Scattering Anisotropies in *n*-Type Silicon

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Measurements have been made of magnetoresistance effects in several relatively pure samples of *n*-type silicon for the purpose of obtaining information on scattering anisotropies. The results indicate that the ratios of relaxation times parallel and perpendicular to a constant-energy-spheroid axis in the six-valley conduction band of silicon are $\tau_{\parallel}/\tau_{\perp}\approx\frac{2}{3}$ for acoustic-mode intravalley lattice scattering and $\tau_{\parallel}/\tau_{\perp}>1$ for ionized-impurity scattering. Intervalley lattice scattering, important at higher temperatures, is isotropic.

I. INTRODUCTION

THIS paper describes an investigation in which the objective has been to learn as much as possible about anisotropies of the scattering of electrons in the conduction band of silicon by making careful measurements of the magnetoresistance effects which are sensitive to these anisotropies.

It is now well established that the bottom edge of the silicon conduction band is composed of six equivalent energy minima, or valleys, located at 0.85 of the way from the center of the Brillouin zone to the [100] zone faces.[1] The surfaces of constant energy ϵ at each valley are spheroids represented by the expression,

$$\epsilon=\frac{\hbar^2}{2}\left(\frac{2k_{\perp}^2}{m_{\perp}}+\frac{k_{\parallel}^2}{m_{\parallel}}\right), \tag{1}$$

where the k's are electron wave numbers, and $m_{\perp}$ and $m_{\parallel}$ are effective masses in directions perpendicular and parallel, respectively, to the spheroid axis. These masses are known from cyclotron resonance experiments. The most recent experiments[2] give $m_{\perp}=(0.192\pm0.001)\,m_0$ and $m_{\parallel}=(0.90\pm0.02)\,m_0$, where m_0 is the mass of a free electron, but earlier experiments[3] gave $m_{\perp}=(0.19\pm0.01)\,m_0$ and $m_{\parallel}=(0.98\pm0.04)\,m_0$. The reason for the discrepancy in the $m_{\parallel}$ values is not yet known.

The only important scattering agents in the samples of *n*-type silicon studied here are lattice vibrations and ionized impurities. Scattering by lattice vibrations can be expected to cause two different types of electronic transitions; viz., transitions between states within a single valley (called intravalley acoustic, or simply acoustic scattering throughout this paper), and transitions between states in different valleys (called intervalley scattering).[4,5] These two mechanisms appear to be of the same order of importance at room temperature in silicon, with intervalley about twice as strong as acoustic scattering according to our estimates.[6] Intervalley scattering decreases in relative importance with decreasing temperature, since it requires high-energy phonons which are excited in appreciable numbers only at the higher temperatures. Scattering by ionized impurities involves only transitions within a single valley, and of course it varies in importance relative to lattice scattering according to the impurity content and temperature of a sample.

Intervalley scattering is expected on reliable theoretical grounds to be isotropic, but acoustic and ionized-impurity scattering will both generally be anisotropic in a conduction band like that of silicon.[4] Herring and Vogt[7] have shown that anisotropic scattering in this case can be described by a relaxation-time tensor diagonal in the principal axes of an energy spheroid, provided that all the scattering processes either conserve carrier energy or randomize carrier velocities. The scattering processes to be considered here all satisfy these requirements, and therefore the anisotropy of the scattering will be describable in terms of relaxation times $\tau_{\perp}$ and $\tau_{\parallel}$ for directions perpendicular and parallel, respectively, to the spheroid axis. Thus, the program of the present study is to determine the ratio of $\tau_{\parallel}$ to $\tau_{\perp}$ for each type of scattering mechanism by analysis of magnetoresistance data. A preliminary report of some of the results has already been made.[6]

II. EXPERIMENTAL RESULTS

We have measured magnetoresistance effects on several samples of rather highly purified *n*-type silicon cut from single crystals grown mostly by the floating-zone method. One sample (SP1D) was cut from a crystal grown by the Czochralski method, but the others were from three different floating-zone crystals, designated as SP6, SP8, and SP4 in order of increasing impurity content. The samples were all of either of two "bridge-type" shapes, shown in Fig. 1, with electrical contacts formed by alloying Sb-doped Au spots to the

[1] G. Feher, Phys. Rev. **114**, 1219 (1959).
[2] C. J. Rauch, J. J. Stickler, H. J. Zeiger, and G. S. Heller, Phys. Rev. Letters **4**, 64 (1960).
[3] See, for example, R. N. Dexter, H. J. Zeiger, and B. Lax, Phys. Rev. **104**, 637 (1956).
[4] C. Herring, Bell System Tech. J. **34**, 237 (1955).
[5] W. A. Harrison, Phys. Rev. **104**, 1281 (1956), has shown that intravalley scattering by optical modes is probably unimportant in *n*-type silicon, and it is therefore neglected here. Actually, it follows the same type of scattering law and has all the same characteristics as intervalley scattering, so that any such scattering can be considered to be included effectively as part of the intervalley contribution.
[6] D. Long and J. Myers, Bull. Am. Phys. Soc. **5**, 195 (1960).
[7] C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).

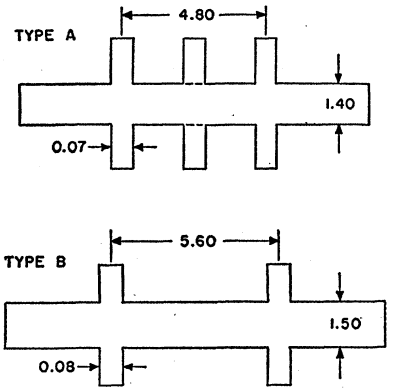

FIG. 1. Diagrams of shapes of silicon samples. Dimensions are in millimeters.

silicon. The type *A* samples had six voltage-probe side-arms to begin, but the middle ones were sometimes removed later. It is necessary to pay attention to sample shape, because the presence of the side-arms generally has an effect on quantities being measured. For example, a sample with side-arms of some finite width will exhibit a slightly lower apparent resistivity than if the side-arms were absent, because the effective sample width is greater. We have measured the difference between these two situations by cutting out stainless steel scale models of our samples (after Herring, Geballe, and Kunzler[8]) and have found that the side-arm error is about 5% for the type *A* sample and about 3% for the type *B*. Removal of the middle side-arms of a type *A* sample cuts the error in half. All of the data reported here were taken on samples with etched surfaces, but some similar measurements on lapped-surface samples gave nearly the same results for the particular effects studied.[8] The measuring equipment and procedures were essentially the same as described previously.[9]

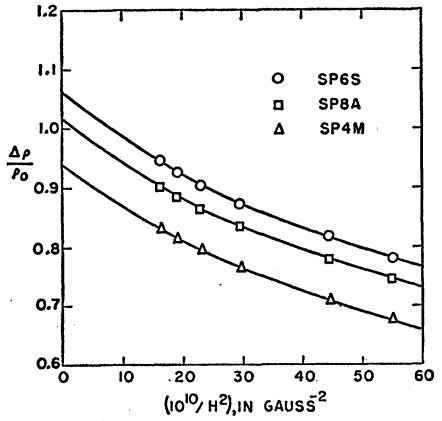

FIG. 2. Plot of [111]-directed longitudinal magnetoresistance vs inverse of square of magnetic field strength in three samples of *n*-type silicon.

[8] C. Herring, T. H. Geballe, and J. E. Kunzler, Bell System Tech. J. **38**, 657 (1959).
[9] D. Long and J. Myers, Phys. Rev. **109**, 1098 (1958).

A list of the samples studied, including the shapes, crystallographic orientations, and the approximate concentrations N_D of donor (phosphorus) and N_A of acceptor (boron) impurities is given in Table I. The impurity concentrations have been determined from Hall data by methods described previously.[10,11] It should be noted that SP6A and SP4A are the same samples on which we had studied the electrical properties quite extensively at temperatures below 100°K in a recent investigation of impurity scattering in *n*-type silicon.[10]

Figure 2 shows the results of measurements of the magnetic field dependences at 77°K of the longitudinal magnetoresistance (field parallel to current) in a [111] direction up to 25 000 gauss on three of the samples of Table I. The curves are plots of the fractional increase of resistivity $\Delta\rho/\rho_0$ vs the inverse of the square of the magnetic field strength H. The important quantity to be obtained from these data is the infinite-field extrapolated value of $\Delta\rho/\rho_0$. Parabolas in $1/H^2$ have been fitted to the strong-field ends of the curves in Fig. 2 to indicate the proper extrapolations to the $H=\infty$ intercepts.[8] The correction for the error due to the side-arms is particularly straightforward for this experiment, because the magnetic focusing effect of the strong field eliminates all bulging of the current into the side-arms in the limit of infinite field.[8] Thus, one need only correct the zero-field resistivity ρ_0. The correction is about 3% for the samples of Fig. 2, and so the saturation values should be reduced from those shown in Fig. 2 to those listed in Table II. Comparison of Tables I and II indicates that the saturation longitudinal magnetoresistance decreases with increasing impurity concentration.

TABLE I. List of samples of *n*-type silicon, including type of sample shape, crystallographic orientation, and concentrations N_D of donors and N_A of acceptors.

Sample designation	Sample shape type	Orientation of current-flow axis	Orientation of magnetic field in Hall measurement	Approximate impurity concentrations, in cm^{-3} N_D	N_A
SP6A	*A*	[110]	[1$\bar{1}$1]	2.8×10^{13}	0.8×10^{13}
SP6X	*A*	[110]	[001]	1.7×10^{13}	0.8×10^{13}
SP6S	*B*	[111]	···	2.1×10^{13}	0.8×10^{13}
SP8A	*B*	[111]	[1$\bar{1}$0]	5.4×10^{13}	1×10^{13}
SP4A	*A*	[110]	[1$\bar{1}$1]	24×10^{13}	1×10^{13}
SP4M	*B*	[111]	[1$\bar{1}$0]	13×10^{13}	1×10^{13}
SP1D	*A*	[110]	[001]	80×10^{13}	40×10^{13}

Weak-field magnetoresistance and Hall mobility (μ_H) data for samples SP6A, SP6X, SP4A, and SP1D at temperatures of 195°K (dry ice and acetone mixture) and 273°K (ice water) are presented in Table III. The results are given for each sample as values of the fractional resistivity increase $\Delta\rho/\rho_0$ and of the quantity $\mu_H^2H^2$ for two different field strengths very nearly in the "weak-field" range, defined by the condition that $\Delta\rho/\rho_0 \propto H^2$. The Hall mobility is defined by the expression, $\mu_H=R_H/\rho_0$, where R_H is the Hall coefficient. The

[10] D. Long and J. Myers, Phys. Rev. **115**, 1107 (1959).
[11] D. Long and J. Myers, Phys. Rev. **115**, 1119 (1959).

subscript and superscript on each $\Delta\rho/\rho_0$ refer, respectively, to the crystallographic directions of the current and magnetic field. There are three independent weak-field magnetoresistance coefficients for a cubic crystal like silicon,[9] and we have measured either two or all three of them on each sample at each temperature. Note that the particular coefficients measured depend on the sample orientation, but that they are all interrelated in such a way as always to be expressible in terms of three independent coefficients. The relations between the two different sets of coefficients appearing in Table III are as follows:

$$\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{001}=2\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{\bar{1}12}-\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{1\bar{1}1}, \tag{2a}$$

$$\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{1\bar{1}0}=2\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{1\bar{1}1}-\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{\bar{1}12}. \tag{2b}$$

Another relation needed later, which follows from the magnetoresistance "symmetry condition" for n-type silicon[4,7] (to be discussed in Sec. III), is

$$\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{1\bar{1}1}+\frac{2}{3}\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{110}=\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{001}. \tag{3}$$

The middle side-arms had been removed from SP6A and SP6X in these experiments, but were left on the other two samples. Side-arm error corrections have not been made in the data presented in Table III.

III. ANALYSIS AND DISCUSSION OF RESULTS

The objective in this section is to deduce the anisotropies of the lattice and ionized-impurity scattering from the magnetoresistance data of Sec. II. Let us first consider the strong-field magnetoresistance results of Fig. 2 and Table II.

The saturation ($H=\infty$) value of the longitudinal magnetoresistance in the [111] direction in n-type silicon can be shown to be related to the effective masses and relaxation times by the expression,[7]

$$\left.\frac{\Delta\rho}{\rho_0}\right|_{111\ (H=\infty)}=\frac{[2\langle\epsilon\tau_\perp\rangle/m_\perp+\langle\epsilon\tau_{\shortparallel}\rangle/m_{\shortparallel}]}{9\left\langle\dfrac{\epsilon}{2m_\perp/\tau_\perp+m_{\shortparallel}/\tau_{\shortparallel}}\right\rangle}-1, \tag{4}$$

where the $\langle\ \rangle$ indicate Maxwellian averages over the carrier energy ϵ. In situations in which the scattering is largely of one type, a very good approximation to Eq. (4) is given by the following expression.

$$\left.\frac{\Delta\rho}{\rho_0}\right|_{111\ (H=\infty)}\cong\frac{(2m_{\shortparallel}\langle\epsilon\tau_\perp\rangle/m_\perp\langle\epsilon\tau_{\shortparallel}\rangle+1)(m_{\shortparallel}\langle\epsilon\tau_\perp\rangle/m_\perp\langle\epsilon\tau_{\shortparallel}\rangle+2)}{9(m_{\shortparallel}/m_\perp)(\langle\epsilon\tau_\perp\rangle/\langle\epsilon\tau_{\shortparallel}\rangle)}-1. \tag{5}$$

TABLE II. Saturation values of the [111]-directed strong-field longitudinal magnetoresistance at 77°K in samples of n-type silicon.

Sample	Saturation ($H=\infty$) value of $\Delta\rho/\rho_0)_{111}$
SP6S	1.00
SP8A	0.955
SP4M	0.88

In the 77°K magnetoresistance data which face us here, the scattering is undoubtedly predominantly acoustic with some small admixtures of intervalley and ionized-impurity scattering.[6] For pure acoustic scattering, for which $\tau\propto\epsilon^{-\frac{1}{2}}$, the ratios of averages in Eq. (5) would reduce to simple ratios of $\tau_\perp$ and $\tau_{\shortparallel}$, and Eq. (5) would then be exact. Thus, the saturation value of the [111]-directed longitudinal magnetoresistance gives a direct indication of the over-all scattering anisotropy, provided that the effective masses are known.

Equations (4) and (5) do not allow for any effects due to orbital quantization in the strong magnetic field, but these effects are expected to be small under the conditions of our experiments. Herring, Geballe, and Kunzler[8] have considered this quantization problem in great detail for n-type germanium, and their conclusions should be equally applicable to n-type silicon with appropriate modifications for differences in effective masses, etc. Our silicon experiments have extended only up to field strengths which give oscillator level spacings no greater than those which Herring, Geballe, and Kunzler found produced a negligible influence on their germanium magnetoresistance results at 77°K. Actually, we do not really require quite as good accuracy in this initial measurement of lattice scattering anisotropy as

TABLE III. Weak-field magnetoresistance and Hall mobility data for n-type silicon samples at temperatures of 195° and 273°K.

Sample	temperature (°K)	H (Gauss)	Coefficients, $\times10^{-3}$: $\left.\frac{\Delta\rho}{\rho_0}\right\|_{110}^{110}$	$\left.\frac{\Delta\rho}{\rho_0}\right\|_{110}^{1\bar{1}1}$	$\left.\frac{\Delta\rho}{\rho_0}\right\|_{110}^{\bar{1}12}$	$\mu_H^2H^2$
SP6A	195	1640	2.49	1.82	···	5.63
		2240	4.63	3.38	···	10.48
	273	3700	2.96	2.42	···	6.74
		4420	4.20	3.41	···	9.56
SP4A	195	1630	2.11	1.44	···	5.12
		2240	3.98	2.73	···	9.73
	273	3690	2.78	2.23	···	6.48
		4420	3.97	3.14	···	9.29
			$\left.\frac{\Delta\rho}{\rho_0}\right\|_{110}^{110}$	$\left.\frac{\Delta\rho}{\rho_0}\right\|_{110}^{001}$	$\left.\frac{\Delta\rho}{\rho_0}\right\|_{110}^{\bar{1}10}$	$\mu_H^2H^2$
SP6X	195	1510	2.12	2.96	1.05	4.69
		1620	2.44	3.43	1.17	5.41
	273	2960	1.89	2.82	1.06	4.28
		3690	2.93	4.33	1.62	6.58
SP1D	195	1630	1.56	2.05	···	4.03
		2240	2.94	3.83	···	7.61
	273	3700	2.39	3.38	···	5.70
		4420	3.38	4.80	···	8.06

did Herring, Geballe, and Kunzler in their work, so that any small quantization error that might still exist despite the above arguments can be ignored without serious consequences.

Now, it is evident upon examination of the results in Fig. 2 and Table II and comparison of them with Eq. (5) that scattering by ionized impurities is noticeable in the samples at 77°K, and furthermore that the anisotropy of this scattering must be different from that of the lattice scattering in such a way that the $\tau_{\parallel}/\tau_{\perp}$ ratio is *higher* for the impurity scattering. In order to deduce the lattice scattering anisotropy, we have plotted the $(m_{\parallel}/m_{\perp})(\langle\epsilon\tau_{\perp}\rangle/\langle\epsilon\tau_{\parallel}\rangle)$ ratios determined from the saturation values of $\Delta\rho/\rho_0)_{111}$ for the three samples as a function of the strength of impurity scattering (represented by the impurity scattering mobility for each sample, calculated under the considerations outlined in the Appendix), and have then extrapolated to vanishing impurity scattering. The extrapolated result, which should give a good approximation to the lattice scattering anisotropy, is $[(m_{\parallel}/m_{\perp})(\langle\epsilon\tau_{\perp}\rangle/\langle\epsilon\tau_{\parallel}\rangle)]_{\text{lattice scatt.}}\cong 6.7$. For a mass ratio of 4.7, corresponding to the latest cyclotron resonance results, the lattice scattering anisotropy would be $\langle\epsilon\tau_{\parallel}\rangle/\langle\epsilon\tau_{\perp}\rangle\cong 0.70$. We estimate that intervalley scattering makes up roughly 15% of the total lattice scattering at 77°K. The acoustic scattering anisotropy would then be somewhat more pronounced than the total lattice scattering anisotropy, because intervalley scattering is isotropic. Our calculations indicate that the acoustic anisotropy is in the vicinity of $\tau_{\parallel}/\tau_{\perp}=\frac{2}{3}$ for the above mass ratio. The anisotropy value deduced for the acoustic scattering is thus not very sensitive to the amount of accompanying intervalley scattering at a level of around 15%, but considerably stronger intervalley scattering could lower the acoustic τ-ratio markedly. This ratio would also be lowered if there were an error due to the measurements not being carried to strong enough fields to give correct saturation values, but this error is probably minor in the present experiments.

After arriving at the above result, we then calculated the Maxwellian averages in Eq. (4) for the three samples from their known impurity concentrations according to the prescription in the Appendix, where it is assumed that $\tau_{\parallel}/\tau_{\perp}\approx 4$ for ion scattering. Substitution of these averages into Eq. (4) gives a fairly accurate reproduction of the results in Table II. The fit is not very sensitive to the exact value of $\tau_{\parallel}/\tau_{\perp}$ for ionized-impurity scattering, but it does indicate that this ratio is considerably higher than that for acoustic scattering, say, at least a factor of 2 higher.

One can also obtain information about the scattering anisotropies from the weak-field magnetoresistance data. Let us define a quantity W in terms of measured effects and also in terms of the relaxation times and effective masses by the following pair of equations.[7]

$$W=\frac{\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{001}+\mu_H^2H^2}{\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{110}}=\frac{2[(m_{\parallel}/m_{\perp})^2\langle\epsilon\tau_{\perp}^3\rangle/\langle\epsilon\tau_{\perp}\tau_{\parallel}^2\rangle+(m_{\parallel}/m_{\perp})\langle\epsilon\tau_{\perp}^2\tau_{\parallel}\rangle/\langle\epsilon\tau_{\perp}\tau_{\parallel}^2\rangle+1]}{[(m_{\parallel}/m_{\perp})^2\langle\epsilon\tau_{\perp}^3\rangle/\langle\epsilon\tau_{\perp}\tau_{\parallel}^2\rangle-2(m_{\parallel}/m_{\perp})\langle\epsilon\tau_{\perp}^2\tau_{\parallel}\rangle/\langle\epsilon\tau_{\perp}\tau_{\parallel}^2\rangle+1]}. \tag{6}$$

Consider the two temperatures of these experiments, 195° and 273°K. The total scattering should be more nearly iostropic in a pure sample at 273° than at 195° ($\tau_{\parallel}/\tau_{\perp}$ closer to unity), since the isotropic intervalley scattering increases in relative importance with increasing temperature. It follows from Eqs. (6) that W will *increase* in going from 195° to 273° if the other contributions to the relaxation time besides intervalley scattering tend to make $\tau_{\parallel}/\tau_{\perp}<1$; whereas, W will *decrease* if they tend to make $\tau_{\parallel}/\tau_{\perp}>1$.

TABLE IV. Experimental values of W for n-type silicon samples at temperatures of 195° and 273°K.

Sample	195°K H (Gauss)	195°K W	273°K H (Gauss)	273°K W
SP6A	1640	3.66	3700	3.76
	2240	3.66	4420	3.75
SP6X	1510	3.61	2960	3.75
	1620	3.62	3690	3.72
SP4A	1630	3.78	3690	3.80
	2240	3.80	4420	3.80
SP1D	1630	3.90	3700	3.80
	2240	3.89	4420	3.81

Table IV lists the experimental values of W determined for samples SP6A, SP6X, SP4A, and SP1D from the data in Table II, using Eq. (3) when necessary. Results are presented for both field strengths at which the data were taken. No side-arm corrections have been made. Any small geometrical-type errors due to side-arms or to inaccurate measurements of sample dimensions will be independent of temperature and therefore not affect the temperature dependence of W. The observed changes in W are believed to be meaningful, since it was possible to measure the relative values at the two temperatures of the effects constituting W to within errors much smaller than these changes. Table IV shows that W is larger at 273° than at 195°K in the two purest (SP6) samples; whereas, it is almost the same at both temperatures in SP4A, and is smaller at the higher temperature in SP1D. Since the other contribution besides intervalley scattering is almost solely acoustic scattering at these relatively high temperatures in the SP6 samples, the results for them imply that $\tau_{\parallel}/\tau_{\perp}<1$ for the acoustic scattering, in agreement with the strong-field magnetoresistance results. The results in

Table IV for the two less pure samples are qualitatively consistent with the earlier conclusion about the ionized-impurity scattering anisotropy, since they indicate a trend toward a $\tau_{\parallel}/\tau_{\perp}>1$ situation with increasing ion scattering. Note that this impurity scattering anisotropy is of the same type that has been observed in n-type germanium, an analogous material.[12]

We have chosen not to try to deduce anything about the scattering anisotropies from the absolute magnitudes of the experimental W's, since such deductions have proven generally unreliable in previous studies.[8] The magnitude of W is susceptible to several different and rather subtle sources of error. This is a subject on which more study is needed to resolve present confusion.[8] Suffice it to point out that the observed magnitudes are not far from what would be expected for the scattering anisotropies already deduced, even without side-arm corrections. The weak-field experiments and analysis in this paper have been arranged so as to circumvent the necessity of correcting for the side-arm and other such errors in deducing scattering anisotropy properties, but the data can perhaps be profitably analyzed further when a better understanding of these errors has been reached.

The last item to be considered is the symmetry condition among the three independent weak-field magnetoresistance coefficients. One can show that for the conduction band structure of silicon and for scattering describable by relaxation times by the procedure used in this paper, the three coefficients are related by the expression,

$$\left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{110} = \left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{001} - \left.\frac{\Delta\rho}{\rho_0}\right|_{110}^{\bar{1}10}, \tag{7}$$

where all the coefficients are to be measured at the same field strength. In the few cases in Table III in which all three coefficients were measured, it is seen that they satisfy Eq. (7) approximately, but that there is a discrepancy of several percent. This discrepancy is possibly caused mostly by the fact that the $\Delta\rho/\rho_0)_{110}^{\bar{1}10}$ coefficient was measured with the magnetic field lying in the plane of the sample side-arms, a situation which is expected to lead to substantial error. There are side-arm, and perhaps other small errors in the other two coefficients, also. The approximate agreement of the data with Eq. (7) is believed to be satisfactory in view of the possible errors, although this subject should be investigated further.[8]

IV. CONCLUSION

The magnetoresistance experiments reported here have shown that one can represent at least the gross features of the scattering anisotropies in n-type silicon by the relaxation-time ratios $\tau_{\parallel}/\tau_{\perp}\approx\frac{2}{3}$ for acoustic lattice scattering (if the latest mass values are used) and $\tau_{\parallel}/\tau_{\perp}>1$ for ionized-impurity scattering. There is still a need for a much better quantitative understanding of the anisotropies, however, particularly in the impurity scattering case. The lattice scattering result found here is used in a study of the lattice scattering mobility of electrons in silicon,[6] which we expect to report in detail at a later data.

V. ACKNOWLEDGMENTS

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APPENDIX

In a recent study we found that the ionized-impurity scattering of electrons in silicon at temperatures below 100°K is fairly well described by the Brooks-Herring formula, at least when ion scattering is not dominant.[10] This formula gives the ion scattering drift mobility as

$$\mu_{dI}=\eta\frac{T^{\frac{3}{2}}}{N_I(\ln b-1)}, \tag{8}$$

where N_I is the density of ionized impurity atoms, $(\ln b-1)$ is a term which effectively weights the ion concentration N_I according to the amount of shielding of an impurity ion by free carriers and by distribution of electrons over adjacent impurity sites, and η is the coefficient specifying the strength of the scattering. Our latest estimate gives $\eta\cong 7\times 10^{17}$ [units for η throughout are (cm-volt-sec-degrees$^{\frac{3}{2}}$)$^{-1}$]. This value is based both on the considerations mentioned in a note added in proof in reference 10 and on the realization that side-arm corrections (see Sec. II) to the data of reference 10, which had not been made there, would lower all the mobility curves by several percent and thus require a slightly stronger ion scattering for the best fit of the data. Note that there is still considerable uncertainty in η for reasons given in reference 10.

The Brooks-Herring formula takes no explicit account of any anisotropy in the ion scattering. Actually, our previous study can be regarded as having indicated the strength of the ion scattering only for conduction perpendicular to an energy spheroid axis, since 90% or more of the conductivity (when lattice scattering is the dominant mechanism) is composed of conduction in that direction, essentially because $m_{\perp}\ll m_{\parallel}$. Thus, in extending considerations to anisotropic ion scattering, one can use the above value of η to give the strength of the scattering for conduction perpendicular to a spheroid axis. Ham[13] has made calculations for anisotropic ion scattering which suggest that $\tau_{\parallel}/\tau_{\perp}\approx 4$ for n-type silicon. The theory of ionized-impurity scattering rests on somewhat unrealistic assumptions,[8] but the conclusions of

[12] See, for example, R. A. Laff, and H. Y. Fan, Phys. Rev. **112**, 317 (1958).

[13] F. S. Ham, Phys. Rev. **100**, 1251 (1955).

Sec. III seem to indicate that Ham's result is nevertheless at least qualitatively correct for n-type silicon.

In the calculations of Maxwellian averages of relaxation times in this paper, impurity scattering has been added to lattice scattering according to the usual rule,

$$\frac{1}{\tau_\alpha}=\frac{1}{\tau_{L\alpha}}+\frac{1}{\tau_{I\alpha}}, \tag{9}$$

where the subscript α refers to the direction with respect to a spheroid axis, either $\parallel$ or $\perp$. These calculations have had to be carried out numerically. The $\tau_{L\alpha}$, which includes acoustic and intervalley scattering, is given by an expression of the form presented by Herring.[4] The $\tau_{I\alpha}$ depends on energy as,

$$\tau_{I\alpha}=A_\alpha\epsilon^{\frac{3}{2}}, \tag{10}$$

where A_α includes the various parameters in the Brooks-Herring formula, which one obtains by averaging $\tau_{I\alpha}$ according to the usual Maxwellian prescription. The magnitude of $A_\perp$ to be used in calculating $\tau_\perp$ for a particular sample at a particular temperature is determined by the obvious requirement that the ratio of the mobility calculated from Eq. (10) and $A_\perp$ to the total mobility calculated from Eq. (9) must be the same as the ratio of the mobility calculated from the Brooks-Herring formula to the observed mobility. Then, $A_\parallel=4A_\perp$. We have neglected the logarithmic function of ϵ which should really be included in the expression for τ_I simply because its presence would make the calculations much too difficult.[10] The resultant error is not important in our cases of weak ion scattering.

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Dispersion Relations for Bloch Functions

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It is shown that the Floquet factor $e^{ik(E)a}$ is analytic in the upper half complex energy plane, thus enabling a set of four dispersion relations to be derived from this expression as a direct result of the application of Cauchy's theorem. These relations are characterized by their ability to relate the wave number k at one energy to the wave number at all others. In particular, the imaginary part of the wave number k_i in the forbidden gap may be equated to an integral of a function of the real part of the wave number k_r over allowed energies. As an application of these dispersion relations a theorem regarding the location of the branch points has been established.

I. INTRODUCTION

THE physical concept of causality has been exploited in many areas of physics and in the majority of cases has shed valuable light on problems hitherto impossibly difficute to calculate.[1] The statement of microscopic causality alone is usually sufficient to guarantee that the scattering amplitude is analytic in the upper half complex energy plane, so that a direct application of Cauchy's theorem enables relations between the real and imaginary parts of the scattering amplitude to be established. For this reason, we have been motivated to extend a similar technique to the problem of a one-dimensional Schrödinger equation possessing a periodic potential. This equation in its three-dimensional form is essentially the starting point for a large class of problems in solid-state physics; however, exact solutions, even in the one-dimensional case are virtually impossible to obtain, except for a very limited class of periodic potentials (e.g., square well, delta function, sinusoidal, etc.). For this reason, it would be desirable to make some statements about the properties of wave functions in solids without recourse to the details of the actual potential other than its periodicity, causal nature, and general mathematical properties.

In problems involving single potential scattering, the outgoing wave function is related to the incoming wave function by the scattering matrix S, defined by the relation $\psi_{\text{out}}=S\psi_{\text{in}}$. Hence, by analogy it is almost obvious that the Floquet factor $[\lambda(E)=e^{ik(E)a}]$ defined by $\psi(x+a)=\lambda\psi(x)$ plays a similar role for periodic potentials. This immediately tempts us to investigate the analytic properties of $\lambda(E)$ with the aim of being able to derive a set of dispersion relations for this quantity. Unfortunately, causality alone is not sufficient to guarantee that $\lambda(E)$ is analytic in the upper half plane, since it appears that a knowledge of the zeros of the corresponding single potential S matrix is also required.[2] However, it is shown in the Appendix, using a direct approach, that $\lambda(E)$ is analytic in the upper half complex energy plane for a large class of potentials; more-

[1] E.g., M. Gell-Mann and M. Goldberger, Phys. Rev. **96**, 1433 (1954).

[2] This statement is almost self-evident as a consequence of the work by D. S. Saxon and R. A. Hutner, Philips Research Repts. **4**, 81–122 (1949).