Proceedings of the

17th International Conference on Low Temperature Physics

LT-17

Part II - Contributed Papers

Universität Karlsruhe and
Kernforschungszentrum Karlsruhe
15–22 August 1984

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Organized under the aegis of
THE INTERNATIONAL UNION OF PURE AND APPLIED PHYSICS
by
Universität Karlsruhe and Kernforschungszentrum Karlsruhe

NHPC

1984
NORTH-HOLLAND
AMSTERDAM · OXFORD · NEW YORK · TOKYO

ISBN: 0 444 86910 7

Published by:

North-Holland Physics Publishing
a division of
Elsevier Science Publishers B.V.
P.O. Box 103
1000 AC Amsterdam
The Netherlands

Sole distributors for the U.S.A. and Canada:

Elsevier Science Publishing Company, Inc.
52 Vanderbilt Avenue
New York, NY 10017
U.S.A.

Printed in The Netherlands

LT-17 (Contributed Papers)
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HYBRIDIZATION EFFECTS BETWEEN d AND s BANDS IN AMORPHOUS MATERIALS

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Measurements of the electrical resistivity and the Meissner penetration depth of superconducting amorphous materials, based in transition metals, show that the d and s bands are strongly hybridized.

In a previus paper (1) we have shown that heat treating amorphous $Zr_{.70}Cu_{.30}$ induces a decrease in the superconducting critical temperature, T_c, and in the electronic density of states, N(0). Together with the decrease in N(0) and T_c, an increase in the electrical resistivity is detected. Fig 1 shows the variation of the electrical resistance for the sample of reference (1), as a function of the changes in critical temperature induced by annealing (1). Although the change in T_c has being understood (1) in terms of the induced variation in N(0) there was no explanation of why a structural relaxation induces an increase in the electrical resistivity.

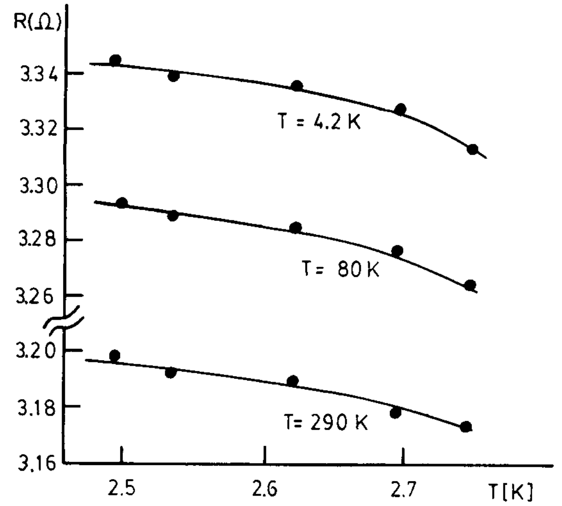

FIGURE 1
Variation of the electrical resistance for the sample of ref.(1) as a function of the changes in critical temperature induced by annealing.

Recent measurements (2,3) of the electrical resistivity of amorphous Zr_xCu_{1-x} as a function of concentration show that for $.50 < x < .80$ the resistivity increases with decreasing Zr concentration. When discussing (2) this results, a two bond (d-s) model (4) has been used, arguing that in the rich Zr region the conduction due to the d band cannot be disregarded. In this model and for the rich Zr concentration region the increase in resistivity is associated (2) with a decrease in the density of states and Zr concentration. Annealing decreases (1) the electronic density of states and then, the increase in resistivity can be qualitatively understood within the same picture. Since the relaxation process is made at constant concentration the change in resistivity, for a given variation of N(0) (or T_c), should be smaller than the corresponding one obtained changing N(0) plus concentration.

From the results in ref.(1) it is seen that the variation in T_c shown in fig.1 is equivalent to the variation of T_c induced by a change in concentration $\Delta x = 0.023$. Following references (2) and (3) this change in concentration corresponds to an increase in resistivity of 2.3% or 1.3% respectively. The rise found with annealing is less than 1% in qualitative agreement with the behavior predicted by the two independent band model. On the other hand, Bosch and Bennemann (5) have indicated the importance of the hybridization between d and s states to understand the transport properties of liquid transition metals. The measurements of the Meissner penetration depth, $\lambda(T)$, in amorphous metals can be used to determine the importance of the proposed d-s bands mixing.

The electrodynamic response of a superconductor to the presence of a weak magnetic field is determined by the superconducting penetration depth. The Gorkov expression for λ in the dirty limit, valid near T_c, is given by

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$$\lambda_d = 0.615\ (\xi_0/\ell)^{1/2}\ \lambda_L(0)(1-t)^{-1/2} \qquad [1]$$

where $\lambda_L(0)$ is related to the normal properties of the material, $\lambda_L(0) = [3c^2/8\pi e^2 v^2{}_F N(0)]^{1/2}$, $\xi_0 = 0.18\ \hbar\ v_F/k_B T_c$ is the superconducting BCS coherence length and ℓ is the elastic electron mean free path. In expression [1] ξ_0 is related to the superconducting interaction potential and consequently to the electronic density of states. The London penetration depth $\lambda_L(0)$ and the electron mean free path are related to the electrodynamic response of the normal material. It is clear that if the independent two bands model is correct, the d band density of states should dominate in the determination of T_c and, consequently, in ξ_0. However the contribution of the s band should not be disregarded when considering the electrodynamic response of the material. On the contrary, if the hybridization is strong enough to consider that the electrons that contribute to the superconducting and transport properties are the same, expression [1] can be reduced to

$$\lambda_d = 1.288\times10^{-2}\ (\rho/T_c)^{1/2}(1-t)^{-1/2} \qquad [2]$$

where ρ is expressed in Ω-cm and T_c in degrees Kelvin.

In a previous publication (6) we have shown that expression [2] is verified by the $Zr_{.70}Cu_{.30}$ amorphous system. In this paper we include the previous data plus another sample of $Zr_{.70}Cu_{.30}$ plus the results corresponding to the La_xM_{1-x} (M = Cu,Au,Al) amorphous systems (see Table 1).

The same Table includes the preliminary results for $Zr_{.76}Cu_{.24}$ sputtered amorphous system (7). The results shown in Table 1 were obtained by measuring the magnetic flux expulsion of the superconducting sample as a function of temperature. The value B shown in Table 1 is obtained by assuming $\lambda(T) = By$ (where $y = (1-t^4)^{-1/2}$) and should be compared with the coefficient $1.288\ 10^{-2}\ (\rho/T)^{1/2}$ of expression [2]. Further details on the experimental technique can be seen in ref.6. A detailed discussion on the temperature dependence of $\lambda(T)$ is not relevant for the discussion presented here and will be published elsewhere.

TABLE I

Electrical resistivity, critical temperature, coefficient B as defined in the text and coefficient of eq.[2].

Sample	ρ [$\mu\Omega$cm]	T_c [K]	B [μm]	Ec.[2] [μm]
$La_{70}Cu_{30}$	170	3.740	0.88	0.87
$La_{70}Cu_{30}$	170	3.583	0.94	0.89
$La_{70}Cu_{30}$	170	3.570	0.84	0.89
$La_{80}Au_{20}$	150	3.608	0.95	0.83
$La_{80}Au_{20}$	150	3.288	0.88	0.87
$La_{70}Al_{30}$	172	2.892	0.83	0.99
$Zr_{70}Cu_{30}$	152	2.610	0.99	0.99
$Zr_{70}Cu_{30}$	186	2.533	1.00	1.10
$Zr_{76}Cu_{24}$	153	3.450	0.97	0.93

It can be seen that the agreement between the value of B and the coefficient in expression [2] is remarkable. We think this agreement is a strong indication that hybridization between bands should be taken into account for a realistic calculation of the transport properties of these amorphous metals.

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