

## Band-structure effects on transport in aluminum<sup>†</sup>

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We present results of calculations of the electrical and thermal conductivity and the phonon-drag thermopower in pure Al including a realistic Fermi surface and multiple-plane-wave electron-phonon matrix elements. Scattering times to electrical and thermal conductivity are computed as a function of position on the Fermi surface at various temperatures. Large anisotropies are observed, particularly at low temperatures. Comparison of our results for the electrical resistivity and the phonon-drag thermopower with previous one-plane-wave calculations show considerable differences and the agreement with experiment is significantly improved.

### I. INTRODUCTION

Transport properties are average properties in that all the electrons at the Fermi surface participate. Since much of the Al Fermi surface is free-electron-like we might expect that multiple-plane-wave effects may not be overly important. Indeed one-plane-wave calculations with a spherical Fermi surface do give a reasonable description of the observed high-temperature resistivity of Al.<sup>1</sup> However at low temperatures it is well known that this is no longer the case.<sup>2</sup>

In polyvalent metals the electronic wave functions near Bragg planes are very different from plane waves. Ignoring this feature leads to an artificial  $1/\omega$  behavior for the square of the electron-phonon coupling for umklapp processes with vanishingly small reduced momentum<sup>3</sup> which means small phonon frequencies  $\omega$ . Since at low temperature ( $T$ ) only these phonons will be present, the low-temperature transport coefficients can be very seriously overestimated in the free-electron model.

It is the main purpose of this paper to make a quantitative study of the effects of band structure on the transport properties of aluminum. Previous work has been done by Pytte,<sup>4</sup> Lawrence and Wilkins,<sup>2</sup> and Chan and Huntington.<sup>5</sup> Our work is more extensive since it covers several transport coefficients and treats the Fermi surface, phonons and electron-phonon matrix elements in greater detail. For the Fermi surface we use the four-plane-wave model of Ashcroft<sup>6</sup> which is known to fit the de Haas-van Alphen data well. For the electron-phonon matrix element we use 15 plane waves to describe the electronic states. The lattice dynamics is calculated from a Born-von Kármán force-constant system fit to the measured phonon dispersion curves.

The microscopic information on the electronic structure, the electron-phonon interaction and the lattice dynamics are related to the transport coef-

ficients through the Boltzmann transport equation. It is out of the question at the moment to try to solve this equation exactly. We will consider two approximate solutions which have frequently been used in the past. The first is the one obtained from a variational principle utilizing the simplest possible trial functions<sup>7</sup> and the second is the scattering time solution used by Robinson and Dow<sup>8</sup> and Chan and Huntington<sup>5</sup> to study the high-temperature resistivity.

The lowest-order trial function largely ignores any anisotropy or energy dependence in the scattering. This is discussed by Lawrence and Wilkins<sup>2</sup> for Al and by Kus and Carbotte<sup>9</sup> for the electrical resistivity of the alkalis. On the other hand, the anisotropy in the scattering can easily and quite naturally be accounted for in an approximate scattering time solution for the Boltzmann equation. We assume the existence of an anisotropic scattering time  $\tau(\vec{k}, T)$  and the Boltzmann transport equation becomes an integral equation for  $\tau(\vec{k}, T)$ . Sorbello<sup>10</sup> has recently given a clear discussion of the concepts associated with  $\tau(\vec{k}, T)$ . If we limit the discussion to a first iteration of the equation for  $\tau(\vec{k}, T)$  we get a simple closed expression for the scattering times at any temperature from which we can calculate the transport coefficients.

In Sec. II we discuss the approximate solution to the Boltzmann equation appropriate to the various transport coefficients. We introduce a scattering time  $\tau_R(\vec{k}, T)$  appropriate to the electrical conductivity and another  $\tau_W(\vec{k}, T)$  for the thermal conductivity. Their relation to the microscopic interactions is described. Two spectral weight functions  $\alpha_{TR}^2 F_{\vec{k}}(\omega)$  and  $\alpha_{\vec{k}}^2 F_{\vec{k}}(\omega)$  will be introduced. The first one is for the electrical resistivity while both are required for the thermal resistivity. In addition two more,  $\alpha_{1L\vec{k}}^2 F_{\vec{k}}(\omega)$  and  $\alpha_{LL\vec{k}}^2 F_{\vec{k}}(\omega)$  are needed to discuss the phonon-drag contribution to the thermopower and the electrical resistivity. These distributions apply to each state  $\vec{k}$  on the Fermi sur-

face and contain all of the details of the Fermi surface, the electronic structure and the electron-phonon interaction as well as the lattice dynamics. The same distributions,  $\alpha_{\text{TR}}^2 F_{\vec{k}}(\omega)$  and  $\alpha_{\vec{k}}^2 F_{\vec{k}}(\omega)$ , are used in both the variational and the scattering-time approximations for the electrical and thermal resistivities. In Sec. III we give the results of the calculations and compare with one-plane-wave results and with experiment. In Sec. IV we draw conclusions.

## II. TRANSPORT COEFFICIENTS

In the presence of an external field the occupation of the state  $\vec{k}$  is given by

$$f_{\vec{k}} \approx f_{\vec{k}}^0 - \Phi_{\vec{k}} \frac{\partial f_{\vec{k}}^0}{\partial \epsilon_{\vec{k}}}, \quad (1)$$

where  $f_{\vec{k}}^0$  is the Fermi-Dirac function and  $\epsilon_{\vec{k}}$  is the energy of the electron in the state  $\vec{k}$ . For the electrical resistivity  $\Phi_{\vec{k}}$  is proportional to the electric field  $\vec{E}$  and the usual lowest order trial variational function is<sup>7</sup>

$$\Phi_{\vec{k}} \propto \vec{v}_{\vec{k}} \cdot \vec{E}, \quad (2)$$

where  $\vec{v}_{\vec{k}}$  is the velocity of the electron in state  $\vec{k}$ . This gives an expression for the resistivity

$$\rho_v(T) = \frac{64\pi^5 \hbar^2}{e^2 k_B T} \int_0^\infty d\omega R(\omega) \alpha_{\text{TR}}^2 F(\omega) \times \left( \frac{1}{3} \left| \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \right|^2 \right)^{-1}, \quad (3a)$$

where  $e$  is the electronic charge,  $k_B$  is the Boltzmann constant,  $\hbar$  is Planck's constant divided by  $2\pi$ , and  $R(\omega)$  is a thermal factor for the phonon frequency  $\omega$

$$R(\omega) = \hbar \omega / (e^{\hbar\omega/k_B T} - 1)(1 - e^{-\hbar\omega/k_B T}). \quad (4)$$

$\alpha_{\text{TR}}^2 F(\omega)$  is the Fermi surface average of  $\alpha_{\text{TR}}^2 F_{\vec{k}}(\omega)$  which is defined below.

In our second approximate solution of the Boltzmann equation, scattering-time approximation, one makes the ansatz

$$\Phi_{\vec{k}} \propto \tau_R(\vec{k}, T) \vec{v}_{\vec{k}} \cdot \vec{E} \quad (5)$$

$$\rho_v(T) = \frac{4\pi^3 \hbar}{e^2} \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \tau_R^{-1}(\vec{k}, T) \left( \frac{1}{3} \left| \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \right|^2 \right)^{-1}. \quad (3b)$$

For the thermal resistivity, the usual lowest-order variation trial wave function is<sup>7</sup>

$$\Phi_{\vec{k}} \propto [(\epsilon_{\vec{k}} - \epsilon_F)/k_B T] \vec{v}_{\vec{k}} \cdot \vec{\nabla} T, \quad (11)$$

where  $\epsilon_F$  is the Fermi energy and  $\vec{\nabla} T$  is the temperature gradient. This gives the following expression for the thermal resistivity:

and obtains an integral equation for  $\tau_R(\vec{k}, T)$  when  $\Phi_{\vec{k}}$  is substituted in the Boltzmann equation.<sup>8</sup> Keeping only the first iteration we get an explicit expression for  $\tau_R(\vec{k}, T)$

$$\frac{1}{\tau_R(\vec{k}, T)} = \frac{4\pi}{k_B T} \int_0^\infty d\omega R(\omega) \alpha_{\text{TR}}^2 F_{\vec{k}}(\omega). \quad (6)$$

$\alpha_{\text{TR}}^2 F_{\vec{k}}(\omega)$  is given explicitly by

$$\alpha_{\text{TR}}^2 F_{\vec{k}}(\omega) = \frac{1}{8\pi^3 \hbar} \int \frac{dS_{\vec{k}'}}{|\vec{v}_{\vec{k}'}|} \left( 1 - \frac{\vec{v}_{\vec{k}} \cdot \vec{v}_{\vec{k}'}}{|\vec{v}_{\vec{k}}|^2} \right) \times \sum_{\lambda} |g_{\vec{k}\vec{k}\lambda}|^2 \delta(\omega - \omega_{\lambda}(\vec{k}' - \vec{k})), \quad (7)$$

where  $\omega_{\lambda}(\vec{k}' - \vec{k})$  is the phonon with wave vector  $(\vec{k}' - \vec{k})$  reduced to the first Brillouin zone, with  $\lambda$  the branch index.  $g_{\vec{k}\vec{k}\lambda}$  is the electron-phonon coupling constant describing the scattering of an electron in a state  $\vec{k}$  to state  $\vec{k}'$  via the emission or absorption of a phonon with frequency  $\omega_{\lambda}(\vec{k}' - \vec{k})$

$$g_{\vec{k}\vec{k}\lambda} = \frac{-i\vec{\epsilon}_{\lambda}(\vec{k}' - \vec{k})}{[2MN\omega_{\lambda}(\vec{k}' - \vec{k})]^{1/2}} \left( \sum_{ij} C_{\vec{k}j}^* C_{\vec{k}i}(\vec{k}' - \vec{k} + \vec{G}_j - \vec{G}_i) \times \langle \vec{k}' + \vec{G}_j | W | \vec{k} + \vec{G}_i \rangle \right), \quad (8)$$

with  $M$  the ionic mass,  $N$  the number of ions per unit volume, and  $\vec{\epsilon}_{\lambda}(\vec{k}' - \vec{k})$  the phonon polarization vector. The coefficients  $C_{\vec{k}i}$  are the mixing coefficients in the plane-wave expansion of the electron state,  $\vec{G}_i$  are the reciprocal-lattice vectors, and  $\langle \vec{k}' + \vec{G}_j | W | \vec{k} + \vec{G}_i \rangle$  is the pseudopotential form factor.<sup>11</sup> The isotropic distribution  $\alpha_{\text{TR}}^2 F(\omega)$  needed in Eq. (3a) is given by

$$\alpha_{\text{TR}}^2 F(\omega) = \frac{1}{4\pi \hbar} \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \alpha_{\text{TR}}^2 F_{\vec{k}}(\omega). \quad (9)$$

In the scattering-time approximation the resistivity is given by

$$\rho_{\text{ST}}(T) = \left( \frac{e^2}{12\pi^3 \hbar} \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \tau_R(\vec{k}, T) \right)^{-1}. \quad (10)$$

We note that  $\rho_v(T)$  can be rewritten in terms of the  $\tau_R(\vec{k}, T)$ . We find

$$W_V(T) = \frac{1}{\mathfrak{L}_0 T} \left( \frac{4\pi}{k_B T} \right) \frac{48\pi^4 \hbar^2}{e^2} \int_0^\infty d\omega R(\omega) \left\{ \left[ 1 - \frac{1}{2\pi^2} \left( \frac{\hbar\omega}{k_B T} \right)^2 \right] \alpha_{\text{TR}}^2 F(\omega) + \frac{3}{2\pi^2} \left( \frac{\hbar\omega}{k_B T} \right)^2 \alpha^2 F(\omega) \right\} \left( \left| \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \right|^2 \right)^{-1} \quad (12)$$

where  $\mathfrak{L}_0$  is the Lorentz number. The distribution function  $\alpha^2 F(\omega)$  is familiar from the theory of strong-coupling superconductivity, and is given by the same expression as  $\alpha_{\text{TR}}^2 F(\omega)$  with the factor

$$[1 - (\vec{v}_{\vec{k}} \cdot \vec{v}_{\vec{k}}) / |\vec{v}_{\vec{k}}|^2]$$

omitted.

In the scattering-time approximation one assumes

$$\Phi_{\vec{k}} \propto \tau_w(\vec{k}, T) [(\epsilon_{\vec{k}} - \epsilon_F) / k_B T] \vec{v}_{\vec{k}} \cdot \vec{\nabla} T, \quad (13)$$

and obtains for  $\tau_w(\vec{k}, T)$  the expression, in lowest order,

$$\frac{1}{\tau_w(\vec{k}, T)} = \frac{4\pi}{k_B T} \int_0^\infty d\omega R(\omega) \left\{ \left[ 1 - \frac{1}{2\pi^2} \left( \frac{\hbar\omega}{k_B T} \right)^2 \right] \alpha_{\text{TR}}^2 F_{\vec{k}}(\omega) + \frac{3}{2\pi^2} \left( \frac{\hbar\omega}{k_B T} \right)^2 \alpha_{\vec{k}}^2 F_{\vec{k}}(\omega) \right\}. \quad (14)$$

This gives, for the thermal resistivity,

$$W_S(T) = \left( \mathfrak{L}_0 T \frac{e^2}{12\pi^3 \hbar} \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \tau_w(\vec{k}, T) \right)^{-1}. \quad (15)$$

We could also rewrite  $W_V(T)$  in terms of  $\tau_w(\vec{k}, T)$  in the same way  $\rho_V(T)$  was written in terms of  $\tau_R(\vec{k}, T)$  in Eq. (3b).

To study the effect of phonon drag on the thermopower and resistivity, one must consider the coupled Boltzmann equation for both the electron and phonon occupation probabilities.<sup>7</sup> In analogy with the case for the electron trial function  $\Phi_{\vec{k}}$ , one writes the phonon occupation as

$$n_{\vec{q}\lambda} = n_{\vec{q}\lambda}^0 - \Psi_{\vec{q}\lambda} \frac{\partial n_{\vec{q}\lambda}^0}{\hbar \partial \omega_\lambda(\vec{q})}, \quad (16)$$

where the simplest choice for  $\Psi_{\vec{q}\lambda}$  is<sup>7</sup>

$$\Psi_{\vec{q}\lambda} \propto \vec{q} \cdot \vec{u}, \quad (17)$$

where  $\vec{u}$  is the unit vector of the electric field.

Using Eq. (2) for  $\Phi_{\vec{k}}$  we obtain for the electrical resistivity<sup>7</sup>

$$\rho^{\text{PD}}(T) = \rho_V(T) (1 - P_{1L}^2 / P_{11} P_{LL}), \quad (18)$$

where  $\rho_V(T)$  is given in Eq. (3) and  $P_{11}$ ,  $P_{1L}$ , and  $P_{LL}$  are as follows:

$$P_{11} = \frac{1}{k_B T} \int_0^\infty d\omega R(\omega) \alpha_{\text{TR}}^2 F(\omega), \quad (19a)$$

$$P_{1L} = \frac{1}{k_B T} \int_0^\infty d\omega R(\omega) \alpha_{1L}^2 F(\omega), \quad (19b)$$

and

$$P_{LL} = \frac{1}{k_B T} \int_0^\infty d\omega R(\omega) \alpha_{LL}^2 F(\omega). \quad (19c)$$

$\alpha_{1L}^2 F(\omega)$  and  $\alpha_{LL}^2 F(\omega)$  are the same as  $\alpha_{\text{TR}}^2 F(\omega)$  except that  $(v_{\vec{k}} - v_{\vec{k}})^2$  is replaced by  $\vec{q} \cdot (v_{\vec{k}} - v_{\vec{k}})$  and

$\vec{q} \cdot \vec{q}$ , respectively.

Using the same approximations for  $\Phi_{\vec{k}}$  and  $\psi_{\vec{q}\lambda}$ , the phonon drag contribution to the thermopower is<sup>7</sup>

$$S^{\text{PD}}(T) = \frac{k_B}{en_a} \frac{C_L(T)}{3Nk_B} \left( -\frac{P_{1L}}{P_{LL}} \right), \quad (20)$$

where  $n_a$  is the number of free electrons per atom and  $C_L(T)$  is the lattice specific heat.

We see that we can write the various transport coefficients in terms of four similar distribution functions. Our first problem is thus to calculate these distributions. The transport coefficients at any temperature may then be obtained by simply doing the frequency integral over the appropriate distribution. Some more details of the method of calculating the  $\alpha_{\vec{k}}^2 F_{\vec{k}}(\omega)$  may be found in the paper by Leung *et al.*<sup>12</sup>

### III. CALCULATIONS AND DISCUSSION

For the electrical resistivity, the results are given in Figs. 1 and 2. In Fig. 1, we show the Fermi-surface variations of  $\tau_R(\vec{k}, T)$  at three different temperatures, namely 20, 50, and 100 K. Entries correspond to three constant  $\phi$  arcs,  $\phi = 1^\circ$ ,  $23^\circ$ , and  $45^\circ$ . The anisotropy at 20 K is very large. For example, the longest time between scatterings entered is  $1 \times 10^{-10}$  sec while the shortest is about  $3.5 \times 10^{-12}$  sec. For  $T = 50$  K all of the entries are of the order of  $10^{-13}$  sec and for  $T = 100$  K of the order of  $10^{-14}$  sec. In this last case there are numbers as small as  $\sim 4$  and as large as  $\sim 9.5$ , showing that there is still a significant amount of anisotropy. Note that we have used a logarithmic scale on the vertical axis. It is very important to realize that the curves fully include the distortions of the Fermi surface from a sphere and the multiple-plane-wave character of the electronic states.

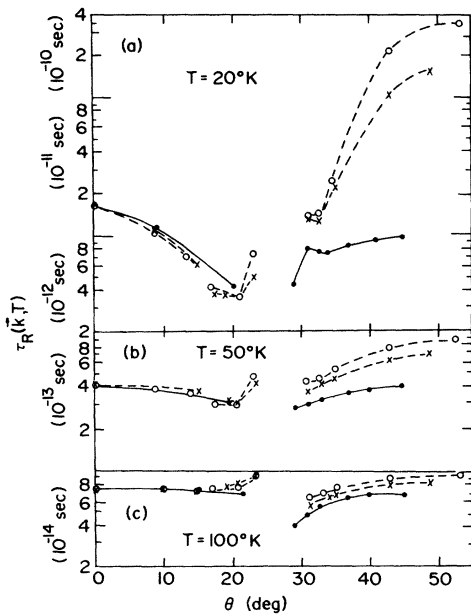


FIG. 1. Variation of the scattering times  $\tau_R(\vec{k}, T)$  over the  $(\frac{1}{48})$  irreducible zone on the Fermi surface. (a)  $T = 20^\circ\text{K}$ ; (b)  $T = 50^\circ\text{K}$ ; (c)  $T = 100^\circ\text{K}$ . Solid line,  $\phi = 1^\circ$ ;  $-x-x-$ ,  $\phi = 23^\circ$ ;  $-o-o-o$ ,  $\phi = 45^\circ$ .

Also, realistic phonons are used throughout.

Using these scattering times  $\tau_R(\vec{k}, T)$ , we get the values of the electrical resistivity in the two different approximations  $\rho_V(T)$  and  $\rho_{ST}(T)$  from Eqs. (3) and (10), respectively. Since in  $\rho_{ST}(T)$  we average  $\tau_R(\vec{k}, T)$ , while in  $\rho_V(T)$  we average  $1/\tau_R(\vec{k}, T)$ , we expect these two quantities to differ most when the anisotropy is greatest, i.e., at low temperature. If  $\tau_R$  is isotropic, both formulas would give the same result, namely

$$\rho(T) = \left( \frac{e^2}{12\pi^3\hbar} \tau_R \int dS_k |v_{\vec{k}}| \right)^{-1}. \quad (21)$$

These expectations are borne out in the calculations which are given in Fig. 2, where  $\rho_V(T)$  is compared with  $\rho_{ST}(T)$  in the range 20–300 K. Above 80 K the values of  $\rho_V(T)$  and  $\rho_{ST}(T)$  agree almost exactly, indicating that the anisotropy in  $\tau_R(\vec{k}, T)$  does not matter much when the Fermi-surface average has been performed. As the temperature decreases below 80 K however, the two results start to diverge, and at 20 K they differ by a factor of nearly 5. This shows that the two approximate solutions to the Boltzmann equation used here are not really adequate at these low temperatures.

The variational solution can be improved by including a more complicated trial wave function  $\Phi_{\vec{k}}$  than Eq. (2). For potassium, this has recently been done by Ekin and Bringer<sup>13</sup> who employ a Kubic harmonic expansion and conclude that correc-

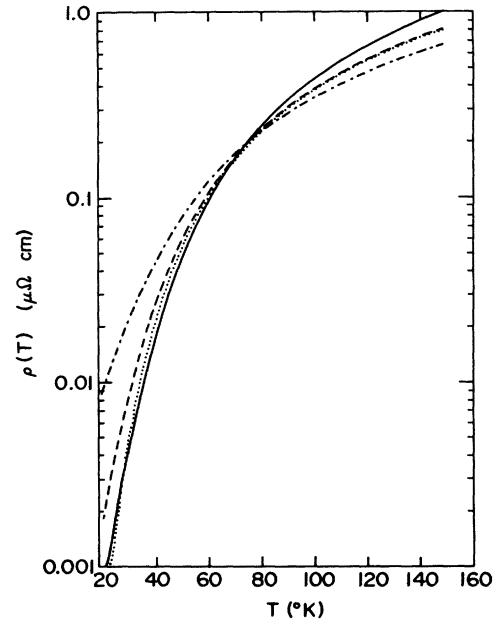


FIG. 2. Electrical resistivity of pure aluminum as a function of temperature. The dotted line denotes  $\rho_{ST}(T)$  using 15 plane waves, the dashed line denotes  $\rho_V(T)$  using 15 plane waves, the dash-dot line is  $\rho_V(T)$  using one plane wave and a spherical Fermi surface, and the solid line is the experimental data.

tions to Eq. (3) are important when the scattering is very anisotropic.

As the temperature is lowered, Eq. (3) certainly becomes less reliable while Eq. (10) gives reasonable agreement with the experimental data<sup>14</sup> (Fig. 2). However the problem is that at such temperature the anisotropy in  $\tau_R(\vec{k}, T)$  becomes very large and the one iteration procedure that we have followed becomes unreliable so that the agreement may be fortuitous. For  $T > 80$  K the theoretical curve lies slightly below experiment. For  $T$  less than 80 K it agrees well until about 20 K. On the whole our calculations are very satisfactory.

Finally in Fig. 2 we have also shown for comparison results obtained in a one-plane-wave theory with spherical Fermi surface. At high temperature the agreement with our sophisticated multiple-plane-wave results is very good as we anticipated in the introduction. As the temperature is lowered the agreement rapidly deteriorates indicating clearly that to obtain meaningful results it is necessary to do a multiple-plane-wave calculation.

Turning now to the thermal resistivity, we give some results for  $\tau_w(\vec{k}, T)$  in Fig. 3 for several points on the Fermi surface. By comparing with the results for  $\tau_R(\vec{k}, T)$  in Fig. 1 we see that while the amount of anisotropy is smaller in  $\tau_w(\vec{k}, T)$  it is still significant. Results for  $W_V(T)$  and  $W_{ST}(T)$  are

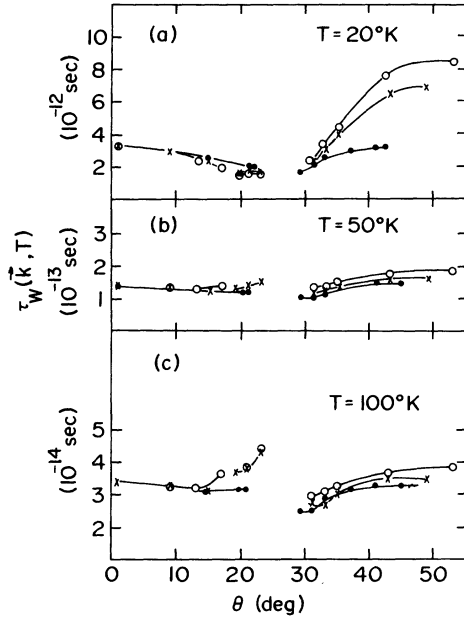


FIG. 3. Variation of the thermal scattering time  $\tau_w(\vec{k}, T)$  of the electronic state on the Fermi surface in the  $(\frac{1}{48})$  irreducible zone. (a)  $T = 20^\circ\text{K}$ ; (b)  $T = 50^\circ\text{K}$ ; (c)  $T = 100^\circ\text{K}$ . Solid line,  $\phi = 1^\circ$ ; -x-x-,  $\phi = 23^\circ$ ; -o-o-,  $\phi = 45^\circ$ .

given in Fig. 4 where we compare with the data of Cook *et al.*<sup>15</sup> At high temperature both formulas agree within a few percent. The agreement with experiment is also satisfactory. It is in this region that our approximate solutions of the Boltzmann equation are expected to be most reliable. On the other hand as the temperature is lowered the agreement with experiment becomes quite poor. For example, at  $T = 20\text{ K}$  the variational formula gives  $1.60 \times 10^{-4}\text{ mK/W}$ , the scattering time is  $1.25 \times 10^{-4}$  while the experimental value is  $6.94 \times 10^{-5}$ . While the scattering time is closer to experiment it is still too large by a factor of 2. This indicates that a better solution to the Boltzmann equation is needed at this temperature. In this context we note that if  $\tau_w(\vec{k}, T)$  was isotropic (which is not the case at 20 K), both Eqs. (12) and (15) would give the same answer. Namely

$$W(T) = \left( \mathcal{L}_0 T \frac{e^2}{12\pi^3 \hbar} \tau_w \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} |\vec{v}_{\vec{k}}|^2 \right)^{-1},$$

where  $\tau_w$  denotes an average scattering time. Since averaging over  $\tau_w(\vec{k}, T)$  as in (12) instead of  $1/\tau_w(\vec{k}, T)$  as in Eq. (15) only reduces the thermal conductivity by about 20%, the anisotropy in the scattering is not likely to be the most important source of error in our calculations at low temperatures. It is more likely that higher corrections due

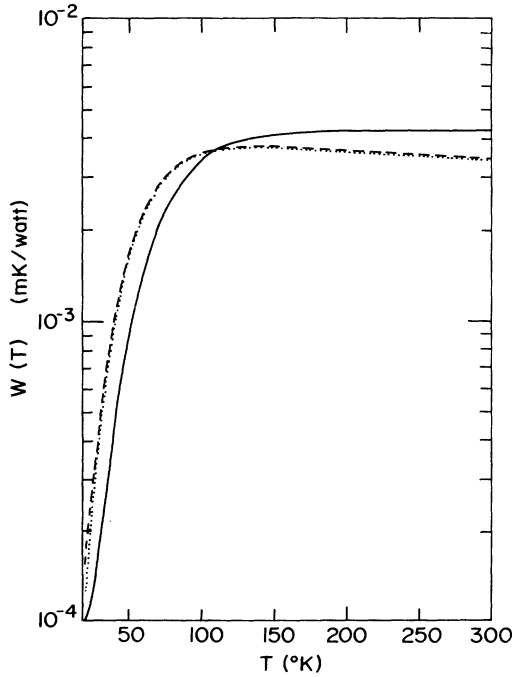


FIG. 4. Thermal resistivity of aluminum as a function of temperature. The dotted line denotes  $W_{ST}(T)$  using 15 plane waves, the dashed line denotes  $W_V(T)$  using 15 plane waves, and the solid line denotes the experimental results.

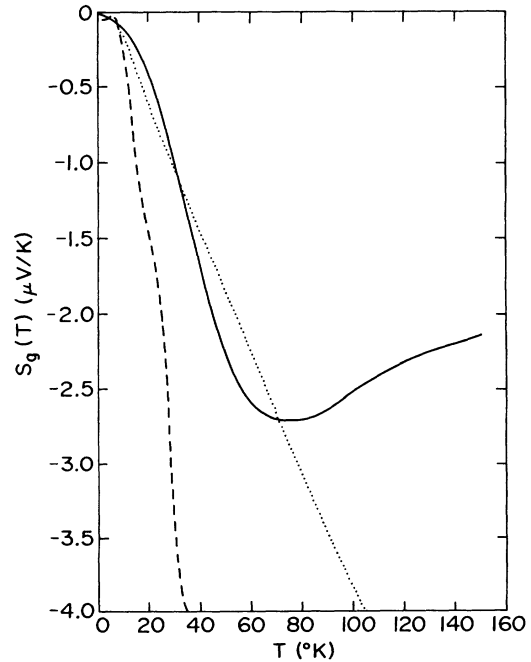


FIG. 5. Phonon-drag contribution to the thermopower. The dotted line denotes the result obtained using 15 plane waves, the dashed line is the one-plane-wave result, and the solid line is the experimental result.

TABLE I. Ratio of the resistivity including phonon drag to the resistivity without phonon drag. The results of the single-plane-wave calculation are compared with the multiple-plane-wave results.

$T$ (°K)	$\rho^{\text{PD}}(T)/\rho_V(T)$ (Single plane wave)	$\rho^{\text{PD}}(T)/\rho_V(T)$ (Multiple plane wave)
20	0.972 44	0.8359
30	0.971 39	0.9238
40	0.976 00	0.9611
50	0.979 48	0.9751
60	0.981 44	0.9807
80	0.982 81	0.9840
100	0.982 88	0.9847

to the energy dependence in  $\Phi_{\vec{k}}$  is the important factor. It would be quite difficult to calculate such corrections while at the same time including band structure and realistic phonons. Yet it is essential to have multiple plane wave at 20 K since the one-plane-wave approximation for the electron-phonon interaction breaks down completely.

We come now to the results for the phonon-drag contributions to the thermopower and the electrical resistivity. For the thermopower, the results of the single-plane-wave calculation  $S_g^{\text{SPW}}(T)$  are compared with the multiple-plane-wave result and with the experimental results of Gripshover *et al.*<sup>16</sup> in Fig. 5. Both calculations agree with experiment qualitatively in sign. However,  $S_g^{\text{SPW}}(T)$  differs by an order of magnitude from the experimental values while the multiple-plane-wave result shows good agreement up to about 80 °K.

The behavior of  $S_g(T)$  depends on the fact that  $\alpha_{L\vec{k}}^2 \vec{k} F_{\vec{k}}(\omega)$  can give negative as well as positive values since  $\vec{g} \cdot (\vec{v}_{\vec{k}} - \vec{v}_{-\vec{k}})$  will be positive for normal processes and negative for umklapp processes. As the temperature is changed, different portions of  $\alpha_{L\vec{k}}^2 \vec{k} F_{\vec{k}}(\omega)$  are sampled by the thermal factors  $R(\omega)$ . That the umklapp processes are responsible for the positive thermopowers was suggested by Ziman<sup>7</sup> and Bailyn.<sup>17</sup>

We conclude this section with some results for the effect of phonon drag on the electrical resistivity. The ratio  $\rho^{\text{PD}}(T)/\rho_V(T)$  is given in Table I. We see that the effect of phonon drag is small at high temperature and that the band structure is only significant below about 40 °K.

#### IV. CONCLUSION

In a polyvalent metal like Al it is essential to include multiple-plane-wave effects in the electronic structure in order to get a quantitative description of the transport properties at low temperature.

For Al a single-plane-wave model with spherical Fermi surface is only reasonable above about 80 K. Below 50 K an additional complication arises which is connected with the solution of the Boltzmann equation. In that temperature region the scattering due to the electron-phonon interaction is very anisotropic so that the usual formula for the resistivity based on the variational principle with simplest possible trial function becomes inadequate. It is necessary to consider higher trial functions in addition to including properly the electronic band structure and real lattice dynamics. Alternatively, one can use a scattering-time formalism in which the Boltzmann equation is solved directly without reference to a variational principle. If only the lowest iteration of the equation for the scattering time is retained, a manageable closed expression for the electrical and thermal resistivity results which includes some effects of the anisotropy in a very natural way. It gives electrical resistivities considerably lower than the variational formula and in quite good agreement with experiment. A complete iteration of the equation for  $\tau_R(\vec{k}, T)$  is desirable and will be attempted in the near future.

For the thermal resistivity, the anisotropy in the scattering time is found to be less important than it is for the electrical resistivity. This is largely due to the fact that, at low temperature  $W(T)$  is largely determined by the  $\alpha_{\vec{k}}^2 F_{\vec{k}}(\omega)$  term, not the  $\alpha_{\text{TR}\vec{k}}^2 \vec{k} F_{\vec{k}}(\omega)$  term. There is however the more important complication of the energy dependence of the trial wave function. Here we have used only the simplest possible choice for it. Clearly a proper solution to this problem involves the necessity of solving the Boltzmann integral equation for both the energy as well as the angular dependence of  $\Phi_{\vec{k}}$ .

For the phonon-drag contributions to the thermopower and the electrical resistivity, obtaining an adequate solution to the coupled electron and phonon Boltzmann equations is a very difficult task. It has recently received much attention in the calculations of  $\rho(T)$  for potassium, particularly by Leavens and Laubitz.<sup>18</sup> They show the inadequacy of the usual lowest-order variational solution. For the phonon drag contribution to the thermopower, the effects of the band structure are very significant, but for  $\rho^{\text{PD}}(T)/\rho_V(T)$ , much less so. For the electrical resistivity, it is the contribution excluding phonon drag, i.e.,  $\rho_V(T)$  or  $\rho_{\text{ST}}(T)$ , that is very sensitive to the details of the band structure.

In conclusion we can state that we have made detailed calculations of the following transport properties: the electrical and thermal resistivities, the phonon-drag contributions to the thermopower, and the electrical resistivity. The calculations involve no adjustable parameters and include in a

realistic fashion the details of the nonspherical Fermi surface, the electronic states, the electron-phonon interaction, and the lattice dynamics. A comparison of the single-plane-wave results with

those obtained in a multiple-plane-wave calculation show the great importance of including such effects if one is to achieve reliable quantitative agreement with experiment.

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