(1955).
[10]K. S. Champlin, D. B. Armstrong, and P. D. Gunderson, Proc. IEEE 52, 677 (1964).
[11]H. Brooks, Advan. Electron. Electron Phys. 7, 128 (1955).
[12]K is a correction factor which would be unity if all holes had the same relaxation time.
[13]M. B. Prince, Phys. Rev. 92, 681 (1953).
[14]D. M. S. Bagguley et al., Proc. Roy. Soc. (London) A262, 340 (1961).

CONDUCTION ELECTRONS AND OPTIC MODES OF IONIC CRYSTALS

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Longitudinal optic (LO) modes of ionic crystals are associated with a macroscopic electric field, E_M. If free carriers are present then they will couple with E_M, and the dispersion relations for both the plasma oscillations of the carriers and the optic modes of vibration will be modified.[1] In this Letter we present a theory of these effects and apply it to the case of the LO modes in n-type lead telluride (PbTe). Experimental measurements of the dispersion relation for the normal modes of vibration of PbTe have revealed an anomalous behavior for the LO modes of long wavelength, which we believe is associated with the presence of free carriers. The measured frequencies of the long-wavelength optic modes in PbTe have already been reported.[2] A complete description of the dispersion curves, and of attempts to fit them with various models, will be published later in a joint communication with W. Cochran and M. Elcombe.

For wavelengths which are longer than the interatomic spacings but shorter than the wavelength of light, the frequency of the LO modes in cubic diatomic crystals is given by[3]

$$\omega_L^2 = \omega_T^2 + CE_M,$$

where ω_T is the frequency of the transverse optic (TO) modes, and C a constant depending upon the masses and effective charges of the ions. Free carriers in the crystal are influenced by the electric field,[4] E_M, and respond in such a way as to modify its effect. This modification can be expressed by dividing the magnitude of the electric field by the longitudinal frequency- and wave-vector-dependent dielectric constant for the carriers, $\epsilon(\vec{q},\omega)$.[5] The frequencies of the LO modes are then given by

$$\omega(\vec{q})^2 = \omega_T^2 + (\omega_L^2 - \omega_T^2)/\epsilon(\vec{q},\omega). \quad (1)$$

The solutions of this equation are in general very complicated and depend upon the detailed electronic band structure of the crystal. A detailed discussion of the form of the solutions will be given in a future publication. If the plasma frequency of the electrons is much greater than the lattice vibration frequencies, the Thomas-Fermi dielectric constant is appropriate for small wave vectors, $\epsilon(\vec{q},0) = 1 + k_S^2/q^2$, and $\omega(0)^2 = \omega_T^2$. However, the carriers will not be able to screen the electric field when the wavelength becomes much shorter than the distance between the carriers, and the frequency of the LO modes will tend to ω_L^2 for $q \gg k_S$. The dispersion relation for the LO modes will therefore show a marked decrease in frequency as the wave vector decreases.

Measurements of the LO mode frequencies have been made by studying the coherent one-phonon scattering of slow neutrons from a single-crystal specimen of n-type PbTe at 296°K, by means of the triple-axis crystal spectrometer at the NRU reactor, Chalk River. The measurements were made for momentum-transfer vectors near the reciprocal lattice points (115), (331), and $(33\bar{3})$, with wave vectors along the [001], [110], and $[11\bar{1}]$ directions, respectively. A marked decrease in frequency was observed in all of these experiments as $aq/2\pi$ decreased from 0.2 to 0 (a is the lattice constant). This decrease, from 3.40 ± 0.04 to 3.24 ± 0.05 in units of 10^{12} cps, was the same for all three directions of q within experimental error, as shown in Fig. 1. Also shown in Fig. 1 are two of the neutron groups. It is believed that this decrease in frequency is not an effect of the instrumental resolution, because it was not observed for the long-wavelength LO modes in KBr.[6]

The band structure of PbTe has ellipsoidal minima of the conduction band at the [111] zone

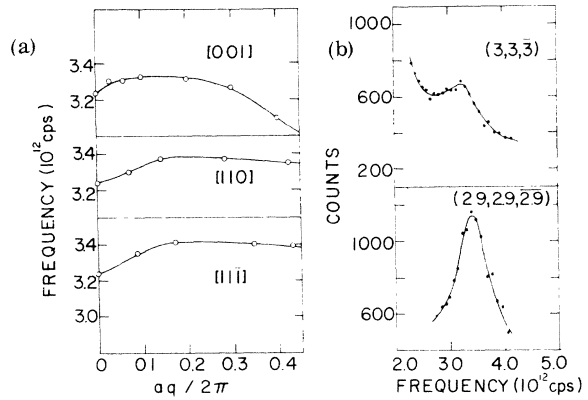

FIG. 1. LO modes in PbTe at 296°K: (a) Measured dispersion curves for [001], [110], and [11$\bar{1}$] directions, showing the dip in frequency near $q = 0$. (b) Vectors $(3, 3, \bar{3})$ and $(2.9, 2.9, \bar{2}.\bar{9})$. The increasing count rate at low frequency in the upper group is due to the nearby TO mode.

boundaries.[7] The dielectric constant can be evaluated readily if these are approximated by spheres and the effective mass taken as its mean value, $m^* = 0.095 m_0$. Measurements of the Hall coefficient for small pieces of the crystal indicated an electron density in the range $(1\text{-}3)\times 10^{19}$ cm^{-3}. Using the value 2×10^{19}, we find the Fermi radius, k_F, of the filled spheres in the conduction band to be 0.054 reciprocal lattice units, and the plasma frequency to be 24.4×10^{12} cps.

Since the plasma frequency is considerably greater than the LO mode frequency, the dielectric constant can be approximated by its static value,[4]

$$\epsilon(q,0) = 1+\frac{k_S^2}{q^2}\left[0.5+\frac{k_F}{2q}\left(1-\frac{q^2}{4k_F^2}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right|\right]. \quad (2)$$

Only intravalley scattering has been included in this expression since this is the dominant contribution for small wave vectors. Intervalley scattering gives rise to effects at much larger wave vectors. The Thomas-Fermi screening length, k_S, for this model of PbTe is 0.043 reciprocal lattice units. The dispersion relation for the LO mode can then be obtained from Eqs. (1) and (2), and is shown in Fig. 2. This figure also shows the singularity in the slope

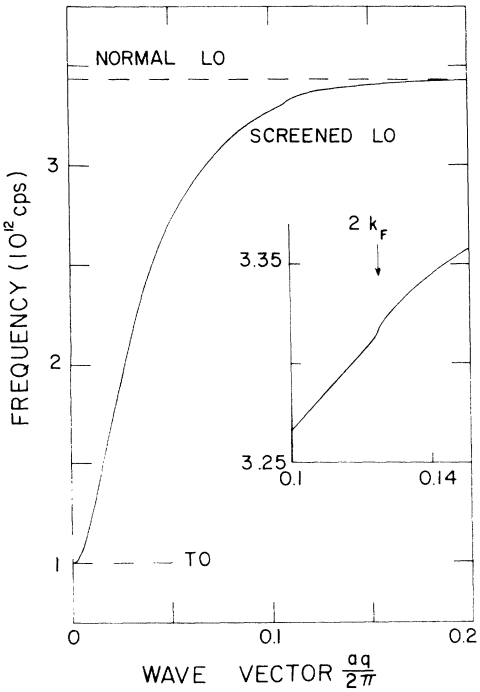

FIG. 2. The calculated LO dispersion curve in doped PbTe. The inset shows the discontinuity in the slope of the curve when the wave vector is equal to the Fermi surface diameter.[8]

of the dispersion curve when $q = 2k_F$.[8]

The neutron scattering from the LO modes with the dispersion curve shown in Fig. 2 is dependent upon the form of the resolution function of the spectrometer. In practice this is a complicated asymmetric function in which the energy and wave-vector resolutions are strongly coupled. The scattering can be calculated, however, if the energy dependence of the resolution function is assumed to be infinitely sharp, while the wave-vector dependence is taken to be a spherically symmetric Gaussian function. An estimate of the half-width of this function gives 0.06 reciprocal lattice units. The results of the calculation for the case in which the mean value of the neutron momentum-transfer vector is equal to a reciprocal lattice point are shown in the lowest curve of Fig. 3. The sharp dip in the scattering cross section at a frequency ~3.29 arises from the discontinuity in slope of the LO mode dispersion curve at $q = 2k_F$. (In the Thomas-Fermi approximation a single smooth curve is obtained.) This sharp dip is not observed experimentally owing to the finite energy resolution of the spectrometer, and the lowest curve would there-

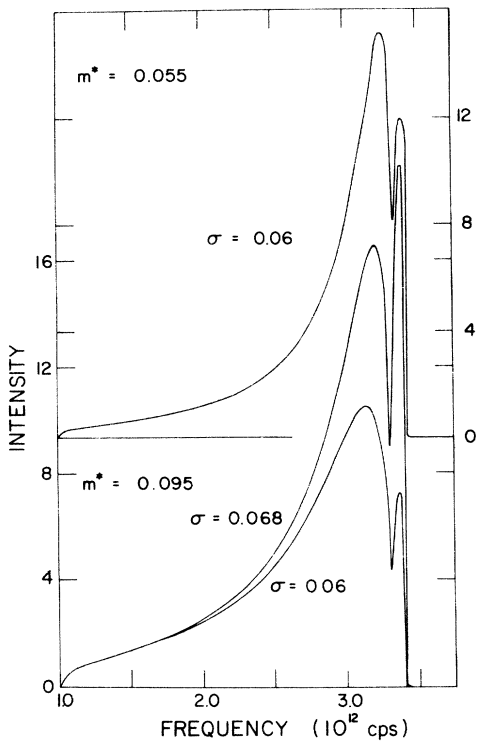

FIG. 3. The calculated shape of the neutron scattering at a reciprocal lattice point. The resolution function is taken to be a spherically symmetric Gaussian of half-width σ (reciprocal lattice units), but infinitely sharp in energy.

fore be interpreted as giving a phonon frequency of 3.1. In view of the approximations made in the present theory, by replacing the ellipsoidal band structure and resolution function by spheres, the agreement with the experimental value of 3.24 is reasonable. Excellent agreement can be obtained if we take $m^* = 0.055m_0$, or if the resolution function of the spectrometer is increased by about 10%, as shown in the upper curves of Fig. 3.

Calculations of the neutron scattering away from reciprocal lattice points have also been made, neglecting the change in the unscreened vibrational frequencies and eigenvectors of the LO mode with wave vector, and the calculated dispersion curve for the LO modes gives reasonable agreement with experiment.

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[1]I. Yokota, J. Phys. Soc. Japan 16, 2075 (1961).
[2]W. Cochran, Phys. Letters 13, 193 (1964).
[3]M. Born and K. Huang, Dynamical Theory of Crystal Lattices (Oxford University Press, New York, 1954).
[4]P. Nozières and D. Pines, Phys. Rev. 109, 762 (1958).
[5]D. Pines, Elementary Excitations in Solids (W. A. Benjamin, Inc., New York, 1963).
[6]A. D. B. Woods, B. N. Brockhouse, R. A. Cowley, and W. Cochran, Phys. Rev. 131, 1025 (1963).
[7]N. Numata and Y. Uemura, J. Phys. Soc. Japan 19, 2140 (1964).
[8]W. Kohn, Phys. Rev. Letters 2, 393 (1959).

OPTICAL QUENCHING OF PHOTOCONDUCTIVITY NEAR THE BAND EDGE IN CdS†

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We have observed the optical quenching of photoconductivity at photon energies slightly less than the band gap in undoped CdS crystals. The purpose of this Letter is to present the results and suggest an explanation.

Previous work[1-5] on the optical quenching of photoconductivity in CdS reports two "bands" at about 0.9 and 1.4 eV, well separated from the band gap at approximately 2.5 eV. The 0.9-eV band, observed only at higher temperatures, is considered to arise from the optical excitation of a trapped hole from its ground state to an excited state close to the valence band. The hole, then, may ionize thermally and subsequently recombine with a trapped electron, emptying an electron trap. The emptied trap is then able to capture a free electron leading to a decrease of photocurrent. The 1.4-eV band, observed at lower temperatures as well, is due to the same mechanism except that the free hole is provided by the direct optical ionization of a trapped hole. The trapped electrons and holes are supplied by previous and simultaneous excitation of the crystal with