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Electrical Resistivity due to Dislocations*

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Regarding a dislocation as a row of weak scatterers, each having spherically symmetric potential, a solution of the linearized Boltzmann equation in the presence of a set of parallel dislocations is obtained. The method consists of expanding the distribution function in terms of spherical harmonics and, as developed here, it is exact for the monovalent metals. For polyvalent metals there are additional contributions to the resistivity tensor which arise from the diffraction peaks which occur when the electron wavelength is smaller than twice the interatomic distance – these terms are estimated by the variational method. By allowing for other mechanisms (impurities) of scattering to be present, it is found that the dislocation resistivity ρ_D depends on the resistivity due to other mechanisms also. Numerical results for these deviations from Matthiessen's rule and for ρ_D for randomly oriented dislocations in aluminum are obtained by taking, after Harrison, the scatterers constituting the dislocations to be vacancies.

I. INTRODUCTION

This paper is mainly concerned with the problem of solving the Boltzmann transport equation, and hence calculating the electrical resistivity, for a set of parallel dislocations treating each dislocation to be a row of weak scatterers each having a spherically symmetric potential. Such an investigation is desirable for several reasons.

First, the preliminary investigation made by Harrison[1] show that, though crude, the above model is not far from reality and it is of interest to obtain a reliable estimate of the resistivity on its basis. Parenthetically, it may be recalled that the calculations,[2–4] which consider the electron scattering to arise primarily from the elastic strain field associated with a dislocation, give values for the resistivity which are at least an order of magnitude smaller than the observed values. Second, if our solution is extended to the case where the potential due to the individual scatterers is allowed to have radial asymmetry in the plane perpendicular to the row, the model would simulate the scattering due to an exact arrangement of the ions near the core of an edge dislocation.[5] Third, an exact solution, if only for a simple model, is important because it can be used as a guide to the reliability of the various approximate procedures which have been in use – or, if one wants to use the variational technique, for constructing a suitable trial function.

The scattering probability of an electron due to a dislocation is anisotropic, i.e., it depends not only on the relative orientation of the incident and scattered wave vectors $\vec{k}$ and $\vec{k}'$, respectively, but also on $\vec{k}$ and $\vec{k}'$ separately. Consequently, the total resistivity of a crystal, when other scattering mechanisms are present, will, in general, not be simply a sum of the resistivities due to the dislocations and these mechanisms (violation of Matthiessen's rule in the present context). To investigate the deviations[6] from Matthiessen's rule, we include in our work scattering from other mechanisms also. However, for simplicity, we assume the scattering from these to be elastic and to depend only on the relative orientation of $\vec{k}$ and $\vec{k}'$.

The method of solving the Boltzmann equation (Sec. II) consists of expanding the electron distribution function f in terms of spherical harmonics and obtaining a difference equation for the coefficients f_{LM} in the expansion. It is found that for the model of the dislocation used here, the task of solving this difference equation reduces to solving a finite number (usually of the order of 5) of linear algebraic equations, if the number of Legendre polynomials needed to represent the relevant pseudopotential matrix elements in the dislocation scattering and the scattering due to the other mechanisms is finite – and it is reasonable to assume that this will be so in a physical problem. Thus it is possible to evaluate f, and hence the resistivity, to any desired degree of accuracy with only a reasonable amount of computation.

The method as described above is here developed only for the monovalent metals, where the electron wavelength is larger than twice the interatomic distance. For polyvalent metals there are additional contributions to the resistivity tensor which are estimated by the variational principle [see discussion following Eq. (11) and Sec. III]. The results of some numerical calculations on the resistivity due to dislocations and the deviations from Matthiessen's rule are presented in Sec. IV. For making the numerical calculations we have taken, following Harrison,[1] the scatterers constituting the dislocations to be vacancies. The scattering due to these vacancies was calculated from the pseudopotential approach.

Finally, in Sec. V, we make some comments on the resistivity due to dislocations when they are oriented at random and on comparison with experiment.

II. BOLTZMANN EQUATION AND ITS SOLUTION

A. Boltzmann Equation

For the case of elastic scattering, the steady-state linearized Boltzmann equation is given by

$$-\frac{e}{k\hbar}(\vec{\epsilon}\cdot\vec{k})\frac{\partial f_k^0}{\partial k}=\frac{\Omega}{8\pi^3}\int P(\vec{k},\vec{k}')\,(f_{\vec{k}}-f_{\vec{k}'})\,d^3k' , \quad (1)$$

where $\vec{\epsilon}$ is the electric field; Ω is the crystal volume; $P(\vec{k},\vec{k}')$ is the probability, per unit time, of the scattering of an electron from a state of wave vector $\vec{k}$ to another state of wave vector $\vec{k}'$; $f_{\vec{k}}$ is the distribution function of the elctrons; and $f_{\vec{k}}^0$ is the equilibrium distribution function. It is assumed that the energy surfaces are spherical in $\vec{k}$ space so that $f_{\vec{k}}^0$ (but not $f_{\vec{k}}$) depends only on the magnitude of $\vec{k}$. We shall also assume that the probabilities $P_1(\vec{k},\vec{k}')$ and $P_2(\vec{k},\vec{k}')$ of scattering due to dislocations and other mechanisms, respectively, are additive. Thus $P(\vec{k},\vec{k}')$ is given by

$$P(\vec{k},\vec{k}')=P_1(\vec{k},\vec{k}')+P_2(\vec{k},\vec{k}') . \quad (2)$$

As mentioned before, $P_2(\vec{k},\vec{k}')$ will be taken to depend only on $|\vec{k}-\vec{k}'|$. We set $\vec{k}'-\vec{k}=\vec{q}$, and will write $P_2(\vec{k},\vec{k}')$ as $P_2(q)$, where $q=|\vec{q}|=2k\sin\frac{1}{2}\theta$, θ being the angle of scattering.

$P_1(\vec{k},\vec{k}')$ is given by

$$P_1(\vec{k},\vec{k}')=\frac{2\pi}{\hbar}\,|M_1(\vec{k},\vec{k}')|^2\,\delta(E_k-E_{k'}) , \quad (3)$$

where $M_1(\vec{k},\vec{k}')$ is the scattering matrix element due to the dislocations and E_k is the energy of an electron of wave vector $\vec{k}$. For our model, where a dislocation is considered as a row of weak scatterers, the scattering matrix element due to one dislocation is

$$(1/N)W(\mathrm{q})\sum_{r=0}^{n-1}\exp[-ikra\,(\cos\alpha-\cos\beta)] ,$$

where N is the total number of ions in the crystal; α and β denote, respectively, the angles which $\vec{k}'$ and $\vec{k}$ make with the dislocation line; n is the number of individual scatterers in the line; a the distance between successive scatterers; and $W(q)$ their scattering form factor in the metal. [If these scatterers are considered as vacancies in an otherwise perfect crystal (no distortions), then $W(q)$ is just the negative of the form factor for the host ions.] $W(q)$ depends on the magnitude of $\vec{q}$ only because of the assumed spherical symmetry of the potential of the individual scatterers. If now there are N_0 such dislocation lines in the crystal, all parallel to one another but distributed at random in space, then $P_1(\vec{k},\vec{k}')$ is given by

$$P_1(\vec{k},\vec{k}')=\frac{2\pi}{\hbar}\,\frac{N_0}{N^2}\,[W(q)]^2 \times\frac{\sin^2[\frac{1}{2}nka\,(\cos\alpha-\cos\beta)]}{\sin^2[\frac{1}{2}ka\,(\cos\alpha-\cos\beta)]}\,\delta(E_k-E_{k'}) . \quad (4)$$

The integral equation (1), with $P_1(\vec{k},\vec{k}')$ given by (4), was considered by one of us[7] many years ago, in connection with a calculation of change in resistance when carbon atoms diffuse into dislocations of a cold-worked iron-carbon alloy of low carbon content. It was shown there that (1) gives for f an analytical expression in the closed form provided $W(q)$ and $P_2(q)$ are independent of the angle of scattering θ. To solve the equation when $W(q)$ and $P_2(q)$ depend on the angle of scattering, we proceed here as follows.

Let the polar coordinates of $\vec{k}$ and $\vec{k}'$, with the polar axis along the dislocation line, be, respectively, (k, β, ψ) and $(k' \ (=k), \alpha, \phi)$. We expand $f_{\vec{k}}$ and $f_{\vec{k}'}$ in spherical harmonics $Y_{LM}(\beta, \psi)$ and $Y_{LM}(\alpha, \phi)$, and $[W(q)]^2$ in terms of Legendre polynomials[8] $P_l(\cos\theta)$. Thus we write

$$f(\vec{k}) = f_0(k) + \sum_{LM} f_{LM} Y_{LM}(\beta, \psi) , \tag{5}$$

$$f(\vec{k}') = f_0(k) + \sum_{LM} f_{LM} Y_{LM}(\alpha, \phi) ,$$

$$[W(q)]^2 = \sum_{l=0}^{\infty} C_l^{(1)}(k) \, P_l(\cos\theta) , \tag{6}$$

and recall that

$$P_l(\cos\theta) = \frac{4\pi}{2l+1} \sum_m Y_{lm}(\beta, \psi) \, Y^*_{lm}(\alpha, \phi) . \tag{7}$$

In (5), the L summation is over all positive integers, excluding zero, and the M summation from $-L$ to L. We also write Eq. (1), for convenience, as

$$\frac{-e}{k\hbar} (\vec{\epsilon} \cdot \vec{k}) \frac{\partial f_0}{\partial k} \equiv I_1 + I_2 , \tag{8}$$

where

$$I_1 = \frac{\Omega}{8\pi^3} \int P_1(\vec{k}, \vec{k}') (f_{\vec{k}} - f_{\vec{k}'}) d^3k' , \tag{9}$$

and I_2 is similar integral with $P_1(\vec{k}, \vec{k}')$ replaced by $P_2(q)$.

Consider first I_1. Substituting Eqs. (4)–(7) into (9), and integrating over $E_{k'}$, one gets

$$I_1 = \frac{N_0 \Omega_0 k^2}{\pi\hbar N} \left(\frac{dE_k}{dk}\right)^{-1} \sum_{lmLM} \frac{C_l^{(1)}}{2l+1} f_{LM} Y_{lm}(\beta, \psi) \times \int Y^*_{lm}(\alpha, \phi) \frac{\sin^2[\frac{1}{2} nka(\omega' - \omega)]}{\sin^2[\frac{1}{2} ka(\omega' - \omega)]} \times [Y_{LM}(\beta, \psi) - Y_{LM}(\alpha, \phi)] \, d\omega' d\phi , \tag{10}$$

where $\omega = \cos\beta$, $\omega' = \cos\alpha$, and Ω_0 denotes the volume per atom. For sufficiently large n, the function $\sin^2 ny/\sin^2 y$ behaves as a series of Dirac δ functions,

$$\frac{\sin^2 ny}{\sin^2 y} = n\pi \sum_m \delta(y - m\pi), \quad m = 0, \ \pm 1, \pm 2, \ \ldots \ . \tag{11}$$

For monovalent metals, where the wavelength of the Fermi electrons is larger than twice the interatomic distance, $k_F a < \pi$ (k_F wave number at the Fermi surface), and hence only the first term in (11) contributes to the integral in (10). For polyvalent metals the terms $m = \pm 1$ have also to be considered and their contribution to resistivity is estimated in Sec. III. Here we confine our attention to the case $k_F a < \pi$, for which Eq. (10), on using (11), reduces to

$$I_1 = \sum_{lLM} C'_l f_{LM} Y_{LM}(\beta, \psi) \{[\mathcal{P}_{l0}(\omega)]^2 - [\mathcal{P}_{lM}(\omega)]^2\} . \tag{12}$$

Here $\mathcal{P}_{LM}$ are defined by

$$\mathcal{P}_{LM}(\omega) = (4\pi)^{1/2} Y_{LM}(\beta, \psi) \, e^{-iM\psi} \equiv N_{LM} P_L^M(\omega) , \tag{13}$$

where $P_L^M(\omega)$ are the associated Legendre polynomials and N_{LM} are given by

$$N_{LM} = \left((2L+1) \frac{(L - |M|)!}{(L + |M|)!}\right)^{1/2} . \tag{14}$$

The coefficients C'_l in (12) are given by

$$C'_l = \frac{N_D \Omega_0^2 k C_l^{(1)}}{(2l+1)\hbar a^2} \left(\frac{dE_k}{dk}\right)^{-1} , \tag{15}$$

where N_D is the dislocation density and is equal to $(N_0 na/\Omega)$.

To evaluate I_2, we note that $P_2(q)$ has a form similar to expression (3) for $P_1(\vec{k}, \vec{k}')$, except that the matrix element now depends on $|\vec{k} - \vec{k}'| = q$ only. Hence we can write

$$(\Omega/8\pi^3) \int k'^2 P_2(|\vec{k} - \vec{k}'|) dk' = k^2 \sum_{l=0}^{\infty} C_l^{(2)}(k) P_l(\cos\theta) . \tag{16}$$

Using (7), one then obtains

$$I_2 = \sum_{LM} (C''_0 - C''_L) f_{LM} Y_{LM}(\beta, \psi) , \tag{17}$$

where $C''_l = C_l^{(2)} 4\pi k^2/(2l+1)$. (18)

Finally, since

$$\frac{(\vec{\epsilon} \cdot \vec{k})}{k} = \epsilon_x \sin\beta \cos\psi + \epsilon_y \sin\beta \sin\psi + \epsilon_z \cos\beta , \tag{19}$$

we find, using Eqs. (12), (17), and (19), that the Boltzmann equation (8) reduces to

$$\sum_{LM} (C''_0 - C''_L) f_{LM} Y_{LM}(\beta, \psi) + \sum_{lLM} C'_l f_{LM} Y_{LM}(\beta, \psi) \times \{[\mathcal{P}_{l0}(\omega)]^2 - [\mathcal{P}_{lM}(\omega)]^2\} = \sum_m A_{1m} Y_{1m}(\beta, \psi) , \tag{20}$$

where $m = 0, \ \pm 1$, and

$$A_{1,\pm 1} = -\frac{e}{\hbar} \frac{\partial f_k^0}{\partial k} (\tfrac{2}{3}\pi)^{1/2} (\epsilon_x \mp i\epsilon_y) ,$$
$$A_{10} = -\frac{e}{\hbar} \frac{\partial f_k^0}{\partial k} (\tfrac{4}{3}\pi)^{1/2} \epsilon_z . \tag{21}$$

Thus the problem of solving the Boltzmann equation may be reduced to one of solving Eq. (20) for f_{LM}. For determining the electrical conductivity we need, of course, to know only f_{10}, $f_{1,\pm 1}$.

B. Difference Equation

Multiplying Eq. (20) by $Y^*_{L'M'}(\beta, \psi)$, integrating, and using the orthogonality property of the spherical harmonics, one sees that all $f_{LM} = 0$, unless $M = 0$ or ± 1, and that

$$f_{L0} = [A_{10}/(C_0'' - C_1'')]\,\delta_{L,1}\ . \tag{22}$$

Further, for $f_{L'\eta}$ $(\eta = \pm 1)$, one obtains the set of equations $(L' = 1, 2, 3, \cdots)$

$$A_{1\eta}\,\delta_{L'1} = (C_0'' - C_{L'}'')\,f_{L'\eta} + \tfrac{1}{2}\int \mathcal{P}_{L'1}(\omega) \times \sum_{Ll} f_{L\eta}\,\mathcal{P}_{L1}(\omega)\, C_l'\{[\mathcal{P}_{l0}(\omega)]^2 - [\mathcal{P}_{l1}(\omega)]^2\}\, d\omega\ , \tag{23}$$

where we have used the fact that $\mathcal{P}_{L1}(\omega) = \mathcal{P}_{L,-1}(\omega)$.

Now let

$$\sum_l C_l'\{[\mathcal{P}_{l0}(\omega)]^2 - [\mathcal{P}_{l1}(\omega)]^2\} = a_0 + a_1\omega^2 + \cdots a_{l_0}\,\omega^{2l_0}, \tag{24}$$

where a_0, a_1, etc., are constants and l_0 is the degree of highest Legendre polynomial occurring in the expansion (6) of $[W(q)]^2$. We shall assume that l_0 is some finite number. We shall also need the expansion

$$\omega^{2n} P_L^1(\omega) = \sum_{r=-n}^{n}{}' k_{nL}^{L+2r} P_{L+2r}^1(\omega)\ , \tag{25}$$

where P_L^1 are associated Legendre polynomials for $M = 1$ and k_{nL}^{L+2r} are constants, the sub- and superscripts being self-explanatory. The prime over the summation sign means that the values of r for which $L + 2r < 0$ (which would be the case for some values of r if $L < 2n$) are excluded from the sum. From the definition of the k's and the normalization properties of $P_L^1(\omega)$, one verifies that

$$\alpha(L)\, k_{nL}^{L-2r} = \alpha(L - 2r)\, k_{n,L-2r}^{L}\ , \tag{26}$$

a relation which will be needed later. In (26)

$$\alpha(L) \equiv \tfrac{1}{2} N_{L1}^2 = (2L+1)/2L(L+1)\ . \tag{27}$$

Substituting (24) and (25) into (23), integrating over ω, and making use of (13) and the relation

$$\int P_{L'}^1(\omega)\, P_L^1(\omega)\, d\omega = \delta_{L,L'}/\alpha(L)\ , \tag{28}$$

one obtains

$$A_{1\eta}\,\delta_{L'1} = (C_0'' - C_{L'}'')\,f_{L'\eta} + (N_{L'1})^{-1}\sum_L (f_{L\eta} N_{L1}) \times \sum_{n=0}^{l_0} a_n \sum_r^{n}{}' k_{nL}^{L+2r}\,\delta_{L',L+2r}\ . \tag{29}$$

Introducing, for brevity,

$$A_{1\eta}' = A_{1\eta} N_{11},\quad f_{L\eta}' = f_{L\eta} N_{L1}\ , \tag{30}$$

and interchanging the role of L' and L, we can write (29) as

$$A_{1\eta}'\,\delta_{L,1} = (C_0'' - C_L'')\,f_{L\eta}' + \sum_{L'} f_{L'\eta}' \sum_{n=0}^{l_0} a_n \times \sum_r^{n}{}' k_{nL'}^{L'+2r}\,\delta_{L,L'+2r} \tag{31}$$

or

$$A_{1\eta}'\,\delta_{L,1} = (C_0'' - C_L'')\,f_{L\eta}' + \sum_m^{l_0}{}' f_{L+2m,\eta} \times \Big(\sum_{n=|m|}^{l_0} a_n k_{n,L+2m}^{L}\Big)\ . \tag{32}$$

A rearrangement enables one to rewrite (32) as

$$A_{1\eta}'\,\delta_{L,1} = (C_0'' - C_L'' + a_0)\,f_{L\eta}' + \sum_{r=1}^{l_0} a_r \Big(\sum_n^{r} k_{r,L+2n}^{L} f_{L+2n,\eta}'\Big)\ . \tag{33}$$

Equation (33) is the required difference equation. Written for $L = 1, 2, 3, \ldots$, it gives a set of linear algebraic recursion relations for $f_{L\eta}'$. We see from (33) that $f_{L\eta}'$, for even L, are neither coupled to the applied electric field $(A_{1\eta}')$ nor to those $f_{L\eta}'$ for which L is odd. Hence $f_{L\eta}' = 0$ $(\eta = \pm 1)$, for all even L.

Our next task is to solve Eqs. (33) for $f_{L\eta}'$ for odd L, or , at least, to cast these equations in a form convenient for numerical work. For this purpose suppose that the coefficients $C_L^{(2)}$ and hence C_L'', in the expansion (16) for $P_2(q)$ are nonzero up to some finite value of L, say L_0, and zero thereafter. We choose L_0 to be an odd integer – the reason for this choice will become evident presently. Then it is not difficult to verify by direct substitution that f_L' given by[9]

$$f_{L\eta}' = \alpha(L)\,[(B_{1\eta} + \beta_1 f_{1\eta}')\,I(L,1) + \beta_3 f_{3\eta}'\,I(L,3) + \beta_5 f_{5\eta}'\,I(L,5) + \cdots \beta_{L_0} f_{L_0\eta}'\,I(L,L_0)] \tag{34}$$

$(L = 1, 3, 5, \ldots)$ is a solution of (33). In (34)

$$I(L, L') = \int_{-1}^{1} \frac{P_L^1(\omega)\, P_{L'}^1(\omega)\, d\omega}{1 + \gamma_1\omega^2 + \gamma_2\omega^4 + \cdots \gamma_{l_0}\omega^{2l_0}} \tag{35}$$

and

$$B_{1\eta} = \frac{A_{1\eta}'}{C_0'' + a_0}\ ,\quad \beta_r = \frac{C_r''}{C_0'' + a_0}\ ,\quad \gamma_r = \frac{a_r}{C_0'' + a_0}\ . \tag{36}$$

Writing (34) for $L = 1, 3, \ldots L_0$, we get $\frac{1}{2}(L_0 + 1)$ linear equations in as many f''s. From these, $f_{1\eta}'$, $f_{3\eta}', \ldots, f_{L_0\eta}'$ may be obtained. Once these f''s are known, $f_{L\eta}'$ for higher L may be evaluated from (34) directly. (For the purpose of electrical resistivity, of course, we need only $f_{1\eta}'$.) Thus the number of equations to be solved depends on the number L_0 of Legendre polynomials necessary to adequately represent the angular dependence of the impurity scattering probability $P_2(q)$. If L_0 is not too large, as is usually the case, these equations can be numerically solved without undue labor. The results of some numerical calculations are presented in Sec. IV. Here we only note that Eqs. (34) are such, as will be clear from inspection, that $f_{1\eta}'/B_{1\eta}$ is independent of the index η. Hence, using (30) and (36), we set, for future convenience,

$$f_{1\eta}=G(C',\ C'')\,A_{1\eta}\ ,\quad \eta=\pm 1 \tag{37}$$

where C' and C'', respectively, stand for the sets $\{C_0',\ C_1',\cdots,\ C_{l_0}'\}$ and $\{C_0'', C_1'',\cdots, C_{L_0}''\}$. The function $G(C', C'')$ is independent of the index η and is determined with the help of (34).

III. RESISTIVITY TENSOR AND SPECIAL CASES

In terms of the distribution function f, the electric current density $\vec{J}$ is given by

$$\vec{J}=(e/4\pi^3)\int f_{\vec{k}}\, v_{\vec{k}}\, d^3k\ , \tag{38}$$

where $v_{\vec{k}}$ $(=\hbar^{-1}\,\mathrm{grad}_{\vec{k}}\, E)$ is the velocity of the electron of wave vector $\vec{k}$. On substituting for $f_{\vec{k}}$ from (5) and using (22), (37), and (21), one obtains

$$J_x=\mathcal{A}^{-1}G_F(C', C'')\,\epsilon_x,\quad J_y=\mathcal{A}^{-1}G_F(C', C'')\,\epsilon_y\ ,$$

$$\text{and}\ \ J_z=\mathcal{A}^{-1}\epsilon_z/(C_0''-C_1'')_F\ , \tag{39}$$

where $\mathcal{A}=(3\pi^2\hbar^2/e^2)(k^2dE_k/dk)_F^{-1}$ and F denotes the value of the subscripted quantity at the Fermi surface. The fact that a given component of $\vec{J}$ depends only on the corresponding component of $\vec{\epsilon}$ means that the axes we have used are the principal axes for the resistivity tensor. Hence the principal resistivities are given by

$$\rho_{xx}=\rho_{yy}=\mathcal{A}/G_F(C',\ C'')\ ,\ \ \rho_{zz}=\mathcal{A}(C_0''-C_1'')_F\,. \tag{40}$$

We see from (40) that the value of ρ_{zz} is the same as in the absence of the dislocations. This result is to be expected for the monovalent metals, where the Fermi wavelength of the electrons is such that in scattering by a dislocation, the component of the electron momentum along the dislocation line (or the z axis) does not change [see discussion following Eq. (11)]. Further, since in the model we are using the dislocation line is an axis of symmetry, we have $\rho_{xx}=\rho_{yy}$. The three principal components of ρ_D, the resistivity due to the dislocations, are thus $[(\rho_D)_1\equiv(\rho_D)_{xx}$, etc.$]$

$$(\rho_D)_3=0\ ,\ \ (\rho_D)_{1,2}=\mathcal{A}\,D(C', C'')\ ,$$

$$D(C', C'')\equiv\{[1/G_F(C', C'')]-(C_0''-C_1'')_F\}\,. \tag{41}$$

For brevity, we shall, at times, suppress the subscripts 1, 2 on ρ_D.

In general, G_F (or D) depends on C' and C'' in a complicated way and its value has to be obtained from (34) numerically (see Sec. IV). Below, we discuss two particular cases of interest where G_F and D can be evaluated analytically in terms of C' and C''.

Case I. $C_l'=C_0'\delta_{l,0}$ (i.e., the individual scatterers constituting the dislocation scatter isotropically): For this case, the integrals $I(L, L')=\delta_{LL'}/\alpha(L)$. Hence $D=a_0$ which is equal to C_0' when other C_l' are zero. This is the same result as that obtained by Bhatia,[7] with the difference that to show this result we have not made any assumption regarding C'' while Bhatia assumed $C_L''=C_0''\times\delta_{L0}$.

Case II.

$$(C_0''+a_0)\gg C_l'\ \text{for}\ l=1,2,\ldots,l_0\,. \tag{42}$$

For this case we get

$$D\simeq\tfrac{3}{4}\int_{-1}^{1}[P_1^1(\omega)]^2(a_0+a_1\omega^2+\cdots a_{l_0}\omega^{2l_0})\,d\omega, \tag{43}$$

where the correction terms are of order $a_l/(C_0''+a_0)$ with $l=1,2,\ldots$. Using (24) and evaluating the integrals, one obtains

$$D\simeq-3\textstyle\sum_l C_l'/[(2l-1)(2l+3)]\,. \tag{44}$$

Substituting for C_l' from (15) and (6), one can then show that $(\rho_D)_{1,2}$ for this case is given by[10]

$$(\rho_D^\infty)_{1,2}=\mathcal{B}\int_0^2[W(x)]^2x^2\,dx\ , \tag{45}$$

where the superscript ∞ on ρ_D signifies that (45) is valid when the resistivity ρ_i due to other mechanisms is much greater than ρ_D, $x=q/k_F$ and

$$\mathcal{B}=\frac{3\mathcal{A}\Omega_0^2N_Dk_F}{8\,\hbar a^2}\left(\frac{dE_k}{dk}\right)_F^{-1}=\frac{9\pi^2(m^*)^2\Omega_0^2N_D}{8e^2a^2\hbar^3k_F^3}\ , \tag{46}$$

where m^* is the electron effective mass.

We may mention that the approximation (42) under which (43), and hence (45), are derived is essentially the same as that used by Mackenzie and Sondheimer[2] for obtaining an expression for the resistivity for their model of the dislocation.

We also note that when the inequalities (42) are satisfied, the distribution function f of the electrons is primarily determined by the electric field and the scattering probability $P_2(q)$ due to other mechanisms (which depends on the magnitude of q only). Consequently, f is of the form of the simplest trial function used in the calculation of resistivity by the variational method (see, for example, Ziman[11]). In fact, as we shall see below, the variational expression for the resistivity, using the simplest trial function, gives just (45), for $k_Fa<\pi$, as it should. Since the variational expression gives for the resistivity values which are greater than or equal to the true resistivity, it follows that the true ρ_D will be less than that given by (45) and that this difference will be the greater, the smaller is the scattering probability $P_2(q)$. Only in the limit when (42) are satisfied is the true ρ_D given by (45). These conclusions are in agreement with the numerical results presented in Table I.

ρ_D^∞ for polyvalent metals. Hitherto we have restricted our discussion to monovalent metals for which $k_Fa<\pi$. For polyvalent metals k_Fa lies between π and 2π, so that the $m=\pm1$ terms in the expansion (11) also contribute to the integral in

(10). An exact analysis similar to that given in Sec. II is difficult for this case. However, as the above discussion suggests, the principal resistivities in the limit $\rho_i \gg \rho_D$ may be obtained from the variational expression for the resistivity using the simplest trial function for the distribution function f, namely, by taking f to be of the form $f(k) = f_0 - \alpha(\vec{k} \cdot \vec{\epsilon})\, \partial f_0/\partial E_k$, where α is a constant. The method for making such a calculation is standard and is described, for example, in Ref. 11. Applied to our problem it gives, for $\pi < k_F a < 2\pi$,

$$(\rho_D^\infty)_{1,2} = \mathcal{B} \int_0^2 W^2(x)\, x^2\, dx + 2\mathcal{B} \int_{2\pi/k_F a}^2 W^2(x)\, x^2\, dx - \frac{8\mathcal{B}\pi^2}{(k_F a)^2} \int_{2\pi/k_F a}^2 W^2(x)\, dx\,, \tag{47}$$

$$(\rho_D^\infty)_3 = \frac{16\mathcal{B}\pi^2}{(k_F a)^2} \int_{2\pi/k_F a}^2 W^2(x)\, dx\,. \tag{48}$$

The last two terms in (47) and $(\rho_D^\infty)_3$ arise from the $m = \pm 1$ terms in the expansion (11) and are to be put equal to zero for the monovalent metals. We observe that in polyvalent metals a dislocation contributes to the resistivity in the direction parallel to itself also. In general $(\rho_D^\infty)_3$ may, however, be expected to be at most a few percent of $(\rho_D^\infty)_{1,2}$.

IV. NUMERICAL RESULTS

The object of this section is to investigate how ρ_D changes as a function of ρ_i/ρ_D and thus estimate deviations from Matthiessen's rule. For this purpose one should ideally choose to make calculations for a monovalent metal since the theory as developed in Sec. II applies to these metals only. Unfortunately, for the monovalent metals for which the dislocation resistivities are experimentally known, namely, the noble metals, the pseudopotential or effective potential matrix elements $W(q)$ are unreliable. We, therefore, choose for our study the metal aluminum, since $W(q)$ for Al^{+3} is known with some reliability. In estimating deviations from Matthiessen's rule, we thus ignore the contribution to ρ_D arising from the polyvalency of aluminum. Hence, throughout this section ρ_D refers to $(\rho_D)_{1,2}$ as given by (41), and $(\rho_D^\infty)_{1,2}$ as given by (45). [The difference between this expression for $(\rho_D^\infty)_{1,2}$ and that appropriate for Al, namely, (47), is about 20%.] ρ_i in our calculations was taken to be due to the impurities. The impurities we tried were Mg, Zn, and Cd whose form factors in Al (host) were calculated by Gupta.[12]

Using the definitions of C_l' and C_l'', we then have

$$C_l' = \frac{N_D \Omega_0^2 k}{2\hbar a^2} \left(\frac{dE_k}{dk}\right)^{-1} I_l'\,,$$

$$C_l'' = \frac{\Omega_0 c k^2}{2\pi\hbar} \left(\frac{dE_k}{dk}\right)^{-1} I_l''\,, \tag{49}$$

where c is the concentration of the impurities and I_l' and I_l'' are integrals given by

$$\begin{aligned} I_l' &= \int_0^2 x[W(x)]^2\, P_l(1 - \tfrac{1}{2}x^2)\, dx\,, \\ I_l'' &= \int_0^2 x[\Delta W(x)]^2\, P_l(1 - \tfrac{1}{2}x^2)\, dx\,. \end{aligned} \tag{50}$$

In (49) W is the form factor of Al and ΔW the difference in the form factors of Al and the impurity ion in Al.

Now $D(C', C'')$, defined in (41), has the property that

$$D(C', C'') = \beta D(C'/\beta, C''/\beta)\,, \tag{51}$$

where $D(C'/\beta, C''/\beta)$ is obtained from $D(C', C'')$ by replacing all C_l' by C_l'/β and C_L'' by C_L''/β, respectively, and where β is a constant independent of l or L. Hence, using (49), one has

$$D(C', C'') = \frac{N_D \Omega_0^2 k_F}{2\hbar a^2} \left(\frac{dE_k}{dk}\right)_F^{-1} D(I', \gamma I'')\,, \tag{52}$$

where

$$\gamma = c k_F a^2/(\pi \Omega_0 N_D)\,. \tag{53}$$

The parameter γ determines the relative value of the resistivity due to the dislocations and impurities: $\rho_i/\rho_D \simeq \gamma I_0''/I_0'$. Therefore, $D(I', \gamma I'')$ was calculated for various values of γ, from where one may obtain ρ_D for the various values of ρ_i/ρ_D. The number of integrals I' used in the calculation was six and that of I'' was ten (l_0 and L_0 equal to five and nine, respectively). The results for $D(I', \gamma I'')$ for various values of $R \equiv \gamma I_0''/I_0'$ are given in Table I. The expression (44) which we recall, corresponds to the limit $R \to \infty$, gives $D = 0.0552$.

We observe from the table that D increases progressively with increasing R so that ρ_D increases as more and more impurities are added,

TABLE I. Values of $D(I', \gamma I'')$ for various values of R for dislocations in Al with Mg, Zn, and Cd as impurities. Here $R = \gamma I_0''/I_0' \simeq \rho_i/\rho_D$, where ρ_i is the resistivity due to impurities, and ρ_D that due to dislocations.

$R \times (1.64)^{-1}$	D in Ry^2		
	Mg	Zn	Cd
0.0	0.0401	0.0401	0.0401
1.0	0.0468	0.0462	0.0472
2.0	0.0492	0.0486	0.0495
3.0	0.0504	0.0499	0.0507
4.0	0.0512	0.0507	0.0514
6.0	0.0522	0.0518	0.0523
8.0	0.0527	0.0524	0.0529
10.0	0.0531	0.0528	0.0532
12.0	0.0533	0.0531	0.0534
16.0	0.0537	0.0535	0.0538
20.0	0.0539	0.0538	0.0540

in agreement with the comments made in Sec. III. The two limiting values of ρ_D are $\rho_D = 0.72\times10^{-19} \times N_D\ \Omega\,\mathrm{cm}^3$ for $R = 0$ and $\rho_D = 1.0\times10^{-19} N_D\ \Omega\,\mathrm{cm}^3$ for $R\to\infty$. At any given R, $\rho_D(R) - \rho_D(R=0)$ is the deviation from Matthiessen's rule, and the maximum deviation is $0.28\times10^{-19} N_D\ \Omega\,\mathrm{cm}^3$ or about 38% of $\rho_D(R=0)$.

V. RESISTIVITY DUE TO RANDOMLY ORIENTED DISLOCATIONS AND DISCUSSION

In terms of ρ_{zz}, $\rho_{xx} = \rho_{yy}$, the resistivity for flow of current in a direction which makes an angle ψ with the dislocation lines (z axis) is given by the ordinary tensorial rule

$$\rho = \rho_{zz}\cos^2\psi + \rho_{xx}\sin^2\psi \ . \tag{54}$$

Hence the average resistivity of a specimen having randomly oriented dislocation lines is $\langle\rho\rangle_{\mathrm{av}} = \frac{1}{3}\rho_{zz} + \frac{2}{3}\rho_{xx}$, and since $\rho_{xx} = \rho_i + (\rho_D)_1$, etc., the average resistivity due to the dislocations is $(R \simeq \rho_i/\rho_D)$

$$\langle\rho_D(R)\rangle_{\mathrm{av}} = \tfrac{1}{3}\left[\rho_D(R)\right]_3 + \tfrac{2}{3}\left[\rho_D(R)\right]_{1,2} \ . \tag{55}$$

For $R\to\infty$, (55) gives, using (47) and (48),

$$\langle\rho_D^\infty\rangle_{\mathrm{av}} = \tfrac{2}{3}\,\mathcal{B}\int_0^2 W^2(x)\,x^2\,dx + \tfrac{4}{3}\,\mathcal{B}\int_{2\pi/k_F a}^{2} W^2(x)\,x^2\,dx. \tag{56}$$

The second term in (56), which exists only for polyvalent metals, is about 20% of the first term for Al. Assuming that this polyvalency effect is of similar magnitude at $R = 0$ also, and using the numerical values obtained in Sec. IV, one sees that the two limiting values of $\langle\rho_D\rangle_{\mathrm{av}}$ for aluminum are $\langle\rho_D\rangle_{\mathrm{av}} = 0.58\times10^{-19} N_D$ and $0.8\times10^{-19} N_D\ \Omega\,\mathrm{cm}^3$ at for $R\to 0$ and $R\to\infty$, respectively, compared to the experimental value[13] of $1.8\times10^{-19}\ N_D\ \Omega\,\mathrm{cm}^3$ at 4.2°K. This is, perhaps, as good an agreement as can be expected in view of the crudeness of the model of the dislocation used in the theory. In this connection it is also relevant to calculate the resistivity ρ_0 which the vacancies would produce if they were distributed at random in the crystal. ρ_0 is given by the standard formula which, in our notation, is

$$\rho_0 = \tfrac{1}{4}\,\mathcal{C}\,\frac{\mathcal{a}}{\pi\hbar}\,k_F^2\,\Omega_0\left(\frac{dE}{dk}\right)_F^{-1}\int_0^2 [W(x)]^2 x^3\,dx \ , \tag{57}$$

where $\mathcal{C}$ ($\ll 1$) is the atomic concentration of the vacancies. For $\mathcal{C} = 0.01$ and the form factor $W(x)$ used in the present work, the formula (57) gives $\rho_0 \simeq 1.4\times10^{-6}\ \Omega$ cm, compared to the corresponding experimental value[14] of $3.0\times10^{-6}\ \Omega$ cm. Thus it appears that at least a part of the discrepancy between our theoretical value and the experimental value for the dislocation resistivity is due to the inadequacy of the form factor.

It will therefore be of interest to repeat the calculations presented here using better estimates of the scattering due to the core region of the dislocations, and also to make calculations by using the actual distribution of the atoms in a dislocation such as that computed by Cotterill and Doyama.[15] It is interesting to mention in this connection that estimates corresponding to $\langle\rho_D^\infty\rangle_{\mathrm{av}}$ for any model of a dislocation can be made much more easily if we note that expression (56) could have been derived simply by first averaging the scattering probability $P_1(\vec{k}, \vec{k}')$ due to the dislocations over all orientations of the dislocations. Since the resulting average depends only on the angle of scattering, the problem of solving the Boltzmann equation becomes a trivial one. Our work shows that such a procedure would give exact results[16] if $\rho_i \gg \rho_D$, and overestimate the dislocation resistivity by about 30 or 40% if $\rho_i \ll \rho_D$.

As regards the deviations from Matthiessen's rule, discussed in Sec. IV, it is of interest to note that although our calculations are carried out by taking other sources of resistivity to be impurities, similar results should be qualitatively expected when the additional resistivity is due to thermal vibrations. A glance at the Table I will then show that in an extremely pure specimen, the dislocation resistivity $\langle\rho_D(R)\rangle_{\mathrm{av}}$ would at first rise sharply as the temperature increased from zero, due to the corresponding rise in ρ_i or $R(\simeq\rho_i/\rho_D)$, and would then gradually tend to an asymptotic value of about 30 to 40% higher than $\langle\rho_D(0)\rangle_{\mathrm{av}}$. Basinski *et al.*[17] have observed such behavior in noble metals, saturation occurring near liquid-air temperatures. The ratio of the two limiting values of the dislocation resistivity is 1.6 for Cu, 1.8 for Ag, and 1.3 for Au. Similar results have been found by Rider and Foxon,[13,18] namely, 1.6 for Al and 1.3 for Cu. Unfortunately the residual resistivity of the undeformed specimens is not reported in these works so that the above qualitative agreement[19] between the theoretical and the observed variation of $\langle\rho_D\rangle_{\mathrm{av}}$ with temperature should be regarded at present as suggestive rather than conclusive.

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[4] For a recent review and complete list of references, see F. R. N. Nabarro, *Theory of Crystal Dislocations* (Oxford U. P., London, 1967).

[5] The simple model used here is designed to simulate the scattering only due to the core of the dislocation. Inasmuch as the core of a screw dislocation also has a dilatation (see, for example, Ref. 4, p. 617), the model provides an estimate for the resistivity due to a screw dislocation also.

[6] These deviations turn out to be quite significant.

[7] A. B. Bhatia, Proc. Phys. Soc. (London) B62, 229 (1949).

[8] No confusion should arise from the use of the symbol P for the probabilities as well as for the Legendre polynomials.

[9] This form of solution is suggested by the fact that for the case where $C_L'' = C_0''\delta_{L,0}$, the solution of Eqs. (33) is simply given by $f_{L\eta}' = \alpha(L) B_{1\eta} I(L,1)$.

[10] Note the weighting factor in the integrand in (45) which is x^2, instead of the usual x^3 occurring in the expressions for the resistivity due to impurities, etc. [cf. Eq. (57)].

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[16] It is not entirely clear whether this is the only condition under which this procedure, i.e., averaging $P_1(\vec{k}, \vec{k}')$ over all orientations first and then solving the Boltzmann equation, will give exact result. For example, if the objects giving rise to anisotropic scattering $P_1(\vec{k}, \vec{k}')$ were of atomic dimensions (i.e., if their linear dimensions were all small compared with the electron mean free path), then one would automatically use this averaging process in preference to the one which averages over the resistivity.

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[19] We may mention that a similar variation of $\langle\rho_D\rangle_{av}$ with temperature can occur even if $\rho_D(R)$ itself is independent of R, provided the dislocations are not quite randomly oriented. Consider the extreme case (perhaps, not likely to occur in practice) where the specimen is such that if it is divided into thin parallel slabs with their lengths along the direction of the current, then all the dislocations in a given slab are oriented parallel to one another while their orientations in different slabs are random. This corresponds to the slab resistances being in parallel, so that the average resistivity is $[\langle 1/\rho\rangle_{av}]^{-1}$, with ρ given by (54). For the case $(\rho_D)_3 = 0$, one then has the result that $\langle\rho_D\rangle_{av} = 0$ $\rho_i = 0$ and $\langle\rho_D\rangle_{av} = \frac{2}{3}(\rho_D)_{1,2}$ when $\rho_i \gg \rho_D$.

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Landau Diamagnetism from the Coherent States of an Electron in a Uniform Magnetic Field

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A complete set of coherent-state wave packets has been constructed for an electron in a uniform magnetic field. These states are nonspreading packets of minimum uncertainty that follow the classical motion. Use was made of the ladder operators that generate all the eigenstates of the Hamiltonian from any one energy eigenstate. The coherent states are the eigenstates of the two ladder operators that annihilate the zero-angular-momentum ground state. We have calculated the partition function, exploiting advantages of the coherent-state basis. The Landau diamagnetism and the de Haas–van Alphen oscillations are contained in the coherent-state framework.

I. INTRODUCTION

Coherent-state wave packets have received renewed attention since the recent article of Glauber.[1] Much of this attention is due to the recognition of their usefulness as a set of basis states for the calculation of observable physical quantities.[1,2] In addition, they have been of value in the theoretical problem of the quantum-mechanical definition of the phase of an oscillator.[3] The