THEORY OF ELECTRON-PHONON
SCATTERING EFFECTS IN METALS

Progress Report

Walter E. Lawrence

Dartmouth College
Hanover, New Hampshire

March 1, 1973 - November 30, 1973

Prepared for the U. S. Atomic Energy Commission under
Contract No. AT(11-1)-2315.

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ABSTRACT

We have investigated electron-phonon scattering anisotropy in metals: A soluble model which relates the resulting relaxation time anisotropy to deviations from Matthiessen's rule in the electrical resistivity is equally applicable to several Fermi surface types and exhibits qualitative behavior in agreement with experiment. The low-temperature resistivity of potassium has been studied in detail to clarify the role of different physical mechanisms at low temperatures. An exact calculation of electron-phonon scattering in aluminum has been undertaken.

I. Introduction

The topics which we have investigated and the results obtained will be discussed only briefly and qualitatively here. The details will be prepared for publication and submitted as a technical report later in this Contract year. In the next section we briefly describe the scope of our investigation to date. The results of that investigation are discussed in sec. III.

II. Scope of Investigation

While our long range goal is to study the effect of anisotropic electron-phonon scattering on transport coefficients of metals in general, we have restricted our study so far to the electrical resistivity. After this case has been studied in detail we shall proceed to treat the others (the magnetoresistivity was named in our original research proposal, and the current proposal includes the thermal conductivity and thermoelectric power). In the electrical resistivity problem we seek to relate the transport relaxation time anisotropy to deviations from Matthiessen's rule⁽¹⁾ (DMR). The investigation proceeds by analytic modeling as described in the next section. The model treats different Fermi surface types on equal footing, so that we can investigate the qualitatively different kinds of behavior exhibited by different types. The model parameters are related explicitly to electron-phonon matrix elements, and because of this the anisotropic transport time can be related to the anisotropic quasiparticle lifetime. The latter can be measured directly and therefore provides an experimental check on our modeling.

We have studied the general problem of the low-temperature resistivity of potassium⁽²⁾. The purpose of this was to clarify the state of agreement between experiment and theory, and to clarify the roles of different physical mechanisms at low temperatures. Potassium is an important test case of our modeling technique, and deserves close attention.

To complement the analytic modeling we are setting up an exact numerical calculation of the quasiparticle properties of aluminum - the quasiparticle lifetime and the mass enhancement (the latter has been calculated,⁽³⁾ but without taking band structure into account). In addition the simple-trial-function resistivity will be calculated (not the full DMR). The Ashcroft pseudopotential⁽⁴⁾ will be used for the Fermi surface and the matrix elements, and the numerical integrations will be performed over the distorted Fermi surface. The routines are now being set up and so no results have yet been obtained.

III. Results

The principal result of our research is a derivation (by approximation) of the diffusion model⁽⁵⁾ from the exact Boltzmann equation for electron-phonon scattering. The model parameters are thereby related explicitly to the electron-phonon matrix elements, and one can therefore in principle obtain quantitative results and compare them with experiment. The derivation exhibits the regimes of validity of the diffusion model; in terms of both the temperature and the impurity concentration. The most important aspect of the derivation, however, is that umklapp processes (the principal mechanism for relaxation time anisotropy⁽⁶⁾) occur explicitly in the model - not implicitly as in the previous diffusion models. It is this aspect which is essential for quantitative accuracy, and for ultimate comparison with experiment. It is also this aspect which permits the treatment of the alkali metal Fermi surfaces to which previous models could not be applied.

The diffusion model approximates the Boltzmann equation (an integral equation for the nonequilibrium electron distribution) by a differential equation. The latter is more amenable to familiar methods of approximation and to modeling. So even though the differential equation is complicated by the highly

anisotropic nature of electron-phonon scattering, and in some cases by the Fermi surface distortion, we have found nevertheless that one can construct models which are more easily solved, and which still represent the physical situation. The results of calculations naturally depend to some extent upon the modeling and upon the degree of sophistication with which electron-phonon scattering is treated. However the qualitative results - in particular the contrast between the alkali metal versus polyvalent metal geometries - are model independent and worth quoting here.

To describe the results we must digress briefly on the diffusion model. The inhomogeneous differential equation has the structure

$$1 = \left(\frac{1}{\tau_{tr}^{(0)}(\vec{k})} - \frac{1}{2} k_F^2 D_{ij}(\vec{k}) \frac{\partial^2}{\partial k_i \partial k_j} \right) \tau_{tr}(\vec{k}),$$

where $\tau_{tr}^{(0)}(\vec{k})$ is a "zeroeth-order" transport time which forces the "true" transport time $\tau_{tr}(\vec{k})$ to be anisotropic, and $D_{ij}(\vec{k})$ is a diffusion constant which prevents $\tau_{tr}(\vec{k})$ from becoming extremely anisotropic. k_i and k_j are locally cartesian Fermi surface coordinates. The solution $\tau_{tr}(\vec{k})$ determines the electrical conductivity

$$\sigma \sim \left\langle \tau_{tr}(\vec{k}) \right\rangle_{\text{Fermi Surface}},$$

and its anisotropy gives rise to the deviations from Matthiessen's rule (DMR).

To compare the typical alkali and polyvalent geometries we tabulate the anisotropy of the "zeroeth-order" transport times $\tau_{tr}^{(0)}(\vec{k})$ and the maximum DMR. We also tabulate the anisotropy of the quasiparticle relaxation times $\tau_Q(\vec{k})$, which can be measured directly.

TABLE

	maximum DMR	anisotropy of $\tau_{tr}^{(0)}(\vec{k})$	$\tau_Q(\vec{k})$
alkali	1/3 - 1/2	10	1/10
polyvalent	2-3	100	10

The two relaxation times are simply different Fermi surface averages of the electron-phonon matrix elements; $\tau_Q(\vec{k})$ can be measured directly and may provide a check for our models - $\tau_{tr}^{(0)}(\vec{k})$ is manifested less directly, through the transport quantities. The interesting relationship between them, suggested by the table, will be dealt with in a future technical report. The qualitative comparison between the DMR is in accord with experimental observations.

Secondary results are described in the appended preprint,⁽²⁾ upon which I collaborated with J. W. Ekin. A study of the general low-temperature resistivity problem^(2,7,8) in potassium shows that the phonon-drag mechanism is not active in the regime where the DMR are largest (4-6°K.). In that regime relaxation time anisotropy is presumably the dominant mechanism of DMR. Our study shows also that the Debye model describes umklapp scattering extremely well (Fig. 2 of ref. 2), and it is reasonable to use the same model to calculate $\tau_{tr}^{(0)}(\vec{k})$ for the diffusion model. It is important that the diffusion model parameters can be deduced from a single resistivity-versus-temperature curve, so that the DMR can be calculated without any additional parameters. This has been done successfully for potassium, and will be reported.

We conclude with a progress report on the numerical calculation in aluminum (sec. II). Mr. Meador has set up a Fermi surface grid and an integration routine. We are beginning now to set up a calculation of the matrix elements, and so no results are available at this point.

References

1. J. Bass, Advances in Physics 21, no. 91 (1972).
2. J. W. Ekin and W. E. Lawrence, report no. C00-2315-1, submitted to Phys. Rev.
3. C. R. Leavens and J. P. Carbotte, Solid State Comm. 9, 75 (1971).
4. N.W. Ashcroft, Philos. Mag. 8, 2005 (1963).
5. See D. Schotte and U. Schotte, Solid State Comm. 10, 131 (1972), for the most recent version.
6. W. E. Lawrence and J. W. Wilkins, Phys. Rev. B 6, 4466 (1972).
7. J. W. Ekin and B. W. Maxfield, Phys. Rev. B 4, 4215 (1971), and D. Guban, Proc. Roy. Soc., Ser. A 325, 223 (1971).
8. M. Kaveh and N. Wiser, Phys. Rev. Letters 29, 1374, (1972).

Level of Activity

There are no significant differences between the level of activity performed and that contemplated in the Contract. The principal investigator has devoted one-third time during the academic year, and full time during the summer term, to the proposed research.

Travel Performed

The principal investigator has used Contract funds for travel to one professional meeting. He has actually attended two such meetings since March 1, 1973.

Technical Report Submitted

"Comment on 'Phonon Drag and the Low-Temperature Electrical Resistivity of the Alkali Metals: Potassium", report no. C00-2315-1, submitted to Phys. Rev.

Co-author, J. W. Ekin.