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## Optical Phonons of $Bi_2Te_3$

By

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Bismuth telluride is a layer-structure crystal belonging to the space group $D_{3d}^5$. The electron band structure of this narrow gap semiconductor is very well known because of the interest in its thermo-electric properties (see for example the references given in (1) and (2)). It was found from studies of the transport phenomena that even at high carrier concentrations greater than $5x10^{19}/cm^3$ (p- and n-type), the scattering of free carriers from acoustical phonons dominates in the temperature region down to 10 K. This would be understandable in spite of the high carrier concentration and hence a high density of charged scattering centres, if the static dielectric constant in $Bi_2Te_3$ were very large.

It is well known that the dielectric constant in the far infrared is dominated by optical phonons which give rise to the "Restrahlbande". In order to obtain information about the dielectric constant in the far infrared region we measured the reflectivity of cleavage planes of $Bi_2Te_3$ crystals between 10 and 600 $cm^{-1}$. At nearly normal incidence the polarization of the light was perpendicular to the trigonal axis of the crystals ($\vec{E} \perp \vec{c}$). The measurements were carried out at room temperature, using a Polytec Fourier spectrometer FIR 30 and a Beckmann Fourier spectrometer FS 720.

The crystals were pulled by the Bridgman-Stockbarger method with carrier concentrations of about $5x10^{17}/cm^3$ and less.

Fig. 1 shows the reflectivity of two samples with different carrier concentrations. The concentration dependence of the reflectivity minima at 39 and 48 μm demonstrates their connection with the plasma resonance. By the step in the reflectivity between 160 and 250 μm wavelength the lattice vibrations were found for the first time in $Bi_2Te_3$.
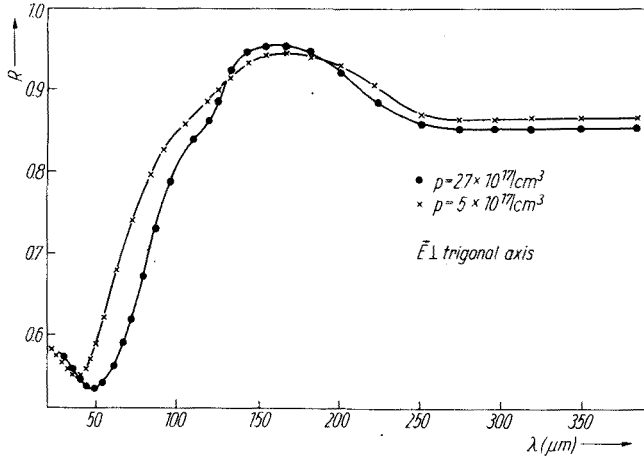
Fig. 1. Reflectivity vs. wavelength at room temperature for two samples with different carrier concentrations

Using the Kramers Kronig transformations we obtained the real and imaginary parts of the dielectric constant $\varepsilon_1 = n^2 - k^2$ and $\varepsilon_2 = 2nk = nK\omega c$.

In Fig. 2 $n^2 - k^2$ and $nK$ are plotted over the wavelength. The absorption cannot be described with only one eigenfrequency at $\lambda_1 = 205$ µm, because there exists an additional peak in the absorption at about $\lambda_2 = 100$ µm wavelength. This might be caused by a second eigenfrequency. Indeed from group theory it follows that there exist two doubly degenerate IR active modes for light polarized perpendicular to the c-axis (3). In view of this fact we tried to fit the optical constants with two classical oscillators:

$$n^2 - k^2 = \varepsilon_\infty + \sum_{i=1,2} \frac{\Delta\varepsilon_i \left(\omega_i^2 - \omega^2\right) \omega_i^2}{\left(\omega_i^2 - \omega^2\right)^2 + \omega^2 \gamma_i^2} - \frac{Ne^2}{m^* \varepsilon_0} \frac{\tau^2}{\tau^2 \omega^2 + 1} \, , \qquad (1)$$

$$n K = \frac{1}{c} \sum_{i=1,2} \frac{\Delta\varepsilon_i \, \omega^2 \, \gamma_i \, \omega_i^2}{\left(\omega_i^2 - \omega^2\right)^2 + \omega^2 \gamma_i^2} + \frac{N e^2}{m^* c \, \varepsilon_0} \frac{\tau}{\tau^2 \omega^2 + 1} \, , \qquad (2)$$

where the $\omega_i$ are the transverse optical frequencies, $\Delta\varepsilon_i$ the contributions of the classical oscillators to the static dielectric constant, and the $\gamma_i$ describe the damping of the lattice vibrations.
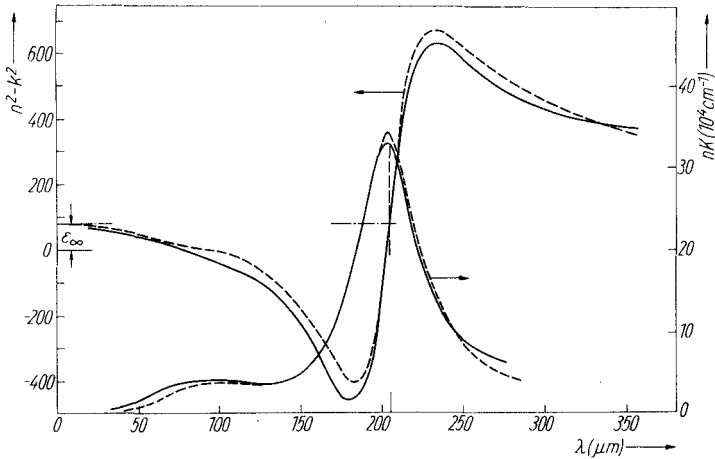
Fig. 2. Dispersion and absorption vs. wavelength for a sample with $p = 2.7 \times 10^{17}/cm^3$ at room temperature.
—— Kramers Kronig transformation,
---- oscillator fit, using equations (1) and (2)

The last terms are free carrier contributions. The best fit to the experimental data - Fig. 2 - was obtained with the following parameters:

$$\Delta\varepsilon_1 = 240, \qquad \gamma_1 = 2.2 \times 10^{12}/s, \qquad \omega_1 = 9.3 \times 10^{12}/s \ ,$$
$$\Delta\varepsilon_2 = 40, \qquad \gamma_2 = 1.9 \times 10^{13}/s, \qquad \omega_2 = 1.9 \times 10^{13}/s \ ,$$
$$N = 2.7 \times 10^{17}/cm^3, \quad \tau = 4 \times 10^{-14}/s, \qquad m^* = 0.085 \, m_o \ .$$

The carrier concentration N and the relaxation time $\tau$ of the electron were determined by galvanomagnetic measurements. The susceptibility mass $m^* = 0.085 \, m_o$ was calculated from the effective mass tensor (4) which was obtained from Shubnikov-de Haas experiments.

The contribution of the two oscillators to the static dielectric constant is $\Delta\varepsilon = 280 \pm 50$. The resulting dielectric constant is then $\varepsilon_{stat} = \varepsilon_\infty + \Delta\varepsilon = 360 \pm 50$ for the polarization $\vec{E} \perp \vec{c}$. This high value implies that the Coulomb potential of charged scattering centres is strongly screened and therefore contributes very little to electron scattering. Hence the transport behaviour dependence upon scattering from acoustical phonons mentioned above is reasonable.

## References

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