PHYSICAL REVIEW VOLUME 106, NUMBER 4 MAY 15, 1957

Internal Friction and Defect Interaction in Germanium: Theoretical

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(Received January 14, 1957)

A model has been constructed in which small vibrations of dislocation line segments cause displacements in the point-imperfection distributions surrounding the dislocations. The energy lost through the motions of the point imperfections is observed as mechanical damping. The motion of the dislocations is obtained from the theory of Koehler. The Cottrell potential is taken as the interaction between dislocations and point defects.

It is shown from the high-frequency expansion of the theoretical energy dissipation that the dependence of the dissipation on strain, frequency, and temperature is essentially the same as that of the normal anelastic relaxation effect, in agreement with the experimental observations. It is further shown that the magnitude of the effect is such as to support the hypothesis that the lattice vacancy, present in a concentration of approximately 10^{10}/cm^3, is the point defect which interacts with dislocations, giving rise to the observed vibrational energy loss. In turn, using the numbers derived from the vacancy hypothesis, it is shown that the cutoff for the purely elastic dislocation potential is several atom spacings from the dislocation line.

INTRODUCTION

An anelastic relaxation effect has been observed in measurements of the internal friction (logarithmic decrement) of germanium single crystals subjected to high-frequency stress in the temperature range from 250 to 750°C. The experimental results are reported in a previous paper,[1] together with a tentative interpretation in terms of the stress-induced migration of lattice vacancies.

The interpretation in I is based on the observed temperature dependence of the logarithmic decrement, on the dependence of the decrement on the number of dislocations in the specimens, and, implicitly, on the assumption that the generally accepted mechanisms for the diffusion of substitutional impurities is the correct one. It was brought out in I that, because of the high degree of symmetry of the diamond lattice, and because of the similarity of the experimental results for both [111] and [100] directions of propagation of the ultrasonic stress, stress-induced diffusion of point defects could take place only in anisotropically strained regions of the crystal. Such regions exist, for instance, in the vicinity of dislocations. Beyond this, no particular mechanism was specified. In addition, the phenomenological interpretation implied that 10^{10} vacancies/cm^3 give rise to the effect at temperatures below 500°C.

In the present paper a definite model is proposed for the energy dissipation caused by the stress induced change in the equilibrium distribution of relatively mobile impurities around dislocations. This model is used to derive numerical results corresponding to those derived from the experiment. The dependence of the dissipated vibrational energy on the frequency and amplitude of the applied stress, on the temperature, on the concentration of dislocations and impurity atoms (or vacancies), and on the diffusion coefficient of the impurity atoms is derived in the limit of high frequencies.

DERIVATION OF THE EQUATIONS

The definition of the logarithmic decrement, δ, states that

$$\delta=\frac{(\text{vibrational energy dissipated/cycle})/\text{cm}^3}{2\times\text{peak vibrational energy stored/cm}^3}$$

$$=\Delta W/2W. \tag{1}$$

For a bar in resonant longitudinal oscillation, one may write

$$W=\sigma^2/2M, \tag{2}$$

where M is Young's modulus and σ is the peak stress.

It is postulated that the energy dissipation, ΔW, arises from the simultaneous presence in the crystal of ν dislocation segments/cm^2, with an average free length of λ cm, and of C point imperfections/cm^3. The concentration C is assumed to be sufficiently small that the pinning of the dislocations, leading to the free length λ, is solely due to the crossing of dislocation lines, and not due to the interaction with the impurities. In addition, any particular point defect is assumed to interact with only the nearest dislocation segment. Then, if p ergs/sec is the average power dissipated by one point defect in the field of one dislocation, the power dissipated, per dislocation ($\perp$), is

$$P_{\perp}=\int_0^{\lambda}dz\int\int p(x,y)C(x,y)dxdy. \tag{3}$$

The z axis is taken along the dislocation line, and the double integral is extended essentially over the cross section of influence of one dislocation segment. Since in a box of volume one cm^3 there are approximately ν/λ dislocation segments, one may write the energy dissipa-

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[1] J. O. Kessler, Phys. Rev. 106, 646 (1957), preceding paper. This paper will be referred to as I.

tion per cycle as

$$\Delta W=\frac{2\pi\nu}{\omega}\iint pCdA. \tag{4}$$

The equation for δ then becomes

$$\delta=\frac{2\pi\nu M}{\omega\sigma^2}\iint pCdA. \tag{5}$$

To find δ, the above integral must be evaluated. Furthermore, if the interpretation of the experimental results described in I is correct, it should be possible to express the resultant δ in terms of the equation

$$\delta=\Delta\omega\tau/[1+(\omega\tau)^2]. \tag{6}$$

This is the equation for the logarithmic decrement arising from an anelastic relaxation effect. In Eq. (6), ω is the applied angular frequency and τ is the relaxation time, which, in the present case, is of the order of atomic jump times. The proportionality factor Δ is π times the relaxation strength. The temperature variation of Δ must be small compared to the temperature variations of $\omega\tau[1+(\omega\tau)^2]^{-1}$.

It has been shown by Cottrell[2] that in an elastic continuum the interaction potential between a unit edge dislocation and a point defect is given by

$$U=-A\sin\theta/|\mathbf{r}|, \tag{7}$$

where $|\mathbf{r}|$ is the magnitude of the radius vector from the dislocation line to the defect, θ is the angle between $\mathbf{r}$ and the Burgers vector of the dislocation, and A is a parameter depending on the elastic constants of the crystal, the lattice constant, and the relative degree of misfit of the defect. Equation (7) is valid only in the region of purely elastic interaction of the dislocation and impurity. The elastic force exerted by the dislocation on the defect is $-\nabla U$. This force may be attractive or repulsive, depending on the size of the defect and on its location with respect to the dislocation.

If the concentration of the point defects far from the dislocation is C_0/cm^3, then, for small C_0, the concentration near the dislocation is given by

$$C_1=C_0e^{-U/kT}. \tag{8}$$

This equation may be derived[3] by considering the drift velocities of defects due to their concentration gradient and due to the interaction force. If D is the diffusion constant of the defects, then the concentration gradient induced drift velocity is

$$\mathbf{v}_1=-D\nabla C/C, \tag{9}$$

while the drift velocity due to the interaction force field is

$$\mathbf{v}_2=-(D/kT)\nabla U. \tag{10}$$

The total drift velocity of the defects is given by $\mathbf{v}=\mathbf{v}_1+\mathbf{v}_2$. The quantity $\mathbf{v}$ vanishes when equilibrium is attained, resulting in Eq. (8).

It is proposed to account for the observed energy dissipation by the perturbation of the atmosphere of point defects normally surrounding dislocation lines through small vibrations of the line segments caused by the applied stress. It will be assumed that Koehler's theory of small motions of edge-dislocation segments, pinned at the ends, is applicable. In this theory, the amplitude of vibration of the dislocation line is proportional to the applied shear stress and to the square of the free dislocation length.

Under these assumptions, then, it is to be expected that the dislocation atmospheres will vibrate with the same frequency as the dislocation, but that the phases and amplitudes of the defect vibrations, relative to those of the dislocations, will depend strongly on the relation between the frequency of the externally applied stress (dislocation vibration frequency) and the jump time for diffusion of the defects, which may be varied, experimentally, by changing the temperature.

Consider now an edge dislocation, having (x,y) as its slip plane, and $\mathbf{x}$ as the slip direction. The dislocation is assumed to undergo small oscillations in its slip plane, under the influence of an externally applied shear stress. The oscillatory amplitude, averaged over the length of the dislocation line, is assumed to be $\mathbf{R}(t)=R_0\mathbf{i}\exp(i\omega t)$, where $\mathbf{i}$ is the unit vector in the $\mathbf{x}$ direction. The point defects located within a small volume, a distance $\mathbf{r}$ from the dislocation, have concentration $C(\mathbf{r},t)$ and drift velocity $\mathbf{v}$. From Eqs. (9) and (10), one may write

$$\mathbf{v}=-\frac{D}{kT}\nabla[U(\mathbf{r},t)+kT\ln C(\mathbf{r},t)]. \tag{11}$$

This equation gives a first relation between C and $\mathbf{v}$. The second relation is given by the conservation of defects:

$$\nabla\cdot[\mathbf{v}(\mathbf{r},t)C(\mathbf{r},t)]=-\frac{\partial}{\partial t}C(\mathbf{r},t). \tag{12}$$

When $|\mathbf{r}|\gg|\mathbf{R}(t)|$,

$$U(\mathbf{r},t)\simeq U(\mathbf{r})-\mathbf{R}(t)\cdot\nabla U(\mathbf{r}), \tag{13}$$

where $U(\mathbf{r})$ is given by Eq. (7). Under static equilibrium conditions, i.e., when $\mathbf{v}=0$ and $R_0=0$, the concentration is $C_1(r)$, as given in Eq. (8). For small perturbations, one may write

$$C(\mathbf{r},t)=C_1(\mathbf{r})[1+\epsilon(\mathbf{r},t)], \tag{14}$$

where $|\epsilon|\ll 1$.

Inserting Eqs. (13) and (14) into Eqs. (11) and (12), one obtains

$$\nabla\cdot[\mathbf{v}(\mathbf{r},t)C_1(\mathbf{r})]=-C_1(\mathbf{r})\frac{\partial}{\partial t}\epsilon(\mathbf{r},t) \tag{15}$$

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[2] A. H. Cottrell, *Report on the Strength of Solids* (The Physical Society, London, 1948), p. 30.

[3] A. H. Cottrell and M. A. Jaswon, Proc. Roy. Soc. (London) **B199**, 104 (1949).

and

$$\mathbf{v}(\mathbf{r},t) = -\frac{D}{kT}\nabla[kT\epsilon(\mathbf{r},t) - \mathbf{R}(t)\cdot\nabla U(\mathbf{r})]. \qquad (16)$$

The zeroth-order terms have been canceled, in virtue of the assumption that equilibrium conditions were established before the dislocation was made to vibrate.

By using Eqs. (10) and (16), an effective force acting on a particle at r may be defined,

$$\mathbf{F} = -\nabla[kT\epsilon(\mathbf{r},t) - \mathbf{R}(t)\cdot\nabla U(\mathbf{r})]. \qquad (17)$$

The effective time-average power put into the particle motion is

$$p = \tfrac{1}{2}[\tfrac{1}{2}\mathbf{v}^*\cdot\mathbf{F} + \tfrac{1}{2}\mathbf{v}\cdot\mathbf{F}^*]$$
$$= \tfrac{1}{2}DkT\left|\nabla\left(\epsilon - \frac{\mathbf{R}\cdot\nabla U}{kT}\right)\right|^2, \qquad (18)$$

where $\mathbf{v}(\mathbf{r},t)$ and $\epsilon(\mathbf{r},t)$ have been assumed to vary sinusoidally with the time, due to the harmonic driving force, $\mathbf{R} = \mathbf{i}R_0 \exp(i\omega t)$. The power dissipated per dislocation is then given by Eqs. (3) and (18). In order to perform the necessary integration it will first be necessary to obtain an expression for $\epsilon(\mathbf{r},t)$ from Eqs. (15) and (16).

To eliminate $\mathbf{v}(\mathbf{r},t)$, Eq. (16) is multiplied by $C_1(\mathbf{r})$ and the result is substituted in Eq. (15), the continuity equation. Then

$$\frac{\partial}{\partial t}\epsilon(\mathbf{r},t) + \frac{D}{kT}\left[\frac{\nabla U(\mathbf{r})}{kT} - \nabla\right] \cdot\nabla[kT\epsilon(\mathbf{r},t) - \mathbf{R}(t)\cdot\nabla U(\mathbf{r})] = 0, \qquad (19)$$

where $\nabla C_1/C_1$ has been replaced by $-\nabla U/kT$, again making use of the equilibrium condition. Equation (19) may be simplified by setting $\epsilon(\mathbf{r},t) = \epsilon(\mathbf{r})\exp(i\omega t)$, and noting that $\nabla^2 U(\mathbf{r}) = 0$,

$$D\nabla^2\epsilon - \frac{D}{kT}(\nabla U)\cdot(\nabla\epsilon) - i\omega\epsilon = -\frac{D}{(kT)^2}(\nabla U\cdot\nabla)(\mathbf{R}\cdot\nabla U). \qquad (20)$$

An approximate solution of this equation may be obtained by rewriting it in a coordinate system based on the equipotentials of $U(\mathbf{r})$. If $\psi = r^{-1}\cos\theta$ and $\eta = r^{-1}\sin\theta$, then $dA = (dxdy) = (\psi^2+\eta^2)^{-2}d\psi d\eta$ and $U = -A\eta$. With the indicated substitutions, Eq. (20) is transformed into

$$\epsilon(\psi,\eta) = -\frac{D}{i\omega}(\psi^2+\eta^2)^2\left\{2R_0\psi\left(\frac{A}{kT}\right)^2 - \left[\frac{\partial^2}{\partial\psi^2} + \frac{\partial^2}{\partial\eta^2} + \frac{A}{kT}\frac{\partial}{\partial\eta}\right]\epsilon(\psi,\eta)\right\}. \qquad (21)$$

By iterating this equation, $\epsilon(\psi,\eta)$ can be obtained as a series expansion in powers of $1/\omega$. The first two terms of the expansion, which approximate the solution in the limit of small D/ω, are given by

$$\epsilon(\psi,\eta) = 2R_0\frac{D}{\omega}\left(\frac{A}{kT}\right)^2\psi(\psi^2+\eta^2)^2 \times\left\{i + \frac{4D}{\omega}(\psi^2+\eta^2)\left(6 + \frac{A}{kT}\eta\right) + \cdots\right\}. \qquad (22)$$

With the aid of Eq. (22), the real and imaginary parts of $\nabla(\epsilon - \mathbf{R}\cdot\nabla U/kT)$ may be constructed. The time-average power dissipated in the cylindrical volume element $\lambda dxdy$ is given by

$$p\lambda dxdy = \{[\mathrm{Re}\nabla(\ )]^2 + [\mathrm{Im}\nabla(\ )]^2\}\frac{\lambda DkTd\eta d\psi}{2(\psi^2+\eta^2)}. \qquad (23)$$

Retaining terms to order $(D/\omega)^2$, this equation becomes

$$p\frac{dxdy}{d\psi d\eta} = \frac{DkT}{2}\left(\frac{2AR_0}{kT}\right)^2\left\{\psi^2+\eta^2+\frac{A}{kT}\left(\frac{D}{\omega}\right)^2 \times\left[\frac{A}{kT}(17\psi^8 - 52\psi^6\eta^2 - 162\psi^4\eta^4 - 100\psi^2\eta^6 - 7\eta^8) - 48(13\psi^6\eta + 27\psi^4\eta^3 + 15\psi^2\eta^5 + \eta^7)\right]\right\}. \qquad (24)$$

It is now possible to evaluate the integral appearing in Eq. (5) if a lower limit of integration can be found. For this it is necessary to assume that there exists a cut-off distance L such that the potential $U(\mathbf{r}) = Ar^{-1}\sin\theta$ becomes invalid for $|\mathbf{r}| \leqslant L$. This is reasonable if it is remembered that $U(\mathbf{r})$ is derived from the strain interaction of a dislocation and an impurity in an elastic continuum. The continuum approximation clearly does not hold when $|\mathbf{r}|$ is of the order of only a few atomic spacings.[4] One may think of L as the distance from the dislocation line at which the potential becomes strongly repulsive. For the case when the impurity is a lattice vacancy, a further argument for the existence of such a cutoff distance may be made. Since a jog is formed when a vacancy condenses on a straight segment of edge dislocation, and since such a jog increases the strain energy of the dislocation, it is expected that the effective force between vacancy and dislocation becomes repulsive at small $|\mathbf{r}|$, regardless of the value of θ. In terms of the variables (ψ,η), then, the limits of integration become $\pm 1/L$.

The further assumption, that the radius of the impurity atmosphere is large compared to the cut-off distance, or that $kTL/A \ll 1$, may be made in evaluating the integral. This assumption is neither strictly correct,

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[4] A. H. Cottrell, *Dislocations and Plastic Flow in Crystals* (Oxford University Press, Oxford, 1953), Chap. II.

nor is it essential to this development. It is introduced only in order to make the final expression for δ more manageable.

The integral to be evaluated, then, is

$$P_{\perp}\equiv\lambda\int\int pCdA=\tfrac{1}{2}DkT\left(\frac{2AR_0}{kT}\right)^2C_0\lambda \times\int_{-1/L}^{1/L}d\psi\int_{-1/L}^{1/L}e^{A\eta/kT}\Big\{\quad\Big\}d\eta, \tag{25}$$

where { } is the expression appearing in brackets in Eq. (24). The result is

$$P_{\perp}=\frac{16AR_0^2C_0}{3L}\left(\frac{D}{L^2}\right)e^{|A|/kTL} \times\left[1-\frac{24\,656}{420}\left(\frac{D}{L^2}\right)^2\left(\frac{A}{kTL}\right)^2\frac{1}{\omega^2}+\cdots\right]. \tag{26}$$

To this approximation, according to Eq. (5), the logarithmic decrement is given by

$$\delta=\frac{2\pi}{\omega}\left(\frac{16AR_0^2C_0\nu M}{3L\sigma^2}\right)\left(\frac{D}{L^2}\right)e^{|A|/kTL} \times\left[1-\frac{24\,656}{420}\left(\frac{D}{L^2}\right)^2\left(\frac{A}{kTL}\right)^2\frac{1}{\omega^2}+\cdots\right]. \tag{27}$$

The assumed expression for the decrement may be similarly expanded for the high-frequency case:

$$\delta=\Delta\left[\frac{\omega\tau}{1+(\omega\tau)^2}\right]\simeq\frac{\Delta}{\omega\tau}\left[1-\frac{1}{(\omega\tau)^2}+\cdots\right]. \tag{28}$$

Taking the corresponding terms of (30) and (29), one obtains

$$\tau=\left(\frac{420}{24\,656}\right)^{\frac{1}{2}}\left(\frac{kTL}{|A|}\right)\frac{L^2}{D} \tag{29}$$

and

$$\Delta=\frac{32\pi}{3}\left(\frac{420}{24\,656}\right)^{\frac{1}{2}}\frac{R_0^2\nu MC_0kT}{\sigma^2}e^{|A|/kTL}. \tag{30}$$

NUMERICAL RESULTS AND DISCUSSION

In order to correlate Eqs. (29) and (30) with the experimentally obtained values for Δ and τ, it is necessary to make some reasonable choice of the constants appearing in these equations. Although the values of several of the constants are in some doubt, due to insufficient experimental evidence, it is believed that at least an order of magnitude may be calculated for the effect.

Koehler[5] has given an expression for the amplitude of deflection of an edge dislocation of free length λ, due to resolved shear stress σ. This amplitude will be used for the average deflection, R_0, which is required in the equations. For the case of germanium, one obtains

$$R_0=5\times10^{-6}\lambda^2\sigma\text{ cm}. \tag{31}$$

Combining Eqs. (30) and (31), it is seen that the decrement is independent of the applied stress, as required for an anelastic relaxation effect. The average free length of a dislocation, λ, is estimated to be 1 micron.[6] Then $R_0=5\times10^{-9}$ cm, or much less than one lattice distance, for a typical strain of 10^{-7}. The density, ν, of dislocations which lie in slip planes and hence are able to take part in the postulated mechanism, is put at $5\times10^4/\text{cm}^2$.[7]

The formula for the impurity-dislocation interaction constant is[4]

$$A=\frac{4}{3}\left(\frac{1+n}{1-n}\right)Mb\eta\rho^3, \tag{32}$$

where b is the Burgers vector, M is Young's modulus, n is Poisson's ratio, ρ is the normal radius of an atomic site, and $(1+\eta)\rho$ is the radius of a site with an impurity atom. The elastic constants of germanium are obtained from the data of Fine[8] and from the experiments described in I. It is further estimated that a vacancy site has an effective radius differing by 10% from that of a normal site. When one uses these values for the subsidiary constants, the derived value of A is 10^{-19} erg cm.

It is now possible to compare the expressions for Δ and τ which were derived in this development with the values found in the experiments. This comparison, the outcome of which bears on both the validity of the model used in the calculations and on the estimates of the numerical constants, is accomplished in the form of a calculation of L, the cut-off parameter, and D, the diffusion coefficient. If the values of A, of R_0, and of the elastic moduli are inserted in Eq. (30), together with the measured value of Δ, which is 3×10^{-5}, and the derived value of C_0, which is approximately $10^{10}/\text{cm}^3$, a value of 5.4×10^{-8} cm is found for L. The cut-off distance for the Cottrell potential is then approximately two lattice spacings, which is certainly quite reasonable.

Equation (29) gives the relation between the diffusion coefficient and the relaxation time, the value of which was found to be $10^{-13\pm1}$ sec.[1] Inserting L and A into that equation, one obtains the magnitude of D_0. This magnitude turns out to be $10^{-4\pm1}$ cm^2/sec, which is smaller by a factor of at least 1000 than the temperature-independent part of the diffusion coefficient for va-

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[5] J. S. Koehler, *Imperfections in Nearly Perfect Crystals* (John Wiley and Sons, Inc., New York, 1952).

[6] S. G. Ellis (private communication).

[7] S. G. Ellis (private communication) and S. G. Ellis, J. Appl. Phys. **26**, 1140 (1955). This density of short, mobile dislocation segments is derived from the apparent density of composite dislocations, most of which do not lie in slip planes.

[8] M. E. Fine, J. Appl. Phys. **24**, 1331 (1953).

cancies derived by Letaw *et al.*[9] from experiments on the self diffusion of germanium and from data on the quenching-in of vacancies.[10]

The discrepancy between the value of D_0 derived in this paper and in that of Letaw *et al.* may be due either to a somewhat faulty estimation of some of the constants entering into Eqs. (29) and (30) or to the uncertainity of the vacancy quenching-in experiments, or to both of these. The latter possibility is of course the most likely. If, for instance, the number of quenched-in vacancies is ten times higher[11] than that reported by Mayburg, and if, in addition, small errors have been made in the estimates of η and λ, leading to changes in A and L by no more than factors of two, a reasonable match in the two values of D_0 is obtained.

SUMMARY

A model has been proposed for the calculation of the vibrational energy dissipated in a crystal subjected to ultrasonic stress, which contains point defects and dislocations. In this model an equilibrium situation is visualized in which the point defects form dilute Cottrell atmospheres around short mobile dislocation segments having some edge component. Under the influence of externally applied stress, these dislocation segments are assumed to deflect in the manner described by Koehler. The impurity atom distribution within the potential of a given dislocation may thus, in a statistical sense, be visualized as "dragged" along by the interaction force, at a rate and to an extent which is determined by the diffusion coefficient and by the opposing force of the concentration gradient. The dissipated power is calculated from the product of the net force and the drift velocity due to the force.

Several approximations are made, but only one of these is of fundamental physical significance. The others either reflect the present state of ignorance concerning the internal state of crystals, or permit simplifications in the mathematics. The fundamental assumption of a cutoff for the dislocation-impurity interaction potential is made in such a way that the numerical value of the cutoff distance is obtained from the calculation and from the experimental constants, rather than from *a priori* reasoning. The validity of the assumption has been discussed by Cottrell, and in itself is not in doubt.

From the present calculations one may draw the general conclusions that very small concentrations of point defects, through their interactions with mobile portions of dislocation lines, may give rise to a measureable effect, which, in the limit of high frequencies, is equivalent to an anelastic relaxation whose relaxation time depends on the diffusion coefficient of the point defects. It has also been shown that the magnitude of the effect is such as to support the hypothesis that the relaxation effect observed in pure germanium crystals is due to lattice vacancies. Furthermore, if the vacancy assumption is allowed, that is, if numerical values corresponding to the vacancy concentration derived in I are inserted into the equations, it is possible to estimate that the cutoff of the purely elastic defect-dislocation interaction potential occurs several atom spacings away from a dislocation. This result is rather interesting, since for covalent crystals a considerably larger cut-off distance might have been expected.

ACKNOWLEDGMENTS

The author is greatly indebted to Dr. L. S. Nergaard and Dr. R. H. Parmenter for their help and advice in the solution of this problem, and to Dr. A. R. Moore and Dr. D. O. North for many stimulating discussions.

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[9] Letaw, Portnoy, and Slifkin, Phys. Rev. **102**, 636 (1956).

[10] S. Mayburg, Phys. Rev. **95**, 38 (1954).

[11] R. A. Logan, Phys. Rev. **101**, 1455 (1956).