

Here we require the additional definitions

$$\gamma_\lambda = K\lambda = \frac{1}{2}y(1-\alpha),$$

$$\gamma_{12} = 4\lambda d\sigma_1^2 = 2\gamma_1 \left( \frac{1-\alpha}{\alpha} \right),$$

and

$$\beta_{12} = \sigma_1 b = -3\alpha(1-\alpha)(\alpha^{-2}\eta_{12}g_{11} + \eta_{22}g_{12}).$$

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## Resonance Scattering and the Electrical and Thermal Resistivities Associated with Extended Defects in Crystals

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The general failure of theory to account for the observed electrical and thermal resistivities associated with dislocations is reviewed in the light of the resonance scattering previously shown to be a characteristic property of linear defects in crystals. Expressions for the scattering width and density of states near a resonance are obtained, and the magnitude of the resonance scattering is shown to be consistent with the observed electrical resistivity of dislocations in a number of metals. Observed stacking-fault electrical resistivities are consistent with the absence of resonance scattering; such scattering is not expected to occur for plane defects. The resonance-scattering mechanism is shown to be capable of accounting for the magnitude of the dislocation thermal resistivity in ionic crystals, and also, possibly, for the much smaller effect in metals. The observed temperature dependence of the thermal resistivity in ionic crystals is rather difficult to explain in terms of resonance scattering, although it would probably be expecting too much for the simple treatment given here to deal adequately with this point. The generally encouraging results would appear to justify the expenditure of more effort, both experimentally and theoretically, on these problems.

### I. INTRODUCTION

**R**ESONANCE scattering of electrons and phonons has been shown<sup>1</sup> to be a characteristic property of linear defects in crystals. In this paper, we attempt to investigate the role of these phenomena in determining the electrical and thermal resistivities associated with dislocations.

Previous theories have severely underestimated these resistivities, and the situation is briefly reviewed in Sec. II; the existence of resonance scattering opens all these theories to a rather more definite criticism than appears to have been previously leveled, and we may feel reasonably confident in suggesting that this mechanism provides a basic reason for the failure of the theory to date.

The remainder of this paper is devoted to the more positive procedure of showing how resonance scattering fits in with the currently available experimental data on the electrical and thermal resistivities associated with line and plane defects. Thus, in Sec. III, we develop simple expressions for the resistivities, in a form convenient for such an analysis, and in Sec. IV develop expressions for the dislocation scattering width near a

resonance, and in particular obtain the phase shifts to be used in the resistivity formulas of Sec. III. The density of states near a resonance is considered in Sec. IV B. The relation of the experimental data to the existence of resonance scattering is discussed in Sec. V.

Analysis of the electrical-resistivity data is particularly encouraging in that resonance scattering is indicated to occur, for the two types of defect, in just the way predicted by the theory<sup>1</sup>; that is to say, it appears to be both necessary and sufficient to explain the data on dislocations, at least for those cases where these data appear most reliable, but is not necessary to explain stacking-fault resistivities. The need for more accurate experimental work on a greater number of metals is evident, and it is hoped that the results of the present analysis are sufficiently promising to encourage such measurements.

The situation with the dislocation thermal resistivity is not quite so happy. On the one hand, the *magnitude* of the observed resistivity in the alkali halides is such as to be consistent with resonance scattering, and also the apparent absence of resonances in the low-temperature phonon scattering from metals<sup>2</sup> is not an insurmountable difficulty, at least at the present shallow level of investigation. On the other hand, it seems impossible,

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<sup>1</sup> R. A. Brown, Phys. Rev. **156**, 889 (1967).

<sup>2</sup> See Ref. 27, however.

at least for ionic crystals, to predict anything like the  $T^{-2}$  temperature dependence of the resistivity, which has played such a large part in establishing the theory of Klemens.<sup>3</sup> Recent experiments have, in fact, indicated a more complex temperature dependence, as discussed in Secs. II and V B, and it is suggested in the latter that a more detailed theoretical analysis could perhaps establish the role of resonance scattering more definitely. Generally speaking, however, it is felt that a more detailed treatment than that given here, both of thermal and electrical resistivities, would better await the acquisition of more accurate data pertaining to a wider range of crystals.

## II. REVIEW

The earliest attempts<sup>4</sup> to calculate the contribution of edge dislocations to the electrical resistivity were concerned with the scattering of free electrons by the first-order elastic-strain field, and involved the use of a first-order perturbation, or Born-approximation approach; the existence of resonance scattering clearly throws doubts on the use of such an approximation, and provides a plausible reason why such calculations yield resistivities typically a factor of 50 or so less than the observed values. Seeger and Stehle<sup>5</sup> considered scattering by the second-order elastic strains about a screw dislocation; the particular form of their perturbing potential enabled them to fairly easily determine the phase shifts without resorting to perturbation theory, but, in common with the above treatments, no account was taken of the electronic-band structure which we have shown<sup>1</sup> to be essential to the obtaining of resonance scattering; thus, it is not surprising that their value for the resistivity due to a screw dislocation in copper was of the same order as the above estimates for edge dislocations. Seeger and Bross<sup>6</sup> obtained much higher estimates for edge dislocations by working to second order in perturbation theory; apart from the apparent inconsistency involved in stopping a perturbation treatment at the second-order stage after having shown the second-order contributions to dominate those of first order, their use of perturbation theory and neglect of band structure subjects their calculation to the same criticisms as the above, and it has also been criticized<sup>7</sup> on somewhat different grounds. This theory also appears to be open to some criticism on the basis of experiment, for the resistivity as calculated by Seeger and Bross owes its large magnitude to its logarithmic dependence

on the range of the strain field, which must be supplied with a cutoff radius. One would therefore expect a considerable dependence of resistivity on dislocation configurations. Cotterill<sup>8</sup> has determined a somewhat higher resistivity associated with dislocation loops in quenched aluminium than has been measured for dislocations in deformed aluminium<sup>9,10</sup>; however, Rider and Foxon<sup>10</sup> have suggested reasons why Cotterill's result may be rather high, and their work combining electron-microscope observations with resistivity measurements at different stages of annealing shows fairly conclusively that resistivity is not sensitive to dislocation arrangement.

As an alternative to strain-field scattering, Harrison<sup>11</sup> considered the volume increase associated with a dislocation to be located in a hollow core which scattered free electrons. Working in the Born approximation, he obtained a resistivity only about a factor of 5 below the observed value for copper. His theory is open to the criticism that the second-order long-range elastic-strain field<sup>12</sup> appears to be responsible for most of the volume change in cold-worked crystals, so that this should not all be assigned to the core region.

Howie<sup>13</sup> considered a diffraction mechanism and obtained the same order of magnitude as Harrison for the resistivity; his calculation is based on an estimate of stacking-fault resistivity which has several uncertainties, and indeed appears to considerably overestimate the stacking-fault resistivity (see below). Ziman<sup>14</sup> has also suggested that diffraction effects may be important, but has not made any estimates. Just the opposite view was taken by Basinski *et al.*,<sup>15</sup> who proposed a semiempirical theory which supposed the residual resistivity to be proportional to the mean-square displacement of the ions from their unperturbed positions, and so amounted to neglecting all interference effects. Having calibrated their theory to agree with the experimental value for copper, their agreement with other data does not appear to be remarkably good, but their paper contains a useful summary of experimental data on dislocation resistivity.

The inability of the early theories to account for the residual resistivity in terms of dislocation scattering led Broom<sup>16</sup> to suggest that the stacking-fault ribbons associated with split dislocations might scatter electrons sufficiently strongly to explain the observations. Different theories gave widely different results for the stacking-fault resistivity, and the situation prior to 1960 was reviewed by Howie,<sup>13</sup> who considered the

<sup>3</sup> P. G. Klemens, *Solid State Phys.* **7**, 1 (1958).

<sup>4</sup> J. S. Koehler, *Phys. Rev.* **75**, 106 (1949); J. K. Mackenzie and E. H. Sondheimer, *ibid.* **77**, 264 (1950); R. Landauer, *ibid.* **82**, 520 (1951); D. L. Dexter, *ibid.* **85**, 936 (1952); **86**, 770 (1952); S. C. Hunter and F. R. N. Nabarro, *Proc. Roy. Soc. (London)* **A220**, 542 (1953); P. G. Klemens, *Can. J. Phys.* **34**, 1212 (1956).

<sup>5</sup> A. Seeger and H. Stehle, *Z. Physik* **146**, 242 (1956).

<sup>6</sup> A. Seeger and H. Bross, *Z. Naturforsch.* **15a**, 663 (1960).

<sup>7</sup> F. R. N. Nabarro and J. M. Ziman, *Proc. Phys. Soc. (London)* **A78**, 1512 (1961).

<sup>8</sup> R. M. J. Cotterill, *Phil. Mag.* **8**, 1937 (1963).

<sup>9</sup> L. M. Clarebrough, M. E. Hargreaves, and M. H. Loretto, *Phil. Mag.* **6**, 807 (1961).

<sup>10</sup> J. G. Rider and C. T. B. Foxon, *Phil. Mag.* **13**, 289 (1966).

<sup>11</sup> W. A. Harrison, *J. Phys. Chem. Solids* **5**, 44 (1958).

<sup>12</sup> H. Stehle and A. Seeger, *Z. Physik* **146**, 217 (1956).

<sup>13</sup> A. Howie, *Phil. Mag.* **5**, 251 (1960).

<sup>14</sup> J. M. Ziman, *Advan. Phys.* **13**, 89 (1964).

<sup>15</sup> Z. S. Basinski, J. S. Dugdale, and A. Howie, *Phil. Mag.* **8**, 1989 (1963).

<sup>16</sup> T. Broom, *Proc. Phys. Soc. (London)* **B65**, 871 (1952).

problem from the point of view of diffraction and obtained a resistivity of about  $10^{-12} \Omega \text{ cm}^2$  per unit stacking-fault density in copper. Freeman<sup>17</sup> showed that a diffraction description of the scattering is not appropriate for the conduction electrons in monovalent fcc metals, and also predicted considerably weaker stacking-fault scattering in zinc. Seeger and Statz<sup>18</sup> presented a fairly complete treatment of the problem, but numerical values<sup>19</sup> based on their theory depended fairly critically on certain parameters which were difficult to determine.

Experimentally, the situation is complicated by the uncertainties involved in separating the resistivity due to stacking faults from that due to dislocations and other defects. Measurements on stacking-fault tetrahedra in gold have relied on the assumption that the dislocations associated with the edges of the tetrahedra do not contribute to the resistivity,<sup>20</sup> and resistivities per unit stacking-fault density in the range  $7\text{--}18 \times 10^{-14} \Omega \text{ cm}^2$  have been obtained<sup>21</sup> at 78°K. More recently, Siegel<sup>22</sup> has obtained the value  $3 \times 10^{-14} \Omega \text{ cm}^2$  at 4.2°K. The applicability of Matthiesen's rule is doubtful.<sup>23</sup> Measurements made on faulted loops in aluminium, attempting to allow for the dislocation contribution to the resistivity, have yielded<sup>24</sup> a stacking-fault resistivity of about  $4 \times 10^{-13} \Omega \text{ cm}^2$ . These determinations serve to show the relative unimportance of stacking-fault scattering compared to that from dislocations, so that the resistivity originally attributed to dislocations was of the right order of magnitude, and Broom's suggestion does not help to cover the discrepancy in the theory. This conclusion is supported by the lack of correlation between residual resistivity and stacking-fault energy,<sup>25</sup> and also by experiments combining resistivity measurements with electron-microscope observations showing dislocations, but no evidence of stacking faults.<sup>8,10</sup> The recent work on dislocation resistivity by Rider and Foxon<sup>10</sup> gives references to previous measurements on aluminium, while Basinski *et al.*<sup>15</sup> give a comprehensive summary of results for a number of metals.

Turning to the effect of dislocations on lattice thermal resistivity, we find a far more complex problem, both theoretically and experimentally, due to the simultaneous influence of a number of scattering mechanisms at low temperatures. In order to separate these effects, one needs to utilize the different temperature dependences

of the resistivity due to different defects, and thus the theory is required to predict the observed temperature dependence as well as the general magnitude of the resistivity. Experimental data on metals (alloys or superconductors), combining thermal-conductivity measurements with reliable estimates of dislocation density, are rather scarce, but the resistivity is observed to vary approximately as  $T^{-2}$ , in accordance with Klemens's theory,<sup>3</sup> and its magnitude<sup>26</sup> has appeared to be in reasonable accord with the theory, provided one makes liberal allowance for the uncertainties involved in the choice of certain constants describing the non-linear interatomic forces essential to the calculations. However, more recent experiments<sup>27</sup> suggest that the magnitude of the dislocation resistivity in alloys may be considerably higher, so that one should perhaps keep an open mind until further experimental data become available. More recent theoretical treatments,<sup>28</sup> taking into account the influence of three-phonon processes on the defect scattering, have found the same order of resistivity as Klemens. All the above theories use perturbation-type approximations, but, as discussed in Sec. VB, the existence of resonance scattering does not necessarily invalidate their use over small temperature ranges.

In ionic crystals, the dislocation thermal resistivity appears to be much larger,<sup>29-32</sup> by a factor of about 100, than the above theories can account for; also, the relaxation time for phonon scattering by dislocations, which should vary inversely with frequency according to Klemens's theory, appears to have a rather more complex frequency dependence.<sup>31,32</sup> These points are discussed further in Sec. VB.

### III. THE TRANSPORT PROBLEMS

In dealing with the electrical- and thermal-transport problems, we find it most convenient to treat the scattering of free (plane-wave) electrons and phonons by point, line, and plane defects characterized, respectively, by spherical, cylindrical, and planar surfaces of constant potential, so that expressions for the resistivities in terms of phase shifts or reflection coefficients can be obtained. As used in Sec. V, the simple expressions obtained by this naive treatment facilitate comparisons between the orders of magnitude of the resistivities due to each of the three types of defect, and more especially

<sup>17</sup> S. Freeman, *J. Phys. Chem. Solids* **26**, 473 (1965).

<sup>18</sup> A. Seeger and H. Statz, *Phys. Status Solidi* **2**, 857 (1962).

<sup>19</sup> H. Statz, *Z. Naturforsch.* **17a**, 994 (1962).

<sup>20</sup> This has been justified by the fact that the long-range strain fields of such dislocations should cancel; it does not seem justified in the light of the resonance-scattering mechanism suggested in this paper.

<sup>21</sup> See references in Ref. 22.

<sup>22</sup> R. W. Siegel, *Phil. Mag.* **13**, 359 (1966).

<sup>23</sup> In this context, see Refs. 10 and 15.

<sup>24</sup> S. Yoshida, M. Kiritani, and T. Yamagata, *J. Phys. Soc. Japan* **20**, 1662 (1965).

<sup>25</sup> L. M. Clarebrough, M. E. Hargreaves, and M. H. Loretto, *Phil. Mag.* **7**, 115 (1962).

<sup>26</sup> K. Mendelssohn and H. M. Rosenberg, *Solid State Phys.* **12**, 223 (1961).

<sup>27</sup> P. Charsley and J. A. M. Salter, *Phys. Status Solidi* **9**, K101 (1965).

<sup>28</sup> A. Seeger, H. Bross, and P. Gruner, *Discussions Faraday Soc.* **38**, 69 (1964); H. Bross, P. Gruner, and P. Kirschenmann, *Z. Naturforsch.* **20a**, 1611 (1965); P. Gruner, *ibid.* **20a**, 1626 (1965), *Phys. Status Solidi* **12**, 679 (1965).

<sup>29</sup> R. L. Sproull, M. Moss, and H. Weinstock, *J. Appl. Phys.* **30**, 334 (1959).

<sup>30</sup> S. Ishioka and H. Suzuki, *J. Phys. Soc. Japan* **18**, Suppl. II, 93 (1963).

<sup>31</sup> A. Taylor, H. R. Albers, and R. O. Pohl, *J. Appl. Phys.* **36**, 2270 (1965).

<sup>32</sup> M. Moss, *J. Appl. Phys.* **36**, 3308 (1965).

enable us to readily see whether a given experimental value would appear to require resonance scattering for its explanation.

### A. Charge Transport

We denote<sup>33</sup> by  $(N\Omega/4\pi^3)f(\mathbf{k},t)d^3k$  the number of electrons in the crystal of volume  $N\Omega$ , which at time  $t$  have wave vectors in the element  $d^3k$  of  $\mathbf{k}$  space. Then, if these are free electrons of mass  $m$ , the current density at time  $t$  is

$$\mathbf{J}(t) = -\frac{e\hbar}{4\pi^3m} \int \mathbf{k}f(\mathbf{k},t)d^3k, \quad (3.1)$$

the integral being over all  $\mathbf{k}$  space.

For a steady state, we require, for all  $t$ ,

$$\left[ \frac{\partial f}{\partial t} \right]_E + \left[ \frac{\partial f}{\partial t} \right]_S = 0, \quad (3.2)$$

where the subscripts  $E$  and  $S$  denote the rates of change of occupation of states due, respectively, to acceleration by the electrical field  $\mathbf{E}$ , applied perpendicular to the defect line or plane, and scattering by the defect.

The first term in (3.2) is written<sup>33</sup> as  $(e/\hbar)\mathbf{E} \cdot \nabla_{\mathbf{k}}f(\mathbf{k})$  and the second term is expressed, as usual, in terms of a scattering probability; the resulting solution of (3.2) is then used in (3.1) to give, for the conductivities normal to the dislocation and stacking fault respectively,

$$\sigma_d = -\frac{N\Omega}{4\pi^3} \left( \frac{e\hbar}{2\pi m} \right)^2 \int_{-\infty}^{\infty} dk_3 \int_0^{\infty} dk_* k_*^3 \left( \frac{\partial f_0}{\partial \mathcal{E}} \right)_k \times P(k_3, k_*) \quad (3.3a)$$

and

$$\sigma_{sf} = -\frac{N\Omega}{4\pi^3} \left( \frac{e\hbar}{2\pi m} \right)^2 \int_{-\infty}^{\infty} dk_3 \int_0^{\infty} dk_* \frac{k_* k_3^2}{W_{sf}(k_3, k_*)} \times \left( \frac{\partial f_0}{\partial \mathcal{E}} \right)_k. \quad (3.3b)$$

Here  $\mathbf{k} = \mathbf{k}_* + \mathbf{k}_3$ , with  $\mathbf{k}_*$  and  $\mathbf{k}_3$  being, respectively, normal and parallel to the dislocation, or parallel and normal to the stacking fault. The equilibrium Fermi distribution function  $f_0$  is a function only of  $\mathcal{E} = \hbar^2 k^2/2m$ , and at  $T=0$  takes the values 0 or 1 according to whether  $\mathcal{E}$  is greater or less than  $\mathcal{E}_f$ , the Fermi level. The quantity  $P(k_3, k_*)$  is given by

$$P(k_3, k_*) = \left\{ \int_0^{2\pi} W_d(k_3, k_*; \phi) (1 - \cos\phi) d\phi \right\}^{-1}, \quad (3.4)$$

where  $(4\pi^3/N\Omega)W_d(k_3, k_*; \phi) d\phi$  is the probability per unit time of an electron in state  $\mathbf{k}_i = \mathbf{k}_3 + \mathbf{k}_i$  being scattered by the dislocation into a state  $\mathbf{k}_f = \mathbf{k}_3 + \mathbf{k}_*$

with  $\mathbf{k}_*$  having its cylindrical polar angle in the range  $d\phi_f$  about  $\phi_f$ , provided the initial state is occupied and the final state empty. Likewise,  $(4\pi^3/N\Omega)W_{sf}(k_3, k_*)$  is the probability per unit time of an electron in state  $\mathbf{k}_* + \mathbf{k}_3$  being scattered by the stacking fault into the state  $\mathbf{k}_* - \mathbf{k}_3$ .

A phase-shift analysis<sup>5,12</sup> of the line-defect scattering shows that  $P(k_3, k_*)$  is, in fact, independent of  $k_3$  (for *free-electron* scattering) and (3.3a) then reduces to

$$\sigma_d = \frac{N\Omega}{L} \frac{e^2}{4\pi^2\hbar} \int_0^{k_f} k_*^3 (k_f^2 - k_*^2)^{-1/2} \times \left\{ \sum_{m=-\infty}^{\infty} \sin^2(\eta_{m+1} - \eta_m) \right\}^{-1} dk_*, \quad (3.5a)$$

for a crystal extending a distance  $L$  in the direction of the defect. Here,  $k_f$  is the wave vector at the Fermi surface, and  $\eta_m(k_*)$  is the phase shift in the  $m$ th radial function involved in the expansion in cylindrical coordinates of the perturbed wave function corresponding to the unperturbed plane wave of wave vector  $\mathbf{k}_3 + \mathbf{k}_*$ .

A similar treatment of the Schrödinger equation for the plane-defect scattering shows  $W_{sf}$  to be independent of  $k_*$ , and (3.3b) reduces to

$$\sigma_{sf} = \frac{N\Omega}{A} \frac{e^2}{2\pi^2\hbar} \int_0^{k_f} \frac{k_3}{r(k_3)} dk_3, \quad (3.5b)$$

where  $A$  is the area of cross section of the crystal parallel to the defect, and the reflection coefficient  $r(k_3)$  is the probability that an electron of wave vector  $\mathbf{k}_* + \mathbf{k}_3$  will be reflected by the fault into the state  $\mathbf{k}_* - \mathbf{k}_3$ ;  $r$  takes values in the range  $0 \leq r \leq 1$ , and is independent of  $k_*$ .

The corresponding procedure for point-defect scattering yields the well-known result

$$\sigma_p = N\Omega \frac{e^2 k_f^4}{12\pi^3\hbar} \left\{ \sum_{l=1}^{\infty} l \sin^2[\eta_l(k_f) - \eta_{l-1}(k_f)] \right\}^{-1}, \quad (3.5c)$$

where  $\eta_l(k_f)$  is the phase shift in the  $l$ th radial wave function, evaluated for electrons at the Fermi surface.

### B. Energy Transport

For scattering by static lattice imperfections, the *electronic* thermal conductivity  $\kappa^{(e)}$  is related to the electrical conductivity  $\sigma$  by the Wiedemann-Franz relation<sup>34</sup>

$$\kappa^{(e)} = (\pi^2 k_B^2/3e^2) T \sigma, \quad (3.6)$$

where  $k_B$  is Boltzmann's constant and  $T$  the absolute temperature. Thus, for each type of defect,  $\kappa^{(e)}$  is readily calculated from the work of Sec. IIIA.

<sup>33</sup> A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, England, 1936), Chap. 5.

<sup>34</sup> J. M. Ziman, *Electrons and Phonons* (Oxford University Press, London, 1962), p. 385.

Of more interest is the *phonon* thermal conductivity  $\kappa^{(p)}$ . In analogy to Sec. IIIA, we find it convenient to consider the scattering of plane-wave phonons by a defect in an otherwise homogeneous and isotropic medium. We expect to lose nothing significant by using this approximation at low temperatures, where only the long-wavelength acoustic modes are occupied. Thus, we set up the equations of elasticity for such a medium, before introduction of the perturbation, in the form<sup>35</sup>

$$\mu \nabla^2 \mathbf{u}^0 + (\lambda + \mu) \nabla \nabla \cdot \mathbf{u}^0 = \rho \partial^2 \mathbf{u}^0 / \partial t^2, \quad (3.7)$$

where  $\lambda$  and  $\mu$  are the Lamé constants,  $\rho$  is the density of the unperturbed medium, and  $\mathbf{u}^0(\mathbf{r}, t)$  is its local elastic displacement.

Equation (3.7) has, for any wave vector  $\mathbf{k}$ , one longitudinal-wave solution satisfying

$$\nabla \times \mathbf{u}_l^0 = 0; \quad \partial^2 \mathbf{u}_l^0 / \partial t^2 + v_l^2 \nabla^2 \mathbf{u}_l^0 = 0, \quad (3.8)$$

and two transverse-wave solutions satisfying

$$\nabla \cdot \mathbf{u}_t^0 = 0; \quad \partial^2 \mathbf{u}_t^0 / \partial t^2 + v_t^2 \nabla^2 \mathbf{u}_t^0 = 0, \quad (3.9)$$

where

$$v_l^2 = (\lambda + 2\mu) / \rho; \quad v_t^2 = \mu / \rho. \quad (3.10)$$

Now, writing each of these solutions in the form

$$\mathbf{u}^0(\mathbf{r}, t) = \mathbf{u}^0(\mathbf{r}) \alpha e^{-i\omega t}, \quad (3.11)$$

where  $\omega = kv^0$  and  $\alpha$  is a unit vector either parallel to, or perpendicular to  $\mathbf{k}$ , we find

$$\nabla^2 \mathbf{u}^0(\mathbf{r}) + k^2 \mathbf{u}^0(\mathbf{r}) = 0. \quad (3.12)$$

On introducing the perturbation, we will consider only the effects of the dilatation  $\Delta(\mathbf{r})$  associated with it, and, following Ziman,<sup>36</sup> write the local velocity of the waves as

$$v(\mathbf{r}) = v^0 \{1 + \gamma \Delta(\mathbf{r})\}, \quad (3.13)$$

where  $\gamma$  is the Grüneisen constant. The perturbed version of (3.12) is then

$$\nabla^2 \mathbf{u}(\mathbf{r}) + k^2 \{1 - 2\gamma \Delta(\mathbf{r})\} \mathbf{u}(\mathbf{r}) = 0. \quad (3.14)$$

Equation (3.14) is now susceptible to the same type of analysis as used on the Schrödinger equation in Sec. IIIA. On carrying through such a treatment, we find, corresponding to Eqs. (3.5), the expressions

$$\begin{aligned} \kappa_a^{(p)} = & \frac{N\Omega}{L} \frac{\hbar v^2}{8\pi^2} \int_0^\infty dk_3 \int_0^\infty dk_* k_*^3 \frac{\partial n_0(k)}{\partial T} \\ & \times \left\{ \sum_{m=-\infty}^{\infty} \sin^2(\eta_{m+1} - \eta_m) \right\}^{-1}, \end{aligned} \quad (3.15a)$$

$$\kappa_{st}^{(p)} = \frac{N\Omega}{A} \frac{\hbar v^2}{4\pi^2} \int_0^\infty dk_3 \int_0^\infty dk_* \frac{k_3 k_*}{r(k_3, k_*)} \frac{\partial n_0(k)}{\partial T}, \quad (3.15b)$$

<sup>35</sup> I. S. Sokolnikoff, *Mathematical Theory of Elasticity* (McGraw-Hill Book Company, Inc., New York, 1956), p. 370.

<sup>36</sup> Reference 34, p. 229.

and

$$\begin{aligned} \kappa_p^{(p)} = & N\Omega \frac{\hbar v^2}{24\pi^3} \int_0^\infty k^5 \frac{\partial n_0(k)}{\partial T} \\ & \times \left\{ \sum_{l=1}^{\infty} l \sin^2(\eta_l - \eta_{l-1}) \right\}^{-1} dk. \end{aligned} \quad (3.15c)$$

These equations apply to each polarization branch by inserting the appropriate value of  $v$ ; the total conductivity is the sum of the three  $\kappa$ 's, one for each polarization. Note that in our approximation the Bose-Einstein occupation number  $n_0$  depends on  $v$  through

$$n_0(k) = \{ \exp(\hbar kv / k_B T) - 1 \}^{-1}, \quad (3.16)$$

but, because Eq. (3.14) does not contain  $v$ , the phase shifts  $\eta$  and reflection coefficient  $r$  are the same for all three polarizations. On the other hand, note that, in contrast to the electronic case,  $\eta$  and  $r$  depend on *both*  $k_3$  and  $k_*$  (3.15a, 3.15b), for phonon scattering by dilata-tions due to line and plane defects; this is due to the involvement of  $k^2$  in the perturbation term in (3.14). The phase shifts in (3.15c) are functions of  $k$ .

#### IV. SCATTERING FROM A LOCALIZED LINE DEFECT

##### A. Resonance Scattering

Using the simple model of a screw dislocation introduced in Sec. IVA of the previous paper,<sup>1</sup> referred to in the following as A, it is a simple matter to carry through a procedure, analogous in every way to that of Callaway,<sup>37</sup> which yields the scattering amplitude, the differential-scattering width, and the probability  $W_d$  of (3.4), each in a form exhibiting the resonant nature of the scattering. We will briefly sketch the procedure; the notation is as in A, unless otherwise defined.

Thus, we substitute

$$V_{qj}(\mathbf{m}^*, \mathbf{n}^*) = \delta_{qj} \delta_{\mathbf{m}^*, 0} \delta_{\mathbf{n}^*, 0} V_0 \quad (4.1)$$

in Eq. (2.9) of A to obtain

$$C_q^{(s)} = N_*^{-1/2} \delta_{qs} \left\{ e^{i\mathbf{k}^* \cdot \mathbf{n}^*} + \frac{V_0 \mathcal{G}_{E,q}(\mathbf{n}^*)}{1 - V_0 \mathcal{G}_{E,q}(0)} \right\}. \quad (4.2)$$

The behavior of  $\mathcal{G}_{E,q}(\mathbf{n}^*)$  for large  $n_*$  is obtained<sup>37</sup> by the method of stationary phase as

$$\begin{aligned} \mathcal{G}_{E,q}(\mathbf{n}^*) \sim & -\sqrt{2\pi^{3/2}} \sigma_* \sum e^{i(\mathbf{k}_0^* \cdot \mathbf{n}^* + \pi/4)} (a_1^2 + a_2^2)^{1/4} \\ & \times \{ n_* (a_1^2 b_2 + a_2^2 b_1) \}^{-1/2}, \end{aligned} \quad (4.3)$$

where the sum is over all points  $\mathbf{k}_0^*$  satisfying

$$E_{0,q}(\mathbf{k}_3; \mathbf{k}_0^*) = E$$

and

$$[\nabla_{\mathbf{k}^*} E_{0,q}(\mathbf{k}_3; \mathbf{k}_0^*)]_{\mathbf{k}_0^*} \parallel \mathbf{n}^*, \quad (4.4)$$

and we have expanded

$$E_{0,q}(\mathbf{k}_3; \mathbf{k}_*) = E_{0,q}(\mathbf{k}_3; \mathbf{k}_{0*}) + \kappa_1 a_1 + \kappa_2 a_2 + 2b_1 \kappa_1^2 + 2b_2 \kappa_2^2, \quad (4.5)$$

where  $\kappa_1, \kappa_2$  are orthogonal components of  $\kappa = \mathbf{k}_* - \mathbf{k}_{0*}$ .

Rather than complicate matters, we assume the simple form

$$E_{0,q}(\mathbf{k}_3; \mathbf{k}_*) = \mathcal{E}_B(\mathbf{k}_3) + \hbar^2 k_*^2 / 2m_q^*(k_3), \quad (4.6)$$

for which (4.3) becomes

$$\mathcal{G}_{E,q}(\mathbf{n}_*) \sim - (2\pi)^{3/2} \sigma_* \frac{m_q^*(k_3) e^{i(k_* n_* + \pi/4)}}{\hbar^2 (k_* n_*)^{1/2}}. \quad (4.7)$$

Now, on using (4.7) in (4.2), we get

$$C_q^{(s)} = N_*^{-1/2} \delta_{q*} \{ e^{i\mathbf{k}_* \cdot \mathbf{n}_*} + f_q(k_3, k_*) e^{i k_* n_*} n_*^{-1/2} \}, \quad (4.8)$$

with

$$f_q(k_3, k_*) = - e^{i\pi/4} (2\pi)^{3/2} \frac{\sigma_* m_q^*(k_3) V_0}{\hbar^2 k_*^{1/2} (1 - V_0 \mathcal{G}_{E,q}(0))}. \quad (4.9)$$

In the same sense as Callaway,<sup>37</sup> we identify  $f$  as the scattering amplitude, and it is a straightforward manner to show the differential-scattering width  $\tau$  is given by

$$\tau_q(k_3, k_*; \phi) = |f_q(k_3, k_*)|^2 = (2\pi)^3 \{ \sigma_* m_q^*(k_3) \hbar^{-2} \}^2 \times \frac{V_0^2}{k_* |1 - V_0 \mathcal{G}_{E,q}(0)|^2}. \quad (4.10)$$

Here,  $\tau$  is defined such that  $\tau(\phi)d\phi$  is the number of electrons per second, per unit length of dislocation, scattered from a beam of unit normal intensity through a cylindrical polar angle lying between  $\phi$  and  $\phi + d\phi$ . We define the "normal intensity" of a beam as the number of electrons in the beam-crossing unit area normal to the  $\mathbf{k}_*$  direction for that beam in unit time, so that the normal intensity of the "free-electron" beam  $(N\Omega)^{-1/2} \exp\{i(\mathbf{k}_3 + \mathbf{k}_*) \cdot \mathbf{r}\}$  is  $\hbar k_* / N\Omega m$ . For our simple model (4.1), we see from (4.8) that  $f$ , and hence  $\tau$ , is independent of  $\phi$ ; i.e., we are restricted to "s-wave" scattering.

From this definition of  $\tau(\phi)$ , we readily find the scattering probability  $W_d(\phi)$  introduced in (3.4):

$$W_d(k_3, k_*; \phi) = L(\hbar k_* / 4\pi^2 m) \tau(k_3, k_*; \phi). \quad (4.11)$$

Likewise, the total scattering width of the dislocation for the  $q\mathbf{k}_3$  subband is

$$Q_q(k_3, k_*) = 2\pi \tau_q(k_3, k_*), \quad (4.12)$$

and if we compare this expression with

$$Q(k_3, k_*) = 4k_*^{-1} \sum_{m=-\infty}^{\infty} \sin^2 \eta_m(k_*), \quad (4.13)$$

obtained from the partial-wave analysis of free-electron scattering, we obtain the useful identification, for our "s-wave" scattering of the Bloch wave of wave vector  $\mathbf{k}_3 + \mathbf{k}_*$ ,

$$\sin^2 \eta_0 = \{ 2\sigma_* \pi^2 V_0 m_q^*(k_3) / \hbar^2 |1 - V_0 \mathcal{G}_{E,q}(0)| \}^2. \quad (4.14)$$

To write the above expressions explicitly in their resonant form, we put

$$\mathcal{G}_E(0) = I(E) - i\pi\eta(E), \quad (4.15)$$

and consider an energy  $E_0$  in the subband, satisfying

$$1 - V_0 I(E_0) = 0. \quad (4.16)$$

Then we look for a solution

$$E = E_R - i\Gamma/2, \quad (4.17)$$

of

$$1 - V_0 \mathcal{G}_E(0) = 0, \quad (4.18)$$

such that  $E_R \simeq E_0$ , and  $\Gamma \simeq 0$ .

Expanding  $\mathcal{G}_E(0)$  about the point  $E_0 + i0$ , we obtain, in the same way as Callaway,

$$E_R = E_0 - \pi^2 \eta(E_0) \eta'(E_0) / \{ I'^2(E_0) + \pi^2 \eta'^2(E_0) \}, \quad (4.19)$$

and

$$\Gamma = -2\pi \eta(E_0) I'(E_0) / \{ I'^2(E_0) + \pi^2 \eta'^2(E_0) \},$$

the primes denoting differentiation. As is shown in A, for a resonance close to a subband edge, we have  $\eta \rightarrow \text{constant}$ ,  $I \rightarrow \infty$ , so that we assume  $I'^2 \gg \eta'^2$ , generally, to obtain

$$E_R \simeq E_0 - \pi^2 \eta(E_0) \eta'(E_0) / I'^2(E_0) \simeq E_0$$

and

$$\Gamma \simeq -2\pi \eta(E_0) / I'(E_0) \simeq 0. \quad (4.20)$$

Writing  $\Delta_0 = E_0 - \mathcal{E}_B$ , the distance of the resonance from the bottom of the subband, we obtain from the second equation of (4.20), for small  $\Delta_0$ ,

$$\Gamma = -2\pi \Delta_0, \quad (4.21)$$

so that there may be some justification in expecting the width of a resonance, positioned well in the interior of a subband, to be an appreciable fraction of the width of that subband.<sup>38</sup> We shall see, from Eq. (4.23) and Sec. V, that the width of the resonance is of importance in determining the likely effect on the resistivity.

By expanding about  $E = E_0$  and using Eqs. (4.20), we obtain

$$1 - V_0 \mathcal{G}_E(0) = 2\pi \eta(E_0) V_0 \Gamma^{-1} \times \{ (E - E_0) + i\Gamma/2 \}, \quad (4.22)$$

<sup>38</sup> Note, however, that, because of the divergence of the Green's function, Eq. (4.14) shows that  $\sin^2 \eta_0 \rightarrow 0$  at the subband edges, in accord with the well-known result  $\eta_0 \rightarrow n\pi$  for the scattering of zero-energy plane waves from a point defect.

<sup>37</sup> J. Callaway, J. Math. Phys. 5, 783 (1964).

which yields in (4.14), using Eq. (3.11) of A for  $\eta(E_0)$ ,

$$\sin^2\eta_0 = \frac{\Gamma^2/4}{(E-E_0)^2 + \Gamma^2/4}. \quad (4.23)$$

Corresponding expressions for the scattering width, etc., are readily obtained.

### B. Density of States near Resonance

Following Klauder,<sup>39</sup> we find for the increase,  $N^*\Delta\eta_{q\mathbf{k}_3}(E)$ , in the density of  $q\mathbf{k}_3$  subband states, brought about by the perturbation  $V$ ,

$$N^*\Delta\eta_{q\mathbf{k}_3}(E) = -\frac{1}{\pi} \mathcal{I} \left\{ \lim_{\epsilon \rightarrow +0} \frac{d}{dE} \times \ln \left[ \det_{q\mathbf{k}_3} \left( I - \frac{1}{E+i\epsilon-H_0} V \right) \right] \right\}, \quad (4.24)$$

where  $\mathcal{I}$  denotes imaginary part, and  $\det_{q\mathbf{k}_3} \mathcal{A}$  indicates the determinant formed from the matrix elements of the operator  $\mathcal{A}$  with respect to all the Wannier functions of the  $q\mathbf{k}_3$  subband. For our simple model (4.1),

$$\lim_{\epsilon \rightarrow +0} \det_{q\mathbf{k}_3} (I - \{E+i\epsilon-H_0\}^{-1}V) = 1 - V_0 \mathcal{G}_E(0), \quad (4.25)$$

and so (4.24) readily yields, near a resonance (cf. Callaway),

$$N^*\Delta\eta_{q\mathbf{k}_3}(E) = \frac{1}{2\pi} \frac{\Gamma}{(E-E_0)^2 + \Gamma^2/4}. \quad (4.26)$$

To find the number of states introduced into the neighborhood of the resonance, we can integrate this expression over an energy interval of order  $\Gamma$  centered on  $E_0$ . Since the integral converges fairly rapidly, we can extend the terminals to  $\pm\infty$  and obtain for the number of states introduced near each resonance,

$$\Delta n(E_0) = \frac{\Gamma}{2\pi} \int_{-\infty}^{\infty} \frac{dE}{(E-E_0)^2 + \Gamma^2/4} = \Gamma/|\Gamma|, \quad (4.27)$$

which, in conjunction with the second equation of (4.20), is the result quoted in the discussion of Fig. 1 of A.

### C. Further Remarks

The procedure of Secs. IVA and IVB can be carried through very similarly for the corresponding model [see Eq. (4.4) of A] of an edge dislocation. The results are rather more complicated, although of a similar form, but of course the phase-shift correspondence (4.23) is no longer meaningful. The density of states near a resonance takes precisely the same form as (4.26), so that (4.27) follows and we have exactly one state either pushed out from, or pulled into, the vicinity of each

resonance; of course, as remarked in A, the edge dislocation gives rise to *pairs* of resonances, arising together from the top and bottom respectively of the subband. The one-one correspondence between resonances and bound states has been discussed in A.

For phonon scattering by a dilatation representing a screw dislocation, we find similar expressions to those above for electron scattering, and, in particular, obtain, corresponding to (4.23), for the phase shift near the resonance at  $\omega = \omega_0$ ,

$$\sin^2\eta_0 = \frac{\gamma^2/4}{(\omega^2 - \omega_0^2)^2 + \gamma^2/4}. \quad (4.28)$$

The width  $\gamma$  is given by

$$\gamma = -2\pi\xi_j(\omega_0^2)/J_j'(\omega_0^2) \quad (4.29)$$

for the  $j$ th polarization branch of the  $\mathbf{k}_3$  acoustic subband; the notation is that of Eq. (3.22) of A.

## V. INTERPRETATION OF THE EXPERIMENTAL DATA

Before attempting any numerical analysis of the data on electrical and thermal resistivities, we should comment on the following basic difference between electron and phonon scattering by defects; thus, on the one hand, the majority of conduction electrons in a metal have wavelengths of the order of a lattice constant, but on the other hand, the dominant phonon wavelength increases with decreasing temperature and is of the order of a hundred lattice constants at the temperatures (10–20°K), at which dislocation scattering, for example, becomes important. This difference leads to two important conclusions. Firstly, the obvious one, that for electron scattering the effects of the defect core should dominate those of the long-range strain field, while for phonon scattering the opposite should be the case; this remark is consistent with the evidence,<sup>10</sup> mentioned in Sec. II, that dislocation electrical resistivity is insensitive to dislocation arrangement, and likewise there is some evidence<sup>31</sup> that the opposite is true for thermal resistivity. Secondly, the effects of the scattering resonances will be much more sensitive to their actual positions in the phonon subbands, and also to the widths of the resonances, than will be the case for electron resonances. The desirability, from the point of view of obtaining a high resistivity, of having the electron resonances near the Fermi energy  $\mathcal{E}_f$  is evident from Eqs. (3.5), but it is clear that only changes of an appreciable fraction of  $\mathcal{E}_f$  in the positions or widths of the resonances will effect the order of magnitude of the resistivity. On the other hand, due to the exponential temperature dependence of  $n_0$ , Eqs. (3.15) show that changes of order  $kT$  in the positions or widths of the phonon resonances can greatly effect the thermal resistivity; this point will be further discussed in Sec. V B.

<sup>39</sup> J. R. Klauder, Ann. Phys. (N. Y.) 14, 43 (1961).

### A. Electron Scattering

For scattering by dislocations, the simple model of Sec. IV suggests that we obtain the resistivity from Eq. (3.5a), retaining only the zeroth-order phase shift. Then, by (4.23), the value of  $\sin^2\eta_0$  will never be far below unity, provided the width of the resonance is not too small, so that, according to the above remarks regarding the relative insensitivity of the resistance to the positions of the resonances, we can take  $\sin^2\eta_0$  outside the integral and replace it by some average value which we expect to be close to unity. Thus, (3.5a) yields, for the resistivity due to a density of  $\beta$  dislocations per unit area,

$$\rho_d = \beta (12\pi^2 \hbar / e^2 k_f^3) \langle \sin^2\eta_0 \rangle_{\text{av}}. \quad (5.1)$$

The same sort of argument applied to (3.5b) yields, for a density of  $\alpha$  stacking faults per unit length,

$$\rho_{\text{st}} = \alpha (4\pi^2 \hbar / e^2 k_f^2) \langle r \rangle_{\text{av}}, \quad (5.2)$$

where we expect the "average" reflection coefficient to be significantly less than unity, since resonance scattering is not predicted<sup>1</sup> as a characteristic property of surface defects.

We take the experimental data for dislocations from Ref. 15, except for a more recent value<sup>10</sup> for aluminium. For stacking-fault resistivity, we take an upper limit of  $1.8 \times 10^{-13} \Omega \text{ cm}^2$  for gold, which appears to be the largest experimental value obtained for this metal,<sup>21</sup> and the value of  $4 \times 10^{-13} \Omega \text{ cm}^2$  for aluminium<sup>24</sup>; the value of Hiki *et al.*,<sup>40</sup> for copper, is unreliable, due to the considerable uncertainties in determining the width of the fault.

Using the above data, the appropriate parameters are evaluated<sup>41</sup> from Eqs. (5.1) and (5.2), taking for  $k_f$  the free-electron value  $(3\pi^2 n)^{1/3}$ , where  $n$  is the electron density. The results are shown in Tables I and II. We see that the value of the reflection coefficient for Au and Al suggests no resonance scattering from stacking faults in these metals; the high value for the specific resistivity in copper must be regarded as very uncertain,<sup>40</sup> particularly since it is so much greater than the apparently more reliable values for gold,<sup>21</sup> so for the present we feel justified in overlooking the high value of  $\langle r \rangle_{\text{av}}$  for Cu. Turning to the data on dislocations, we first of all note that the estimates of dislocation density leading to the experimental values quoted for the five metals in the left-hand segment of Table II have been made<sup>10,15</sup> by one or more of the techniques of thin-film electron microscopy, stored energy measurement, and density change measurement; such techniques are known to be reasonably self-consistent. On the other

TABLE I. Electrical resistivity of stacking faults.

Metal	Au	Al	Cu
$(\rho_{\text{st}}/\alpha) \Omega \text{ cm}^2 \times 10^{-13}$	1.8	4.0	60
$\langle r \rangle_{\text{av}}$	0.02	0.08	0.86

hand, the estimates of dislocation density associated with the remaining five values of Table II do not seem to be so well-founded.<sup>15</sup> We can therefore be reasonably satisfied, from the results for Cu, Ag, Au, and Al, that resonance scattering appears to be capable of explaining dislocation electrical resistivities.

The need for more accurate experimental determinations of dislocation and stacking-fault resistivities for a wider range of metals is apparent. The values quoted in Table II for Ni, Fe,<sup>42</sup> W, and Zr would appear to be unthinkably high, since, even allowing for the undoubted oversimplifications of a model which gives rise to only "s-wave" scattering, it is difficult to see how the more general expression

$$\sum_{m=-\infty}^{\infty} \sin^2(\eta_{m+1} - \eta_m)$$

could average a value so much greater than unity. By way of some support for this contention, we note that if Eq. (3.5c) is applied to the analysis of the alloy data of Linde, as tabulated by Blatt,<sup>43</sup> the values obtained for

$$\sum_{l=1}^{\infty} l \sin^2\{\eta_l(k_f) - \eta_{l-1}(k_f)\}$$

do not exceed 2.5, and most are less than unity.

### B. Phonon Scattering

The need to consider the temperature dependence of the dislocation thermal resistivity was mentioned in Sec. II. The peak in the conductivity curve usually occurs at around 10–20°K, and at higher temperatures the effects of dislocations are not important; thus, any successful theory should account for the magnitude and temperature dependence of the dislocation scattering up to about 20°K. Now this range of temperatures corresponds to a range of phonon energies extending up to only about one-tenth of the total width of the acoustic

TABLE II. Electrical resistivity of dislocations.

Metal	Cu	Ag	Au	Al	Ni	Pt	K	Fe	W	Zr
$(\rho_d/\beta) \Omega \text{ cm}^2 \times 10^{-10}$	2.0	1.9	2.6	1.8	9.4	9	4	20*	19	100
$\langle \sin^2\eta_0 \rangle_{\text{av}}$	1.0	0.7	0.9	2.0	10	3.6	0.3	24	15	52

\* See Ref. 42.

<sup>40</sup> Y. Hiki, T. Suzuki, and K. Yajima, J. Phys. Soc. Japan 18, Suppl. II, 105 (1963).

<sup>41</sup> The "experimental" values of  $r$  and  $\sin^2\eta_0$  shown in Tables I–III, having been deduced from Eqs. (5.1)–(5.3), apply to an array of parallel stacking faults or dislocations. For a random distribution of orientations, these values will be approximately twice those shown.

<sup>42</sup> The value of  $\rho_d/\beta = 1.7 \times 10^{-10} \Omega \text{ cm}^2$ , quoted by I. Y. Dekhtyar, S. G. Litovchenko, and R. G. Fedchenko [Ukr. Fiz. Zh. 6, 233 (1961)] for Fe-Mo alloys, leads to a value of  $\langle \sin^2\eta_0 \rangle_{\text{av}} = 2.0$ , and so would seem more reasonable than the value quoted in Ref. 15.

<sup>43</sup> F. J. Blatt, Solid State Phys. 4, 199 (1957).



TABLE III. Thermal resistivity of dislocations.

Crystal	$(\beta t)^{-1}$ cm <sup>2</sup> sec <sup>-1</sup>	$T_p$ deg K	$\sin^2\eta_0(T_p)$ Expt. <sup>a</sup> Klemens	
KCl	$2.65 \times 10^{-1}$	7	0.6	0.008
NaCl	$2.76 \times 10^{-13} \omega$	9	0.8	0.01
NaCl	$4.40 \times 10^{-1}$	9	1.0	0.01
NaF	$0.93 \times 10^{-13} \omega$	12	0.3	0.008
LiF	$1.67 \times 10^{-13} \omega$	20	0.8	0.01
LiF	$2.61 \times 10^{-13} \omega$	20	1.3	0.01
LiF	$4.75 \times 10^{-1}$	20	0.9	0.01
CaF <sub>2</sub> <sup>b</sup>	$8.75 \times 10^{-26} \omega^2$	18	2.3	0.04
Cu	$0.97 \times 10^{-14} \omega$	20	0.1	0.03

<sup>a</sup> Deduced by inserting the experimental relaxation time in Eq. (5.3).

<sup>b</sup> There is some uncertainty (Ref. 32) in the estimate of dislocation density for CaF<sub>2</sub>.

energy band. This fact provides a *prima facie* link with resonance scattering, since we can suppose the wide difference in the magnitude of the scattering which appears to exist between metals and ionic crystals to be due to the phonon resonances in metals falling, for some reason, fairly well into the subbands, and thus not influencing the energies of interest, while the opposite is supposed for ionic crystals. One cannot be at all definite without performing the presumably complex calculations necessary to actually estimate the positions of the resonances for different crystals, but at least the suggestion appears plausible. This argument would explain the reasonable success of the perturbation-based approaches for metals, and its failure for ionic crystals; its weakness lies in the complex frequency dependence, Eq. (4.28), associated with the resonance scattering. However, there does appear to be some evidence<sup>31,32</sup> for a different frequency dependence of the scattering in ionic crystals to that predicted by Klemens,<sup>3</sup> and perhaps one should not rule out resonance scattering on these grounds without some sort of detailed curve-fitting analysis.<sup>31,32</sup>

Before devoting a great deal of effort to the subject of temperature dependence, it is of obvious relevance to inquire whether the *magnitude* of the resonance scattering is compatible with the observations on ionic crystals. To decide this we use a treatment similar to that of Sec. VA.

Thus, with the phonon scattering width  $\tau(k_3, k_*)$

being given in terms of the relaxation time  $t$ , by  $\tau = k/\beta v k_* t$ , and in terms of our zero-order phase shift, by  $\tau = 4k_*^{-1} \sin^2\eta_0$ , we have

$$\sin^2\eta_0 = (\omega/4v^2)(\beta t)^{-1}, \quad (5.3)$$

where we have used the Debye approximation,  $\omega = vk$ . Using Eq. (5.3) and putting  $\omega = k_B T_p/h$ ,  $k_B$  being Boltzmann's constant, we have evaluated<sup>41</sup>  $\sin^2\eta_0$  at the temperature  $T_p$  corresponding to the peak of the conductivity curve in the annealed crystal. We have used the experimental data on ionic crystals from Refs. 31 and 32, and have included figures for copper<sup>44</sup> for comparison. The results are shown in Table III, together with the corresponding values according to the theory of Klemens<sup>45</sup>; it is clear that the resonance scattering ( $\sin^2\eta_0 \simeq 1$ ) is considerably stronger than that given by Klemens, and is of the right order of magnitude to be a possible explanation of the experimental observations on ionic crystals. Although the question of temperature dependence remains a problem, the promise, magnitude wise, of the resonance mechanism would seem to justify the expenditure of some effort on a more detailed treatment of this problem.

There appear to be no quantitative data pertaining to the effects of internal-surface imperfections on the thermal conductivity, but there is some indication that dislocation scattering decreases when dislocation wall formation occurs.<sup>46</sup> This is consistent with our theory, which does not expect resonance scattering from surface defects, although it can also be explained on the basis of other theories.<sup>47</sup>

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<sup>44</sup> W. R. G. Kemp, P. G. Klemens, and R. J. Tainsh, *Phil. Mag.* **4**, 845 (1959).

<sup>45</sup> Based on Eq. (5.23) of Ref. 3.

<sup>46</sup> R. L. Sproull and R. O. Pohl, *J. Phys. Soc. Japan* **18**, Suppl. II, 89 (1963).

<sup>47</sup> P. G. Klemens, in discussion of Ref. 30.