

Infrared Absorption Spectrum of Germanium*

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WE have calculated the optical absorption by valence electrons in pure germanium for "direct" and "indirect" transitions to the conduction band. The "direct" transitions are those in which the valence electron absorbs a photon, the propagation vector \mathbf{k} of the electron remaining essentially constant. In the case of the "indirect" transitions the electron absorbs a photon and also suffers a substantial change of its \mathbf{k} vector, momentum conservation being achieved by the absorption or emission of a phonon.

The band structure which was assumed for this calculation is shown in Fig. 1, and is based on previous calculations of Herman,¹ and Herman and Callaway,² and on cyclotron resonance experiments.^{3,4} It is evident from this structure that the long wavelength absorption limit for the direct transitions occurs at a wavelength $\lambda_d = 0.86$ microns, corresponding to the energy difference $E_{c0} - E_v = 1.45$ ev, and that this wavelength is shorter than the long-wavelength limit for the indirect transitions $\lambda_i = 1.8$ microns, corresponding to the energy difference $E_c - E_v = 0.7$ ev.

Because the indirect transitions are of second order as compared to the direct transitions, one may expect that the probability for the former is less than the probability for the latter. If the probability for the indirect transitions is many orders of magnitude smaller than for the direct transitions, the former could not be observed, and the long wavelength limit of the absorption spectrum would appear at $\lambda = \lambda_d$. If, however, the probability for indirect transitions is reduced by only a few orders of magnitude in relation to the direct transitions, a tail at the long wavelength end of the spectrum should appear, the ultimate absorption limit being at $\lambda = \lambda_i$.

The calculation follows the usual time-dependent perturbation procedure. One obtains the following expressions for the rate of absorption of energy by direct and indirect transitions, respectively:

$$W_d = \iint \left\{ \frac{2\pi t}{\hbar^2} \left[(E_f - E_0 - \hbar\omega) \frac{t}{\hbar} \right] \right\} \{ |H'|^2 \} \left\{ \frac{8\pi\omega^2 d\omega}{(2\pi c)^3} \right\} \left\{ \frac{1}{4\pi^2} \left(\frac{2m_v}{\hbar^2} \right)^{\frac{3}{2}} (E_v - E_0)^{\frac{1}{2}} dE_0 \right\}, \quad (1)$$

$$W_i = N \iiint \left\{ \frac{2\pi t}{\hbar^2} \left[(E_f - E_0 - \hbar\omega) \frac{t}{\hbar} \right] \right\} \{ |H''|^2 \} \left\{ \frac{8\pi\omega^2 d\omega}{(2\pi c)^3} \right\} \\ \times \left\{ \left(\frac{1}{4\pi^2} \right)^2 \left(\frac{2m_v}{\hbar^2} \right)^{\frac{3}{2}} \left(\frac{2m_c}{\hbar^2} \right)^{\frac{3}{2}} [(E_v - E_0)(E_f - E_c)]^{\frac{1}{2}} dE_0 dE_f \right\}. \quad (2)$$

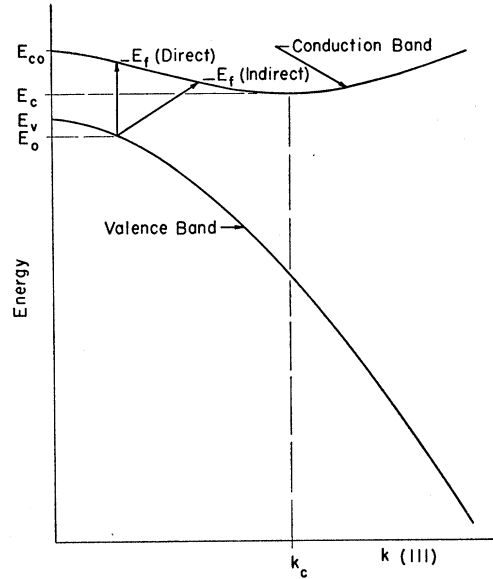


FIG. 1. Assumed band structure of germanium.

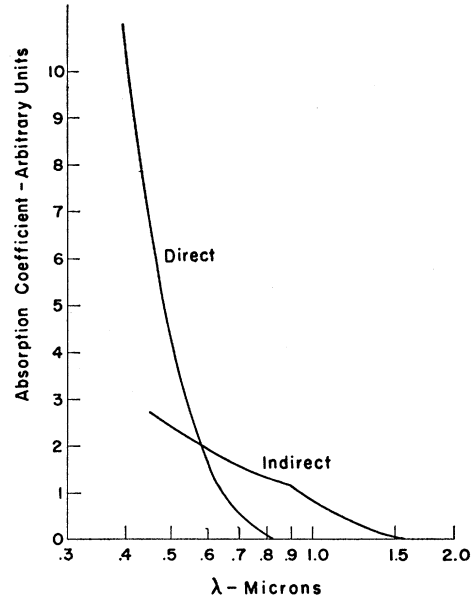


FIG. 2. Absorption coefficients for "direct" and "indirect" transitions as functions of wavelength. The ordinates have been chosen such that $A_d(\lambda_d - \Delta\lambda)/A_i(\lambda_i - \Delta\lambda) = 10$.

The factor N gives the number of minima in the energy surfaces of the conduction band, of which, according to recent cyclotron resonance experiments,⁴ there are either eight as illustrated in Fig. 1, or four if the energy minima occur at the band edges. In the above expressions the first factor in the curly brackets expresses,

through the delta function, the conservation of energy requirement; the second factor is the square of the matrix element for the transition, the third factor gives the density of photon states, and the final factor the appropriate density of electron states. These expressions can be reduced to

$$W_d(\omega)d\omega = C_1 \frac{2m_v}{\hbar} (E_v - E_0)^{\frac{1}{2}} \omega d\omega, \quad (3)$$

$$W_i(\omega)d\omega = C_1 C_2 \left\{ \left[k_c^2 + \left(\frac{m_c + m_v}{\hbar^2} \right) (E_v + \hbar\omega - E_c) \right] B + \frac{2(m_v - m_c)}{3\hbar^2} [(E_{c0} - E_c)(E_v + \hbar\omega - E_{c0})]^{\frac{1}{2}} \right\} \frac{d\omega}{\omega} \quad (4a)$$

$$B = \frac{1}{4} \left\{ [3(E_v + \hbar\omega) - 2E_{c0} - E_c] [(E_{c0} - E_c)(E_v + \hbar\omega - E_{c0})]^{\frac{1}{2}} + (E_v + \hbar\omega - E_c)^2 \tan^{-1} \left(\frac{E_{c0} - E_c}{E_v + \hbar\omega - E_{c0}} \right)^{\frac{1}{2}} \right\}$$

$$W_i(\omega)d\omega = C_1 C_2 \frac{\pi}{8} \left\{ k_c^2 + \left(\frac{m_c + m_v}{\hbar^2} \right) (E_v + \hbar\omega - E_c) \right\} (E_v + \hbar\omega - E_c)^2 \frac{d\omega}{\omega}; \lambda \geq \lambda_d. \quad (4b)$$

The constant C_1 involves only known physical constants; C_2 contains a factor characterizing the strength of the electron-phonon interaction in the conduction band and also the quantity N already referred to above. Free electron wave functions have been used throughout.

By using Eqs. (3) and (4) and the following parametric values²⁻⁴: $E_{c0} - E_c = 0.75$ eV, $E_{c0} - E_v = 1.45$ eV, $m_v = 0.3m_e$, $m_c = 0.2m_e$, the shapes of the absorption spectra for the direct and indirect transitions have been obtained, and these curves are shown in Fig. 2. An estimate for the ratio of the absorption coefficients for the direct and indirect transitions at wavelength

$\lambda_d - \Delta\lambda$ and $\lambda_i - \Delta\lambda$, respectively, gives

$$A_d(\lambda_d - \Delta\lambda)/A_i(\lambda_i - \Delta\lambda) \sim 10.$$

These results appear to be in qualitative agreement with experimental observations of absorption in thin films of germanium by Brattain and Briggs.⁵ Details of the calculation will soon be published in this journal.

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Some Properties of Germanium-Silicon Alloys

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PREPARATION of homogeneous alloys of germanium-silicon has been reported by Stöhr and Klemm¹ and by Wang and Alexander.² We have prepared a series of germanium-silicon alloys by a process of homogenization at high temperatures and have determined composition, density, lattice constant, and forbidden band gap. All alloys were homogeneous within the precision of the x-ray measurements. Absolute values of composition of the material were determined by analyzing for germanium polarographically.³ This method of analysis, with silicon as the sole chemical impurity, is believed to be accurate to better than

± 1 percent. Forbidden band widths were determined optically, on samples normalized to 0.020-in. thickness. The band width was taken as the energy corresponding to the value of the absorption which is exhibited by germanium at its accepted band width (0.72 eV). At this point the absorption coefficient was 22.7 cm^{-1} . All absorption curves had slopes which were similar to that of pure germanium.⁴

In Table I is summarized the data obtained on these alloys. Figure 1 shows the variation of lattice constant with composition and agrees within experimental error with that obtained by Stöhr and Klemm.¹ Lattice constant measurements indicate that one should observe a nonlinear variation of density with composition due to the small volume difference between germanium and silicon. However, our measurements of density and composition are not sufficiently sensitive to detect this. Consequently, a plot of density *versus* composition