Scattering of electrons in bismuth

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An analysis is made of the mechanism of electron scattering in bismuth. A calculation is made of the probability of electron scattering by phonons allowing for the anisotropy of the deformation potential and of the phonon spectrum. A comparison of the calculated and experimental results shows that the temperature dependence of the electrical conductivity of bismuth is described satisfactorily by the intravalley scattering of electrons by phonons, whereas the results of a study of relaxation by the cyclotron resonance method cannot be fully explained by such scattering or by the electron-electron scattering and intervalley scattering by phonons. Further possible investigations are considered.

The Fermi surface of bismuth is relatively simple and has been studied thoroughly.[1] Investigations have also been made of the phonon spectrum of bismuth[2,3] and reliable measurements have been made of the deformation potential.[4] Nevertheless, investigations of the relaxation of carriers in bismuth have revealed disagreements between theory and experiment.

Most investigators have determined the temperature dependences of the electrical resistivity of bismuth single crystals. It has been established that the dependence $\rho(T)$ is nearly quadratic in the 2–16°K range. Hartman[5] gives the most accurate data on the temperature dependence of the transport relaxation time of electrons in the 4–16°K range. At higher temperatures the dependence $\rho(T)$ becomes linear[6] and the intermediate range lies at 15–30°K. Fenton et al.[7] and Fischer and Kao[8] have reported that the quadratic dependence extends up to 77–100°K, but their results may have been affected by the poor quality of the samples employed and the associated indeterminacy in the identification of the temperature-dependent component of the resistivity.

The available data are insufficient for the unambiguous determination of the electron scattering mechanism. The dependence $\rho \propto T^2$ is typical of the electron-electron interaction but, in the case of bismuth, it can also be explained by the scattering of electrons on phonons. In fact, since only those phonons whose wave vector is $q < 2k_F$ participate in the scattering and the momentum of a phonon whose energy is 1°K is comparable with the minimum diameter of the electron ellipsoid, the phase volume of the phonons interacting with electrons at higher temperatures is governed by the dimensions of the Fermi surface[9] and this may reduce the power exponent in the dependence $\rho(T)$.

Thus, in order to determine the predominant electron scattering mechanism it has become necessary to measure the relaxation times at $T \lesssim 1$°K. Recent investigations include the determination of the cyclotron resonance line width for very high quality bismuth single crystals at $0.35°K \leq T \leq 4.2°K$[10] and of the electrical conductivity of similar single crystals at $1.2°K \leq T \leq 7°K$.[11]

The present paper reports the results of a numerical calculation concerned with the electron-phonon scattering in bismuth. These calculations were carried out on a BÉSM-6 computer at the Computing Center of the USSR Academy of Sciences. The results are compared below with the experimental data. The necessary theory is well known.[12] The calculations were based on the elastic moduli measured at 77°K,[2] the Fermi surface parameters given by Edel'man,[13] and the deformation potential tensor Λ deduced from the amplitude of the quantum oscillations of the attenuation of ultrasound.[4]

PROBABILITY OF SCATTERING BY PHONONS

We calculated the probability $P(\nu)d(\nu)$ of the scattering of electrons by phonons of frequency ν, where

$$P(\nu)=\frac{\nu}{2ds^3}\left[\Lambda_{ik}\frac{1}{2}(e_iq_k+e_kq_i)\right]^2\delta(E-E'\pm h\nu)\,do$$

(s is the velocity of sound, q is the wave vector of a phonon, e is the polarization vector of a phonon, d is the density of the lattice, E and E′ are the energies of an electron before and after collision, o is the solid angle).

We found that the scattering was dominated by one of the transverse phonon branches. Figure 1 shows the total scattering probability (for three phonon branches) on the direction of the phonon wave vector obtained in the low-frequency limit (in this case, all the phonons interact with electrons and the electron scattering angles are small).

Next, we integrated $P(\nu)$ over the angles and averaged it over the central section of the electron ellipsoid, perpendicular to its major axis. If the phonon momentum exceeded the minimum diameter of the Fermi surface, the conservation of momentum in the scattering was not satisfied for all the directions of q and, therefore, this condition was checked separately for each frequency and each direction of the phonon wave vector.

In the integration of $\delta(E - E' - h\nu)$ it was necessary to allow for the fact that the scattering angles of electrons could not be regarded as small under the experimental conditions:[10,11]

$$\delta(E-E'-h\nu)=\frac{2\pi}{hqv_F}\delta\left(\cos\psi-\frac{q}{2k_F}-\frac{s}{v_F}\right)$$

(ψ is the angle between the electron momentum before the scattering and the phonon momentum). After the integration over the angles we were left with the factor $(2\pi/hqv_F)\sin\psi$. At $q = 2k_F$ the value of $\sin\psi$ vanished and this corresponded to a Migdal-Kohn singularity in the electron-phonon interaction. The value of $P(\nu)$ at such a singularity was governed by the electron relaxation time:[14]

$$P\propto(\sin\psi+1/\omega\tau)^{-1}.$$

In our calculations we assumed that $\omega\tau = 100$.

The value of the parameter $\omega\tau$ was not critical due to the relative weakness of the interaction between the electrons and phonons whose momentum was located in

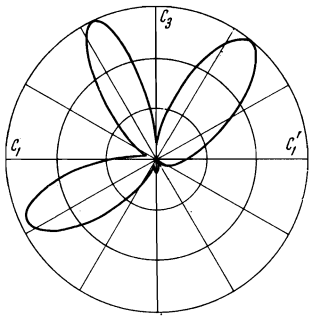

FIG. 1

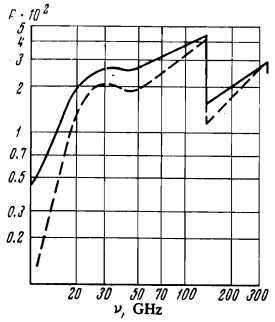

FIG. 2

FIG. 1. Anisotropy of the probability of the scattering of electrons by phonons (arbitrary scale).

FIG. 2. Dependence of the scattering probability on the phonon frequency. The dashed curve represents the transport scattering probability.

the C_2C_3 plane: the main lobes of the scattering diagram (Fig. 1) were located in the C_1C_3 plane and the angle between the momenta was $\psi \approx 50°$. The dependence of the scattering probability on the frequency of the scattering phonons obtained in this way is plotted in Fig. 2. The transport probability of the scattering $P_t = P(1 - \cos\theta)$, where θ is the scattering angle depending on the phonon frequency, was calculated in a similar manner. The dependence $P_t(\nu)$ is shown dashed in Fig. 2.

TRANSPORT RELAXATION TIME

The temperature dependence of the transport relaxation time was calculated from the formula[13]

$$\tau^{-1}=4\int_0^\infty \frac{h\nu}{kT}\frac{P_t(\nu)\,d\nu}{[\exp(h\nu/kT)-1][1-\exp(-h\nu/kT)]}.$$

The results of this calculation are plotted in Fig. 3. For the sake of comparison, Fig. 3 includes the experimentally determined temperature dependence of the conductivity of bismuth.[11] We can see that the main contribution to the conductivity of bismuth is made by the light electrons[7] so that the results of the calculation should be compared with the total conductivity without any attempt to distinguish the various groups of carriers. The experimental points in Fig. 3 are plotted on the assumption that $\tau = A\sigma$ with the coefficient A selected so that the relaxation times in the 4–7°K range are in agreement with the rigorous conversion of the conductivity to the relaxation time given by Hartman in[5].

The calculated and experimental values of the relaxation time differ by a constant factor ≈1.3, which lies within the limits of the error in the absolute determination of the deformation potential and the method adopted to determine τ from the results of Kopylov and Mezhov-Deglin.[11] The temperature dependence of the resistivity agrees very well with the theoretical calculations in the 1.2–7°K range and the characteristic deviations from the quadratic law are also in good agreement with calculations (it is assumed in[11] that $\rho \propto T^{1.7}$).

According to the calculations, the dependence $\rho(T)$ should be linear and $T > 10°K$, whereas it is found experimentally that the linear dependence begins from 15–30°K. This discrepancy can be explained by, for example, the intervalley scattering of electrons by phonons of ≈40°K energy,[5] whose contribution is exponentially small in the $T \lesssim 5°K$ range. The most convincing results would have been obtained by a comparison of a calculated curve with the experimental results for the 0.3–2°K range, but such experiments have not yet been carried out.

WIDTH OF CYCLOTRON RESONANCE LINE

We compared the results reported in[10] with the width of the Landau levels of electrons corresponding to the minimal central section of the Fermi ellipsoid calculated as a function of temperature and the distance to the Fermi level:

$$\Gamma=\int_0^\infty (1+f_+-f_-+2N)P(f)\,df,$$

$$f_\pm=[\exp(E\pm hf)/kT+1]^{-1}.\quad N=[\exp(hf/kT)-1]^{-1}.$$

The amplitude of the quantum oscillations of the scattering probability in the investigated range of frequencies and temperatures was known to be negligibly small[15] and the calculations could be carried out ignoring the magnetic field.

The width of the cyclotron resonance line is governed by the sum of the widths of the upper and lower levels participating in resonance. The main contribution is made by the electrons undergoing transitions between the Landau levels located symmetrically with respect to the Fermi level so that $\tau(f) \approx 1/2\Gamma(f/2)$. Allowance for the other levels, whose width is greater, results in a slight broadening of the cyclotron resonance line. This broadening depends on the nature of the function $\Gamma(f)$ and does not exceed 15%.

The experimental dependence[10] in the frequency range $f \leq 40$ GHz is

$$\tau^{-1}[\text{nsec}^{-1}]=\left(\frac{f[\text{GHz}]}{26.5}\right)^3+KT^2,\ K=\left(\frac{f[\text{GHz}]}{42}\right)\ [\text{nsec}^{-1}\cdot°\text{K}^{-2}].$$

At higher frequencies the coefficient K ceases to vary with the frequency and the dependence $\tau^{-1}(f)$ becomes linear. The linear fall of τ with increasing frequency is observed at least up to 1000 GHz.[16] The calculated dependence differs considerably from these experimental results. The calculations yield a quadratic temperature dependence of the relaxation time:

$$\tau^{-1}=0.11T^2\ \text{nsec}^{-1}\cdot°\text{K}^{-2},$$

where the coefficient in front of T^2 is practically independent of the frequency. A coefficient of this order of magnitude has been observed experimentally at 10 GHz.

The calculated frequency dependence of the Landau level width is plotted in Fig. 4. The same figure in-

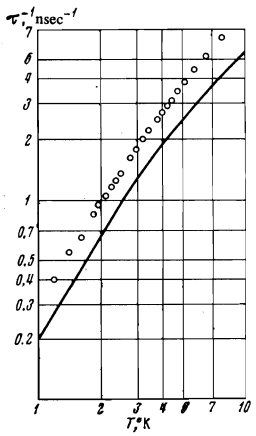

FIG. 3. Temperature dependence of the transport relaxation time. The continuous curve represents calculations and the points are experimental values (taken from [11]).

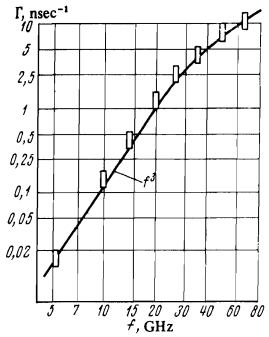

FIG. 4. Frequency dependence of the Landau levels. The continuous curves represent calculated values multiplied by 125. The rectangles are the experimental values taken from [10].

cludes the experimental dependence $\Gamma(f)$.[10] The calculated values of the level width are 125 times smaller than the experimental widths; the agreement between the nature of the dependence is thus surprising.

It should be pointed out that the ratio of the electron and hole relaxation times is equal to that expected for the electron-phonon interaction. In fact, the average deformation potential of electrons is 3 eV and that of holes is 1 eV.[4] The corresponding scattering probabilities are proportional to the square of the deformation potential and should differ by one order of magnitude, in agreement with the experimental observations.[10]

DISCUSSION

Thus, the intravalley scattering of electrons by phonons explains the temperature dependence of the dc resistivity of bismuth and the width of the cyclotron resonance line at 10 GHz as well as the ratio of the electron and hole relaxation times. The frequency dependence of the relaxation time is stronger than that predicted theoretically; moreover, the frequency dependence of the coefficient in front of the square of the temperature cannot be explained.

Our analysis shows that no modification of the function P(f) can yield a value of the ratio of the frequency and temperature contributions to the scattering of bismuth which would agree with the experimental results. Consequently, it is not possible to explain fully the observed dependences on the basis of the model assumed above.

Goy and Castaing[17] analyzed the isotropic model of the electron-phonon scattering for $q \ll k_F$ and obtained the interpolation formula

$$\tau^{-1} \propto (kT)^3 + (hf/3.9)^3 + 0.34hf(kT)^2.$$

The results of a study of the carrier relaxation in lead and indium[17,18] can be described satisfactorily by this formula. The ratio of the frequency and temperature contributions to the scattering obtained in our calculations is of the same order of magnitude, which shows that this ratio depends weakly on the nature of the model.

According to Gurzhi,[19] the scattering of electrons by electrons (holes) can be described approximately by the formula

$$\tau^{-1} \propto (kT)^2 + (hf/2\pi)^2.$$

Consequently, the electron-electron scattering model also fails to explain the observed ratio of the frequency and temperature contributions to the observed scattering. Moreover, this model cannot explain the deviation of the temperature dependence of the resistivity of bismuth from the quadratic form or the observed kink in the frequency dependence of the width of the cyclotron resonance line because these effects occur at 50 GHz ($\approx 2.5^\circ$K), which is much less then the characteristic frequency (energy) which governs the electron-electron interaction: $E_F/h \approx 7000$ GHz.

The intervalley scattering on 40°K phonons ($f \approx 800$ GHz) is characterized by an exponential temperature dependence of the relaxation time at $T < 5^\circ$K (when the temperature is raised from 0.3 to 1°K the intervalley relaxation time changes by 4—5 orders of magnitude) and the temperature contribution to the scattering exceeds considerably the frequency contribution even at $T = 0.5^\circ$K. These dependences differ greatly from those observed experimentally.

In principle, we can explain all the observed dependences by introducing different models of the inelastic scattering of electrons by impurities. If we select a sufficiently complex spectrum of the scattering particles (three or four energy levels separated by 20—50 GHz), we can obtain practically any ratio of the frequency and temperature contributions to the scattering. However, we must then assume that the probability of the inelastic scattering is at least two orders of magnitude higher than the probability of the elastic scattering by the same impurities, which is only possible if the impurity charge is identical with the charge of bismuth ions. A strong broadening of the cyclotron resonance line has been observed at high frequencies in various laboratories[10,16] for bismuth samples of different origin which, obviously, have different compositions and concentrations of impurities, and the relaxation times obtained are in agreement.

It follows from this agreement that the introduction of such very complex hypotheses on the nature of the scattering of electrons by impurities cannot be justified. On the other hand, it is difficult to solve this problem by an experimental study of the influence of impurities on the scattering of electrons by increasing the impurity concentration because it would not be possible to observe the cyclotron resonance below 30 GHz since the relaxation time would be too short. The scattering mechansim might be determined unambiguously by investigating the cyclotron resonance at frequencies of 1–3 GHz at temperatures $T \lesssim 0.1^\circ$K in single crystals with a residual relaxation time of 10–20 nsec but it is not clear how one could improve the quality of the samples so as to increase the relaxation time from 1–2 nsec reported in[10].

It would be very interesting to study in detail the dependences of the hole relaxation time on the temperature and energy above the Fermi level. The most convenient method for studies of the hole relaxation time would be the measurement of the damping of magnetoplasma waves.[12] However, it is not clear whether this would give the relaxation time of excited carriers or those at the Fermi level. This requires a further theoretical study.

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