

## 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  $RT_2B_2C$  ( $T = Ni, Pd, Pt$ , etc.) 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.

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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-of-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 based anisotropy (CFA) [2–4]. There are several additional possible sources for  $H_{c2}$ -anisotropies: anisotropic Fermi velocities  $v_F$ , 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  $v_F$ -anisotropy on individual Fermi surface sheets (FSSs) and what is the specific role of those FSSs 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 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  $H_{c2}$ -peculiarities in  $Y(Lu)Ni_2B_2C$ . To a first approximation their main contribution to  $H_{c2}(0)$  and their interplay with FSSs 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  $v_F$ -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

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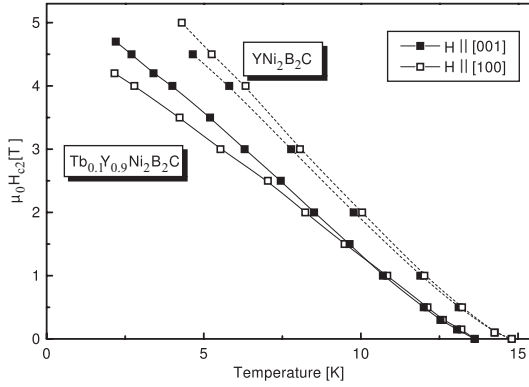


Fig. 1.  $H_{c2}$ -anisotropy in single crystals of nonmagnetic  $YNi_2B_2C$  and  $Y_{1-x}Tb_xNi_2B_2C$  with magnetically active Tb.

borocarbides. For the group of isolated nesting electrons and no other sources of anisotropy we would arrive at a large  $\gamma_{Hc2} = H_{c2}^{ab}/H_{c2}^c$ . Anyhow, its net effect is reduced by the interaction with other FSSs with  $\gamma_v > 1$ .

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 Ref. [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, 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 FSSs 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  $v_F$ -anisotropy  $\gamma_v \sim 2$ –2.4 (see Fig. 2) is comparable with the reversed value  $1/\gamma_{Hc2}^{exp} \approx 2$  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 in terms of strong-coupling theory of multi-band superconductivity 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].

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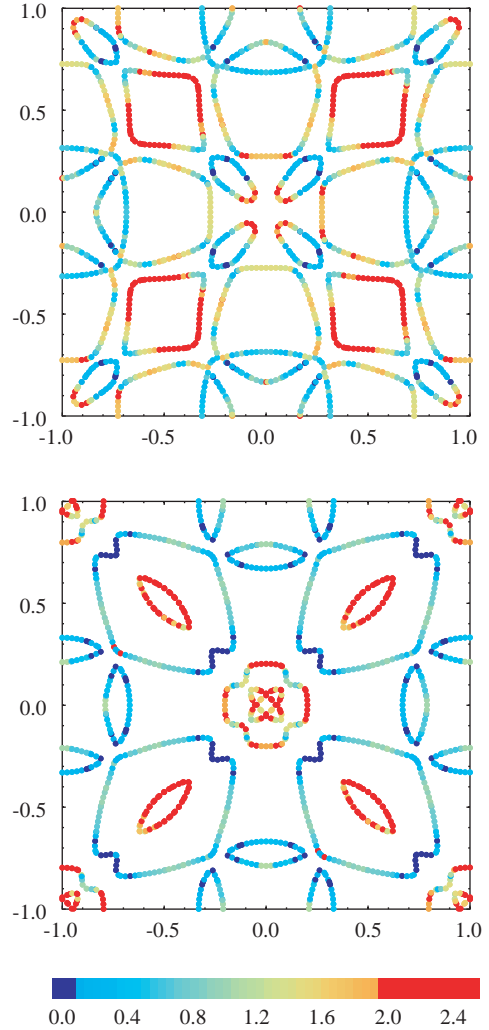


Fig. 2. Anisotropy of Fermi velocities in  $LuNi_2B_2C$ . Cuts through the Fermi surface sheets at  $k_z = 0.55 \pi/c$  (upper panel) and  $0.7\pi/c$  (lower panel).  $k_x$ - and  $k_y$ -axis are measured in units of  $\pi/a$ . The pillow FSSs are centered at  $(\pm 0.5, \pm 0.5)\pi/a$ . The color table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

## References

- [1] S.V. Shulga, S.-L. Drechsler, G. Fuchs, K.-H. Müller, 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: K.-H. Müller, V. Narozhnyi (Eds.), Rare Earth Transition Metal Borocarbides (Nitrides): Superconducting, Magnetic, and Normal State Properties, Kluwer Academic Publishers, Dordrecht, 2001, p. 33.
- [4] K.-H. Müller, G.Fuchs, S.-L. Drechsler, V. Narozhnyi, Magnetic and superconducting properties of rare earth

- borocarbides of the type  $RNi_2B_2C$ , in: K.H.J. Buschow (Ed.), *Handbook of Magnetic Materials*, Vol. 14, North-Holland-Elsevier, Amsterdam, 2002, chap. 3, pp. 200–305.
- [5] K. Koepf, H. Eschrig, *Phys. Rev. B* 59 (1) (1999) 14762.
- [6] I. Opahle, Ph.D. Thesis, University of Technology Dresden, 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.