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Journal of Magnetism and Magnetic Materials 272–276 (2004) e177–e178
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Free energy analysis of the magnetic and superconducting phases in thulium borocarbide☆

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Abstract

The competition between superconducting and magnetic ordering in thulium borocarbide is analyzed in terms of a rough estimate of the different contributions to the free energy. The theory accounts for the anisotropy of the upper critical field, the field dependence of the flux-core radius, and the jump in the derivative of the magnetization at the superconducting transition. The exchange energy gap in the conduction-electron bands induced by the localized moments is estimated to become four times larger than the superconducting energy gap.

PACS: 74.70.Dd; 74.25.Ha; 75.10.−b

Keywords: Borocarbide; Phase diagram; Magnetic; Superconductor

The rare-earth borocarbides RNi_2B_2C, with R = Dy, Er, Ho, and Tm, may be classified as unconventional superconductors in their own right, since superconductivity coexists and competes with antiferromagnetic ordering. The localized magnetic rare-earth moments are coupled indirectly through the conduction electrons. The uniform component of the RKKY interaction is reduced in proportion to the superconducting order because of the Anderson–Suhl [1] screening of the electronic bulk susceptibility. The screening implies that the upper critical field depends on the magnetization induced by the applied field and thereby reflects the anisotropy of the magnetic system, see Ref. [2]. Here, we present a coarse-grained free-energy analysis of the competition between superconducting and magnetic order in these systems with focus on the Tm case. Due to low-lying excited vortex states the screening is assumed to be absent within the core of the vortices in the type-II phase. This implies an excess magnetization of the flux lines in comparison with their surroundings and a radius of the cores, which increases with field. The magnitude of the screening in the Tm system is derived from the stability of the antiferromagnetic ordering in a *c*-axis field [2]. In terms of this estimate, it is found that the exchange splitting between the spin-up and spin-down states of the conduction electrons, just below the upper critical field, is four times the superconducting gap. This finding suggests that the superconducting state in the Tm compound may involve triplet rather than singlet Cooper pairs close to the upper critical field.

The total free energy per Tm-ion of the type-II superconductor is assumed to be interpolated by

$$F = X_\kappa\{(B_i - B_{c2}) + \tfrac{1}{2}B^0_{c2}|\psi|^2\}B^0_{c2}|\psi|^2 + (F^s_M - F^n_M)|\psi|^2/|\psi_0|^2 + F^n_M \tag{1}$$

valid, at least, close to the upper critical field. B_{c2} is the upper critical field in the non-magnetic case, and B^0_{c2} is its value at $T = 0$. The averaged superconducting order parameter $|\psi|^2$ is equal to $|\psi_0|^2 = B_{c2}/B^0_{c2}$ at zero field, when the magnetic part is neglected. $X_\kappa = [1.16 \cdot 4\pi(2\kappa^2 - 1)N]^{-1}$ is determined from the free energy of the hexagonal Abrikosov vortex lattice. The approximately uniform field experienced by the Cooper pairs is $B_i = B + B^0_D(1-D)\langle\langle J_z\rangle\rangle$, $B^0_D = 4\pi g\mu_B N = 2.1$ kOe, D is the demagnetization factor, and $\langle\langle J_z\rangle\rangle = (\langle J^s_z\rangle - \langle J^n_z\rangle)|\psi|^2/|\psi_0|^2 + \langle J^n_z\rangle$ is the averaged value of the

☆Work supported by the Danish Technical Research Council via the Framework Programme on Superconductivity.

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doi:10.1016/j.jmmm.2003.12.1174

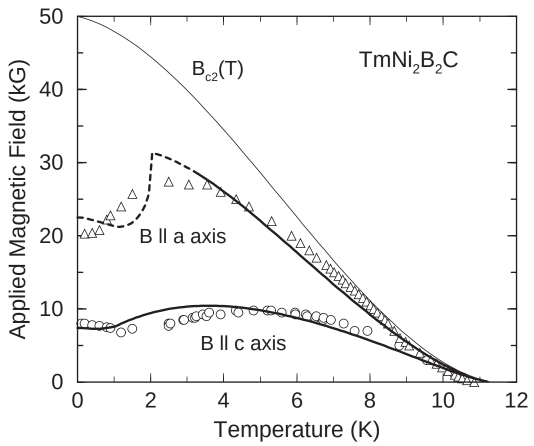

Fig. 1. Upper critical field in $TmNi_2B_2C$. The experimental results are from Ref. [4]. The thin line denotes the assumed value of B_{c2}. The solid lines are the calculated results ($\kappa = 7.23$, $\Delta\mathscr{J} = 8.6$ μeV, and $D_c = 0.64$). Part of the line in the a-axis case is dashed, because the calculated and experimental antiferromagnetic moments are different.

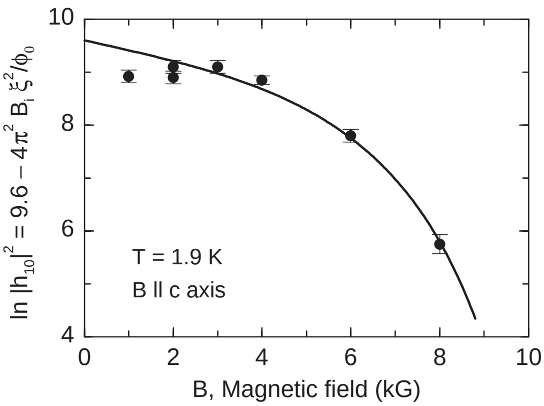

Fig. 2. The field dependence of the logarithm of the flux-line-lattice form factor in $TmNi_2B_2C$. The neutron-diffraction results are from Ref. [3]. The solid line is obtained using $\xi(B) = \xi(0)\sqrt{B_{c2}/B^*_{c2}}$ with $\xi(0) = 89$ Å, and $\xi(B) = 2.2\xi(0)$ at the upper critical field of ~ 9 kG.

angular momentum. $F^s_M = F^s_M(B,T)$ is the free energy of the magnetic system, when $|\psi|^2 = |\psi_0|^2$, and F^n_M is the similar normal-phase quantity. The scaling of the magnetic energy difference by $|\psi|^2/|\psi_0|^2$ in Eq. (1) may be derived directly in the limit $T \to T_C$.

The difference between F^s_M and F^n_M derives from the RKKY contribution $-\frac{1}{2}\sum\mathscr{J}(ij)\mathbf{J}_i\cdot\mathbf{J}_j$ in which the Fourier-transform coupling at zero wave vector is $\mathscr{J}(\mathbf{0})$ in the normal phase and

$$\mathscr{J}_s(\mathbf{0}) = \mathscr{J}(\mathbf{0}) - \Delta\mathscr{J}[1 - \chi_s(\mathbf{0},T)/\chi(\mathbf{0})] \tag{2}$$

in the superconducting phase. $\chi_s(\mathbf{0},T)$ is the screened bulk susceptibility of the superconducting electrons [1,2]. In addition, the antiferromagnetic magnetization reduces the effective density of states and thereby B^0_{c2}, as discussed in Ref. [2]. The predictions of the theory is compared with experiments in Figs. 1 and 2, where $B^*_{c2} = B_{c2} - (F^s_M - F^n_M)/(X_\kappa B_{c2})$. The calculated jump in the derivative of the magnetization at the upper critical field is $0.27\times10^{-4}\,\mu_B$/Oe at 2 K, when the field is applied along the c-axis, in agreement with the experimental value of about $0.3\times10^{-4}\,\mu_B$/Oe [5]. In case the field is applied perpendicular to the c-axis, the calculated and experimental values are both a factor of 5 smaller.

In $TmNi_2B_2C$ at the critical field along the c-axis in the low temperature limit, $\mathscr{N}(0)h^2_{ex} = \frac{1}{2}\Delta\mathscr{J}\langle J^s_z\rangle^2 \approx 0.5\times0.0086\times2.5^2$ meV. Furthermore, $2\mathscr{N}(0)\approx4.6$ eV^{-1} per Tm ion and $\Delta_c \simeq 1.764T_c \simeq 1.7$ meV implying that half the exchange energy gap is $\Delta_{RKKY}/2 = h_{ex} \approx 2\Delta_c$.

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