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Superconductivity and electronic structure in $MgCNi_3$

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Abstract

In polycrystalline samples of superconducting $MgCNi_3$, the critical temperature and the specific heat were measured as a function of magnetic field. A Wertheimer–Helfand–Hohenberg (WHH)-like shape of $H_{c2}(T)$ is observed. The $H_{c2}(T)$ and specific heat data are discussed on a qualitative level in terms of effective single- and multi-band models based on an orbital assignment of the disjoint Fermi surface sheets (FSS) derived from LDA full potential electronic structure calculations.

Keywords: Superconductivity; Electronic structure; Upper critical field; Specific heat

Superconductivity and ferromagnetism have been believed to be incompatible over any extended temperature range until few specific examples—$RuSr_2GdCu_2O_8$, $ZnZr_2$ and UGe_2—have arisen in the past 2–3 years. The discovery of superconductivity above 8 K in $MgCNi_3$ [1], which is primarily the ferromagnetic metal Ni, could provide a new and different example. This compound was shown to be near ferromagnetism [2], requiring only small hole-doping. This system provides an interesting mean to probe coupling, and possible coexistence, of these two forms of collective behavior without the requirement of pressure.

To understand the character of the quasiparticles involved in the superconductivity, we have first carried out LDA electronic structure calculations using a full potential minimum basis local orbital scheme (FPLO) [4] as well as an FLAPW code [3], leading to almost identical results, in good agreement with the results of Ref. [6]. Furthermore, some thermodynamic properties have been measured on a polycrystalline sample which will be reported below. The LDA calculational details are given in Ref. [2]. To describe the steep singularity near the Fermi energy E_F accurately, 1771 k-points in the IBZ were used. The band-wise decomposed density of states (DOS) and the corresponding Fermi surface sheets (FSS) are shown in Fig. 1. The peak at about 50 meV below E_F reveals predominantly (about 90%) Ni 3d character and is related to a single-band forming the clover leaf shaped FS (see topleft panel Fig. 1). For the DOS derived bare Sommerfeld constant we find 11.1 mJ/mol K^2, with about 85% contribution from FSS 1.

Polycrystalline samples of $MgCNi_3$ were prepared by a solid state reaction. A pellet pressed from Mg, C and Ni powders was wrapped in a Ta foil and sintered in a quartz vial in Ar atmosphere at 600 and 900 °C. In this study, a sample with the nominal formula $Mg_{1.2}C_{1.6}Ni_3$ was investigated. The lattice constant of the prepared sample was determined as $a = 0.38107$ nm by a Rietveld analysis being consistent with previous reports [1,5]. A superconducting transition temperature of $T_c = 7.0$ K was found by ac susceptibility, electrical resistance and specific heat measurements. In Fig. 2 specific heat data, c_p/T vs. T^2 are shown for applied magnetic fields up to 8 T.

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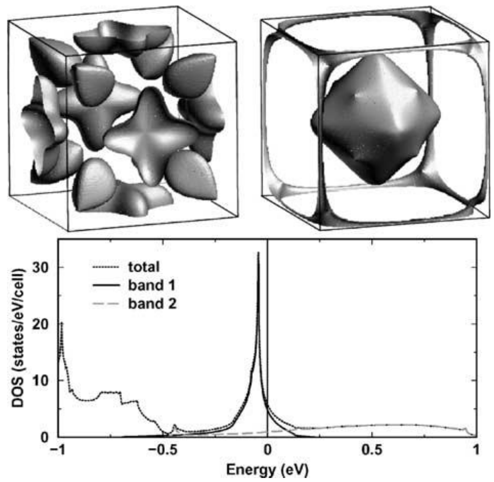

Fig. 1. The two Fermi surfaces of $MgCNi_3$ and the corresponding band resolved DOS near the Fermi level. "Band 1" corresponds to the FSS in the topleft panel, "band 2" to the topright FSS.

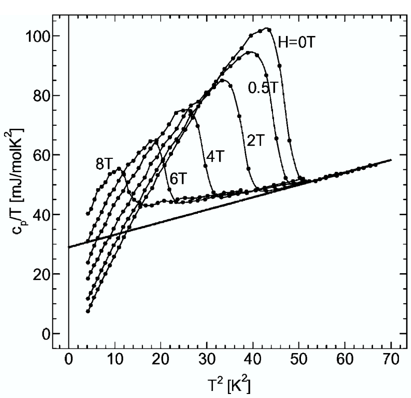

Fig. 2. Measured specific heat of $MgCNi_3$ in magnetic field up to 8 T. The intersection of the solid line gives the Sommerfeld parameter $\gamma_S(H=0)$.

With the experimentally measured renormalized Sommerfeld constant γ_S at a value of $\approx$29 mJ/mol K^2 or even 40 mJ/mol K^2 at $H=8$ T (see Fig. 2), we arrive at a sizable coupling constant averaged over all FSS of about $\bar{\lambda}=1.6$ (2.6 at $H=8$ T), if corrections due to the strong energy dependence of $N_1(E)$ (see Fig. 1) are neglected. Referring to the partial DOS $N_i(0)$ mentioned above, that total coupling constant can be decomposed into the contributions from the two bands:

$$\bar{\lambda}=1.6\text{–}2.6=\frac{1}{N(0)}\sum_i N_i(0)\lambda_i=0.85\lambda_1+0.15\lambda_2,$$

where $\lambda_{1(2)}$ is the coupling constant for FSS 1 (2), respectively. According to Ref. [6], λ_2 is large ($\sim$3) due to strong coupling with low-frequency rotational modes of the Ni-octahedra. Due to the small prefactor for band 2, we arrive at strong coupling in both bands even for a large value, say $\lambda_2=2$. The origin of the strong coupling $\lambda_1\approx 1.5$–2.7 in band 1 is unclear at present. If it corresponds to strong coupling with ferromagnetic spin fluctuations, p-wave superconductivity with a T^3 contribution at low T in the c_p-data would be expected. However, the data shown in Fig. 2 point to s-wave superconductivity since we observe a small but finite gap $\approx 3.1T_c$ slightly below $3.52T_c$ (BCS). Another unresolved problem is the large ratio of the specific heat jump at $T_c:\Delta c_p/\gamma_S T_c\approx 2.3$–$1.67$ compared with 1.43 (BCS). It cannot be explained within a standard two-gap (band) model even for strong coupling [7]. Anyhow, the jump ratio might be enhanced by the strong E-dependence of $N_1(E)$ (see Fig. 1).

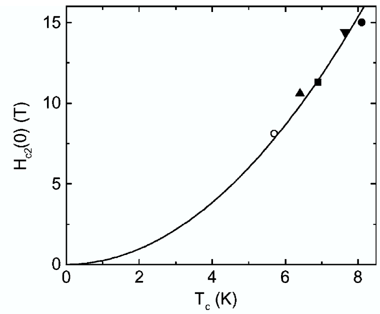

Fig. 3. The $T=0$ upper critical field vs. transition temperature T_c; data available from the literature have been included. The filled square denotes our sample.

Finally, the $H_{c2}\propto T_c^2$ dependence of the upper critical field points to a clean limit regime (see Fig. 3). This is somewhat surprising in view of the mesoscopic disorder which is responsible for the high resistivity. The Werthheimer–Helfand–Hohenberg (WHH)-shape of $H_{c2}(T)$, i.e. without a clear upward curvature at T_c [7], is ascribed to weak interband scattering between FSS 1 and 2. Then the value of $H_{c2}(0)\approx 12$ T stems mainly from strongly interacting electrons on FSS 2.

In conclusion, we arrive at a picture where two strongly competing orderings, superconductivity and magnetism, coexist in almost decoupled FSS's. This resembles the behavior in magnetic borocarbides [8].

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