

maintain the condition $H = H_c$ along the boundaries, and show two such structures. These structures indicate that, as the current increases, so does the axial width of the normal regions, and it follows that the supercooling required near the center of the normal regions would increase and become unacceptably large. An alternative possibility is shown in Fig. 1: As i increases over i_c , a fully normal sheath is formed surrounding an intermediate state core: within the core, the structure will be determined by the same equilibrium conditions as are valid at $i = i_c$, and we may therefore assume that the axial periodicity of the structure decreases so as to maintain the optimum $n - s$ boundary shape which allows H to equal H_c on the boundary. It follows that the supercooling called for in the normal regions is not greater than it was at $i = i_c$.

In Fig. 3(a) the resistance transition predicted by the present model is compared with the London

model and with experimental values obtained for "thick" wires (diameter ≥ 1 mm). For thinner wires secondary effects occur; these have been discussed by BM and the treatment given there remains valid.

In addition to the usual consideration of resistance transitions, an independent check on the validity of any model of the intermediate state in current-carrying type-1 superconductors is provided by Rinderer's measurements of the radius of the intermediate-state core as a function of applied current.⁷ Figure 3(b) shows that the values obtained by Rinderer are in good agreement with the present model, whereas they do not agree well with the values predicted by London.

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Thermal Conductivity in Pure Two-Band Superconductors in High Magnetic Fields

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The theory proposed by Maki, for the electronic thermal conductivity in the gapless region of a pure type-II superconductor, is extended to include the presence of a second superconducting band so that it can be used to describe the mixed-state thermal conductivity in clean transition-metal superconductors near H_{c2} . The general features of Maki's one-band expression remain in the two-band expression.

I. INTRODUCTION

The qualitative features of the theory proposed by Maki,¹ for the thermal conductivity in the gapless region of a pure type-II superconductor, have been seen in the recent measurements^{2,3} of the thermal conductivity in the mixed state in clean niobium superconductors near the upper critical field, i. e., the $(H_{c2} - H)^{1/2}$ field dependence and the anisotropy of the conductivity with respect to the relative angle between the direction of the heat flow and the external magnetic field were seen. Quantitative agreements were achieved by treating the density of states as an adjustable parameter.

Because this treatment of the density of states would imply a false behavior of the magnetic properties, many authors^{4,5} have questioned the parametrization of the density of states. They believe that quantitative agreements would be achieved by the proper treatment of the anisotropy of the Fermi surface. However, it has been shown⁶ that the proper treatment of the anisotropy will lead only to a small enhancement of the results based on a spherical Fermi surface (e. g., the enhancement factor for Nb is⁷ 1.13).

The recent discovery of a second energy gap⁸ and a second transition temperature⁹ in clean niobium superconductors indicates that the usual one-

band model of superconductivity may not be adequate to describe the transition-metal superconductors. A two-band model, which included possible Cooper-pair formation in the overlapping band regions in the transition metals, was introduced by Suhl, Matthias, and Walker¹⁰ (SMW). Using this model to analyze their experimental data, several authors have obtained values for the second energy gaps in pure vanadium¹¹ and molybdenum.¹² The SMW model has been used successfully to explain the behavior of the magnetic properties of the transition-metal superconductors.¹³

The purpose of this addendum is to extend Maki's theory by using the SMW two-band model as the basis for the superconductivity in the transition metals. The resulting two-band expression for the thermal conductivity in the gapless region of a pure type-II transition-metal superconductor will exhibit the same field dependence and anisotropy as the one-band expression. Because the two bands in the transition metals are affected by the impurities in different ways, the transport properties, which are dominated by the lighter electrons from the *s* band, and the thermodynamical properties, dominated by the electrons from the more densely populated *d* band, may behave in quite different ways. A purity dependence in the thermal conduc-

tivity need not show up in a similar dependence in the magnetic properties.

II. TWO-BAND THERMAL CONDUCTIVITY

As was done in Maki's paper, the thermal conductivity can be obtained from the Kubo formula

$$K_S = \text{Im}\{(\omega T)^{-1} P(i\omega)\}_{\omega=0}, \quad (1)$$

where $P(i\omega)$ is obtained from the heat-current correlation function $P(\omega_\nu)$ by analytical continuation. Using the Hartree-Fock factorization, the correlation function in the two-band system is given by

$$P(\omega_\nu) = \langle [u_s, u_s] \rangle_{0\omega_\nu} + \langle [u_d, u_d] \rangle_{0\omega_\nu}, \quad (2)$$

where u_s and u_d are the heat currents associated with the different bands. By assuming that the effects of the magnetic field on the two energy gaps in the clean transition-metal superconductors near H_{c2} are similar to those of a uniform transport current in both bands, the techniques developed by Maki in Ref. 1 can be used to evaluate the individual correlation functions. Performing the steps in Ref. 1, the thermal conductivity in the mixed state in a clean transition-metal superconductor near H_{c2} takes the asymptotic following forms.

Case (a) for the temperature gradient parallel to the magnetic field:

$$\frac{K_{S\parallel}}{K_n} = 1 - \frac{K_n^{(s)}}{K_n} \frac{\Delta_s}{2\pi^2 T} \left(\frac{\epsilon_s}{T}\right)^2 \left[\frac{3}{5} - \frac{18}{35} \left(\frac{\epsilon_s}{2T}\right)^2 + \frac{4}{7} \left(\frac{\epsilon_s}{2T}\right)^4 \right] - \frac{K_n^{(d)}}{K_n} \frac{\Delta_d}{2\pi^2 T} \left(\frac{\epsilon_d}{T}\right)^2 \left[\frac{3}{5} - \frac{18}{35} \left(\frac{\epsilon_d}{2T}\right)^2 + \frac{4}{7} \left(\frac{\epsilon_d}{2T}\right)^4 \right] \quad \text{for } T \lesssim T_c, \quad (3)$$

$$\frac{K_{S\parallel}}{K_n} = 1 - \frac{K_n^{(s)}}{K_n} \frac{3\sqrt{\pi}}{2} \frac{\Delta_s}{\epsilon_s} \left[1 - \frac{108\zeta(3)}{\pi^{5/2}} \left(\frac{T}{\epsilon_s}\right) - \frac{14}{5} \left(\frac{\pi T}{\epsilon_s}\right)^2 \right] - \frac{K_n^{(d)}}{K_n} \frac{3\sqrt{\pi}}{2} \frac{\Delta_d}{\epsilon_d} \left[1 - \frac{108\zeta(3)}{\pi^{5/2}} \left(\frac{T}{\epsilon_d}\right) - \frac{14}{5} \left(\frac{\pi T}{\epsilon_d}\right)^2 \right] \quad \text{for } T \ll T_c. \quad (4)$$

Case (b) for the temperature gradient perpendicular to the magnetic field:

$$\frac{K_{S\perp}}{K_n} = 1 - \frac{K_n^{(s)}}{K_n} \frac{\Delta_s}{\pi^2 T} \left(\frac{\epsilon_s}{T}\right)^2 \left[\frac{3}{5} - \frac{27}{35} \left(\frac{\epsilon_s}{2T}\right)^2 + \frac{8}{7} \left(\frac{\epsilon_s}{2T}\right)^4 \right] - \frac{K_n^{(d)}}{K_n} \frac{\Delta_d}{\pi^2 T} \left(\frac{\epsilon_d}{T}\right)^2 \left[\frac{3}{5} - \frac{27}{35} \left(\frac{\epsilon_d}{2T}\right)^2 + \frac{8}{7} \left(\frac{\epsilon_d}{2T}\right)^4 \right] \quad \text{for } T \lesssim T_c, \quad (5)$$

$$\frac{K_{S\perp}}{K_n} = 1 - \frac{K_n^{(s)}}{K_n} \frac{3\sqrt{\pi}}{4} \frac{\Delta_s}{\epsilon_s} \left(\left[1 - \frac{14}{5} \frac{\pi T}{\epsilon_s} \right]^2 + \frac{1800\zeta(5)}{\pi^{5/2}} \left(\frac{T}{\epsilon_s}\right)^3 \right) - \frac{K_n^{(d)}}{K_n} \frac{3\sqrt{\pi}}{4} \frac{\Delta_d}{\epsilon_d} \left(\left[1 - \frac{14}{5} \frac{\pi T}{\epsilon_d} \right]^2 + \frac{1800\zeta(5)}{\pi^{5/2}} \left(\frac{T}{\epsilon_d}\right)^3 \right) \quad \text{for } T \lesssim T_c. \quad (6)$$

All of the above expressions except for $K_n^{(s)}$ and $K_n^{(d)}$, which are the normal-state thermal conductivities for the *s* and *d* electrons, respectively,

are defined in Ref. 1.

As was the case for the one-band expression, the field dependence in the thermal conductivity in

the gapless region of a pure transition-metal superconductor arises from the behavior of the two energy gaps in a magnetic field. Since the d band can be treated as a BCS band,¹³ the d -band energy gap can be written as

$$\begin{aligned} \Delta_d^2 &= \langle |\Delta_d(r)|^2 \rangle \\ &= \frac{1}{2\pi N_d} \frac{H_{c2}(t) - H}{116(2\kappa_2^2 - 1) + 1} \left[H_{c2}(t) - \frac{1}{2}t \frac{dH_{c2}(t)}{dt} \right], \end{aligned} \quad (7)$$

where κ_2 is the second Ginzburg-Landau parameter and t is the reduced temperature. By analogy to the temperature behavior of the two energy gaps, i. e., the ratio of the two gaps in niobium is constant over a wide temperature range,⁸ it will be assumed that the ratio between the two gaps remains constant in the presence of a magnetic field. By making these assumptions about the forms of the two energy gaps, the two-band thermal conductivity will exhibit the $(H_{c2} - H)^{1/2}$ field dependence.

The anisotropy of the two-band thermal conductivity will also be the same as that of the one-band expression, i. e.,

$$K_{S\perp} \leq K_{S\parallel} \text{ for } T \lesssim T_c \text{ and} \quad (8)$$

$$K_{S\perp} \geq K_{S\parallel} \text{ for } T \ll T_c .$$

III. CONCLUSION

As was mentioned previously, recent measurements^{2,3} of the thermal conductivity in the mixed state in pure niobium superconductor near H_{c2} have confirmed the general features of both Maki's expressions and the two-band expressions. Of particular interest is the work of Noto³ who measured the thermal conductivity in a niobium superconductor having a residual resistivity ratio 1900 over a wide temperature range. To achieve a quantitative agreement between the experimental values and Maki's one-band expression, Noto used a value 1.6×10^{33} states/cm³erg for the density of states. As was noted, this value differs from the value 5.6×10^{34} states/cm³erg obtained by van der Hoeven and Keesom¹⁴ from the specific-heat data on niobium. The discrepancy between the experimental and the theoretical values which grew worse as the purity of the niobium superconductor increased could be accounted for by a purity dependence in the density of states. However, the implied purity dependence in the density of state would imply an

unobserved purity dependence in the magnetic properties of niobium. This has led Noto and others to discount this explanation of the discrepancy.

In the two-band model, the dichotomy in the purity dependence of the thermal conductivity and the magnetic properties present no problems. Since these two properties are dominated by electrons from two different bands which are affected by the impurities in different ways, their behavior may be quite different from each other. The two-band effects can also explain why Maki's expression even with an adjusted density of states predicts a thermal conductivity which is higher than the observed values at temperatures close to T_c and which are too low at low temperatures (see Fig. 8 in Ref. 3). To see this, one rewrites (3) and (4) in the form

$$\begin{aligned} \frac{\Delta K_{\parallel}}{K_n} &= 1 - \frac{K_{S\parallel}}{K_n} = \frac{\Delta_d}{2\pi^2 T} \left(\frac{\epsilon_d}{T} \right)^2 \left[\frac{3}{5} - \frac{18}{35} \left(\frac{\epsilon_d}{2T} \right) + \frac{4}{7} \left(\frac{\epsilon_d}{2T} \right)^4 \right] \\ &\quad - \frac{K_n^{(s)}}{K_n} \left\{ \frac{\Delta_s}{2\pi^2 T} \left(\frac{\epsilon_s}{T} \right)^2 \left[\frac{3}{5} - \frac{18}{35} \left(\frac{\epsilon_s}{2T} \right) + \frac{4}{7} \left(\frac{\epsilon_s}{2T} \right)^4 \right] \right. \\ &\quad \left. - \frac{\Delta_d}{2\pi^2 T} \left(\frac{\epsilon_d}{T} \right)^2 \left[\frac{3}{5} - \frac{18}{35} \left(\frac{\epsilon_d}{2T} \right) + \frac{4}{7} \left(\frac{\epsilon_d}{2T} \right)^4 \right] \right\} \end{aligned} \quad \text{for } T \lesssim T_c \quad (9)$$

and

$$\begin{aligned} \frac{\Delta K_{\parallel}}{K_n} &= \frac{3\sqrt{\pi}}{4} \frac{\Delta_d}{\epsilon_d} \left[1 - \frac{14}{5} \left(\frac{\pi T}{\epsilon_d} \right)^2 - \frac{108\zeta(3)}{\pi^{5/2}} \left(\frac{T}{\epsilon_d} \right) \right] \\ &\quad - \frac{K_n^{(s)}}{K_n} \frac{3\sqrt{\pi}}{4} \left\{ \frac{\Delta_d}{\epsilon_d} \left[1 - \frac{108\zeta(3)}{\pi^{5/2}} \left(\frac{T}{\epsilon_d} \right) - \frac{14}{5} \left(\frac{\pi T}{\epsilon_d} \right)^2 \right] \right. \\ &\quad \left. - \frac{\Delta_s}{\epsilon_s} \left[1 - \frac{108\zeta(3)}{\pi^{5/2}} \left(\frac{T}{\epsilon_s} \right) - \frac{14}{5} \left(\frac{\pi T}{\epsilon_s} \right)^2 \right] \right\} \end{aligned} \quad \text{for } T \ll T_c. \quad (10)$$

The first terms on the right-hand side of the above equations are the terms in Maki's one-band expressions. The remaining terms on the right-hand side reflect the presence of the second band. In niobium where $\Delta_d = 10\Delta_s^8$ and $\epsilon_s \gg \epsilon_d$, one can see that the two-band effect will decrease the thermal conductivity at the higher temperatures and increase the thermal conductivity at the lower temperatures (cause $\Delta K_{\parallel}/K_n$ to be larger for $T \lesssim T_c$ and to be smaller for $T \ll T_c$).

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Positron Annihilation in a Zirconium Single Crystal*

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The angular distribution of the γ quanta emitted in the two-photon annihilation of positrons in zirconium has been measured along the (0001) direction of a single crystal. The results are compared with calculations by Gupta and Loucks in the augmented-plane-wave approximation. The data confirm that the curve at small angles falls significantly below the parabola expected for a free-electron gas and that there is a conspicuous contribution at large angles from the high-momentum components of the electron wave function. A small hump predicted near the zone boundary was not resolved.

Gupta and Loucks¹ calculated the angular distribution of the radiation from the two-photon annihilation of positrons in yttrium and zirconium. The work was based on a study of the electronic structure of these transition metals in an augmented-plane-wave approximation.^{2,3}

The interest of a comparison between zirconium and yttrium lies in the fact that the calculations for yttrium show a pronounced hump in the angular correlation curve at angles of 2.5 mrad which corresponds to the position of the zone boundary, whereas for zirconium with one more electron in the d shell, the hump is predicted to almost disappear. The theory for yttrium is in reasonable agreement with the measurements by Williams and Mackintosh,^{4,5} but no data on zirconium were available until now.

We have measured the angular correlation curve for a zirconium single crystal in a standard angular correlation instrument with a resolution of about 0.5 mrad. The crystal, approximately 3 mm diam and 2 mm thick, was cut such that the (0001) direction was parallel to p_z , the momentum component measured by the angle $\theta = p_z/mc$. The small area of the crystal made it necessary to resort to very intense positron sources for adequate counting statistics. The data presented here are the averages of several runs, each obtained with a 5 Ci source of ⁶⁴Cu without any change in the position of the Zr sample.

The result is shown in Fig. 1 and compared with the predictions by Gupta and Loucks.¹ For reference, the parabola of the free-electron gas is indi-

cated also.

The experiment confirms that at small momenta the angular correlation curve of zirconium falls sig-

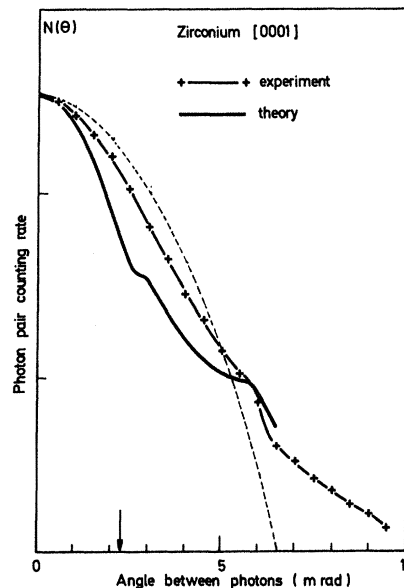


FIG. 1 Angular distribution of two- γ annihilation radiation of positrons in a zirconium crystal along the (0001) direction. Crosses indicate the experimental points and their statistical uncertainty. Solid curve is the results of the calculation by Gupta and Loucks (Ref. 1). Arrow indicates the position of the zone boundary. For comparison, the dashed curve presents the parabola of the corresponding free-valence-electron gas.