

those operations which send \mathbf{k}_0 into $-\mathbf{k}_0$ (i.e., J and $3C_2$). This follows since $\exp(-i2\mathbf{k}_0 \cdot \mathbf{r}_\alpha) = -1$ and $\exp(i\mathbf{k}_0 \cdot \mathbf{r}_\alpha) = \pm i$ when the origin is chosen at one of the β sites. Relating these transformation properties of the functions $X^\alpha(L)$, $Y^\alpha(L)$, and $Z^\alpha(L)$ to the transforma-

tion properties of R and S_\pm given in Table II, we obtain

$$R = iZL^\alpha, \quad S_+ = +(X_L^\alpha + iY_L^\alpha)/\sqrt{2}$$

and

$$S_- = -(X_L^\alpha - iY_L^\alpha)/\sqrt{2}.$$

Magnetoresistance of n -Type Germanium in the Phonon-Assisted Hopping Conduction Range at High Magnetic Fields*

J. A. CHROBOCZEK† AND R. J. SLADEK

Department of Physics, Purdue University, Lafayette, Indiana

(Received 24 June 1966)

The transverse magnetoresistance ρ/ρ_0 of phonon-assisted hopping conduction in n -type germanium samples having phosphorus concentrations N_d between 5×10^{15} and 2×10^{16} cm^{-3} has been measured at 4.2°K as a function of the strength and orientation of the magnetic induction \mathbf{B} in a (110) plane up to much higher values of B (78 kG) than used in previous work (30 kG). It is found that ρ/ρ_0 is an increasing function of B^2/N_d up to the highest values of B and depends on the direction of \mathbf{B} , the anisotropy being more complicated at higher B . For $\mathbf{B} \parallel [001]$, ρ/ρ_0 increases most rapidly (almost exponentially) with B . Following Sladek and Keyes these effects are explained qualitatively in terms of the influence of the magnetic field on the donor wave functions. A simple extension of the magnetoresistance theory of Mikoshiba is made and compared with our anisotropy curves. A reasonably good fit requires that the difference in phase between wave functions on adjacent donors have a much smaller effect than expected of following Mikoshiba's method of choosing a certain parameter ϵ . A more reasonable choice of ϵ , which also includes the influence of the decrease in size of the donor wave functions due to the magnetic field, greatly reduces the calculated phase effect. A final choice of values for ϵ and a parameter relating the spacing to the concentration of impurities yields a calculated anisotropy curve which reproduces the main features of the experimental curve in remarkable detail.

MAGNETORESISTANCE of n -type Ge in the phonon-assisted hopping conduction range has been observed previously by Sladek and Keyes (SK),¹ Yamanouchi,² and Lee and Sladek³ at magnetic fields up to 30 kG. The observations of SK were shown to be consistent with the theory of Mikoshiba,⁴ which appeared shortly after their experiment. Our present results concern the region of higher magnetic fields, up to 78 kG. The magnitude of the magnetoresistance in this region is much larger, and the anisotropy of the effect is larger by an order of magnitude and has more complicated structure, than at lower fields. In this paper we compare our observations with the theory of Mikoshiba and show that the new features of the effect are compatible with the previous observations.

Miller and Abrahams⁵ showed that the transition rate for phonon-induced tunneling of an electron between

two donors, differing slightly in energy due to the presence of an ionized acceptor in their vicinity (Mott's⁶ model), is proportional to the square of its resonance energy, $|W|^2$. Mikoshiba⁴ followed essentially the treatment of Miller and Abrahams in his calculations of the resonance energy but used wave functions derived by including in the Hamiltonian a term quadratic in the magnetic field \mathbf{H} . His wave functions decreased in spatial extent as the magnetic field increased (size effect). The magnetic field also introduces a phase difference between the wave functions of neighboring donors (phase effect). Because of mathematical difficulties Mikoshiba treated the size and phase effects separately and considered only the component of the donor wave function derived from one conduction-band valley. The resonance energies for the size effect $W^{(s)}$ and the phase effect $W^{(f)}$ were then squared and averaged over pairs of donors to yield quantities proportional to the transition rate for electron jumping, i.e.,

$$\langle |W_p^{(s)}|^2 \rangle_{\text{av}} \cong \langle |W_{p0}|^2 \rangle_{\text{av}} \exp \left\{ -\frac{1}{48} \frac{\kappa R^3}{m_i^* c^2} H^2 \cos^2 \varphi_p \right\} f_1, \quad (1)$$

$$f_1 = \frac{9}{16} \left\{ \int_0^1 dx (1+x^2) \exp \left[-\frac{1}{32} \frac{\kappa R^3 x^2}{m_i^* c^2} H^2 \cos^2 \varphi_p \right] \right\}^2,$$

⁶ N. F. Mott and W. D. Twose, *Advan. Phys.* **10**, 107 (1961).

* Work supported by the Advanced Research Projects Agency.

† On leave of absence from Institute of Physics, Polish Academy of Sciences, Warsaw, Poland.

¹ R. J. Sladek and R. W. Keyes, *Phys. Rev.* **122**, 437 (1961).

² C. Yamanouchi, *J. Phys. Soc. Japan* **18**, 1775 (1963).

³ W. W. Lee and R. J. Sladek, *Bull. Am. Phys. Soc.* **10**, 546 (1965); W. W. Lee, thesis, Purdue University, 1966 (unpublished).

⁴ N. Mikoshiba, *Phys. Rev.* **127**, 1962 (1962).

⁵ A. Miller and E. Abrahams, *Phys. Rev.* **120**, 745 (1960).

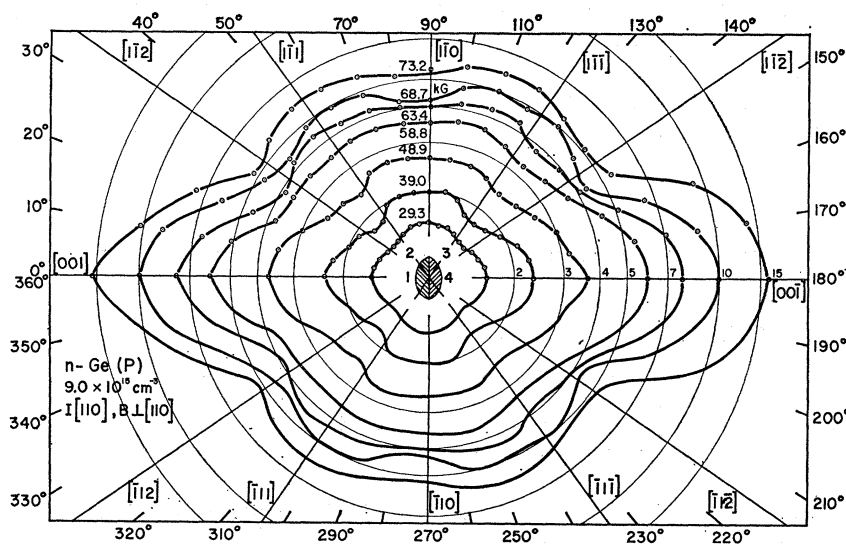


FIG. 1. Magnetoresistance ρ/ρ_0 as a function of the direction of the magnetic field relative to the crystallographic axes in P-doped, *n*-type Ge having 9×10^{15} donors/cm³ for different magnetic-field strengths at 4.2°K. Logarithmic polar coordinates are used. The donor wave function in the center is indicated schematically in the center as being comprised of four pancake-like components.

and

$$\langle |W_p^{(f)}|^2 \rangle_{av} \cong \langle |W_{p0}|^2 \rangle_{av} \exp \left\{ -\frac{1}{16} \frac{\epsilon \kappa R^3}{m_i^* c^2} H^2 \sin^2 \varphi_p \right\} f_2, \quad (2)$$

$$f_2 = \frac{4}{\pi} \int_0^1 dx (1-x^2)^{1/2} \exp \left[-\frac{1}{16} \frac{\epsilon \kappa R^3 x^2}{m_i^* c^2} H^2 \sin^2 \varphi_p \right],$$

where W_{p0} is the zero-field resonance energy, κ is the dielectric constant, φ_p is the angle between the direction of the magnetic field \mathbf{H} and the p th valley axis \mathbf{a}_p , R is the average distance between neighboring donors, and m_i^* is the effective mass perpendicular to the valley axis. Involved in Eqs. (1) and (2) is the assumption, which is known to be quite good for the conduction band of Ge,⁷ that $m_i^* \ll m_i^*$, the effective mass parallel to the valley axis. The quantity ϵ appearing in (2) is defined by the relation

$$(\epsilon a^{*2}/\hbar c)^2 = \epsilon (a^{*3} \kappa / m_i^* c^2);$$

a^* is an effective Bohr radius about which we shall be more explicit later.

Since Mikoshiba treated the influence of the magnetic field on the size and the phase of the wave functions independently of one another, he assumed that the total transition probability for hopping between donors is given by the product of the transition probabilities calculated separately for each effect.

Our experimental results were obtained at 4.2°K for 3 phosphorus-doped, *n*-type Ge samples having donor concentrations from 5.4×10^{15} to 2.0×10^{16} cm⁻³. The donor concentrations were deduced from the Hall coefficients at room temperature and Lee's estimates of

the compensation.⁸ For this concentration range at 4.2°K hop conduction is the dominating mechanism of charge transfer.⁸

We measured the dc magnetoresistance as a function of the magnetic-field strength up to 78 kG and of the orientation of the magnetic field in the plane perpendicular to the current direction [110]. The magnetic field was provided by a 1-in.-diam-bore Westinghouse superconducting solenoid. Voltages were measured with an Applied Physics Corporation Model 30 vibrating-reed electrometer, and Leeds and Northrop type K-2 potentiometer, and a recording potentiometer.

The dependence of the magnetoresistance ρ/ρ_0 on crystallographic orientation of the magnetic field was found to be similar for all three samples, and representative results (for one sample) at various field strengths are given in Fig. 1. The shapes of the curves can be interpreted qualitatively by considering that the effective magnetic field $H \cos \varphi_p$ shrinks the p th component of the wave function, that the jumping probability is appreciable only for components of the wave functions of the same p , as was shown to be the case of zero magnetic field,⁵ and jumping takes place only in the direction in which a component of the wave function is large in the spatial extent,¹ i.e., in the direction transverse to the valley axis since $m_i^* \ll m_i^*$. Thus, one can readily see that for \mathbf{H} in the [001] direction, $H \cos \varphi_p$ is equal for all the valleys since they are located along $\langle 111 \rangle$ directions in *n*-type Ge, and all the components of the wave function are affected equally by the relatively strong effective field $H/\sqrt{3}$. For some directions the effective field can even be zero for particular valleys. For example, for the [110] direction, the effective field is zero for two valleys. This explains qualitatively the existence of a maximum magnetoresistance in the [001] direction and

⁷ See for example, W. Kohn, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 257.

⁸ H. Fritzsche, *J. Phys. Chem. Solids* 6, 69 (1958).

a relative minimum in the $[1\bar{1}0]$ direction. In general, since the magnetic field affects each constituent of the donor wave function in a different way, depending on the direction of the magnetic field, the distortion of the donor wave function will depend on the direction and strength of the field. The qualitative explanation of the phase effect is more difficult because of the more complicated averaging operations involved in it. However, with the same assumptions as used above, the difference in phase of the wave functions of donors in a given pair would be influenced only by the component of the magnetic field along the p th valley axis. This component equals $H \cos \varphi_p$ and the discussion for the size effect is fully applicable. However, due to the different orientations of donor pairs, the average influence of the magnetic field on the p th component of a donor wave function passes through a nonzero minimum for $\mathbf{a}_p \perp \mathbf{H}$. This explains the appearance of the factor α in Eq. (4) given below.

This rather satisfactory explanation of the main features of the effect encouraged us to apply the single-valley theory of Mikoshiba to the many-valley case. Following the method of SK, the conductivity tensor was assumed to be a linear combination of the conductivity tensors derived from particular components of the donor wave functions. Thus

$$\sigma = \sum_p \alpha_p (1 - \mathbf{a}_p \mathbf{a}_p) \langle |W_p|^2 \rangle_{av}. \quad (3)$$

The coefficients α_p were assumed to be field-independent and equal in magnitude. The transition rate for a particular component of the donor wave function was assumed to be given by

$$\langle |W_p|^2 \rangle_{av} = \langle |W_p^{(s)}|^2 \rangle_{av} \langle |W_p^{(f)}|^2 \rangle_{av},$$

where $\langle |W_p^{(s)}|^2 \rangle_{av}$ and $\langle |W_p^{(f)}|^2 \rangle_{av}$ are given by Eqs. (1) and (2), respectively.

The results deduced thus from the theory do account for the main features of our data, although complete quantitative agreement is not obtained.

First of all, H and R appear in W_p always in the combination $H^2 R^3 \propto H^2 N_d^{-1}$, and Fig. 2 shows that the data for different field strengths, and for samples having different concentrations of donors, do indeed fall on one curve for a particular direction of magnetic field.

Second, the magnetic field parallel to the $[001]$ direction has equal projections on all the valley axes. The summation of the transition probabilities is particularly simple in this case and the calculated ρ/ρ_0 is related simply to the expressions for $|W_p|^2$ given in Eqs. (1) and (2), and is almost an exponential function of H^2 . This is also found experimentally, as can be seen from Fig. 2. For comparison ρ/ρ_0 for the $[1\bar{1}0]$ direction is also shown in Fig. 2. As explained before, ρ/ρ_0 should grow slower and should deviate from the exponential form due to the asymmetric positioning of the magnetic-field vector in relation to the components of the wave function.

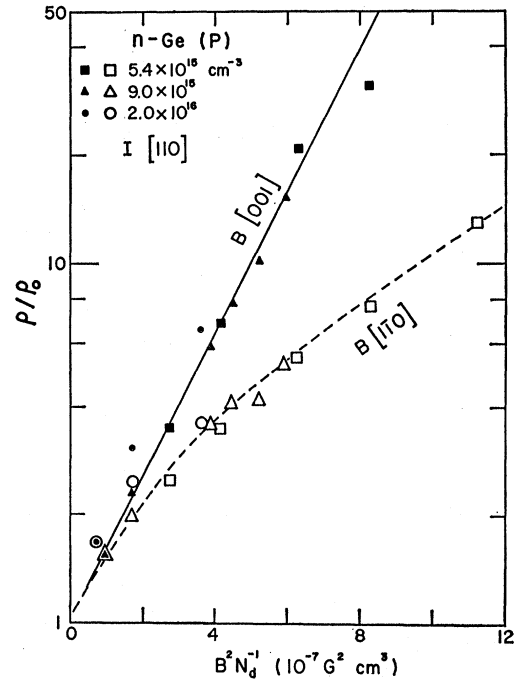


Fig. 2. Magnetoresistance ρ/ρ_0 as a function of $B^2 N_d^{-1}$ for three samples having different concentrations of donors for the magnetic field in the $[1\bar{1}0]$ and $[001]$ directions.

It should be noted that the empirical formulas of SK given by Eqs. (3) and (4) can also account for many features of our data, as can be seen from Fig. 3.

Direct computations of ρ/ρ_0 from Eq. (3) present some difficulties mainly because the values of the constants in Eqs. (1) and (2) are not well known. The constant s in the relation $R = s N_d^{-1/3}$ is estimated to have quite different values by various investigators.^{1,4,6} The constant ϵ which appears in Eq. (2) depends on the value of the effective Bohr radius a^* .

In our first calculations we used $s=1$ and $\epsilon=0.62$ for P-doped Ge, as deduced following Mikoshiba's method.⁴ The function ρ/ρ_0 obtained with these parameters closely resembled the experimental orientation dependence, the positions of the extrema coincided and their relative heights were very similar. However, the absolute value of the magnetoresistance obtained from the calculations was higher than the observed magnetoresistance by as much as a factor of 5.5 for the highest field.

The size effect alone gave values lower than the experimental results suggesting that the phase effect might have been overestimated by the theory. Additional computations based on the results of SK and the low-field theory of Mikoshiba⁹ confirmed this hypothesis. This can be seen as follows. The SK empirical formula for the single-valley magnetoresistance function,

$$f_p(B) = f_p(0) \exp\{\alpha + \beta |\cos \varphi_p|\}, \quad (4)$$

⁹ N. Mikoshiba, J. Phys. Chem. Solids 24, 341 (1963).

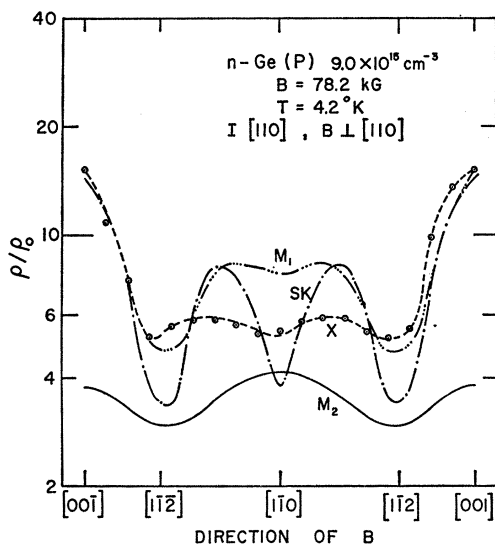


FIG. 3. Comparison of experimental data with computed magnetoresistance. Curve X, experimental results; SK, calculated from the empirical formula of Sladek and Keyes for $\alpha = 6.4 \times 10^{-6}$, $\beta = 8.5 \times 10^{-4}$; M_1 , calculated from a multivalley adaptation of Mikoshiba's theory with $R = N_d^{-1/3}$, $\epsilon = 0.13$; M_2 , same as M_1 except $R = 0.7N_d^{-1/3}$, $\epsilon = 0.23$.

$[f_p(B)]$ corresponds to $\langle |W_p|^2 \rangle_{av}$ in Eq. (3), was fitted to the data using a nonlinear regression method, and the ratio α/β was found to be about 10^{-2} . This indicates that the phase effect plays a less important role than the size effect.

From the intermediate field theory,⁴ at 10 kG the ratio $W_p^{(s)}/W_p^{(f)}$ was about 0.8, while from the low-field theory⁹ $W^{(s)}/W^{(f)}$ was about 1.1. This implies that the value of ϵ deduced following Mikoshiba is too large. If we estimate the effective Bohr radius from the ionization energy, ϵ_I , the value of ϵ is much smaller. If $\epsilon_I = 12.76$ meV is used for a P donor¹⁰ to estimate a^* ,

¹⁰ J. H. Reuszer and P. Fisher, Phys. Rev. 135, 1125 (1964).

we obtain $a^* = 35.3 \text{ \AA}$ and thereby the value of $\epsilon = 0.34$. If we further assume that the magnetic field increases the ionization energy of a donor, following Yafet *et al.*,¹¹ for $B = 75 \text{ kG}$, $a^* = 24 \text{ \AA}$, we obtain $\epsilon = 0.23$.¹² Furthermore, according to Mott and Twose,⁶ a value of $s = 0.7$ gives the best fit between theoretical and experimental resistivity values. The curve M_2 in Fig. 3 gives the calculated values of magnetoresistance for the constants $s = 0.7$, $\epsilon = 0.23$. A series of consecutive adjustments of the constants gave finally the results indicated by curve M_1 , for $s = 1$ and $\epsilon = 0.13$.

The value of ϵ is surprisingly small, indicating that the contribution of the phase factor is relatively small, at least for high magnetic fields.

The rather poor fit of the calculated results in the vicinity of the $[\bar{1}\bar{1}0]$ direction indicates that the wave functions most strongly affected by the magnetic field contribute less strongly to the conductivity than predicted by Eq. (3). This may indicate that the coefficients α_p are decreasing functions of the effective field. This seems to be consistent with a possible energy shift of the valleys induced by the magnetic field. The constants on which the single-valley theory depends, as well as its correctness, might be most easily established experimentally by measuring the magnetoresistance on a sample subjected to $[111]$ uniaxial compression since the experimental data could be compared directly to the single-valley theory.

We wish to acknowledge experimental assistance of Dr. W. W. Lee, useful discussions with Dr. W. W. Lee, Professor S. Rodriguez, and Professor H. M. James, and help in computer programming by J. Cavanagh and by the high-energy physics group at Purdue.

¹¹ Y. Yafet, R. W. Keyes, and E. N. Adams, J. Phys. Chem. Solids 1, 137 (1956).

¹² This corresponds to the assumption that the size effect has an influence on the phase effect through the change of a^* .