PHYSICAL REVIEW VOLUME 97, NUMBER 6 MARCH 15, 1955

Theory of the Infrared Absorption of Carriers in Germanium and Silicon*

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(Received November 8, 1954)

The Drude-Zener theory of optical absorption by free carriers is applied to the infrared absorption of n-type germanium and p-type silicon. Average effective masses so determined are: for electrons in germanium $\langle(m^*/m)\rangle_{\text{Av}}$ ranges from 0.11 to 0.22; for holes in silicon $\langle(m^*/m)\rangle_{\text{Av}}$ ranges from 0.19 to 0.55. The average effective mass values of electrons in germanium are in good agreement with those measured by cyclotron resonance. The infrared absorption bands of p-type germanium are explained on the basis of transitions of holes between three energy bands lying near the top of the valence band. This band structure is suggested by cyclotron resonance experiments. Application of the theory to p-type silicon leads to the prediction of an absorption peak near 25μ and two lesser ones near 33μ.

1. INTRODUCTION

RECENT experiments on infrared absorption in germanium and silicon have shown that there is a marked dependence of the absorption on the type and concentration of the carriers present. In n-type germanium[1,2] and in samples of silicon[3,4] indicated to be p-type, the absorption follows the Drude-Zener frequency dependence, but the magnitudes of the absorption coefficients calculated using the free electron mass are too small by factors between 10^2 and 10^3. We attribute this to effective masses lighter than that of the free electron. In p-type germanium[2,5–7] absorption bands are observed. It has been suggested that this absorption is caused by interband transitions of holes.[6]

In Sec. 2, we estimate from the infrared data the effective masses of carriers in germanium and silicon which follow the Drude-Zener behavior. In Sec. 3, we consider the optical absorption of p-type germanium by interband transitions using a simple model suggested by the results of cyclotron resonance experiments.[8–11]

2. OPTICAL ABSORPTION BY FREE CARRIERS

The Drude-Zener theory of free carrier absorption[12] predicts an absorption coefficient

$$K=\frac{4\pi}{nc}\cdot\frac{Ne^2\tau}{m^*(1+\omega^2\tau^2)},\tag{1}$$

where $\omega=2\pi\nu$ is the angular frequency of the radiation, n the refractive index of the medium, m^* the effective mass of the carriers of concentration N, and τ the mean relaxation time of the carriers. This is developed on the assumption of a spherically symmetric, nondegenerate energy surface. In the case of germanium the lowest conduction band has minima along the (111) directions of $\mathbf{k}$ space, near which the energy surfaces are prolate spheroidal.[11] The longitudinal effective mass is denoted by m_l and the transverse by m_t. If the relaxation time is isotropic, Eq. (1) is still valid if we replace m^* by $\langle m^*\rangle_{\text{Av}}$ where

$$\frac{1}{\langle m^*\rangle_{\text{Av}}}=\frac{1}{3}\left(\frac{1}{m_l}+\frac{2}{m_t}\right).$$

The mobility $\mu=e\tau/\langle m^*\rangle_{\text{Av}}$ is introduced. In the region where $\omega^2\tau^2\gg1$ the absorption coefficient can then be written

$$K=Ne^3/(nc\pi\langle m^*\rangle_{\text{Av}}{}^2\nu^2\mu).\tag{2}$$

Figure 1 shows typical absorption coefficients of n-type germanium samples in the infrared, as determined by Fan and Becker.[1] The sharp rise at about 1.8μ

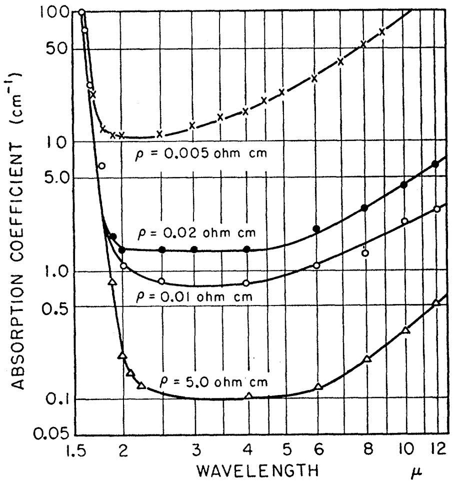

FIG. 1. Absorption coefficient of samples of n-type germanium as observed by Fan and Becker[1] (log-log plot).

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[*] Supported in part by the U. S. Office of Naval Research and the U. S. Signal Corps.

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[1] H. Y. Fan and M. Becker, Proceedings of the Reading Conference (Butterworth Scientific Publications, London, 1951), pp. 132–147.

[2] Kaiser, Collins, and Fan, Purdue Semiconductor Research Progress Report, January 1, 1953 (unpublished), pp. 55–69.

[3] M. Becker and H. Y. Fan, Phys. Rev. **76**, 1531 (1949).

[4] H. B. Briggs, Phys. Rev. **77**, 727 (1950).

[5] H. B. Briggs and R. C. Fletcher, Phys. Rev. **87**, 1130 (1952).

[6] H. B. Briggs and R. C. Fletcher, Phys. Rev. **91**, 1342 (1953).

[7] Kaiser, Collins, and Fan, Phys. Rev. **91**, 1380 (1953).

[8] Dresselhaus, Kip, and Kittel, Phys. Rev. **92**, 827 (1953).

[9] Dresselhaus, Kip, and Kittel, Phys. Rev. **95**, 568 (1954).

[10] Dexter, Zeiger, and Lax, Phys. Rev. **95**, 557 (1954).

[11] Lax, Zeiger, Dexter, and Rosenblum, Phys. Rev. **93**, 1418 (1954).

[12] F. Seitz, *Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), pp. 638–640.

is associated with electronic transitions from the highest valence band to the lowest conduction band. At wavelengths longer than 6μ, the absorption is found to vary directly with $1/\nu^2$.

The data of Conwell[13] were used for the determination of N and μ in Eq. (2). By using Fig. 7 of reference 13, which gives conductivity *vs* temperature for specimens of known carrier concentration, it was possible to estimate N when the conductivities of the samples were given. Figure 5 of reference 13 gives mobility as a function of temperature for the various carrier concentrations. With these values, we find values of $\langle m^*\rangle_{\mathrm{Av}}/m$ by fitting Eq. (2) to the observed absorption curves. The values so determined range from 0.11 to 0.22, as shown in Table I.

The values of m_1^* and m_2^* for n-type germanium in cyclotron resonance experiments[11] near 4°K are $1.3m$ and $0.08m$ respectively. This predicts for $\langle m^*\rangle_{\mathrm{Av}}/m$ the value 0.12, which is close to the values given in Table I.

The infrared absorption of p-type silicon has the same characteristics as that of n-type germanium. On the long wavelength side of the energy gap transition, the absorption appears to be that of the Drude-Zener type. Equation (12) is fitted to the experimental curves and values of $\langle m^*\rangle_{\mathrm{Av}}$ obtained. Mobilities and concentrations for p-type silicon were obtained from the paper of Pearson and Bardeen.[14] The values of $\langle m^*\rangle_{\mathrm{Av}}/m$ so obtained are listed in Table II with the sources of the data. Values range from 0.19 to 0.55.

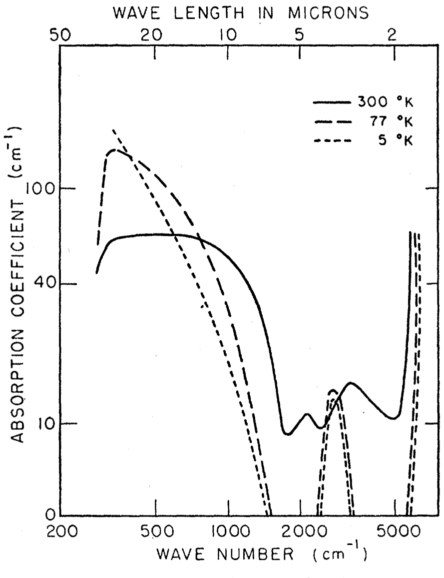

FIG. 2. Absorption coefficient of a sample of p-type germanium of resistivity 0.07 ohm-cm, after Kaiser, Collins, and Fan[7] (log-log plot).

TABLE I. Average effective masses of electrons in germanium as determined by Eq. (2).

Samples of Fan and Becker[a]	Temperature °K	Resistivity (Ω-cm)	Calculated values of $\langle m^*\rangle_{\mathrm{Av}}/m$
	300	0.005	0.11
		0.02	0.12
		0.1	0.20
		5.0	0.14

Sample of Collins and Fan.[b] $N=2.8\times10^{17}$ electrons/cm^3 at all temperatures given.

Temperature °K	Calculated values of $\langle m^*\rangle_{\mathrm{Av}}/m$
77	0.22
300	0.16
353	0.16
379	0.16
439	0.15

[a] See reference 1.
[b] See reference 2.

Tolpygo[15] finds the free carrier absorption by solving the Boltzmann equation for the electronic velocity distribution with radiation present. The current is calculated with the use of a relaxation time inversely proportional to the velocity. He obtains expressions for the optical constants and interprets the results of Briggs to give a value of $\langle m^*\rangle_{\mathrm{Av}}/m=0.25$.

Cyclotron resonance experiments on p-type silicon[16] indicate that there are two bands at the top of the valence band, degenerate at $\mathbf{k}=0$ and having approximate effective masses of 0.17 and 0.50. If both bands have the same relaxation time the cyclotron resonance values would predict a value of $\langle m^*\rangle_{\mathrm{Av}}/m=0.38$, which is within our spread of values. One should expect such a band structure to have an absorption band, as shown in Sec. 3. It is there shown that the peak of this band is expected to occur at 25μ, which is outside the range of experimental values quoted by Becker and Fan[3] and Briggs.[4]

3. OPTICAL ABSORPTION BY INTERBAND TRANSITIONS

The problem of electronic transitions from one energy band to another induced by electromagnetic radiation has been treated by Wilson.[17] He finds the average of the current density in the presence of radiation, to the first order in the applied fields. We adapt his results to obtain the conductivity caused by transitions from band i to band j. Wilson's Eq. (194) gives for the conductivity the expression

$$\sigma=\frac{\pi e^2\hbar}{m^2\omega}\int\delta(\omega_{ij}-\omega)\left|\int\psi_i\boldsymbol{\varepsilon}\cdot\nabla\psi_j d\tau\right|^2 N_i(\mathbf{k})d\mathbf{k}. \quad (3)$$

In the above, ω is the angular frequency of the applied radiation which has polarization vector $\boldsymbol{\varepsilon}$, $\omega_{ij}=[E_i(\mathbf{k})$

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[13] E. M. Conwell, Proc. Inst. Radio Engrs. **40**, 1327 (1952).
[14] G. L. Pearson and J. Bardeen, Phys. Rev. **75**, 865 (1949).
[15] K. B. Tolpygo, Zhur. Eksptl. i Teort. Fiz. **22**, 378 (1952).
[16] Dexter, Lax, Kip, and Dresselhaus, Phys. Rev. **96**, 222 (1954).
[17] A. H. Wilson, *Theory of Metals* (University Press, Cambridge, 1936), first edition, pp. 126–131, especially Eq. (194).

$-E_j(\mathbf{k})]/\hbar$ is the frequency difference between bands i and j, the ψ's are the respective Bloch functions, and $N_i(\mathbf{k})d\mathbf{k}$ is the number of electrons of band i per unit volume lying in volume $d\mathbf{k}$ of $\mathbf{k}$-space. The transitions are vertical, that is, $\mathbf{k}$ is not changed in the transition. The frequency difference ω_{ij} is to be looked upon as a function of $\mathbf{k}$. One integration may be performed by setting $d\mathbf{k}=dSd\omega_{ij}/|\nabla_{\mathbf{k}}\omega_{ij}|$, where dS is an element of surface of constant ω_{ij}. The conductivity at frequency ω becomes

$$\sigma=\frac{\pi e^2}{m^2\hbar\omega}\left[\int\left|\int\psi_i{}^*\boldsymbol{\varepsilon}\cdot\mathbf{p}\psi_j d\tau\right|^2\frac{N_i(\mathbf{k})dS}{|\nabla_{\mathbf{k}}\omega_{ij}|}\right]_{\omega_{ij}=\omega}. \quad (4)$$

The integral is to be evaluated at $\omega_{ij}=\omega$. The absorption coefficient is then obtained through the relation $K_{ij}=4\pi\sigma_{ij}/nc$.

In p-type germanium the infrared absorption spectrum consists of bands. Typical curves are shown in Fig. 2. At 300°K, there are peaks near 500 cm^{-1}, 2200 cm^{-1}, and 3500 cm^{-1}. As the temperature is lowered the band in the neighborhood of 2200 cm^{-1} diminishes and has disappeared at 77°K; the band at 3500 cm^{-1} becomes sharper and higher with the peak moving toward longer wavelengths; the long wavelength band beginning at about 1800 cm^{-1} becomes narrower and higher. In addition the strong absorption near 1.8μ is observed as in n-type germanium. This is due to the energy gap jump as before. It will be shown that the model for p-type germanium proposed by Dresselhaus, Kip, and Kittel[9] will predict infrared absorption of the observed character and of the correct order of magnitude.

According to this model, the top edge of the valence band consists of two bands, almost spherically symmetric, with effective masses $m_1{}^*=0.3m$ and $m_2{}^*=0.04m$. These bands touch at $\mathbf{k}=0$ at a point of symmetry of type $\Gamma_8{}^+$ in the notation of Elliott.[18] Each of these bands is twofold degenerate if we consider spin. The four wave functions at $\mathbf{k}=0$ have the symmetry properties of atomic $p_{\frac{3}{2}}$ orbitals arranged with opposite signs on the two fcc sublattices of the diamond lattice. At an energy ΔE lower is another band, spherically symmetric and doubly degenerate. The wave functions at $\mathbf{k}=0$ are of type $\Gamma_7{}^+$, having the symmetry of $p_{\frac{1}{2}}$ orbitals with opposite signs on the two sublattices. The separation ΔE is caused by spin-orbit interaction. This structure is illustrated in Fig. 3. Optical transitions between these bands are forbidden at $\mathbf{k}=0$. Away from $\mathbf{k}=0$, this selection rule breaks down and electric dipole transitions can occur. From such a model, it is easy to understand the origin of absorption bands. Near $\mathbf{k}=0$, few transitions can occur because of the selection rule. Farther from $\mathbf{k}=0$, absorption can take place if irradiation of the proper frequency is present. Still farther from $\mathbf{k}=0$, the Maxwellian distribution function for the holes will become small and few holes will be present to make transitions. Thus one should expect to find absorption bands with widths strongly dependent on temperature.

TABLE II. Average effective masses of holes in silicon as determined by Eq. (2).

Samples of Fan and Becker,[a] $T=300°\text{K}$		Resistivity (ohm-cm)	$\langle m^*\rangle_{\text{Av}}/m$
		0.014	0.55
		0.032	0.30
		0.075	0.19
		0.5	0.31
Samples of Briggs,[b] $T=300°\text{K}$	Impurity content (percent B)	Resistivity (ohm-cm)	$\langle m^*\rangle_{\text{Av}}/m$
	0.0005	0.03	0.31
	0.001	0.012	0.22
	0.002	0.007	0.27
	0.003	0.005	0.36
	0.005	0.004	0.30
	0.01	0.0015	0.36

[a] See reference 1.
[b] See reference 4.

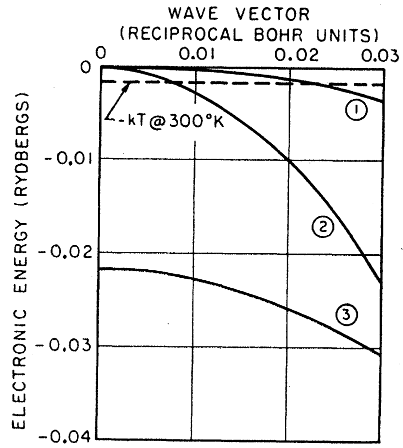

FIG. 3. Proposed structure of the uppermost valence bands of germanium in the neighborhood of $\mathbf{k}=0$. The Bohr unit of length is $a_0=0.529$ A.

We now calculate the absorption coefficients K_{ij} according to Eq. (23) with some simplifying assumptions concerning the band structure and matrix elements. First we treat transitions from band 1 to band 2.

An expression for the matrix element will be obtained. The one-electron Schrödinger equation for the stationary states with spin-orbit interaction included is

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V(\mathbf{r})\psi+\frac{\hbar}{2m^2c^2}\mathbf{S}\cdot[\boldsymbol{\nabla}V(\mathbf{r})\times\mathbf{p}]\psi=E\psi.$$

Since $\boldsymbol{\nabla}V$ has the same periodicity as V, the Bloch form $\psi=u_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$ is preserved. The equation for the u function is

$$-\frac{\hbar^2}{2m}\nabla^2u_{\mathbf{k}}+V(\mathbf{r})u_{\mathbf{k}}+\frac{1}{2m^2c^2}\mathbf{S}\cdot(\boldsymbol{\nabla}V\times\mathbf{p})u_{\mathbf{k}}+\hbar\mathbf{k}$$
$$\cdot\left[\frac{\mathbf{p}}{m}+\frac{1}{2m^2c^2}(\mathbf{S}\times\boldsymbol{\nabla}V)\right]u_{\mathbf{k}}=\left[E(\mathbf{k})-\frac{\hbar^2k^2}{2m}\right]u_{\mathbf{k}}. \quad (5)$$

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[18] R. J. Elliott, Phys. Rev. 96, 266, 280 (1954).

We are interested in points near $\mathbf{k}=0$ and accordingly treat the left-hand term of Eq. (5) enclosed in square brackets as a perturbation. The second term in the square brackets is of order v/c while the first is of order 1 in the nonrelativistic approximation. Hence, we use only the first term. In any event, the two terms have the same symmetry and will admix the same wave functions.

The Schrödinger equation will be considered solved for $\mathbf{k}=0$. We proceed away from $\mathbf{k}=0$ by applying the perturbation $(\hbar/m)\mathbf{k}\cdot\mathbf{p}$. Let $|\lambda_i^0\rangle$ be a u function at $\mathbf{k}=0$ belonging to energy E_λ^0. A Latin subscript will indicate the degenerate states of level λ. The first order u function is

$$|\lambda_i^{\mathbf{k}}\rangle=|\lambda_i^0\rangle+\frac{\hbar}{m}\sum_{\mu j}\frac{\langle\mu_j^0|\mathbf{k}\cdot\mathbf{p}|\lambda_i^0\rangle}{E_\lambda^0-E_\mu^0}|\mu_j^0\rangle. \tag{6}$$

To apply this standard perturbation theory, the $|\lambda_i^0\rangle$ functions must be the correct linear combinations: in this case those which diagonalize the energy to second order in $\mathbf{k}$. This has been treated by Shockley.[19] The condition is

$$\frac{\hbar^2}{m^2}\sum_{\alpha m}\frac{\langle\lambda_j^0|\mathbf{k}\cdot\mathbf{p}|\alpha_m^0\rangle\langle\alpha_m^0|\mathbf{k}\cdot\mathbf{p}|\lambda_l^0\rangle}{E_\lambda^0-E_\alpha^0}=\delta_{il}W_j(\mathbf{k}). \tag{7}$$

$W_j(\mathbf{k})$ is the second-order change of energy produced by the operator $(\hbar/m)\mathbf{k}\cdot\mathbf{p}$. Dresselhaus *et al.*[9] and Elliott[18] have found $W(\mathbf{k})$ for diamond-type crystals in terms of a few fundamental parameters. They obtain for holes:

$$E(\mathbf{k})=\left[\frac{\hbar^2}{2m}+\frac{A+2B}{3}\right]k^2\pm\left[\left(\frac{A-B}{3}\right)^2k^4+\frac{C^2-(A-B)^2}{3}(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2\right]^{\frac{1}{2}}, \tag{8}$$

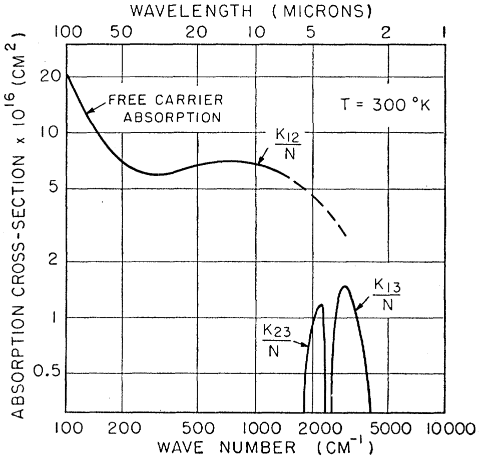

FIG. 4. Calculated optical absorption cross section of holes in germanium at 300°K (log-log plot).

where the constants A, B, and C are determined by matrix elements and energy differences between the initial band and bands of other symmetry. These same constants appear in the expression for the matrix element for interband transitions. The matrix element for transitions between bands degenerate at $\mathbf{k}=0$ is obtained from Eq. (6). It is given by

$$\langle\lambda_l^{\mathbf{k}}|\boldsymbol{\varepsilon}\cdot\mathbf{p}|\lambda_i^{\mathbf{k}}\rangle=\langle\lambda_l^0|\boldsymbol{\varepsilon}\cdot\mathbf{p}|\lambda_i^0\rangle+\frac{\hbar}{m}\sum_{\mu j}\left[\frac{\langle\lambda_l^0|\boldsymbol{\varepsilon}\cdot\mathbf{p}|\mu_j^0\rangle\langle\mu_j^0|\mathbf{k}\cdot\mathbf{p}|\lambda_i^0\rangle}{E_\lambda^0-E_\mu^0}+\frac{\langle\lambda_l^0|\mathbf{k}\cdot\mathbf{p}|\mu_j^0\rangle\langle\mu_j^0|\boldsymbol{\varepsilon}\cdot\mathbf{p}|\lambda_i^0\rangle}{E_\lambda^0-E_\mu^0}\right]. \tag{9}$$

For diamond-type lattices, the term of zero order in $\mathbf{k}$ of Eq. (9) will vanish. This follows from the presence of inversion symmetry which causes all wave functions belonging to a degenerate level at $\mathbf{k}=0$ to have the same parity.

One can obtain a selection rule for the direction of polarization $\boldsymbol{\varepsilon}$. If $\boldsymbol{\varepsilon}$ is parallel to $\mathbf{k}$, the terms in Eq. (9) become proportional to the sum in Eq. (7). Thus the transition element between different bands will vanish.

We make the approximation that bands 1 and 2 are spherically symmetric.

$$E_1=\hbar^2k^2/(2m_1^*),\quad E_2=\hbar^2k^2/(2m_2^*). \tag{10}$$

For the case of germanium, this assumption will correspond to a spread of absorption frequencies of 10 percent. With this assumption, it is then possible to carry out the integration of Eq. (4). For $N_1(\mathbf{k})$ we use the Maxwellian distribution function,

$$N_1(\mathbf{k})=\frac{N_1\hbar^3}{(2\pi m_1^*kT)^{\frac{3}{2}}}\exp(-E_1/kT), \tag{11}$$

where N_1 is the total number of holes in band 1. In evaluating Eq. (4) we need $|\nabla_{\mathbf{k}}\omega_{12}|$ which is given by $\hbar k(m_1^*-m_2^*)/m_1^*m_2^*$. All of these factors are introduced and the integration carried out. The matrix element is proportional to k and the square of its absolute value averaged over all directions is written $\hbar^2k^2A_{12}^2$, where A_{12} is a dimensionless parameter. The absorption coefficient is then found to be

$$\frac{16\pi^{\frac{3}{2}}e^2\hbar^{\frac{3}{2}}}{nc}A_{12}^2N_1\frac{m_1^*m_2^{*5/2}}{m^2(m_1^*-m_2^*)^{5/2}}\times\frac{\omega^{\frac{1}{2}}\exp[-(\hbar\omega/kT)m_2^*/(m_1^*-m_2^*)]}{(kT)^{\frac{3}{2}}}.$$

In this expression, the induced emission from band 2 to band 1 has been omitted. This is calculated by similar application of Eq. (4) and subtracted from the above absorption. N_1 and N_2 are given in terms of N, the total

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[19] W. Shockley, Phys. Rev. **78**, 173 (1950).

number of carriers by the relations:

$$N_1=\frac{N}{1+(m_2^*/m_1^*)^{\frac{3}{2}}};\quad N_2=\frac{N(m_2^*/m_1^*)^{\frac{3}{2}}}{1+(m_2^*/m_1^*)^{\frac{3}{2}}}.$$

The absorption coefficients for all transitions between bands 1, 2, and 3 are given by

$$K_{12}=\frac{16\pi^2(2)^{\frac{1}{2}}e^2\hbar^{\frac{3}{2}}A_{12}{}^2m_1{}^*m_2{}^{*5/2}N\tilde{\nu}^{\frac{1}{2}}}{nc^{\frac{1}{2}}[1+(m_2^*/m_1^*)^{\frac{3}{2}}]m^2(m_1^*-m_2^*)^{5/2}(kT)^{\frac{3}{2}}}\times\left[\exp\left(-\frac{hc\tilde{\nu}}{kT}\frac{m_2^*}{m_1^*-m_2^*}\right)-\exp\left(-\frac{hc\tilde{\nu}}{kT}\frac{m_1^*}{m_1^*-m_2^*}\right)\right],\quad(\tilde{\nu}>0)\qquad(12)$$

$$K_{13}=\frac{16\pi^2(2)^{\frac{1}{2}}e^2\hbar^{\frac{3}{2}}A_{13}{}^2m_1{}^*m_3{}^{*5/2}N(\tilde{\nu}-\tilde{\nu}_0)^{\frac{3}{2}}}{nc^{\frac{1}{2}}[1+(m_2^*/m_1^*)^{\frac{3}{2}}]m^2(m_1^*-m_3^*)^{5/2}\tilde{\nu}(kT)^{\frac{3}{2}}}\times\exp\left[-\frac{hc(\tilde{\nu}-\tilde{\nu}_0)}{kT}\frac{m_3^*}{m_1^*-m_3^*}\right],\quad(\tilde{\nu}>\tilde{\nu}_0)\qquad(13)$$

$$K_{23}=\frac{16\pi^2(2)^{\frac{1}{2}}e^2\hbar^{\frac{3}{2}}A_{23}{}^2(m_2^*/m_1^*)^{\frac{3}{2}}m_2{}^*m_3{}^{*5/2}N(\tilde{\nu}_0-\tilde{\nu})^{\frac{3}{2}}}{nc^{\frac{1}{2}}[1+(m_2^*/m_1^*)^{\frac{3}{2}}]m^2(m_3^*-m_2^*)^{5/2}\tilde{\nu}(kT)^{\frac{3}{2}}}\times\exp\left[-\frac{hc(\tilde{\nu}_0-\tilde{\nu})}{kT}\frac{m_3^*}{m_3^*-m_2^*}\right],\quad(\tilde{\nu}<\tilde{\nu}_0).\qquad(14)$$

In the above, $\tilde{\nu}=\nu/c$ is the wave number of the incident light. The energy gap at $k=0$ between bands 1 and 3 is $\Delta E=hc\tilde{\nu}_0$. The restrictions given in the parentheses indicate the ranges of $\tilde{\nu}$ to which the formulas apply. They follow from the energy separations between bands. Going away from $\mathbf{k}=0$, ν_{12} increases from zero; ν_{13} increases, starting at $\Delta E/h$; ν_{23} decreases, starting at $\Delta E/h$. No induced emission occurs from band 3 as we shall set ΔE at a value much greater than kT. Equations (12), (13), and (14) are evaluated using $m_1^*=0.3m$, $m_2^*=0.04m$, as determined by cyclotron resonance. It is not possible to get an exact fit to the bands found experimentally, but a qualitative agreement is obtained if we take $\Delta E=2400$ cm$^{-1}=0.3$ ev and $m_3^*=0.1m$. If the spin-orbit splitting, ΔE, is small compared to the energy gap between valence and conduction bands, then

$$m_3^*=\left[\frac{1}{2}\left(\frac{1}{m_1^*}+\frac{1}{m_2^*}\right)\right]^{-1}.$$

Estimating the correction due to ΔE, we get $m_3^*\cong 0.1m$. The A constants of Eqs. (12) to (14) are chosen to fit the maxima at $T=300$°K. The values chosen are

$$A_{12}=5.2,\quad A_{13}=2.99,\quad A_{23}=90.$$

An estimate of the matrix element for transition 1 to 2 based on the form of the wave functions at $k=0$ is estimated approximately by

$$|\langle 1|\boldsymbol{\varepsilon}\cdot\mathbf{p}|2\rangle|\gtrsim\frac{-C}{(3)^{\frac{1}{2}}}\frac{m}{\hbar}k\sin\theta,\qquad(15)$$

where C is the same constant as in Eq. (8). Lax *et al.* find by cyclotron resonance $C=-32$ in units of $\hbar^2/2m$. From these figures we obtain $A_{12}=6.4$, which is in excellent agreement with the value obtained by interpretation of the optical absorption.

Plots of the computed absorption coefficients at 300°K and 77°K are given in Figs. 4 and 5. The absorption coefficients are expressed per unit total carrier concentration, giving them the dimensions of a cross section. Also included in these figures is the free carrier absorption of the holes in bands 1 and 2. This absorption is found in the same way as was done in Sec. 2 with the added assumption that both bands have the same relaxation time τ. The relaxation time was taken to be of the order of 10^{-12} sec for both bands. For samples as highly doped as those reported on, τ will not change by more than a factor of 2 as T varies from 300°K to 77°K.

When we compare Fig. 4 with the experimental curve, we see that the correct number of peaks occur, but that the peak of K_{12} overlaps the other peaks. This overlap is at about 2000 cm^{-1}, a region for which the transition is for holes with wave vector $k\sim 0.03a_0{}^{-1}$, where a_0 is the Bohr unit of length (0.529 A). This point is quite far out from the center of the Brillouin zone and it is likely that the energy there is no longer proportional to k^2 as we have assumed. If the effective mass of band 2 were to increase from the very small value of $0.04m$, bands 1 and 2 would not diverge so rapidly and the K_{12} peak would fall of more rapidly on the short wavelength side, in better agreement with experiment. At 77°K, Fig. 5, we

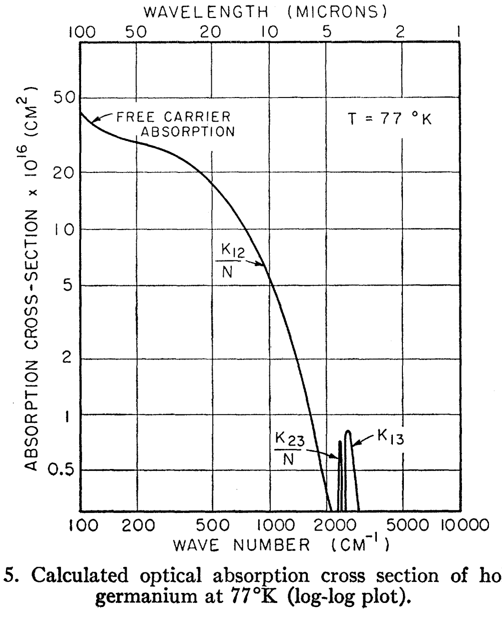

FIG. 5. Calculated optical absorption cross section of holes in germanium at 77°K (log-log plot).

see that the peak of K_{23} has become very narrow and lower in magnitude. In the experimental plot, the band with which we identify K_{23} actually disappears at 77°K. The other bands have the correct qualitative form. The K_{12} peak goes to a higher maximum than at 300°K and falls off more sharply on the short wavelength side. Absorption band K_{13} narrows and decreases in magnitude.

From Fig. 2 it is seen that the absorption at 5°K is very much like that at 77°K. At liquid helium temperatures the carriers lie bound in impurity levels. An acceptor level in germanium has a mean radius of about $13a_0$. We have here used an effective mass of $0.3m$. This impurity state, when analyzed into plane waves, will principally contain $\mathbf{k}$'s lying within a sphere of radius $0.2a_0^{-1}$ in $\mathbf{k}$ space. This spread of $\mathbf{k}$ is of the same order of magnitude as the spread of occupied states of band 1 at $T=77$°K, as seen from Fig. 3. If the Bloch functions are at all like plane waves, we may expect the matrix elements for absorption from band 1 to be of the same magnitude as those for absorption from the impurity levels. Hence we should expect the absorption at liquid helium temperatures to be similar to that[20] at 77°K.

We see from Fig. 5 that at about 80 microns and farther in the infrared the free carrier absorption dominates. This is a possible explanation of the rise in the absorption coefficient at this wavelength as observed by Johnson and Spitzer.[21]

From the above theory, it appears that we should expect p-type silicon to have infrared absorption bands. Application of Eq. (12) with effective masses $0.50m$ and $0.17m$, as determined by Lax *et al.*,[16] predicts a maximum for band K_{12} at 25μ for $T=300$°K. From their data we find $A_{12}{}^2\sim 2.56$, which leads to an absorption coefficient $K_{12}=5\times 10^{-16}N$ at the maximum of the band. Reported measurements of infrared absorption coefficient of p-silicon extend only as far as 10μ and are of the Drude-Zener type. In the region between 10μ and 4μ the band K_{12} falls off rapidly but has the same order of magnitude as the observed absorption. In the case of germanium it was found that the band K_{12} did not fall off rapidly enough on the high frequency side. If this fault is a result of the approximations made and if it also occurs in application to silicon, we may expect that further experimental investigation will locate this band. Spin-orbit splittings in atomic silicon are roughly $\frac{1}{8}$ those of germanium.[22] Hence we should expect bands K_{13} and K_{23} to occur near 33μ in p-type silicon if they are sufficiently high to be seen.

ACKNOWLEDGMENTS

The author wishes to thank Professor C. Kittel for suggesting this problem and for helpful discussions concerning it. He is also grateful to G. Dresselhaus for discussions concerning the band structure of germanium. The Purdue Semiconductor Research Group was kind enough to provide unpublished material on the infrared absorption of semiconductors. This research was performed during the tenure of a National Science Foundation Predoctoral Fellowship.

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[20] This argument is due to Dr. C. Herring (private communication).

[21] E. J. Johnson and W. G. Spitzer, Phys. Rev. **94**, 1415 (1954); Purdue Semiconductor Research Progress Report, October 1, 1953 (unpublished), pp. 50–54.

[22] C. E. Moore, *Atomic Energy Levels*, National Bureau of Standards Circular 467 (U. S. Government Printing Office, Washington, D. C., 1949), Vols. I and II, p. 467.