lattice expansion. The smaller lattice contraction may be caused by aggregation, perhaps in the form of colloids. The fact that there is any contraction at all points to one of two possibilities:

(1) F' centers in equilibrium with other defects; or

(2) less lattice strain associated with the centers responsible for the red absorption, as might be the case for defects intermediate in size between single oxygen vacancies and colloids.

In this connection, it should be emphasized that red BaO crystals are grown at about 900°C, while blue crystals are colored at about 1100°C.

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Classical Theory of Cyclotron Resonance for Holes in Ge

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Cyclotron resonance line shapes for holes have been calculated in the classical limit. The magnetic field was taken in the (001) direction. Because the cyclotron resonance frequency depends on the component of k parallel to the magnetic field (k_H), the line is shifted and broadened as compared to the simple theory with $k_H=0$. The shift of the maximum is about 3%, and the broadening (which is asymmetric) is about 40% for Ge, if $\omega\tau$ is taken as 7.5.

The shape of cyclotron resonance absorption lines for Ge has been calculated treating the holes as classical particles. Quantum effects[1] become important at low temperatures and will be considered in a separate publication. It is easily shown that for a constant magnetic field H, the component of the quasi-momentum in the direction of H (k_H) is a constant of the motion. Thus for H in the (001) direction (the only case considered here), k_z is a constant. The equations of motion for k_x and k_y are then given by

$$\begin{aligned}\dot{k}_x&=\partial\mathcal{H}/\partial k_y\\ \dot{k}_y&=-\partial\mathcal{H}/\partial k_x,\end{aligned}\tag{1}$$

where for holes

$$\mathcal{H}=\frac{eH}{c}(\bar{A}k^2\pm[\bar{B}^2k^2+\bar{C}^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]^{\frac{1}{2}}).\tag{2}$$

The plus and minus refer to the light and heavy holes, respectively. The constants $\bar{A}$, $\bar{B}$, $\bar{C}$ are those reported by Dresselhaus, Kip, and Kittel[2] as A, B, C. One sees from Eq. (1) that k_x and k_y are canonically conjugate variables. The equations of motion for k_x and k_y will depend parametrically on k_z, and there will of course be a thermal distribution of k_z.

In order to estimate the effect of the thermal distribution of k_z a transport theory with a constant relaxation time τ was used. The theory is essentially that of Van Vleck and Weisskopf.[3] The formalism of the theory is similar to that used by Karplus and Schwinger.[4]

The calculations were performed starting with the following expression for the absorbed power per unit volume ρ:

$$\mathcal{P}=Ne\{\langle v_x(t)\rangle E_x(t)\}_{\text{Av}}\tag{3}$$

where E_x refers to an electric rf field in the [100] direction. N is the number of holes per unit volume and $v_x(t)$ is the velocity of a hole in the x direction. The brackets $\langle\,\rangle$ indicate an averaging over the time of collision and an averaging over the Boltzmann distribution. The braces refer to an average over time. Since k_x and k_y are canonically conjugate a new set of canonical coordinates P and Q, where $\mathcal{H}=P$, can be found. This leads to a considerable simplification. In terms of these new variables the averaging procedure gives

$$\mathcal{P}=\tfrac{1}{2}Ne^2E^2\tau\int_{-\infty}^{+\infty}dk_z\int_{P_0}^{\infty}dP\rho\beta\sum_{n=-\infty}^{+\infty}\frac{|v_x(n,P)|^2}{1+\tau^2(\omega+\omega_0 n)^2}.\tag{4}$$

ρ is the Boltzmann factor

$$\rho=\frac{\exp\left(-\dfrac{\beta c}{eH}P\right)}{\Delta},$$

where

$$\Delta=\int_{-\infty}^{\infty}dk_z\int_{P_0}^{\infty}dP\int_0^{2\pi/\omega_0}dQ\exp\left(-\frac{\beta c}{eH}P\right),$$

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[2] Dresselhaus, Kip, and Kittel, Phys. Rev. **98**, 368 (1955).
[3] J. H. Van Vleck and V. F. Weisskopf, Revs. Modern Phys. **17**, 227 (1945).
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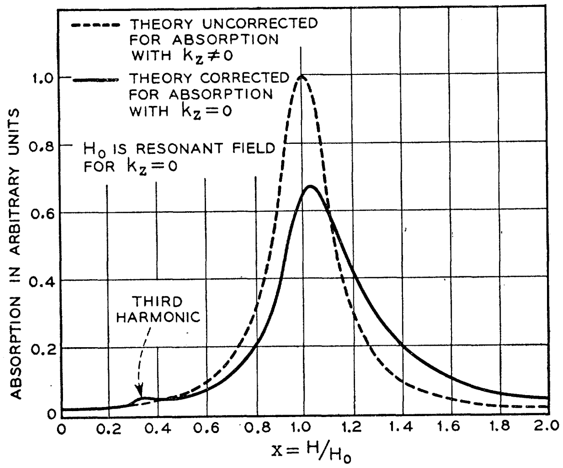

FIG. 1. Cyclotron resonance line shape for holes in Ge.

and $\beta = 1/kT$. P_0 is determined by the minimum value of $\mathcal{H}$ for a given k_z. ω is the frequency of the rf field and $\omega_0 = \omega_0(k_z,P)$ is the frequency of the periodic motion of k_x and k_y for a given P and k_z. The $v_x(n,P)$ are the Fourier coefficients of a Fourier expansion of $v_x(P,Q)$ in terms of $e^{in\omega_0 Q}$. It is easily shown that $v_x = -(c/eH)\dot{k}_y$. Thus, if k_y is expressed as a Fourier series

$$k_y = \sum_{n=-\infty}^{+\infty} C_n e^{i\omega_0 n t}$$

and if η is defined as $\eta = P/k_z^2$, Eq. (3) becomes (after an integration over k_z)

$$\mathcal{P} = \frac{3eE^2\tau c}{4H\delta(\eta_0)} \int_{\eta_0}^{\infty} d\eta \eta^{-5/2} \omega_0(\eta) \sum_{n=-\infty}^{+\infty} \frac{n^2 |C_n|^2}{1+\tau^2(\omega+n\omega_0)^2}, \quad (5)$$

where

$$\delta(\eta_0) = \int_{\eta_0}^{\infty} d\eta \eta^{-\frac{3}{2}} \omega_0^{-1}(\eta),$$

and η_0 is the smallest value of $\mathcal{H}$ for $k_z = 1$.

The C_n and $\omega_0(\eta)$ can in principle be determined exactly by integration of the equations of motion for k_x and k_y. In fact, the results may be expressed as elliptic integrals of the third kind. These exact solutions turn out to be quite impractical for computation, and we have only used them for checking purposes. The results reported here were obtained by means of an analog computer, which integrated the equations of motion of k_x and k_y directly. The values of $\bar{A}$, $\bar{B}$, and $\bar{C}$ taken were those reported by Dresselhaus *et al.*[2] The final integration over η was performed numerically. A variational method was also used to determine the values of C_n and ω_0. There is good agreement between the results of the variational method and the results given by the computer.

In order to determine the values of $\bar{A}$, $\bar{B}$, and $\bar{C}$, Dresselhaus, Kip, and Kittel[2] also used classical methods; however, they used the approximation that $k_H = 0$.[5] The results of calculations using $k_H = 0$, and of our theory may be seen in Fig. 1 (where we have taken $\omega = 1.5 \times 10$ in. rad/sec and $\omega\tau = 7.5$). The corrected curve may be seen to have its maximum shifted by about 3% from that of the $k_H = 0$ curve.[6] In addition an asymmetrical broadening of about 40% occurs. It should be mentioned that Zeiger[7] has reported similar calculations. He has, however, treated the asphericity of the energy surface as a perturbation on the main spherical term, and in addition limited himself to the neighborhood of resonance. His results seem to be in substantial agreement with those reported here.

With the above method it is possible to redetermine the constants $\bar{A}$, $\bar{B}$, and $\bar{C}$ more accurately. The change in their values will be not more than a few percent, and, at present, many other experimental and theoretical uncertainties overwhelm this correction.

It is also possible to calculate the effect of extra resonances due to higher harmonics. From Fig. 1 it can be seen that the third harmonic contribution is quite small for H in the [001] direction. The fifth harmonic was found to be much smaller. Further calculations are being made for H in the [111] direction, and for Si.[8]

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[5] These authors mention an attempt to correct for the $k_H = 0$ assumption [see discussion following their Eqs. (79) and (80)]. No indication of their method is given, and, especially for Si, their corrections seem somewhat high to us.

[6] The larger the $\omega\tau$, the less the maximum is shifted.

[7] H. J. Zeiger, Phys. Rev. **98**, 1560(A) (1955). Also private communication.

[8] In Si the effects discussed here will certainly be larger because of the greater asphericity of the energy surface.