

zone electron surface is centered at Γ and has a nearly uniform extremal cross section (see the modified surface in Fig. 9) which we associate with the α period of TJ. Their γ period corresponds to the central extremal orbit of the fourth-zone hole surface which is also shown in Fig. 9. Possible shapes of this hole surface are indicated by both the broken line and the line of squares in Fig. 9. It is not possible to distinguish between these surfaces because the experimental dHvA periods are not observed beyond about 30° from the $[00.1]$ direction.

The β , δ , and ϵ periods are associated with the multiply connected fifth-zone electron surface centered at H . The areas of the extremal orbits based on the APW surface are consistently too large by a factor of about 1.4, but have approximately the correct angular dependence. The sixth-zone electrons are very small pieces which have not been observed experimentally.

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Damping of Phonons in Aluminum

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The damping of phonons in Al due to the electron-phonon interaction has been calculated using an effective ion-electron interaction potential given recently by Vosko *et al.* The results show that this effect is essential, although not sufficient, to account for the experimental data of Nilsson and Stedman.

I. INTRODUCTION

RECENTLY, very precise measurements of the phonon dispersion curves for Al at 80°K were reported by Nilsson and Stedman.¹ The lifetimes of the individual phonons were also measured. In order to explain the significantly larger damping of the longitudinal phonons compared with the transverse phonons, Nilsson and Stedman conjectured that at these low temperatures the major part of the damping of the phonons arises from electron-phonon interaction and to a lesser extent from anharmonic effects. Several authors have given order-of-magnitude estimates of the phonon lifetimes arising from electron-phonon interaction^{2,3} as well as anharmonicity,^{3,4} but to our knowledge no quantitative calculations of the lifetimes in Al have been reported. On the other hand, several calculations of the phonons dispersion curves have been carried out, based on pseudopotential methods.^{5,6}

We have taken advantage of this in our calculations by using the same pseudopotential as given by Vosko *et al.*⁶ in their calculations of the phonon dispersion curves in Al, which shows quite good agreement with the experimental results.¹ Our aim has been to carry out a sufficiently accurate calculation of the phonon lifetimes as a function of the phonon wave vector and compare with the experimental data in order to ascertain whether the electron-phonon coupling gives the main contribution or not.

II. THEORY

Our calculations are essentially a repetition of earlier calculations by Woll and Kohn,⁷ but with a more realistic effective ion-electron interaction.

The basic quantity entering into the theory of lattice vibrations is the dynamical matrix, which can be written in the following form⁸:

$$D(\mathbf{q}) = \frac{1}{M v_a} \sum_{\mathbf{K}} [(\mathbf{q} + \mathbf{K})(\mathbf{q} + \mathbf{K}) v_{\text{eff}}(\mathbf{q} + \mathbf{K}) - \mathbf{K} \mathbf{K} v_{\text{eff}}(\mathbf{K})], \quad (1)$$

¹ R. Stedman and G. Nilsson, *Phys. Rev.* **145**, 492 (1966).

² J. J. J. Kokkedee, *Physica* **28**, 893 (1962); J. J. J. Kokkedee, in *Proceedings of the Conference on Inelastic Scattering of Neutrons in Solids and Liquids* (International Atomic Energy Agency, Vienna, 1963), Vol. I, p. 15. M. A. Krivogla, *Fiz. Tverd. Tela* **3**, 2761 (1963) [English transl.: *Soviet Phys.—Solid State* **3**, 2015 (1962)].

³ R. J. Elliott and H. Stern, in *Proceedings of the Conference on Inelastic Scattering of Neutrons in Solids and Liquids* (International Atomic Energy Agency, Vienna, 1961), p. 61.

⁴ J. J. J. Kokkedee, *Physica* **28**, 374 (1962); A. A. Maradudin and A. E. Fein, *Phys. Rev.* **128**, 2589 (1962).

⁵ W. A. Harrison, *Pseudopotentials in the Theory of Metals* (W. A. Benjamin, Inc., New York, 1966); W. A. Harrison, *Phys. Rev.* **129**, 2522 (1963).

⁶ S. H. Vosko, R. Taylor, and G. H. Keech, *Can. J. Phys.* **43**, 1187 (1965).

⁷ E. J. Woll and W. Kohn, *Phys. Rev.* **126**, 1693 (1962). A factor $\frac{1}{2}$ seems to be missing in their Eq. (4.4). It should be noted that their expression for $1/\tau$ refers to the damping rate of the phonon energy and thus by definition corresponds to $2/\tau$ in our notation.

⁸ See, for instance, A. Sjölander, in *Symposium on Inelastic Scattering of Neutrons by Condensed Systems*, edited by L. M. Corliss (BNL, Upton, New York, 1966), p. 29.

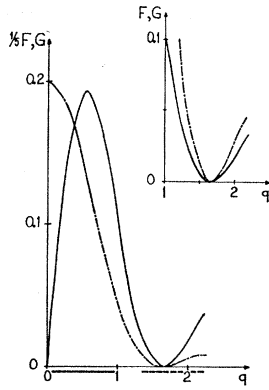


FIG. 1. The functions $F(\mathbf{q})$ (dashed curve) and $G(\mathbf{q})$ (full curve) in Eqs. (4) and (5). q is given in units of $2\pi/a_L$, a_L being the lattice parameter. The lines along the q axis indicate the main regions for giving damping of longitudinal (full line) and transverse (dashed line) phonons.

where M is the ionic mass and v_a denotes the volume of a lattice cell. The summation extends over the reciprocal lattice vectors \mathbf{K} . The effective interaction potential between the ions consists of a direct interaction $v_{ii}(\mathbf{q})$, essentially a pure Coulomb interaction and an interaction which is induced by the conduction electrons. We may write the Fourier transform of the effective interaction in the form

$$v_{\text{eff}}(\mathbf{q}) = v_{ii}(\mathbf{q}) + [v_{ie}(\mathbf{q})]^2 \frac{h_0(\mathbf{q}, 0)}{1 - v^*(\mathbf{q})h_0(\mathbf{q}, 0)}, \quad (2)$$

where $v_{ie}(\mathbf{q})$ represents the unscreened ion-electron interaction and $h_0(\mathbf{q}, \omega)$ is the familiar Lindhard free-electron irreducible response function. The Fourier transform of the interaction potential between the conduction electrons, corrected for exchange effects, is written as

$$v^*(\mathbf{q}) = \frac{4\pi e^2}{q^2} \left[1 - \frac{q^2}{2q^2 + \xi k_F^2} \right], \quad (3)$$

where ξ is an adjustable parameter and k_F the Fermi wave number. Vosko *et al.* express the phonon frequencies in the form

$$\omega_s^2(\mathbf{q}) = \omega_p^2 \sum_{\mathbf{K}} \left\{ \frac{|\mathbf{e}_s \cdot (\mathbf{q} + \mathbf{K})|^2}{(\mathbf{q} + \mathbf{K})^2} [1 - F(\mathbf{q} + \mathbf{K})] - \frac{|\mathbf{e}_s \cdot \mathbf{K}|^2}{\mathbf{K}^2} [1 - F(\mathbf{K})] \right\}, \quad (4)$$

$$G(\mathbf{q}) = \frac{qF(q)}{u(q/2k_F) \{ q^2 + (1 - \frac{1}{2}(q^2/[q^2 + \xi k_F^2])) k_{TF}^2 u(q/2k_F) \}}, \quad (6)$$

where

$$u(x) = \frac{1}{2} \left[1 + \frac{1-x^2}{2x} \ln \left| \frac{1+x}{1-x} \right| \right],$$

and k_{TF} is the Thomas-Fermi screening constant. $G(\mathbf{q})$ is shown graphically in Fig. 1.

III. RESULTS AND DISCUSSIONS

In Fig. 2 the calculated values for $2/\tau(\mathbf{q})$ are compared with the experimental results of Nilsson and Stedman. We see from the figures that the theoretically calculated lifetimes are larger than the observed ones

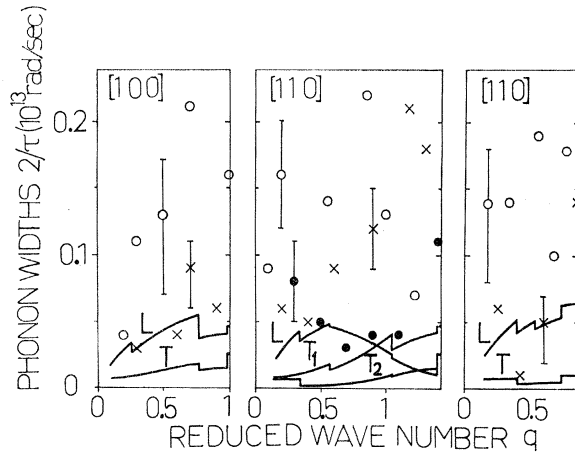


FIG. 2. Phonon linewidth as a function of q . The full lines give the theoretical curves and are compared with some typical experimental points [\circ longitudinal phonons (L), \times or \bullet transverse phonons (T_1, T_2)]. The error bars indicate the average experimental uncertainty. q is in units of $2\pi/a_L$, a_L being the lattice parameter, and $2/\tau$ is in units of 10^{13} rad/sec. $2/\tau$ gives the full phonon linewidth measured in neutron-scattering experiments and refers to the damping rate of the phonon energy.

and the basic function $F(\mathbf{q})$ is given numerically and is shown in Fig. 1. ω_p denotes the ionic-plasma frequency and \mathbf{e}_s the phonon polarization direction of branch s .

When one goes beyond the adiabatic approximation the dynamical matrix becomes complex. The phonon lifetime is obtained from the imaginary part of this matrix which in turn is related to the imaginary part of the electron response function $h_0(\mathbf{q}, \omega)$. This depends linearly on ω for $q < 2k_F$, and vanishes for $q > 2k_F$. Using Eqs. (1) and (2), we arrive at a phonon lifetime $\tau(\mathbf{q})$ given by the expression

$$\frac{1}{\tau_s(\mathbf{q})} = -\frac{1}{2\omega_q} \{ \mathbf{e}_s \cdot \text{Im} \mathbf{D}(\mathbf{q}, \omega_q) \cdot \mathbf{e}_s \} \quad (5)$$

$$= \frac{\omega_p^2 a_L}{8v_F} \sum_{\mathbf{K}} \frac{|\mathbf{e}_s \cdot (\mathbf{q} + \mathbf{K})|^2}{(\mathbf{q} + \mathbf{K})^2} G(\mathbf{q} + \mathbf{K}),$$

where ω_q is the real phonon frequency, a_L the lattice parameter, and v_F the Fermi velocity. The function $G(\mathbf{q})$ stands for

by a factor of 2 or more. In Eq. (5) the main contribution to the longitudinal phonon damping comes from the term $\mathbf{K}=0$. The phonon wave vectors range over a region where the ion-electron pseudopotentials given by various authors agree very well (indicated by the solid horizontal line in Fig. 1). For the transverse phonons, on the other hand, the term $\mathbf{K}=0$ vanishes and the $(\mathbf{q}+\mathbf{K})$ vectors of main importance (broken horizontal line in Fig. 1) lie in a region where the pseudopotential is most uncertain. We have also made calculations using Bardeen's model,⁹ which is expected to give values too small for the pseudopotential at $q \sim 2k_F$. We found significantly longer lifetimes for the transverse phonons whereas the change for the longitudinal ones was smaller. In Kreb's model,¹⁰ the lifetimes are still longer.

Whereas the lifetimes obtained for transverse phonons may be in error by a factor of 2 or more, we feel confident that for the longitudinal phonons the results should be quite good.¹¹ Therefore, our conclusion is that at least half of the contribution to the damping $1/\tau$ comes from anharmonic effects, and that the damping

⁹ J. Bardeen, Phys. Rev. **52**, 688 (1937).

¹⁰ K. Kreb, Phys. Rev. **138**, A143 (1965).

¹¹ We have taken for granted that the dielectric function used above is sufficiently accurate for Al.

arising from electron-phonon coupling is by no means negligible.

In principle measurements of particularly the transverse phonon lifetimes after subtraction of the anharmonic contribution should give quite detailed information about the ion-electron interaction in the region where it is most uncertain. However, because of the extreme difficulties in carrying out such measurements, it does not seem feasible at present to pursue such a program.

Concerning the conjecture of Nilsson and Stedman, we stress that the anharmonic contribution should also give longer lifetimes for the transverse phonons than for the longitudinal phonons. At very low temperatures, the transverse phonons are less likely to decay into two or more phonons compared to the longitudinal phonons because of the conservation laws for energy and momentum.¹²

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¹² R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, London, 1955), pp. 43-45.

Some Effects of Sample Size on Electrical Transport in Bismuth

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The effects of sample size on the electrical conductivity and Hall constant of single crystals of bismuth have been measured between 2 and 10°K. In addition, both components of the conductivity tensor and the Hall tensor component $\rho_{23,1}$, with magnetic field \parallel to the trigonal axis, have been measured between 2 and 77°K in samples which are among the purest reported in the literature. This work was done to determine the proportion of specular reflection of carriers from the electropolished sample surface. The nature of the experimental results, however, has made it impossible to fit observation to any sort of theory with mean free path as the internal parameter. Analysis of these data, however, has shown the following: The scattering is, indeed, partially specular; the scattering time of electrons is highly anisotropic, being of the order of ten times longer in the bisectrix direction than in the binary direction; and both electron and hole mobilities have been shown to have an approximate T^{-2} dependence down to 4.2°K.

I. INTRODUCTION

BISMUTH, a semimetal with electrical properties midway between insulators and metals, has long proven interesting to experimenters. As a result, phenomena such as the de Haas-van Alphen effect and the Azbel-Kaner resonance, which have proven to be valuable tools in the investigation of Fermi surfaces, were first observed in this material. As early as 1939,

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rather detailed models of the bismuth electron Fermi surface were beginning to appear in the literature¹ and investigations of the galvanomagnetic properties of this material and its alloys date back to 1928.²

The conduction electrons, produced by the small overlap of nearly filled 5th Brillouin zone with the 6th, lie within three nearly ellipsoidal regions of momentum space with one major axis of each in each of the binary directions. Directions in the bismuth crystal are specified with respect to three mutually perpendicular direc-

¹ D. Schoenberg, Proc. Roy. Soc. (London) **A170**, 341 (1939).

² P. Kapitza, Proc. Roy. Soc. **A119**, 358 (1928).