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Ultrasonic Attenuation Due to Electron-Phonon Interaction in Potassium

T. M. Rice

Bell Telephone Laboratories, Murray Hill, New Jersey 07974

and

L. J. Sham*

University of California at San Diego, La Jolla, California 92037

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The electron-phonon contribution to the ultrasonic attenuation and the electrical resistivity of potassium at low temperatures is calculated using a number of different pseudopotentials. Serious discrepancies are found between the calculated values and the experimental data reported by Natale and Rudnick.

I. INTRODUCTION

For the simple metals, the method of pseudopotentials has been widely used to calculate the electron-phonon interaction matrix elements which, in turn, determine various properties of the metals such as phonon spectra, resistivity, superconducting transition temperature, the effective mass, and the Landau interaction parameters for the quasiparticles. The references are by now too numerous to list here. We report, in this paper, the first calculation of the ultrasonic attenuation due to electron-phonon scattering by use of the method of pseudopotentials.

In the hydrodynamic regime, that is, when the electron "mean free path" is short compared with the wavelength of the sound wave, the attenuation of the sound wave is proportional to a relaxation time τ_2. It is well known[1] that this relaxation time τ_2 involves a different average over the electron-phonon matrix element from that for the relaxation time τ_1 which enters into the electrical resistivity. Therefore, if we obtain the electron-phonon matrix element from the pseudopotential, a comparison of the resulting electrical resistivity and ultrasonic attenuation over a range of temperature with the experimental measurements will yield some information on the shape of the pseudopotential. This, as we shall see, is a much more stringent test for the correct shape of a pseudopotential than the results obtained by comparing the temperature dependence of resistivity alone.

Potassium is a suitable metal for such a calculation, because (1) it is a "simple metal" for which the pseudopotential approximation is believed to be good, and (2) a measurement of the ultrasonic attenuation as a function of temperature is available.[2]

In Sec. II, we shall describe the calculation of the electron-phonon contribution to the ultrasonic attenuation and the electrical resistivity. In Sec. III, we shall compare our results with the experimental values of Natale and Rudnick.[2]

II. TWO RELAXATION TIMES

The electrical resistivity is given by the well-known expression

$$\rho = m/ne^2\tau_1 \ , \tag{1}$$

where m is the bare electron mass, e the electronic charge, and n the number of electrons per unit volume. In the hydrodynamic regime, the amplitude attenuation constant of a longitudinal sound wave is[2]

$$A = (2/15)(\omega^2/Ms^3)(\hbar^2 k_F^2 \tau_2/m) \ , \tag{2}$$

where ω is the angular frequency of the sound wave, s is its speed, M is the ionic mass, and k_f is the Fermi wave vector.

The two relaxation times τ_1 and τ_2 due to the electron-phonon scatterings at temperature T are given by

$$\begin{aligned} \frac{1}{\tau_l} = \frac{2\pi\hbar}{k_B T}\,\frac{\nu m^*}{m} \sum_j \int \frac{d\Omega_k}{4\pi} \int \frac{d\Omega_{k'}}{4\pi}\, g^{eph} \\ \times(\vec{\mathrm{k}}, \vec{\mathrm{k}}'; j)[\omega_j(\vec{\mathrm{k}} - \vec{\mathrm{k}}')]^2 N_j(\vec{\mathrm{k}} - \vec{\mathrm{k}}') \\ \times [N_j(\vec{\mathrm{k}} - \vec{\mathrm{k}}') + 1][1 - P_l(\hat{k}\cdot\hat{k}')] \ , \end{aligned} \tag{3}$$

where $\nu = m^* k_F/\pi^2$ is the density of states of the quasiparticles, m^* is the effective mass, $g^{eph}(\vec{\mathrm{k}}, \vec{\mathrm{k}}'; j)$ is the scattering probability of a quasiparticle from state $\vec{\mathrm{k}}$ to state $\vec{\mathrm{k}}'$ by a phonon in the j branch, $\omega_j(\vec{\mathrm{k}} - \vec{\mathrm{k}}')$ is the phonon frequency, and $N_j(\vec{\mathrm{k}} - \vec{\mathrm{k}}')$ is its thermal distribution function. The two integrals are angular averages of the quasiparticle momenta $\vec{\mathrm{k}}$ and $\vec{\mathrm{k}}'$ over the spherical Fermi surface. $P_l(\hat{\mathrm{k}}\cdot\hat{\mathrm{k}})$ denotes the Legendre polynomial and is the weighting factor in the integral which distinguishes the two relaxation times.

In order to include any possible effects of quasiparticle interaction, we have obtained Eqs. (1) and (3) from the Landau transport equation by Kohler's variational method. We note that with the relaxation times defined by Eq. (3), the formulas for the resistivity and ultrasonic attenuation are the same as the ones usually obtained from the Boltzmann equation without the quasiparticle interaction, provided that the factor in A which is usually written as mv_F^2, v_F being the Fermi velocity, is replaced by $\hbar^2 k_F^2/m$ with the bare electron mass, rather than with the effective mass.[3]

The expression of the quasiparticle scattering function $g^{eph}(\vec{\mathrm{k}}, \vec{\mathrm{k}}')$ due to phonon exchanges has been given by one of us[4] in terms of the pseudopotential with proper many-body renormalization. The calculation of the relaxation times in terms of $g^{eph}(\vec{\mathrm{k}}, \vec{\mathrm{k}}')$ is very similar in procedure to that of the calculation of Landau parameters carried out in Ref. 4, and we follow the steps in that reference for our computation. Since τ_1 and τ_2 are very sensitive to umklapp processes, we have used the force-constant fit to obtain the phonon spectrum rather than the Kubic harmonic interpolation procedure used in Ref. 4.

In order to study the effect of varying the pseudopotential, we have calculated the two relaxation times, using four different pseudopotentials. These were, respectively, (I) the Bardeen[5] formula for the electron-phonon matrix element (This form was used by Hasegawa[6] to calculate resistivity.),[7] (IV) the local pseudopotential fit to the Fermi-surface data by Ashcroft,[8] and (II) and (III) based on the detailed fit of Lee and Falicov[9] to the Fermi surface, using a nonlocal form for the pseu-

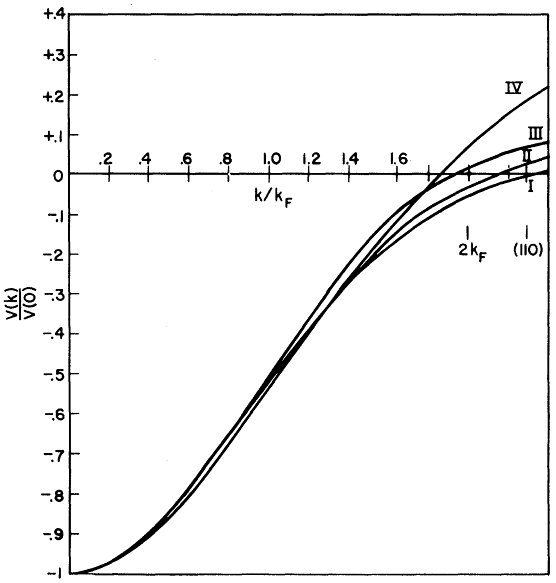

FIG. 1. Various pseudopotentials as a function of momentum: (I) Bardeen, Ref. 5; (II) lower Lee-Falicov, Ref. 9 and text; (III) higher Lee-Falicov, Ref. 9 and text; (IV) Ashcroft, Ref. 8.

dopotential. We used two sets of values corresponding to the extremal values reported by these authors as follows: (II) "Lower" has parameters $U_0 = -1.5$ eV, $U_1 = +3.00$ eV, $U_2 = -32.4$ eV, and $V_L(110) = 0.337$ eV and (III) "Upper" is the same as (II) but with $U_2 = -33.5$ eV and $V_L(110) = 0.41$ eV. The notation we use is that of Ref. 4 and, as in that reference, the local part was interpolated by using the Ashcroft form. The values used for the Lee-Falicov potential in Ref. 4 were an intermediate set which, in fact, are quite close to (II). The four potentials (I)-(IV) are plotted in Fig. 1.

The calculated resistivity and the ratio of the relaxation times, τ_2/τ_1, over the range of temperature 2-20 °K where the ultrasonic attenuation was measured, are tabulated in Table I. We defer comparison with experiment to Sec. III. We note here that the ratio of the relaxation times is very sensitive to the shape of the pseudopotential. (This is in contrast to the effective mass and Landau parameters calculated in Ref. 4.) From Fig. 1, we see that the pseudopotentials used are very close to each other except for momentum transfer greater than $1.6\,k_F$. Since the integral for the relaxation time is over a momentum transfer of only $2k_F$, the differences in the umklapp processes in the range $1.6-2k_F$ account for the differences in τ_2/τ_1 for the four pseudopotentials. Thus, a reliable measurement of τ_2/τ_1 will easily determine which pseudopotential is to be preferred.

The variation of τ_2/τ_1 over the different pseudopotentials and the variation of τ_2/τ_1 for each pseudopotential over the temperature are easily understood in terms of the weighting factors $1-P_l(\hat{k}\cdot\hat{k})$ in the integral (3). In Fig. 2, we show the two weighting factors as a function of the momentum transfer so that we can visualize the difference between the two relaxation times. For example, at extremely low temperatures where the forward scatterings of the electrons be very-long-wavelength phonons dominate, the resistivity varies as T^5 and τ_2/τ_1 equals $\frac{1}{3}$ since the initial slopes of $1-P_l$ are $3:1$ for $l=2$ to $l=1$. At more moderate temperatures, the contributions to $1/\tau_1$ and $1/\tau_2$ from the scatterings at various momentum transfers are different. Roughly speaking, the normal processes contribute more to $1/\tau_2$ while the umklapp processes contribute more to $1/\tau_1$. This is the reason why a determination of τ_2/τ_1 is such a sensitive test for the shape of the pseudopotential or any other theory for the electron-phonon matrix element. The variation of τ_2/τ_1 with respect to different pseudopotentials reflects the variation of the pseudopotentials, especially near the backward scattering region. For example, the Ashcroft potential underestimates the umklapp processes compared with

TABLE I. Calculated values of low-temperature resistivity and ratio of relaxation times pseudopotentials: (I) Bardeen, (II) lower Lee-Falicov, (III) upper Lee-Falicov, (IV) Ashcroft.

	$\rho(\Omega\,\mathrm{cm})$				τ_2/τ_1			
(°K)	I	II	III	IV	I	II	III	IV
2	2.75×10^{-12}	2.41×10^{-12}	1.72×10^{-12}	2.41×10^{-12}	0.57	0.46	0.37	0.50
3	6.11×10^{-11}	3.96×10^{-11}	•••	3.68×10^{-11}	1.27	0.88	•••	0.87
4	4.02×10^{-10}	2.53×10^{-10}	0.77×10^{-10}	2.12×10^{-10}	1.55	1.09	0.42	1.01
6	3.29×10^{-9}	2.11×10^{-9}	0.64×10^{-9}	1.44×10^{-9}	1.52	1.13	0.48	0.96
8	1.08×10^{-8}	0.72×10^{-8}	0.24×10^{-8}	0.46×10^{-8}	1.38	1.06	0.51	0.87
10	2.42×10^{-8}	1.65×10^{-8}	0.61×10^{-8}	1.05×10^{-8}	1.27	1.00	0.53	0.81
12	4.42×10^{-8}	3.10×10^{-8}	1.23×10^{-8}	2.01×10^{-8}	1.18	0.94	0.54	0.75
14	7.11×10^{-8}	5.12×10^{-8}	2.21×10^{-8}	3.37×10^{-8}	1.09	0.89	0.55	0.72
16	1.04×10^{-7}	0.77×10^{-7}	0.35×10^{-7}	0.52×10^{-7}	1.03	0.85	0.55	0.69
18	1.44×10^{-7}	1.08×10^{-7}	0.52×10^{-7}	0.75×10^{-7}	0.98	0.81	0.55	0.67
20	1.88×10^{-7}	1.44×10^{-7}	0.73×10^{-7}	1.02×10^{-7}	0.94	0.79	0.55	0.66

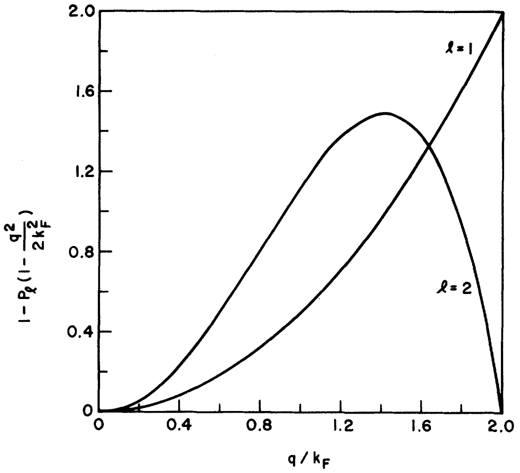

FIG. 2. The weighting factors in the integrals for the inverse relaxation times.

the Bardeen potential, and the latter gives τ_2/τ_1 about 50% higher.

Our low-temperature values for τ_2/τ_1 in Table I show that the forward scatterings of electrons by phonons are not entirely dominant. This is in agreement with the calculation by Hasegawa,[6] who found that down to 3 °K there is still a sizable contribution to ρ or $1/\tau_1$ from the umklapp processes. We find that the T^5 region in ρ arising from the purely forward scatterings is confined to $T \lesssim 2$ °K. Garland and Bowers[10] have measured the resistivity in the region 2.4 °K< T< 4.2 °K and found that ρ quite accurately obeys a T^5 law. However, our calculation shows that this cannot be the T^5 behavior due to purely forward scatterings.

III. COMPARSION WITH EXPERIMENT

Natale and Rudnick[2] have measured the resistivity and ultrasonic attenuation in the same samples of potassium over the range of temperature 2.5–20 °K beyond which the electron-phonon component of the ultrasonic attenuation is too small for reliable measurements. However, two complicating factors make it inaccurate to determine the relaxation time τ_2 from the measured attenuation by means of Eq. (2): (1) the polycrystalline nature of the samples and (2) the finite diameter of the bars used.

The elastic properties of polycrystalline samples are described by the Young's modulus and Poisson ratio of the isotropic medium which is obtained by suitably averaging the cubic crystal elastic constants rather than the elastic constants of the cubic crystal.[11] The most appropriate way of averaging is the one due to Kroner.[12] This is the method used by Natale and Rudnick.[2] However, the Young's modulus and Poisson ratio which we determine by Kroner's method[13] from the elastic constants of single-crystal potassium[14] are somewhat different from the values used by Natale and Rudnick (see Table II). The differences are sufficient to cause a difference of 20% in the determination of τ_2/τ_1, Natale and Rudnick's values giving the lower ratio. In the column of Table II under "Expt, " the elastic constants of the polycrystal are determined from the group velocity of the sound wave measured by Natale and Rudnick, as follows: The Poisson ratio σ is related to the Young's modulus Y by the relation

$$\sigma = \tfrac{1}{2}(1 - Y/3B) \ , \tag{4}$$

where B is the bulk modulus of the cubic crystal.[14] The sound wave which propagates through the cylindrical sample of radius a is a Young's modulus wave with phase velocity[15] given by

$$s_Y = (Y/nM)^{1/2}(1 - \sigma^2 a^2 \omega^2/4 s_Y^2) \ , \tag{5}$$

where ω is the angular frequency of the sound wave. The measured sound velocity is the group velocity

$$s_g = (Y/nM)^{1/2}(1 - 3\sigma^2 a^2 \omega^2/4 s_Y^2) \ , \tag{6}$$

where the term proportional to $a^2\omega^2$ is the leading correction in the ratio of the radius of the sample to the wavelength. In these three relations (4)–(6), s_g, B, ω, and a are known and hence Y, σ, and s_Y are determined.

Including the correction to leading order of the radius of the sample over the wavelength of the sound wave, the attenuation coefficient of the Young's modulus wave is[16]

$$A_Y = A(s/s_Y)^3(1+\sigma)^2[1 + \tfrac{1}{2}a^2q^2\sigma(1 - 2\sigma)] \ , \tag{7}$$

where A is given in Eq. (2). Compared with Filson's expression[15] which was used in Ref. 2, Eq. (7) contains, in the square bracket, the correction due to the finite radius of the cylinder in addition to the correction through the sound velocity s_Y. The factor in the square bracket introduces a correction of about 10%.

We use Eq. (7) to determine τ_2 from the mea-

TABLE II. Elastic properties needed to determine the ultrasonic attenuation.

	Expt	Kroner	Natale and Rudnick
Young's modulus Y (10^{10} dyn/cm^2)	3.517	3.629	3.294
Poisson ratio σ	0.340	0.335	0.350
C (at 3.68×10^5 Hz) (in units of 10^{-12} Ω Np)	5.563	5.273	6.478
C (at 2.77×10^5 Hz)	2.837	2.703	3.257
C (at 2.19×10^5 Hz)	1.690	1.613	1.929

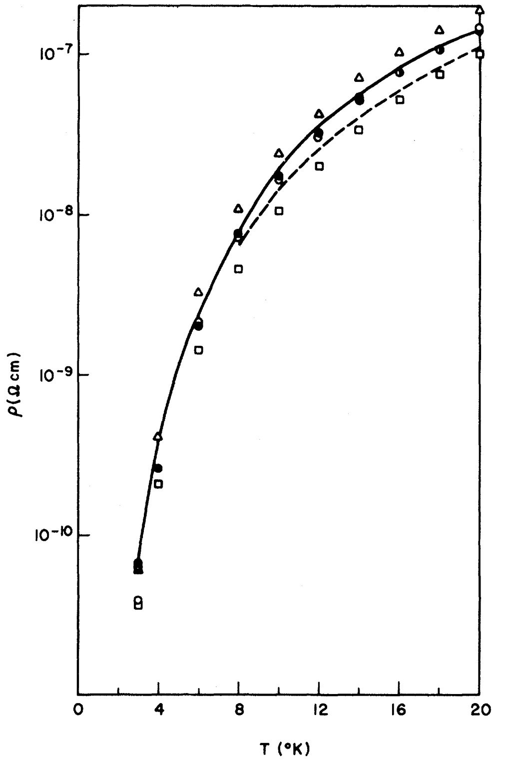

FIG. 3. Ideal resistivity as a function of temperature. —— Natale and Rudnick, Ref. 2; ---- Dugdale and Gugan, Ref. 18; ● Hasegawa, Ref. 6; ▵ from Bardeen pseudopotential (I); ⊙ from lower Lee-Falicov pseudopotential (II); ⊡ from Ashcroft potential (IV).

sured attenuation A_Y. Let us introduce

$$\rho_2 = m/ne^2\tau_2 \tag{8}$$

as a convenient measure of the relaxation time τ_2 in comparison with the measured electrical resistivity. The conversion factor to get ρ_2 from A_Y,

$$C = A_Y \rho_2 \ , \tag{9}$$

is given by Eq. (7) independent of temperature for each frequency of the sound wave and is tabulated in Table II. From this we note that the uncertainty in the elastic constants of the polycrystal alone leads to a variation of about 20% in the determination of ρ_2.

By comparing the measured attenuation coefficient and the resistivity, Natale and Rudnick[2] concluded that τ_2 and τ_1 have similar temperature dependence and have a ratio of about 1.65. In this comparision, the scatterings due to electron phonon and electron impurity are lumped together. The temperature dependence of τ_2/τ_1 is then somewhat masked by the residual value at the lowest temperature. The deviation of τ_2/τ_1 from unity at the lowest temperature due to electron-impurity scatterings alone is for the same reason as in the electron-phonon component.[17,3] However, the unknown nature of the impurities prevents us from a more quantitative investigation. We use Mattheissen's rule to subtract out the residual component of both ρ and ρ_2 and we study the electron-phonon component only.

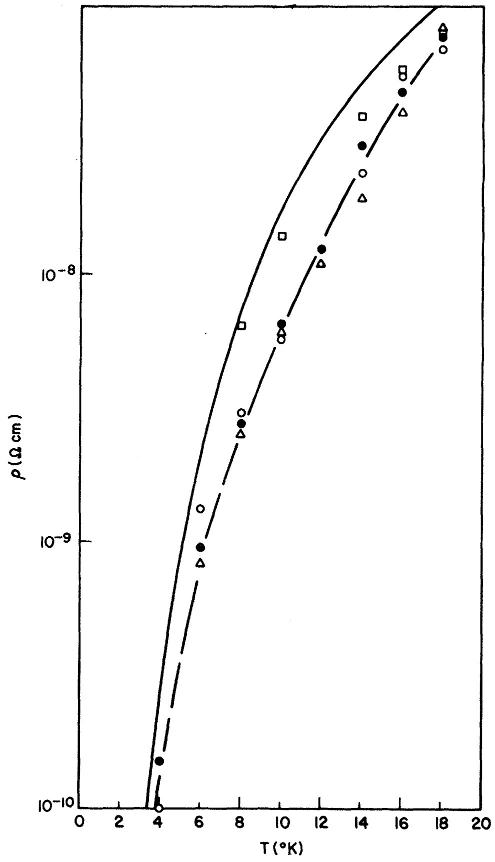

FIG. 4. Relaxation time as measured by ρ_2 from the ultrasonic attenuation: ● at 3.68×10^5 Hz, ⊙ at 2.77×10^5 Hz, ▵ at 2.19×10^5 Hz. Compared with resistivity ρ: —— Natale and Rudnick, Ref. 2; ☐ Dugdale and Gugan, Ref. 18.

In Fig. 3, we plot the ideal resistivity from various calculations and the two sets of measured val-

TABLE III. Experimental values of τ_2/τ_1 due to electron-phonon scatterings.

T (°K)	τ_2/τ_1 (3.68×10^5 Hz)	τ_2/τ_1 (2.77×10^5 Hz)	τ_2/τ_1 (2.19×10^5 Hz)
4	1.80	2.70	3.86
6	2.13	1.52	2.43
8	2.78	2.51	3.02
10	2.63	2.97	2.82
12	2.64	2.96	2.91
14	1.72	2.18	2.71
16	1.61	1.42	1.93
18	1.40	1.56	1.30

ues by Natale and Rudnick[2] and by Dugdale and Gugan.[18] There is a significant discrepancy between the two sets of experimental values. In Fig. 4, we plot ρ_2 obtained, as described above, from the ultrasonic attenuation at three different frequencies and compare it with the measured ρ. Here, we have used the value of the conversion factor C [Eq. (9)] in Table II under the column "Expt." In Table III, we list the ratio of τ_2/τ_1 from experimental measurements.

The temperature dependence of the measured τ_2/τ_1 roughly follows the theoretical prediction. It is small at low temperature, rises to a maximum in the neighborhood of about 8 °K and then diminishes slightly. However, even taking the largest calculated set of τ_2/τ_1, which comes from Bardeen's electron-phonon matrix element, and allowing for the uncertainty in the experimental values due to the uncertainty in the elastic constants of the polycrystal, we find that there is significant disagreement. This discrepancy cannot be ascribed to many-body effects since the attenuation formula which we have used correctly includes all such effects, nor can the discrepancy be ascribed to uncertainties in the phonon spectrum since we have used the phonon frequencies measured at 9 °K by Cowley *et al.*[19] It would clearly be desirable to have more measurements of the ultrasonic attenuation and electrical resistivity at low temperatures, preferably on single crystals, in a number of simple metals. Should the discrepancy persist between the calculated and experimental values, we may have to question the validity of our Kohler solution of the transport equation and the concomitant Matthiessen's rule and, perhaps, also the equivalence of the pseudopotentials needed to fit the Fermi surface and the transport coefficients.

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One-Electron Potential-Energy Functions for Calculating Wave Functions at Solid Surfaces*

D. S. Boudreaux

Department of Physics, Polytechnic Institute of Brooklyn, Brooklyn, New York 11201

(Received 25 August 1969)

An expression is given for the potential energy seen by an electron near a crystal surface including both potential periodicity and exchange and correlation effects among electrons. The possible usage of such a function for determining wave functions and charge distributions is discussed.