Anisotropic electronic structure and orbital analysis of borocarbides

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Abstract

The anisotropy of the Fermi velocities and the orbital character of various parts of the Fermi surface of rare earth (R) transition metal (T) borocarbides RT_2B_2C (T=Ni,Pd,Pt,..) are investigated by full-potential relativistic band structure calculations. Their relationship to the anisotropy of the upper critical field and the coexistence of magnetism and superconductivity is discussed on a qualitative level within the multiband Eliashberg theory.

Key words: upper critical field; borocarbides; electronic structure

As a fundamental property of a clean limit type-II superconductor the upper critical field $H_{c2}(T)$ with its value, shape and anisotropy provides deep insight into the electronic structure and the superconductivity [1]. The nonmagnetic borocarbides YNi_2B_2C and $LuNi_2B_2C$ exhibit weak ($\sim 10\%$) in- and out-of-plane H_{c2}-anisotropies. However, in recent measurements on closely related magnetic and nearly magnetic systems a sizable *reversed* out-off plane anisotropy (up to $\sim 100\%$) of $H_{c2}(T)$ at low temperatures T has been observed (see Fig. 1) and ascribed to crystal field anisotropy (CFA) [2–4]. There are several additional possible sources for H_{c2}-anisotropies: anisotropic Fermi velocities $\mathbf{v}_F$, the electron-phonon (el-ph) interaction including anisotropy of the phonon dispersion itself, and that of the order parameter. To get some insight, we address the questions to what extent the H_{c2}-anisotropy might be related to the $\mathbf{v_F}$-anisotropy on individual Fermi surface sheets (FSS's) and what is the specific role of those FSS's in the superconductivity including also the coexistence with rare earth induced magnetism and pair breaking?

We have performed relativistic and scalar relativistic (pseudo-core for $4f$ electrons) full-potential band structure calculations for a large number of rare earth transition metal compounds of the $LuNi_2B_2C$-type structure using the FPLO-code [5,6]. In cases with experimentally unknown boron position z it has been calculated by minimizing the total energy.

All considered borocarbides exhibit a relatively complex Fermi surface which consists of up to five sheets. However there are relatively uniform qualitative features for all superconducting members among the $3d$ to $5d$ transition metal series. The largest FSS exhibits a

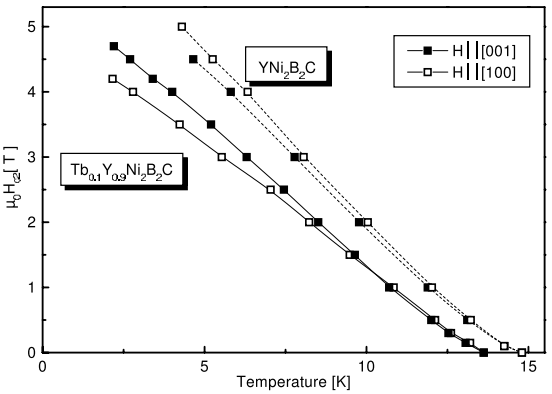

Fig. 1. H_{c2}-anisotropy in single crystals of nonmagnetic YNi_2B_2C and $Y_{1-x}Tb_xNi_2B_2C$ with magnetically active Tb.

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relatively small nested part most strongly pronounced for Ni derived compounds with a partial weight of about 5% of the total density of states (DOS) at the Fermi energy (the dark blue regions in Fig. 2 (lower panel)). These slow electrons with strong el-ph interaction prove to be responsible for the H_{c2}-pecularities in Y(Lu)Ni_2B_2C. To a first approximation their main contribution to $H_{c2}(0)$ and their interplay with FSS's of weakly interacting fast electrons in determining the upward curvature near T_c have been described by a semi-microscopic effective two-band model [1]. The $\mathbf{v_F}$-anisotropy of the nested parts on the large FSS is large $1/\gamma_v \approx 10$ (see Fig. 2) and this way it dominates the sign of the total H_{c2}-anisotropy for nonmagnetic borocarbides. For the group of isolated nesting electrons and no other sources of anisotropy we would arrive at a large $\gamma_{Hc2} = H^{ab}_{c2}/H^{c}_{c2}$. Anyhow, its net effect is reduced by the interaction with other FSS's with γ_v>1.

The orbital analysis of the states near E_F shows that these nested parts of the large FSS contain significant admixtures of rare earth 5d states whereas the central, second-largest, FSS (in red, see Fig. 2) inside the lemon-like features is formed almost only by transition metal $3d_{x^2-y^2}$ and $3d_{xy}$ derived states. This FSS (called pillow-like in [7]) contributes about 70% to the total DOS $N(0)$. In view of the absence of a clear correlation between the empirical T_c-value and the calculated DOS one may conclude that these electrons play a minor role in the superconductivity of nonmagnetic borocarbides. However, in the case of magnetic borocarbides that FSS is least affected by the magnetic moments of the rare earth elements since the magnetism is transferred from the rare earth f electrons to the conducting electrons via the local polarization of the rare earth 5d states. On some FSS's the latter show significant hybridizations with all other states admixed, notably except just that central pillow-FSS. Thus these pillow FSS derived electrons should be of main interest for the coexistence of magnetism and superconductivity. Naturally, the significant opposite $\mathbf{v}_F$-anisotropy $\gamma_v \sim 2$ to 2.4 (see Fig. 2) is comparable with the reversed value $1/\gamma^{exp}_{Hc2} \approx 2$ observed for $Y_{0.8}Tb_{0.2}Ni_2B_2C$ and RNi_2B_2C, where R= Ho, Dy, Er. Possible deviations resulting from a more accurate calculation might be ascribed to the ignored CFA [2–4]. The latter is especially important for the case of R=Tm which exhibits an enhanced normal anisotropy $\gamma_{Hc2} \approx$2.5 [3,4]. In contrast for R=Gd, where is no CFA, we would expect $\gamma_{Hc2} \approx 0.7$ to 0.8 for a mixed $Y_{1-x}Gd_xNi_2B_2C$ crystal ($0.1 < x < 0.2$).

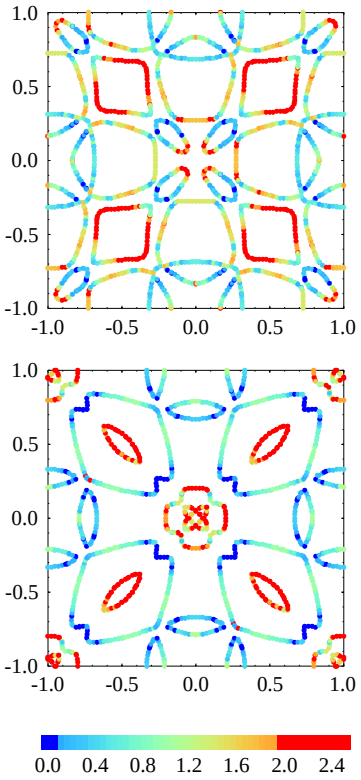

Fig. 2. (color) Anisotropy of Fermi velocities in $LuNi_2B_2C$. Cuts through the Fermi surface sheets at k_z=0.55 π/c (upper panel) and $0.7\pi/c$ (lower panel). k_x- and k_y-axes are measured in units of π/a. The pillow FSS's are centered at $(\pm 0.5, \pm 0.5)\pi/a$. The color table shows the anisotropy measure of the v_F components defined as $\gamma_v = \sqrt{2}v_z/\sqrt{v_x^2 + v_y^2}$.

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References

[1] S.V. Shulga. S.-L. Drechsler, G. Fuchs, K.-H. MIler, K. Winzer, K. Krug, Phys. Rev. Lett. **80** (1998) 1730.

[2] H. Bitterlich, W. Löser, G. Behr, S.-L. Drechsler, K. Nenkov, G. Fuchs, K.-H. Müller, L. Schultz, K.-H. Müller, Phys. Rev. B**65** (2002) 224416.

[3] P.C. Canfield, S.L. Bud'ko, in "Rare earth transition metal borocarbides(nitrides): Superconducing, magnetic, and normal state properties" (Eds. K.-H. Müller and V. Narozhnyi), Kluwer Acad. Publ., Dordrecht, (2001) 33.

[4] K.-H. Müller, G. Fuchs, S.-L. Drechsler, V. Narozhnyi, "Magnetic and Superconducting Properties of Rare Earth Borocarbides of the Type RNi2B2C" , in "Handbook of Magnetic Materials" v. **14** (Ed. K.H.J. Buschow) North-Holland Elsevier, Amsterdam (2002) (in press).

[5] K. Koepernik, H. Eschrig, Phys. Rev. B **59** 1 (1999) 14762.

[6] I. Opahle, PHD-Thesis, University of Technology Dresden (2001).

[7] S.-L. Drechsler, H. Rosner, S. Shulga, I. Opahle, H. Eschrig, J. Freudenberger, G. Fuchs, K. Nenkov, K.-H. Müller, H. Bitterlich, W. Löser, G. Behr, D. Lipp, A. Gladun, Physica C **364-365** (2002) 31.