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Abstract. Superconductivity in the layered yttrium diboride dicarbide, YB_2C_2, has been revisited by means of specific heat, magnetic susceptibility and resistivity measurements down to 50 mK revealing a bulk superconducting transition at 1.0 K. Analysing the low temperature specific heat we obtain a Sommerfeld coefficient of the normal state electonic contribution, $\gamma = 3.1(1)\,\mathrm{mJ/mol\,K^2}$, and a Debye temperature, $\Theta_D^{LT} = 680(10)\,\mathrm{K}$. The specific heat anomaly at T_C, $\Delta C \simeq 4.5\,\mathrm{mJ/mol\,K}$, thus, yields a thermodynamic ratio $\Delta C/\gamma T_C \simeq 1.4$ in close agreement with the BCS value. For polycrystalline $Y^{11}B_2C_2$ prepared by inductive melting we observe a pronounced resistive anomaly near 3.6 K which, however, corresponds to a rather spurious specific heat anomaly and is thus attributed to traces of YC_2 present in this sample.

1. Introduction

The discovery of superconductivity in $R\mathrm{Ni_2B_2C}$ (R = rare earth and Y) and MgB_2 [1, 2] attracted attention on metal borides and intermetallic borocarbides and especially on the low dimensional character of certain features of their electronic structure. An interesting intermetallic borocarbide with laminar structure [3, 4] is YB_2C_2 with a tetragonal lattice build by alternating layers of yttrium and B−C sheets. The latter are a flat network formed by distorted interconnected cyclobutadiene-like B−C rings which are markedly different from the hexagonal boron planes in MgB_2. A recent study of the electronic structure by Khmelevskyi *et al.* [6] suggested that the metallic conductivity of YB_2C_2 is due Y d-bands partially hybridized with p_z-states from the B−C planes and that large portions of the Fermi surface exhibit distinctive two-dimensional features which may cause interesting features of a superconducting state. Superonductivity of YB_2C_2 was reported by Sakai *et al.* [5] with $T_C \sim 3.6\,\mathrm{K}$ which, however, is close to the T_C of YC_2 [7]. In the present paper we re-investigated the appearance of bulk superconductivity in single phase YB_2C_2 by means of specific heat and magnetic susceptibility measurements down to 50 mK.

2. Experimental details

Polycrystalline material of $Y^{11}B_2C_2$ prepared by high frequency induction melting of ultra high purity elements: yttrium (Ames MPC [8], USA: 99.999%), isotope enriched boron ^{11}B (Eagle-Pichler, USA: 99.9999%, isotope purity 99.97%) and carbon (Alpha Aesar, USA: 99.9995%). Thereby, in a first step YC_2 ingots have been prepared and in a second step boron was added. The phase purity of the polycrystalline as cast material (sample ♯1) has been checked via powder x-ray diffraction (XRD). For $Y^{11}B_2C_2$ XRD reveals essentially single phase samples

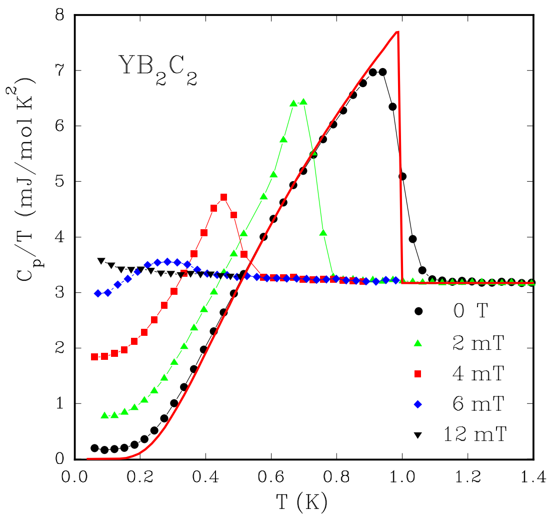

Figure 1. Low temperature specific heat, C/T vs. T, of $Y^{11}B_2C_2$ sample ♯2 measured at various fields as labeled; the solid line represents the BCS model.

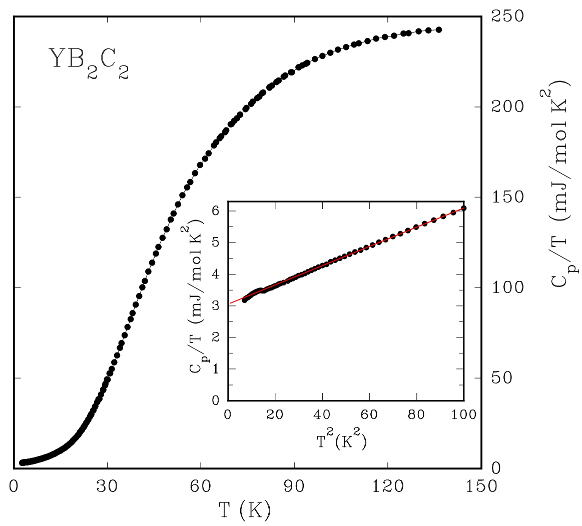

Figure 2. Zero-field specific heat, C/T vs. T, of $Y^{11}B_2C_2$ sample ♯1 measured above 3 K; inset shows C/T vs. T^2 with a $\gamma + \beta T$ fit indicated by the solid line.

with minor traces of YC_2. The latter is evident also from a spurious superconducting transition at 3.6 K visible in resistivity, susceptibility and specific heat data. In order to improve the phase purity, $Y^{11}B_2C_2$ was grown from the melt via the Czochralski method using a tri-arc furnace by Centorr Vacuum Industries. The $Y^{11}B_2C_2$ material obtained thereby (sample ♯2) showed clean single phase x-ray pattern (also magnetic susceptibility reveals a large reduction of the YC_2 diamagnetic impurity signal), significant texture and better mechanical stability.

X-ray studies were carried out on a Siemens D-5000 diffractometer equipped with a graphite monochromator. Ac susceptibility and specific heat measurements (using a relaxation method [9]) in the temperature range 0.1 K – 1.6 K were each carried out on on a bar-shaped 100 mg piece from the Czochralski grown $Y^{11}B_2C_2$ sample ♯2 in two different ^{3}He/^{4}He cryostat systems equipped with 15/17 T superconducting magnets. For experimental reasons the field was in different orientations, parallel and orthogonal to the longitudinal edge of the sample in ac susceptibility and specific heat measurements, respectively. This implies two markedly different demagnetization factors, a relatively small one for ac susceptibility and a larger one for specific heat. Zero-field specific heat measurements in the temperature range 3 K-130 K were carried out on $\sim$ 1.1 g sample ♯1 of $Y^{11}B_2C_2$ employing an adiabatic step-heating technique. Temperature dependent resistivity of $Y^{11}B_2C_2$ sample ♯2 was measured in a ^{3}He cryostat (0.5 K up to 230 K) with current parallel to the Czochralski growth direction revealing a room temperature to normal state residual resistivity ratio, $RRR \sim 15$ and zero-resistance below 1 K.

3. Experimental results and discussion

The low temperature specific heat of $Y^{11}B_2C_2$ shown as C/T vs. T in figure 1 reveals a sharp bulk superconducting transition at 1.0 K. The specific heat anomaly at T_c $\Delta C_p/T \simeq$ 4.5mJ/molK^2 and the normal state specific heat with linear-T electronic Sommerfeld coefficient $\gamma = 3.15\,(5)$ mJ/mol K^2 yields the thermodynamic ratio $\Delta C_p/(\gamma_n T_c) \simeq 1.43$ which matches the figure expected from BCS theory. A direct comparison of the zero-field specific heat data (superconducting magnet demagnetized by a thermal cycle) with the weak coupling BCS result [10] indicated as solid line in figure 1 reveals remarkably close over-all agreement. The

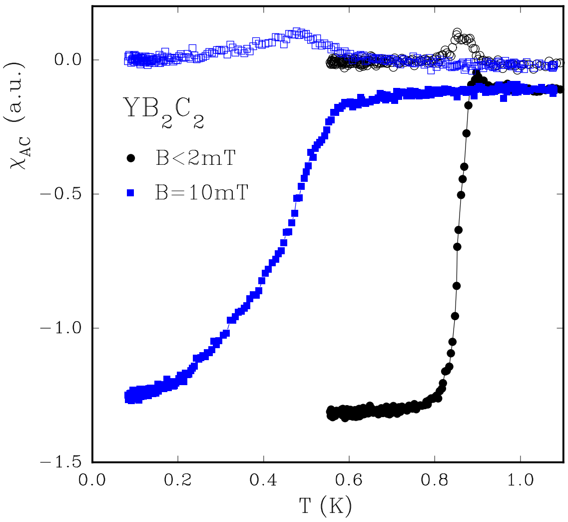

Figure 3. Temperature dependent real part χ' (full symbols) and imaginary part χ'' (open symbols) of the ac susceptibility of $Y^{11}B_2C_2$ sample ♯2 measured at an ac field amplitude of about 1 mT and superimposed dc fields as labeled.

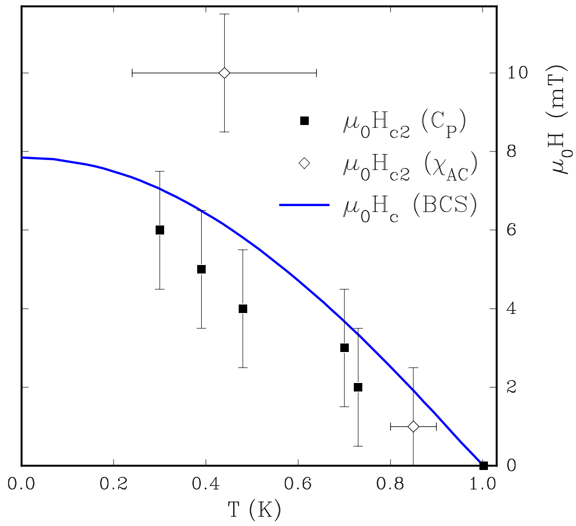

Figure 4. Upper critical field $\mu_0 H_{c2}(T)$ as obtained from specific heat and ac susceptibility; the solid line indicates the thermodynamic critical field $\mu_0 H_c(T)$ as obtained from the BCS idealization of the zero-field specific heat data.

superconducting gap $\Delta(0) \simeq 1.76 k_B T_c$ and thermodynamic critical field $\mu_0 H_c(0) \approx 7.8\,(4)$ mT is, thus, obtained from the BCS values as corresponding to the experimental Sommerfeld coefficient γ and T_c of $Y^{11}B_2C_2$. As the magnetic field strength increases (see some selected field values in figure 1), both the transition temperature and the anomaly right at T_c are suppressed, constituting the temperature dependent upper critical field $\mu_0 H_{c2}(T)$ (see below the discussion and the phase diagram in figure 4).

Figure 2 displays temperature dependent specific heat C/T vs. T measured on $\sim$ 1.1 g sample ♯1 of $Y^{11}B_2C_2$ from 3 to 130 K and the corresponding low temperature C/T vs. T^2 data in the inset. The latter is analyzed in terms of electronic and lattice contributions, $C_p = C_e + C_{ph} \simeq \gamma T + \beta T^3$ where γ is the Sommerfeld coefficient and β is related to the low temperature value of the Debye temperature by $\Theta_D^{LT} = (1944 \cdot n/\beta)^{1/3}$ ($n = 5$ is the number of atoms per formula unit). From the linear fit of the C/T vs. T^2 data (16 K^2 – 120 K^2) we obtain $\gamma = 3.05(1)$ mJ/mol K^2 (LT) and $\Theta_D^{LT} = 680(10)$ K. A more detailed analysis of the overall temperature dependence of the specific heat in terms of Debye- and Einstein contributions reveals a marked deviation of $C_{ph}(T)$ from a simple Debye-function above about 20 K presumably due to yttrium modes with Einstein temperatures near 200 K, which cause the marked kink in C/T seen in figure 2 at about 25 K. The spurious anomaly visible in the inset of figure 2 at about 16 K^2 is attributed to the superconducting transition of YC_2 impurities.

The temperature dependent ac susceptibility of $Y^{11}B_2C_2$ sample ♯2 measured at a frequency of 40 Hz and an ac field amplitude of about 1 mT is displayed in figure 3. The slightly lower value of $T_c \simeq 0.85$ K measured in zero dc-field (as compared to the zero-field specific heat result) is attributed to a small remanent field of about 1 − 2 mT in the 17 T magnet after field demagnetization. The ac susceptibility data obtained with additional dc field of 10 mT on the other hand yield a larger value of the field dependent T_C as compared to the field dependent specific heat data in figure 1 and, thus, imply a slightly larger value of the upper critical field $\mu_0 H_{c2}(0)$. Figure 4 compares these $\mu_0 H_{c2}(T)$ data with the thermodynamic critical field $\mu_0 H_c(T)$

as obtained from the free energy difference between the superconducting and normal state, $\Delta F(T) = F_n - F_s = \mu_0 H_c^2(T)/2$. The thermodynamic critical field $\mu_0 H_c(T)$ indicated by the solid line in figure 4 lies close to the upper critical field data obtained from specific heat, thus, pointing towards type-I superconductivity. The fact that $\mu_0 H_{c2}(T)$ obtained from field dependent specific heat data lies slightly below $\mu_0 H_c(T)$ obtained from zero-field thermodynamic data may be the consequence of the limited resolution of the magnet power supply in this very low field regime (vertical error bars in figure 4 indicate a rough estimate) and/or a consequence of the relatively large demagnetization factor of the sample geometry with field oriented perpendicular to the longitudinal edge. The ac susceptibility data obtained with a different magnet system and a sample geometry with a small demagnetization factor $N \sim 0.15$, lie above the $\mu_0 H_c(T)$ line, thus, indicating weak type-II superconductivity with an upper critical field $\mu_0 H_{c2}(0)$ still being very close to the thermodynamic critical field $\mu_0 H_c(0)$.

In order to obtain an estimate for the electron-phonon mass enhancement factor we compare the experimental Sommerfeld coefficient $\gamma = 3.14\,\mathrm{mJ/mol\,K^2}$ with bare Sommerfeld coefficient $\gamma_b \sim 2.1\,\mathrm{mJ/mol\,K^2}$. The latter corresponds to the bare electronic density of states at the Fermi energy, $N(E_F) \simeq 0.9\,\mathrm{states/eV\,f.u.}$, as obtained from electronic structure calculations reported in reference [6] via $\gamma = \pi^2 k_\mathrm{B}^2 N(E_F)/3$. The relation $\lambda = \gamma_b/\gamma - 1$, thus, yields a value for the electron phonon mass enhancement $\lambda \sim 0.4$ which is in close agreement with the value obtained with the Mc Millan formula [11]

$$T_c = \frac{\Theta_\mathrm{D}}{1.45} \exp\left(- \frac{1.04(1+\lambda)}{\lambda - \mu^\star(1+0.62\lambda)} \right). \tag{1}$$

Taking the experimental values of $T_c = 1.0\,\mathrm{K}$ and $\Theta_\mathrm{D} = 680\,\mathrm{K}$ and assuming a typical value $\mu^\star = 0.13$ for the Coulomb pseudopotential, Mc Millan formula yields almost exactly $\lambda = 0.4$. The close agreement of these two independent estimates of the electron-phonon mass enhancement corroborates the reliability of the *ab initio* results.

4. Conclusions

The re-investigation single phase YB_2C_2 by means of specific heat and magnetic susceptibility measurements revealed bulk superconductivity with weak coupling BCS features below a transition temperature $T_C = 1$ K. The observation of type-I or at least weak type-II superconductivity with $H_{c2}(0) \sim H_c(0)$, i.e. Ginzburg-Landau parameter $\kappa \sim 1/\sqrt{2}$ is rather exceptional among multinary compounds. Earlier reported signatures of a superconducting transition near 4 K have been identified as spurious anomalies also in the present samples which, however, are clearly related to the presence of YC_2 impurities and, thus, extrinsic.

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