{2h} symmetry group. The basis functions, given by Eqs. (5a) and (5b), do not mix

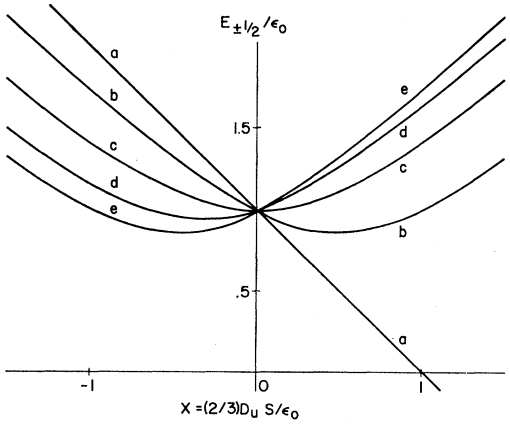


FIG. 3. Variation of hole energies with external stress. The energy is plotted against $x=2D_uS/3\epsilon_0$. (a) $\cos\alpha=1$, ⟨111⟩; (b) $\cos\alpha=(\frac{2}{3})^{1/2}$, ⟨110⟩; (c) $\cos\alpha=(\frac{1}{3})^{1/2}$, ⟨100⟩; (d) $\cos\alpha=\frac{1}{3}$, ⟨111⟩; (e) $\cos\alpha=0$, ⟨110⟩.

[15] The problem could also be solved by computing the potential produced by the applied stress in the original coordinate system.

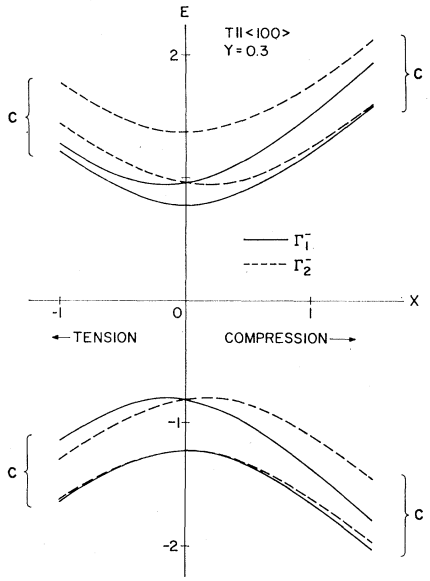


FIG. 4. Variation of the exciton energies with external stress in the ⟨100⟩ direction. The energy is plotted against $x=2D_uS/3\epsilon_0$ for $y=\Delta/2\epsilon_0=0.3$. The units are ϵ_0.

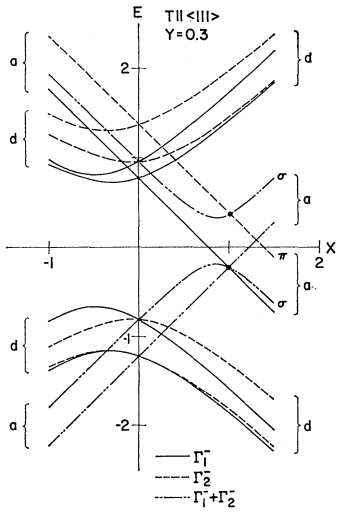


FIG. 5. Exciton energies as in Fig. 4 but for external stress in the ⟨111⟩ direction.

and remain degenerate when the external stress is applied.

The eight exciton wave functions are formed from products of the functions (14) with (5a) and (5b). They have integral spin and belong to the irreducible representations Γ_1^- (from $\Gamma_3^+\times\Gamma_4^-$ or $\Gamma_3^-\times\Gamma_4^+$) and Γ_2^- (from $\Gamma_3^+\times\Gamma_3^-$ or $\Gamma_4^+\times\Gamma_4^-$) of the (single) group C_{2h}.[12] The Γ_2^- states are even on reflection $y\leftrightarrow -y$, while the Γ_1^- states are odd. Since functions of different representations are not mixed by the j-j coupling interaction, each of the two sets can be studied separately.

1. Γ_2^- (*Symmetric*) *States*

The functions which belong to the Γ_2^- representation are e_-h_{1+}, e_-h_{3+}, $e_+h_{1-}e_+h_{3-}$. The $j\cdot j$ interaction matrix based on these functions can be derived from Eqs. (3), (5), and (6). For the order given, it is

$$\mathbf{T}_{js}'=\tfrac{1}{2}\Delta\begin{pmatrix} \frac{1}{2} & i\frac{1}{4}\sqrt{3} & -\frac{3}{4} & -i\frac{1}{4}\sqrt{3} \\ -i\frac{1}{4}\sqrt{3} & 0 & -i\frac{1}{4}\sqrt{3} & -\frac{3}{4} \\ -\frac{3}{4} & i\frac{1}{4}\sqrt{3} & \frac{1}{2} & -i\frac{1}{4}\sqrt{3} \\ i\frac{1}{4}\sqrt{3} & -\frac{3}{4} & i\frac{1}{4}\sqrt{3} & 0 \end{pmatrix}. \quad (15)$$

The energies of the excitons subject to both strains are the eigenvalues of the sum of $\mathbf{T}_{ex}'$ from Eq. (10), $\mathbf{T}_i'$ from Eq. (12), and $\mathbf{T}_{js}'$ from Eq. (15). The solutions can be obtained analytically in this case. The energies are given in Appendix B.

These expressions have been evaluated for certain directions of stress and are plotted against strain energy in Figs. 4–7. If the stress is along a ⟨100⟩ axis, all ⟨111⟩ impurity pairs are equivalent and the cosine of the angle between any ⟨111⟩ direction and the stress is $1/\sqrt{3}$—curve (c) in Fig. 3. The energies of these states are shown in Fig. 4. If the stress is applied in a ⟨111⟩ direction, there are two cases (a) and (d). One-fourth of the impurity pairs are oriented with $\cos\alpha=1$, (a), while the remainder have $\cos\alpha=\frac{1}{3}$, (d). In Fig. 5, these energies are plotted. When the stress is in a ⟨110⟩ direction, either $\cos\alpha=0$, (e), or $\cos\alpha=\sqrt{\frac{2}{3}}$, (b). These two cases which occur with equal probability are shown in Figs. 6 and 7.

In general, when one of the states of the Γ_2^- representation decays, the light emitted is polarized in the x-z plane with components both parallel (π) and perpendicular (σ) to the direction of the stress. In the special case (e), however, when $\cos\alpha=0$ there is higher symmetry and one of the lines of the spectrum is

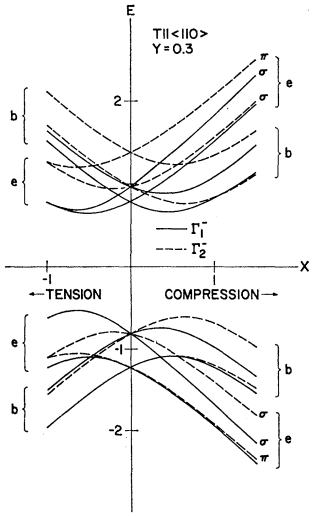


FIG. 6. Exciton energies as in Fig. 4 but for external stress in the ⟨110⟩ direction. The polarizations of the allowed transitions are indicated for case *e*. Figures 6 and 7 show the isotropic case $\beta=1$.

TABLE II. Summary of selection rules and polarization.

Function if strain=0	Polarization if strain=0	Polarization if strain≠0	Total polarization if cosα=0
Γ_1 states[a]			
Is: $\|2,2\rangle-\|2,-2\rangle$	forbidden	x, z	z
IIs[b]: $a[\|2,1\rangle+\|2,-1\rangle]+b[\|1,1\rangle-\|1,-1\rangle]$	x	x, z	x
IIIs[b]: $b[\|2,1\rangle+\|2,-1\rangle]-a[\|1,1\rangle-\|1,-1\rangle]$	x	x, z	x
IVs: $\|1,0\rangle$	z	x, z	z
Γ_2 states[a]			
Ia: $\|2,2\rangle+\|2,-2\rangle$	forbidden	y	forbidden
IIa[b]: $a[\|2,1\rangle-\|2,-1\rangle]+b[\|1,1\rangle+\|1,-1\rangle]$	y	y	y
IIIa[b]: $b[\|2,1\rangle-\|2,-1\rangle]-a[\|1,1\rangle+\|1,-1\rangle]$	y	y	y
IVa: $\|2,0\rangle$	forbidden	y	forbidden

[a] Wave function is given as $|J,M\rangle$. [b] $a/b=(1/\sqrt{3})(\epsilon_j+\epsilon_0+\frac{1}{2}\Delta)/(\epsilon_j+\epsilon_0-\frac{1}{2}\Delta)$, $\epsilon_j=(\epsilon_0^2-\frac{1}{2}\epsilon_0\Delta+\frac{1}{4}\Delta^2)^{1/2}$.

polarized parallel and the other perpendicular to the stress as indicated in Figs. 6 and 7. (See Table II and Appendix B.)

2. Γ_1^-(*Antisymmetric*) *States*

The functions which belong to the Γ_1^- representation are e_+h_{1+}, e_+h_{3+}, e_-h_{1-}, e_-h_{3-}. The $j\cdot j$ interaction matrix for these functions, obtained from Eq. (3) is

$$\mathbf{T}_{ja}'=\tfrac{1}{2}\Delta\begin{bmatrix} -\frac{1}{2} & -i\frac{1}{4}\sqrt{3} & \frac{1}{4} & i\frac{1}{4}\sqrt{3} \\ i\frac{1}{4}\sqrt{3} & 0 & i\frac{1}{4}\sqrt{3} & -\frac{3}{4} \\ \frac{1}{4} & -i\frac{1}{4}\sqrt{3} & -\frac{1}{2} & i\frac{1}{4}\sqrt{3} \\ -i\frac{1}{4}\sqrt{3} & -\frac{3}{4} & -i\frac{1}{4}\sqrt{3} & 0 \end{bmatrix}, \quad (16)$$

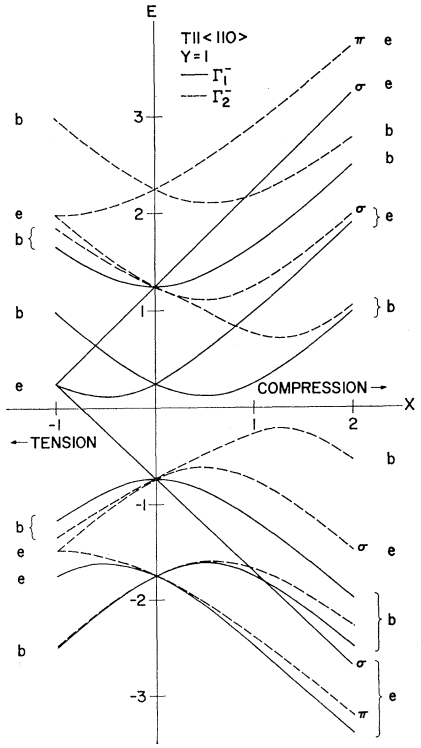


FIG. 7. Same as Fig. 6 but with $y=1$.

and the energies of the excitons are the eigenvalues of the sum of $\mathbf{T}_{ja}'$, $\mathbf{T}_i'$ and $\mathbf{T}_{ex}'$. The solution of this problem has been obtained numerically and the eigenvalues plotted for the principal directions in Figs. 4–7. Light emitted during decay of one of these states is polarized in the y direction, perpendicular to the direction of stress. Because of the higher symmetry of case (e), $\cos\alpha=0$, transitions from two of the Γ_1^- states are forbidden, as shown in Figs. 6 and 7. (Table II and Appendix B.)

IV. LOW STRAIN

Since experiments are frequently performed using only small stresses, expansions of the energy eigenvalues to lowest order in the stress are useful. These expressions are given in Eqs. (18) and (19) below in terms of the following parameters [see Eq. (11)]:

$$x=\tfrac{2}{3}D_u S/\epsilon_0, \quad (17a)$$

$$y=\Delta/2\epsilon_0, \quad (17b)$$

$$p=\tfrac{1}{4}(1+3\cos 2\alpha), \quad (17c)$$

$$k=\tfrac{1}{4}\sqrt{3}(1-\cos 2\alpha). \quad (17d)$$

The energies for the Γ_2^- states are

$$E_{Is}=-(1+\tfrac{3}{4}y-px)\epsilon_0, \quad (18a)$$

$$E_{IIs}=\left[\tfrac{1}{4}y-(1-y+y^2)^{1/2}\times\left(1+x\frac{-p+\frac{1}{2}py-\frac{1}{2}\sqrt{3}ky}{1-y+y^2}\right)\right]\epsilon_0, \quad (18b)$$

$$E_{IIIs}=\left[\tfrac{1}{4}y+(1-y+y^2)^{1/2}\times\left(1+x\frac{-p+\frac{1}{2}py-\frac{1}{2}\sqrt{3}ky}{1-y+y^2}\right)\right]\epsilon_0, \quad (18c)$$

$$E_{IVs}=\left(1+\frac{5}{4}y-px\right)\epsilon_0, \quad (18d)$$

and the energies for the Γ_1^- states are

$$E_{Ia}=-(1+\tfrac{3}{4}y-px)\epsilon_0, \tag{19a}$$

$$E_{IIa}=\left[\tfrac{1}{4}y-(1-y+y^2)^{1/2}\times\left(1+x\frac{-p+\frac{1}{2}py+\frac{1}{2}\sqrt{3}ky}{1-y+y^2}\right)\right]\epsilon_0, \tag{19b}$$

$$E_{IIIa}=\left[\tfrac{1}{4}y+(1-y+y^2)^{1/2}\times\left(1+x\frac{-p+\frac{1}{2}py+\frac{1}{2}\sqrt{3}ky}{1-y+y^2}\right)\right]\epsilon_0, \tag{19c}$$

$$E_{IVa}=(1-\tfrac{3}{4}y-px)\epsilon_0. \tag{19d}$$

The values of p and k for the principal directions of strain are given in Table III.

V. STRESS ANISOTROPY

In Secs. I–IV, we have assumed as a first approximation that the stress-induced splitting ΔE of the valence band is independent of the orientation of the stress relative to the crystallographic axes. In a cubic crystal, however, this splitting is, in general, not isotropic and requires two deformation potential constants for its description.[4,9,14] In the conventional notation, a uniaxial stress T in a $\langle 100\rangle$ direction produces a strain $S=T/(c_{11}-c_{12})$ and a valence band splitting

$$\Delta E=\tfrac{4}{3}D_uS=\tfrac{4}{3}D_uT/(c_{11}-c_{12})\equiv\tfrac{4}{3}BT, \tag{20a}$$

while an equal stress in a $\langle 111\rangle$ direction produces a strain

$$S=T/2c_{44}$$

and an energy splitting of

$$\Delta E=\tfrac{4}{3}D_u'T/2c_{44}=\tfrac{4}{3}B'T. \tag{20b}$$

The factor of $\frac{2}{3}$ in these expressions reflects the fact that the hydrostatic part $\frac{1}{3}T$ of the stress produces only uniform shifts of the bands. For these two stress directions, the stress part of the Hamiltonian has the same symmetry as the stress itself and hence in our approximation is uniaxial. For stress in any other direction the effective potential for the holes possesses a lower symmetry unless the ratio

$$\beta=B'/B \tag{21}$$

equals one.

On the basis of the above discussion, we conclude that the analysis Secs. I–IV remains valid in the anisotropic case $\beta\neq 1$, when the stress lies in either a $\langle 100\rangle$ or a $\langle 111\rangle$ direction, but that the case of a $\langle 110\rangle$ stress is more complex. The latter can be analyzed by resolving the stress into a sum of three stress components—one in a $\langle 100\rangle$ direction and two in $\langle 111\rangle$ directions—and adding the three potential terms they generate. Thus, a compressive stress T applied in the $\langle 110\rangle$ direction—along the z' axis—generates (in addition to the hydrostatic part $\frac{1}{3}T$) a stress field described by a diagonal stress tensor $\boldsymbol{\tau}$,

$$\tau_{ii}=\tfrac{1}{3}(-1,-1,2)T, \quad i=x',y',z' \tag{22}$$

whose transformation properties under rotation are equivalent to those of $Y_2^0(\theta)$. When $\boldsymbol{\tau}$ is expressed relative to the $\langle 100\rangle$ (unprimed) axes it takes the form

$$\boldsymbol{\tau}=\tfrac{1}{3}T\begin{bmatrix}\frac{1}{2} & \frac{3}{2} & 0\\ \frac{3}{2} & \frac{1}{2} & 0\\ 0 & 0 & -1\end{bmatrix}, \quad \langle 110\rangle \tag{23}$$

which can be interpreted very simply. We note that a compressive shear stress in the $[u_1,u_2,u_3]$ direction (where $u_i=\pm 1$) when expressed relative to $\langle 100\rangle$ axes has the form

$$(u_1u_2u_3)\times\begin{bmatrix}0 & u_3 & u_2\\ u_3 & 0 & u_1\\ u_2 & u_1 & 0\end{bmatrix}.$$

Hence, Eq. (23) represents the sum of a uniaxial tension along the [001] axis and two compressions—one along the [111] direction and one along the $[-1\ -1\ 1]$ direction. Thus, symbolically,

$$T(110)=-\tfrac{1}{2}T(001)+\tfrac{3}{4}T(111)+\tfrac{3}{4}T(-1\ -1\ 1), \tag{24}$$

where the coefficients give the magnitudes and signs of the stress components along each direction. The directions are indicated in Fig. 8.

TABLE III. Coefficients of Sec. IV for three principal strain directions (see Fig. 3). The labels used in the figures are indicated.

Direction	Label	$\cos\alpha$	P	k
$\langle 100\rangle$	c	$1/\sqrt{3}$	0	$1/\sqrt{3}$
$\langle 111\rangle$	a	1	1	0
	d	$\frac{1}{3}$	$-\frac{1}{3}$	$4\sqrt{3}/9$
$\langle 110\rangle$	e	0	$-\frac{1}{2}$	$\frac{1}{2}\sqrt{3}$
	b	$\sqrt{2}/\sqrt{3}$	$\frac{1}{2}$	$\sqrt{3}/6$

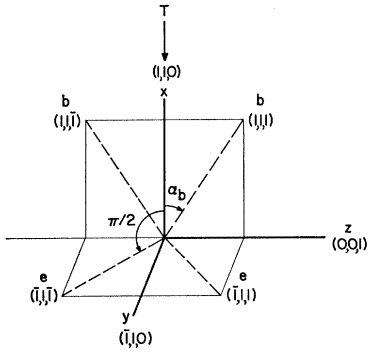


FIG. 8. Coordinate axes showing the decomposition of the $\langle 110\rangle$ stress. A compression along the [110] direction (x axis) is equivalent to the sum of tension along the [001] direction (z axis) and compressions along the [111] and [11$\bar{1}$] directions (b). The internal stress relative to this coodinate system can be either along the (e) ($\cos\alpha=0$) or (b) ($\cos\alpha=(\frac{2}{3})^{1/2}\langle 111\rangle$ axes.

We now proceed to calculate the hole energies in a basis quantized along the [001] axis using the hole functions $h_{1\pm}$ and $h_{3\pm}$ introduced in Eq. (6). In this representation, the effect on the hole energies of the stress $-\frac{1}{2}T(001)$ is given by

$$\tfrac{1}{2}B\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{bmatrix}\tfrac{2}{3}T, \tag{25}$$

where the order of the states is h_{1+}, h_{3+}, h_{1-}, and h_{3-}. The effect of the two stresses $\frac{3}{4}T(111)+\frac{3}{4}T(-1\ -1\ 1)$ is [cf. Eq. (10) with $\cos\alpha=1/\sqrt{3}$ and the states reordered as noted]

$$\tfrac{3}{4}(2/\sqrt{3})B'\begin{bmatrix}0 & -i & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & i\\ 0 & 0 & -i & 0\end{bmatrix}\tfrac{2}{3}T. \tag{26}$$

The hole energies given by the eigenvalues of the sum of these two matrices are

$$E=\pm\tfrac{1}{2}(B^2+3B'^2)^{1/2}\tfrac{2}{3}T, \tag{27}$$

so that a deformation potential can be defined for the $\langle 110\rangle$ direction:

$$B''=(\tfrac{1}{4}B^2+\tfrac{3}{4}B'^2)^{1/2},\quad \langle 110\rangle \text{ stress} \tag{28a}$$

or

$$D_u^{(110)}=(\tfrac{1}{4}D_u^2+\tfrac{3}{4}D_u'^2)^{1/2}. \tag{28b}$$

Because of the reduced symmetry of the potential, the corresponding eigenfunctions are, in general, mixtures of hole states with $|m|=\frac{1}{2}$ and $|m|=\frac{3}{2}$; though the symmetry indicated by $\pm$ is preserved:

$$h_{a-}=\mu h_{1-}-i\nu h_{3-},\qquad E_a=|E|, \tag{29a}$$

$$h_{b-}=-i\nu h_{1-}+\mu h_{3-},\qquad E_b=-|E|, \tag{29b}$$

$$h_{a+}=\mu h_{1+}+i\nu h_{3+},\qquad E_a=|E|, \tag{29c}$$

$$h_{b+}=i\nu h_{1+}+\mu h_{3+},\qquad E_b=-|E|, \tag{29d}$$

where E is given by Eq. (27) above and

$$\nu=\tfrac{1}{2}\sqrt{3}B'/N',$$
$$\mu=(B''+\tfrac{1}{2}B)/N',$$

and

$$N'^2=2B''(B''+\tfrac{1}{2}B).$$

The internal strain axis may lie either in one of the two $\langle 111\rangle$ directions (e) perpendicular to the applied stress or in one of the remaining two $\langle 111\rangle$ directions, (b) which lie in a plane containing the stress axis and the perpendicular [001] direction. These two possibilities are indicated in Fig. 8, where (b) corresponds to the case $\cos\alpha=\sqrt{\frac{2}{3}}$ of Sec. III, while (e) corresponds to $\cos\alpha=0$. For either of these cases the matrix may be obtained from Eq. (10) by setting $\cos\alpha=1/\sqrt{3}$. For case (e), however, since the desired rotation is about (110), the x axis, and Eq. (10) refers to a rotation through α about the y axis, an additional transformation is needed to rotate x into y. In this latter case, the internal strain will couple the h_+ and h_- functions.

In the representation of Eqs. (25) and (26), the internal strain matrices are

$$\begin{bmatrix}0 & -2i & 0 & -2i\sqrt{2}\\ 2i & 0 & +2i\sqrt{2} & 0\\ 0 & -2i\sqrt{2} & 0 & 2i\\ +2i\sqrt{2} & 0 & -2i & 0\end{bmatrix}\frac{\epsilon_0}{\sqrt{3}} \tag{30a}$$

for strain along (e), $\cos\alpha=0$, and

$$\begin{bmatrix}0 & \sqrt{2}+i & 0 & 0\\ \sqrt{2}-i & 0 & 0 & 0\\ 0 & 0 & 0 & \sqrt{2}-i\\ 0 & 0 & \sqrt{2}+i & 0\end{bmatrix}\frac{\epsilon_0}{\sqrt{3}} \tag{30b}$$

for strain along (b), $\cos\alpha=\sqrt{\frac{2}{3}}$. The diagonal elements vanish since the quantization axis is along [001] and $p=0$.

The form of the matrix representing j-j coupling is independent of the particular orientation of axes used and can be obtained directly from Eq. (3) using the transformations of Eqs. (5) and (6). With the Γ_2^- and Γ_1^- states grouped together, this matrix is

$$\tfrac{1}{8}\Delta\begin{array}{c}\begin{matrix}e_-h_{1+} & e_-h_{3+} & e_+h_{1-} & e_+h_{3-} & e_+h_{1-} & e_+h_{3+} & e_-h_{1-} & e_-h_{3-}\end{matrix}\\ \begin{bmatrix}2 & i\sqrt{3} & -3 & -i\sqrt{3} & 0 & 0 & 0 & 0\\ -i\sqrt{3} & 0 & -i\sqrt{3} & -3 & 0 & 0 & 0 & 0\\ -3 & i\sqrt{3} & 2 & -i\sqrt{3} & 0 & 0 & 0 & 0\\ i\sqrt{3} & -3 & i\sqrt{3} & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & -2 & -i\sqrt{3} & 1 & i\sqrt{3}\\ 0 & 0 & 0 & 0 & i\sqrt{3} & 0 & i\sqrt{3} & -3\\ 0 & 0 & 0 & 0 & 1 & -i\sqrt{3} & -2 & i\sqrt{3}\\ 0 & 0 & 0 & 0 & -i\sqrt{3} & -3 & -i\sqrt{3} & 0\end{bmatrix}\end{array}. \tag{31}$$

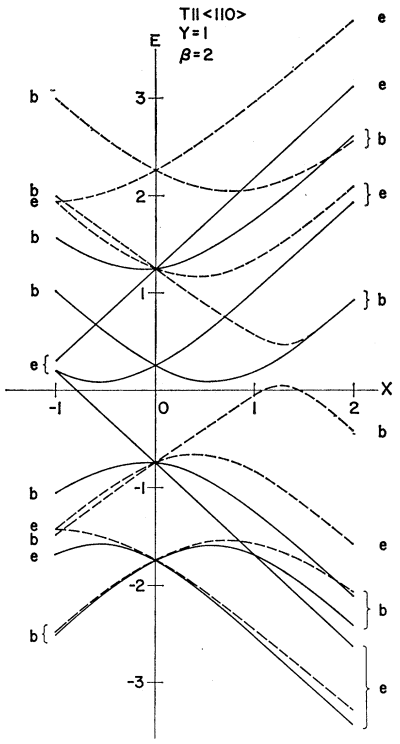


FIG. 9. Same as Fig. 7 but with the anisotropy ratio $\beta=2$.

To express the matrices of Eqs. (25), (26), (30a), and (30b) in this basis we note that states involving different electron wave functions are not connected by the strain, so that the resulting 8×8 matrices have the form

$$\begin{matrix} e_+h_{i\pm} & e_-h_{i\pm} \end{matrix} \qquad \begin{pmatrix} \mathbf{T} & 0 \\ 0 & \mathbf{T} \end{pmatrix}, \tag{32}$$

where $\mathbf{T}$ represents one of the 4×4 matrices of (25), (26), and (30). The rows and columns of the matrices must then be reordered to coincide with the order used in Eq. (31). In case (b), Eq. (30b), the problem reduces to two 4×4 matrices, while in case (e), Eq. (30a), the Γ_2^- and Γ_1^- states are connected by the internal strain and no reduction of the matrix occurs.

The eigenvalues of the resulting 8×8 matrix of the total problem are plotted in Fig. 9 for $\beta=B'/B=2$. All of the symmetry which occurred for the $\cos\alpha=0$ case (e) has now been destroyed, all of the lines are of mixed polarization, and the degeneracies at $x=-1$ have been split. In case (b) $[\cos\alpha=\sqrt{\frac{2}{3}}]$, the symmetry has not been altered (since all four stresses lie in a plane), and there is only a small quantitative difference from the isotropic case, $\beta=1$.

APPENDIX A: SPINOR TRANSFORMATIONS

In identifying the representations to which the functions defined in Eqs. (5) and (6) belong, it is necessary to know the behavior of the hole wave functions under various transformations of the coordinate axes. To obtain this information we start with the spinor functions representing particles of spin $s=\frac{1}{2}$.[16] The function which represents spin directed in the $+z$ direction is $\begin{pmatrix}1\\0\end{pmatrix}$, while the function representing spin in the $-z$ direction is $\begin{pmatrix}0\\1\end{pmatrix}$.

If the coordinate axes are rotated through an angle ϕ around the z axis the function which represents the same spin but which is referred to the new axes is obtained from the old spinor by operating on it with the matrix

$$\mathbf{R}_z(\phi)=\begin{bmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{bmatrix}. \tag{A1}$$

For example, a rotation through an angle of $\frac{1}{2}\pi$ would transform the spinor $\begin{pmatrix}1\\1\end{pmatrix}1/\sqrt{2}$ representing spin directed in the $+x$ direction into the function $(e^{i\pi/2}/\sqrt{2})\begin{pmatrix}1\\-i\end{pmatrix}$ representing spin in the $-y$ direction.

The corresponding matrices for rotations about the y and x axes are

$$\mathbf{R}_y(\theta)=\begin{bmatrix} \cos\tfrac{1}{2}\theta & \sin\tfrac{1}{2}\theta \\ -\sin\tfrac{1}{2}\theta & \cos\tfrac{1}{2}\theta \end{bmatrix}, \tag{A2}$$

and

$$\mathbf{R}_x(\chi)=\begin{bmatrix} \cos\tfrac{1}{2}\chi & i\sin\tfrac{1}{2}\chi \\ i\sin\tfrac{1}{2}\chi & \cos\tfrac{1}{2}\chi \end{bmatrix}. \tag{A3}$$

For inversion the matrix is the identity

$$\mathbf{R}_I=\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{A4}$$

A reflection is equivalent to the inversion followed by a rotation through an angle of π. For example, the reflection $\sigma(y\rightarrow -y)$ is represented by

$$\mathbf{R}_\sigma=\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{A5}$$

From this it follows immediately that the operation σ affects the spin-$\frac{1}{2}$ functions in the following way:

$$\sigma\begin{pmatrix}1\\0\end{pmatrix}=-\begin{pmatrix}0\\1\end{pmatrix},$$

and

$$\sigma\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}1\\0\end{pmatrix}.$$

Equations (5) follow from these relationships.

[16] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* (Addison-Wesley Publishing Co., Inc., Reading, Mass., 1965), Vol. III.

The $j=\frac{3}{2}$ hole wave functions are

$$h^{3/2}=Y_1^1\begin{pmatrix}1\\0\end{pmatrix}, \tag{A6a}$$

$$h^{1/2}=\sqrt{\tfrac{1}{3}}Y_1^1\begin{pmatrix}0\\1\end{pmatrix}+\sqrt{\tfrac{2}{3}}Y_1^0\begin{pmatrix}1\\0\end{pmatrix}, \tag{A6b}$$

$$h^{-1/2}=\sqrt{\tfrac{1}{3}}Y_1^{-1}\begin{pmatrix}1\\0\end{pmatrix}+\sqrt{\tfrac{2}{3}}Y_1^0\begin{pmatrix}0\\1\end{pmatrix}, \tag{A6c}$$

$$h^{-3/2}=Y_1^{-1}\begin{pmatrix}0\\1\end{pmatrix}, \tag{A6d}$$

where

$$Y_1^{\pm1}=(\tfrac{3}{8}\pi)^{1/2}(\mp X-iy)/r, \tag{A7a}$$

$$Y_1^0=(\tfrac{3}{4}\pi)^{1/2}z/r. \tag{A7b}$$

Now we can see that under the operation σ,

$$\sigma h^{3/2}=+h^{-3/2},$$
$$\sigma h^{-3/2}=-h^{3/2},$$
$$\sigma h^{1/2}=-h^{-1/2},$$
$$\sigma h^{-1/2}=+h^{1/2},$$

while under I,

$$Ih^{m_j}=-h^{m_j},$$

and Eqs. (6) follow immediately.

If the crystal field or the Cd-O pair introduced a potential which in some way was not symmetric for $z\rightarrow -z$, the symmetry group would be $C_s=(E,\sigma)$. Then $\Gamma_3^{\pm}$ would map onto Γ_3 of C_s, $\Gamma_4^{\pm}$ onto Γ_4, $\Gamma_1^{\pm}$ onto Γ_2, and $\Gamma_2^{\pm}$ onto Γ_2. As $+$ and $-$ representations never occur together in our problem, there is no difference in the results of Sec. III for these two groups.

To derive Eq. (8b), we must rotate the coordinate axes through an angle $\theta=\alpha$ and operate with $\mathbf{R}_y(\alpha)$ on the spinor parts of the hole wave functions Eqs. (A6) while at the same time using

$$\begin{bmatrix}x'\\y'\\z'\end{bmatrix}=\begin{bmatrix}\cos\alpha & 0 & -\sin\alpha\\ 0 & 1 & 0\\ \sin\alpha & 0 & \cos\alpha\end{bmatrix}\begin{bmatrix}x\\y\\z\end{bmatrix} \tag{A8}$$

to transform the Y_1^m parts. If these operations are carried out on $h^{3/2}$, for example, the resulting function will be represented by a hole whose angular momentum quantum number in the z direction is still $\frac{3}{2}$, but the form of the function will be determined by the fact that it is referred to the primed axes. The relative amounts of the various eigenfunctions relative to the z' axis can be projected out by multiplying the new function by $h^{m'}(z')^*$ and integrating over all angles.

APPENDIX B: WAVE FUNCTIONS

An investigation of the exciton wave functions in the presence of both external and internal strain gives information about selection rules and polarization of the emission spectrum. The solution for the Γ_2^- states can be accomplished by first transforming $\mathbf{T}_{js}'$, Eq. (15) into $\mathbf{T}_{js}''$ in the representation $e_{\pm}h_{\pm}'$ and $e_{\pm}h_{\pm}''$ based on the hole functions (14). To find the eigenfunctions of the sum of $\mathbf{T}_{js}''$ and the diagonal total strain matrix $\mathbf{T}_s$, we introduce the functions

$$X_1=(e_+h_-'-g^*e_-h_+')/\sqrt{2}, \tag{B1a}$$

$$X_2=(e_+h_-'+g^*e_-h_+')/\sqrt{2}, \tag{B1b}$$

$$Y_1=(e_+h_-''-ge_-h_+'')/\sqrt{2}, \tag{B1c}$$

$$Y_2=(e_+h_-''+ge_-h_+'')/\sqrt{2}, \tag{B1d}$$

which diagonalize the 2×2 submatrices along the diagonal. The quantity g is a phase factor defined by

$$g=G/|G|,$$

with

$$G=[-3(1+\gamma^2)+i2\sqrt{3}\gamma]/N^2 \tag{B2}$$

and $\gamma=\rho+i\mu$ defined by Eq. (14e). This leads to a matrix in which the functions are coupled only in pairs, so that the complete solution is easily obtained. The energy eigenvalues are given by

$$\begin{aligned}E_{Is}&=\tfrac{1}{8}\Delta[1-M_1],\\ E_{IIs}&=\tfrac{1}{8}\Delta[1-M_{-1}],\\ E_{IIIs}&=\tfrac{1}{8}\Delta[1+M_{-1}],\\ E_{IVs}&=\tfrac{1}{8}\Delta[1+M_1],\end{aligned} \tag{B3}$$

where

$$\begin{aligned}M_{\pm1}&=\{(|G|/\sqrt{3}\pm P)^2+[1-A\pm|G|+8\epsilon/\Delta]^2\}^{1/2},\\ P&=[-\sqrt{3}(1-|\gamma|^2)+6\mu]/N^2,\end{aligned} \tag{B4}$$

and

$$A=(2|\gamma|^2+2\sqrt{3}\mu)/N^2.$$

In the final step of the solution, two new pairs of functions are formed, one of which is

$$\psi_I=a_1X_1+b_1Y_2, \tag{B5}$$

$$\psi_{IV}=a_4X_1+b_4Y_2, \tag{B6}$$

where b_1/a_1 and a_4/b_4 are of order D_uS/ϵ_0 for small stress. The function X_1 can be expanded:

$$\begin{aligned}X_1\propto{}&(1-g^*)[(e^{1/2}h^{3/2}-e^{-1/2}h^{-3/2})\\ &+\rho(e^{1/2}h^{1/2}+e^{-1/2}h^{-1/2})-\mu(e^{1/2}h^{-1/2}-e^{-1/2}h^{1/2})]\\ &+(1+g^*)i[(e^{-1/2}h^{+3/2}+e^{1/2}h^{-3/2})\\ &+\rho(e^{-1/2}h^{1/2}-e^{1/2}h^{-1/2})\\ &-\mu(e^{1/2}h^{1/2}+e^{-1/2}h^{-1/2})].\end{aligned} \tag{B7}$$

For small stress, $1+g^*$ is proportional to D_uS/ϵ, while $1-g^*$ is of order unity.

The function Y_2 is

$$Y_2 \propto (1-g)i[(e^{-1/2}h^{1/2}-e^{1/2}h^{-1/2}) -\rho(e^{1/2}h^{-3/2}+e^{-1/2}h^{3/2})-\mu(e^{1/2}h^{3/2}-e^{-1/2}h^{-3/2})] +(1+g)[(e^{1/2}h^{1/2}+e^{-1/2}h^{-1/2}) -\rho(e^{1/2}h^{3/2}-e^{-1/2}h^{-3/2}) +\mu(e^{1/2}h^{-3/2}+e^{-1/2}h^{3/2})]. \quad \text{(B8)}$$

If there is no external stress, all terms except the first vanish in these expansions and ψ_{I0} (the subscript 0 indicates no external stress) is simply the combination of the states $J=2$, $M=\pm 2$:

$$\psi_{I0}=|2,2\rangle-|2,-2\rangle. \quad \text{(B9)}$$

In the same notation

$$\psi_{IV0}=|1,0\rangle. \quad \text{(B10)}$$

Transitions from ψ_{I0} to the ground state, which has $J=0$, are forbidden while those from ψ_{IV0} result in the emission of light polarized parallel to the internal strain axis, i.e., in the z direction. (See Fig. 2.)

When a small external stress is applied, ψ_I is modified to include small amounts of the states $|2,1\rangle+|2,-1\rangle$, $|1,1\rangle-|1,-1\rangle$, and $|1,0\rangle$. Transitions are now no longer forbidden but occur with a probability proportional to the square of the strain. The light emitted has components polarized in both the x and z directions. ψ_{IV} also includes all four states and when it decays light is emitted which has a small component polarized in the x direction in addition to the principal component polarized in the z direction.

The states ψ_{II} and ψ_{III} are linear combinations of X_2 and Y_1. When there is no external stress they are

$$\psi_{II0}=a_2[|2,1\rangle+|2,-1\rangle] +b_2[|1,1\rangle-|1,-1\rangle], \quad \text{(B11)}$$

$$\psi_{III0}=a_3[|2,1\rangle+|2,-1\rangle] +b_3[|1,1\rangle-|1,-1\rangle], \quad \text{(B12)}$$

where

$$a_2/b_2=-b_3/a_3=(1/\sqrt{3})(\epsilon_j+\epsilon_0+\tfrac{1}{2}\Delta)/(\epsilon_j+\epsilon_0-\tfrac{1}{2}\Delta) \quad \text{(B13)}$$

and

$$\epsilon_j=(\epsilon_0{}^2-\tfrac{1}{2}\epsilon_0\Delta+\tfrac{1}{4}\Delta^2)^{1/2}.$$

Their decay results in light polarized in the x direction. A small external stress introduces into each state a small amount of the states $|2,2\rangle-|2,-2\rangle$, and $|1,0\rangle$ and adds to the emitted light a small component polarized in the z direction. When $\cos\alpha=0$, the problem has higher symmetry and the wave functions are simpler. G is real and negative and R is zero. The functions X_1 and Y_2 include only the states $|2,2\rangle-|2,-2\rangle$, and (1,0). No other functions are mixed with these even when the external stress is applied, so that ψ_I and ψ_{IV} decay with the emission of light polarized in the z direction. A study of ψ_{II} and ψ_{III} shows that their emission is always polarized in the x direction.

The problem of finding the exact eigenfunctions for the Γ_1^- states has not been solved. The interaction matrix did not simplify after the first step so the solution was carried out numerically. For small stress, however, the Γ_1^- states can be treated in the manner just described for the Γ_2^- states. The $|J,M\rangle$ states which belong to the Γ_1^- are $|2,2\rangle+|2,-2\rangle$, $|2,1\rangle-|2,-1\rangle$, $|1,1\rangle+|1,-1\rangle$, and $|2,0\rangle$. Decay from the third of these states results in light polarized in the y direction while decay from the others is forbidden. In the absence of external stress ψ_{II0} and ψ_{III0} include the $|1,1\rangle+|1,-1\rangle$ state while ψ_{I0} and ψ_{IV0} do not. When the external stress is applied, each of the states includes all four of the $|J,M\rangle$ states and in general all of the transitions become allowed. When $\cos\alpha=0$, the mixing is not complete. ψ_I and ψ_{IV} include $|2,2\rangle+|2,-2\rangle$ and $|2,0\rangle$ and emission is forbidden for all values of strain. The nature of all the wave functions and the selection rules are summarized in Table II.