

substitution in this equation, the result $E_2^{(L_1)} - E_2^{(L_{3'})} = \Xi_u^{(L_1)} - \Xi_u^{(L_{3'})} = 3.5 \pm 3.5$ eV is obtained. The known deformation potentials associated with the L_1 minima^{3,5,11} may then be used in conjunction with the previously determined value of $E_1^{(L_{3'})} - E_1^{(L_1)}$ to deduce the highly approximate values of the deformation potentials of the $L_{3'}$ minima, $\Xi_u^{(L_{3'})} = 14 \pm 3.5$ eV and $\Xi_d^{(L_{3'})} = 1.5 \pm 3$ eV.

Since pressure coefficients associated with band gaps involving the same points in the Brillouin zone in many of the group 4 and 3-5 semiconductors are nearly the same,¹⁰ it would be of interest to perform similar experiments on the 3-5 compounds. Because of this similarity, piezoreflectance experiments would aid in the identification of observed reflectance structure.

PHYSICAL REVIEW

VOLUME 127, NUMBER 3

AUGUST 1, 1962

Energy Dependence of Indirect Optical Absorption in Semiconductors

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(Received February 12, 1962)

Formulas are obtained for the indirect absorption coefficient as a function of photon energy, for both degenerate and nondegenerate semiconductors, taking into account the dependence of the energy denominator on the energy of the intermediate states. The light-hole and heavy-hole contributions and the total absorption were computed for germanium. The results are displayed as a function of photon energy, in graphs, for the nondegenerate case and for several Fermi energies. The results show that, for degenerate material, absorption edges obtained by extrapolation of the experimental absorption spectrum are liable to be too low.

IN a semiconductor, indirect optical absorption¹ connects an initial state in the valence band, through the optical matrix element M_R , to an intermediate state in the conduction band near the zone center, and then by the scattering matrix element M_S to a final state near the conduction band edge^{2,3} (see Fig. 1). The states are designated, respectively, i , a , and f . The probability of this transition determines dN/dt , the number of quanta of incident radiation absorbed per unit time per unit volume. The indirect optical absorption coefficient is $\alpha = (n/Nc)dN/dt$, where n is the index of refraction.

The interaction represented by M_S may be due to phonon scattering or to impurity scattering. In either case $|M_S|$ will be taken here as independent of the state, in the range of states contributing. When M_S is due to phonon scattering, a term $\pm E_p$ (energy of the phonon) appears in the formulas for dN/dt , on account of conservation of energy.³ This will have the effect of shifting the absorption spectrum's edge by an amount $\pm E_p$, and can be taken into account by replacing ΔE_g (see Fig. 1) by $E_{g \text{ phonon}} = \Delta E_g \mp E_p$ in the results

[Eq. (7), etc.] below. The energy variation of M_R may be neglected compared to the variation of the denominator in Eq. (2) below, since M_R is proportional to $(E_a + \Delta E_g + E_g)$ whereas the denominator is proportional to $(E_a + \Delta E_g - E_f)$, so that a change in E_a affects the energy denominator much more than it does M_R . Furthermore, $|M_R|^2$ is independent of the direction of \mathbf{k} for unpolarized incident radiation.⁴ By assuming a spherical energy surface for each hole band we can write α as an integral over the energies only, as in (2)

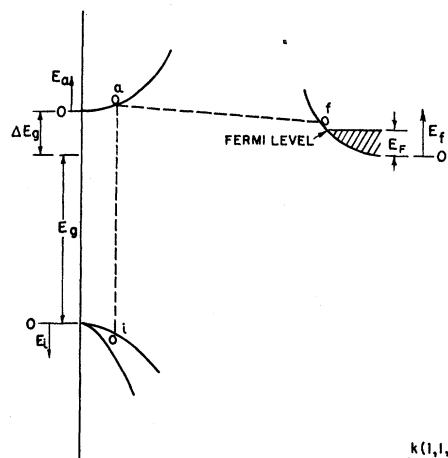


FIG. 1. The conduction and valence bands illustrating the transition discussed in this paper. This figure defines the various energies used in this paper and their zeros.

¹ J. Bardeen, F. J. Blatt, and L. H. Hall, in *Proceedings of the Conference on Photoconductivity, Atlantic City, 1954* (J. Wiley & Sons, Inc., New York, 1956), p. 146.

² The other process given in reference 1, scattering of a hole from a valence band edge, involves a larger energy denominator than the transition considered here and therefore is considered a negligibly smaller contribution to α . Processes in which an exciton is created, also not considered here, are thought to contribute to α in the immediate neighborhood of the indirect absorption edge for pure material, reference 3, and presumably have their analog for degenerately doped material.

³ G. G. MacFarlane, T. P. McLean, J. E. Quarrington, and V. Roberts, Phys. Rev. **108**, 1377 (1957).

⁴ M. Tiersten (private communication).

below. Let the energy of the photon be $E_g + E$. Then¹

$$\alpha = (\pi/2)^2 (n/\hbar c) |M_R|^2 |M_S|^2 A^2 B_i B_f, \quad (1)$$

where

$$A^2 = - \frac{8}{\pi} \int \int \frac{E_i^{3/2} E_f^{3/2} \delta[E_f - (E - E_i)] dE_i dE_f}{(\Delta E_g + E_i + E_a - E)^2}, \quad (2)$$

and where the density of states are $\rho_i = B_i E_i^{1/2}$, $\rho_f = B_f E_f^{1/2}$. Here $B_i = 2^{1/2} V (m_L^{3/2} + m_H^{3/2}) / \hbar^2$, where m_L and m_H are the density of states masses for the light and heavy holes, and $B_f = V (2m_f^{3/2}) / \hbar^2$.

In reference 1 an average value ΔE_g is substituted for the energy denominator so that (2) is replaced by

$$A_t(X, C_t, a)^2 = \frac{8}{\pi C_t^2} \left\{ \frac{-C_t [a(X-a)]^{3/2}}{X(C_t-1) + 1 - aC_t} - \sin^{-1} \left(1 - \frac{2a}{X} \right) - \frac{\pi}{2} \right. \\ \left. + \frac{\{2 + (C_t-2)X\} \{ \sin^{-1}(1 - 2a(1-X)/X[X(C_t-1) + 1 - aC_t]) + \pi/2 \}}{2[1 + (C_t-2)X + (1-C_t)X^2]^{3/2}} \right\}. \quad (5)$$

The corresponding result from Eq. (3) is

$$A_B^2 = \frac{X^2}{\pi} \left\{ \frac{2}{X} \left(1 - \frac{2a}{X} \right) [a(X-a)]^{3/2} \right. \\ \left. + \sin^{-1} \left(1 - \frac{2a}{X} \right) + \frac{\pi}{2} \right\}. \quad (6)$$

For nondegenerate material ($a=0$), $A_B = X$, and Eq. (5) reduces to

$$A_t^2 = \frac{8}{C_t^2} \left[\frac{2 + (C_t-2)X}{2[1 + (C_t-2)X + (1-C_t)X^2]^{3/2}} - 1 \right]. \quad (7)$$

In the limit of small X and $a=0$, A_t is just X . To calculate α , we combine A_L^2 and A_H^2 by

$$A^2 = \frac{m_L^{3/2} A_L^2 + m_H^{3/2} A_H^2}{m_L^{3/2} + m_H^{3/2}}. \quad (8)$$

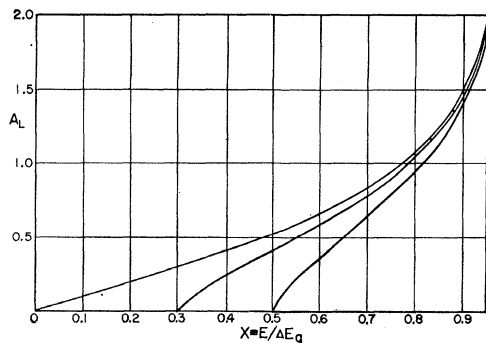


FIG. 2. A plot of the factor A for the light holes vs the energy of the photon (in units of ΔE_g) for three Fermi energies (in the same units).

$$A_B^2 = \frac{8}{\pi (\Delta E_g)^2} \int_0^{E-E_F} E_i^{3/2} (E-E_i)^{1/2} dE_i. \quad (3)$$

In place of this assumption, we integrate (2) directly. Since $\mathbf{k}_i \simeq \mathbf{k}_a$ we have $m_a E_a = m_i E_i$, where $i=L$ or H . Defining $C_t = 1 + m_i/m_a$, Eq. (2) becomes

$$A_t^2 = \frac{8}{\pi C_t^2} \int_0^{E-E_F} \frac{E_i^{3/2} (E-E_i)^{1/2} dE_i}{[(\Delta E_g - E)/C_t + E_i]^2}. \quad (4)$$

Setting $X \equiv E/\Delta E_g$, $a \equiv E_F/\Delta E_g$ we find

The functions (5), (7), and (8) have been calculated on an IBM 610 computer, for the values applying to germanium. These curves A_L , A_H , and A are plotted in Figs. 2-4. (The intercepts $A=0$, are at $X=a$.) The values used in computing these functions were $C_L = 2.2$ and $C_H = 10.45$ obtained from $m_L = 0.043m_0$, $m_H = 0.34m_0$, and $m_a = 0.036m_0$, where m_0 is the free-electron mass.^{5,6}

These curves show the increase in A_t , and hence of α , as $X \rightarrow 1$, which is to be expected when the energy denominator approaches zero. At the other limit, for small $X-a$, the energy denominator increases rapidly

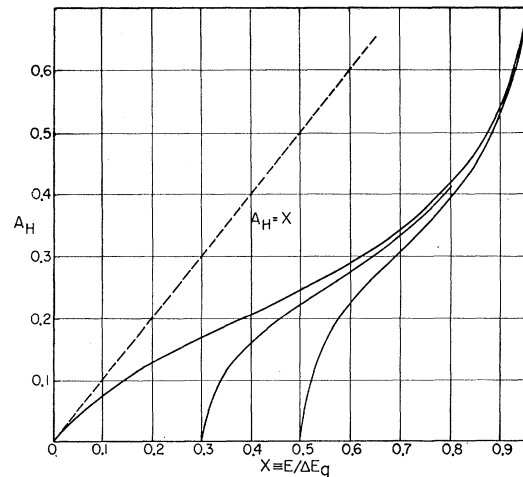


FIG. 3. Similar to Fig. 2 except that this is for the case of heavy holes. The dashed line $A_H = X$ is the result for the constant energy denominator ΔE_g and $E_F = 0$.

⁵ R. N. Dexter, H. J. Zeiger, and B. Lax, Phys. Rev. **104**, 647 (1956).

⁶ S. Zwerdling, B. Lax, and L. M. Roth, Phys. Rev. **108**, 1402 (1957).

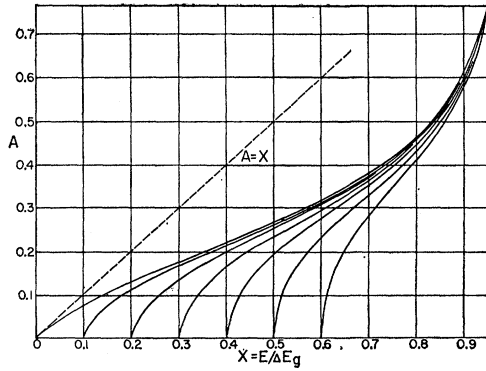


FIG. 4. A vs the excess photon energy, with the Fermi energies as parameters, with energies in units of ΔE_g . The dashed line $A = X$ is for the constant energy denominator ΔE_g and $E_F = 0$.

enough to decrease A from the value given by setting the energy denominator equal to ΔE_g , which is $A = X$ for $a = 0$ (see Fig. 4). This effect is more vividly illustrated by comparing Figs. 2 and 3. The initial increase in the energy denominator, and the curvature, is more pronounced for A_H , where C_H is large. Writing the square of the energy denominator in the form

$$C_i^2(\Delta E_g)^2[(1-X)/C_i + E_i/\Delta E_g]^2, \quad (9)$$

it is seen that (9) will change more rapidly with $E_i/\Delta E_g$ for large C_i (and for $X - a$ small compared to 1). So the departure of α at low energies from (6) is related to the electron and hole masses, since a large m_i means E_a large and hence the denominator becomes effectively larger with increasing E , so the variation of (9) does become physically significant.

The curves in Figures 2-4 also exhibit straight regions about their inflexion points. In the case of nondegenerate material (see Fig. 4, $a = 0$), $\sqrt{\alpha}$ varies linearly with X in the region $0.18 \leq X \leq 0.55$. For this region it should be noted that the slope of the straight line is considerably less than that predicted in reference 1, i.e., $dA/dX = 1$. This range of values of X ($a = 0$) is commensurate with the published results of reference 3, Fig. 2 (for small $\sqrt{\alpha}$ and low temperatures) if the

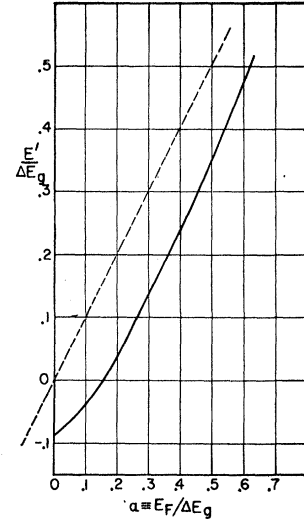


FIG. 5. The energy intercepts, $E'/\Delta E_g$ (determined by a linear extrapolation of the inflection points of Figure 4), plotted against the Fermi energies in units of ΔE_g . The dashed line is $E'/\Delta E_g = E_F/\Delta E_g$.

“phonon knees” are taken into account, and one assumes $E_g \approx 750$ meV, and $\Delta E_g \approx 150$ meV at 4.2°K .^{3,6} In fact in these published data, for small $\sqrt{\alpha}$, a slight curvature can be detected (except for $T = 4.2^\circ\text{K}$, in which case small $\sqrt{\alpha}$ is not plotted) similar to the curvature seen in Fig. 4 as $X \rightarrow 0$.

Another feature of interest in Fig. 4 is the linear extrapolation of the straight-line region for each Fermi energy to $A = 0$. (These points, called $E'/\Delta E_g$, are plotted against a in Fig. 5.) Figure 5 shows that E' is less than E_F , that is to say, the extrapolated photon energy is less than the thermal gap, by the difference between the dashed line $E' = a\Delta E_g$ and the solid curve.⁷ This correction cannot be applied to experimental data unless a value is assumed for ΔE_g or E_g . The change of ΔE_g and of E_g with doping are not yet known.

I wish to express my appreciation to Dr. P. J. Price for many enlightening discussions.

⁷ Note added in proof. These remarks apply to the experimental energy gaps determined by C. Haas, Phys. Rev. **125**, 1965 (1962), Fig. 4; and J. I. Pankove and P. Aigrain, Phys. Rev. **126**, 956 (1962), Fig. 11.