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A brief comparison of superconductivity in borocarbides and cuprates

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Abstract

The challenge of the present knowledge of the electronic structure and selected thermodynamic properties on the mechanism of superconductivity in rare-earth transition metal borocarbides (nitrides) is discussed with respect to somewhat unexpected similarities with as well as to clear differences from the cuprate superconductors. The effect of substitutional nonmagnetic and magnetic disorder in the rare-earth intermediate layer in between the transition metal boron networks as well as in the network itself upon various thermodynamic properties in the superconducting state of $Y_xR_{1-x}C(Ni_{1-y}Pt_yB)_2$ R = Lu or Tb is studied theoretically as well as experimentally. The suppression of the upper critical field and its positive curvature near T_c can be used as highly sensitive measures of the degree of disorder.

Keywords: Transition metal borocarbides; Cuprates Electronic structure; Disorder; Superconductivity

1. Introduction

The possibly exotic nature of superconductivity in rare-earths (R) transition metal borocarbides (nitrides) (RTBC[N] with T = Ni, Pd, Pt, Ru, Re), is still under an intensive debate [1–5] with respect to unusual features not observed for ordinary superconductors. Hence, a comparison of the available data for RTBC[N] with that of other exotic superconductors, especially with the cuprates might be helpful to improve our present incomplete understanding of both challenging novel members of the rich and rapidly growing family of superconductors. Our conventional approach is based on (i) local density approximation (LDA) band structure calculations, (ii) a multiband Eliashberg analysis of selected properties, and on (iii) the present day knowledge of the cuprates taken from the literature. Here we consider briefly some RTBC[N] peculiarities which resemble those of the cuprates, namely, the upper critical field $H_{c2}(T)$, the electronic specific heat c_p in the mixed state, as well as the isotope effect (IE) and their possible relationship to the electronic structure. Disorder

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and site specific partial substitutions are also briefly considered.

Similarly to cuprates with CuO_2 planes, the RTBC[N] can be divided into two electronic subsystems: the main extended R($5d_{(x,y)z}$)-$(TB)_2$-C[N]-($2p_z$) network and the remaining R-C[N]($2p_{x,y}$) layer(s) acting as a charge reservoir. Since the position of the Fermi energy within the sharply peaked density of states is strongly affected by nonisoelectronic substitutions at the T-site, isoelectronic ones can be used as convenient tools to study disorder effects.

2. The upper critical field

$H_{c2}(T)$ provides in many cases an insight into the electronic structure relevant for superconductivity and into the special role of disorder. All attempts to describe $H_{c2}(0)$ within an effective isotropic single-band model (including also its disorder dependence) for the prototypical compounds $RC(NiB)_2$ with R = Y, Lu using averaged Fermi velocity failed. This points to a special role of the electronic anisotropy and/or of that of a relatively small group (band) of strongly interacting electrons with a low Fermi velocity. A minimal two-band model with medium coupling between slow and fast electrons describes reasonably well most peculiarities including also the positive curvature (PC) near T_c

$$H_{c2}(T) = H^*_{c2}\left(1 - \frac{T}{T_c}\right)^{1+\alpha}, \quad 0.3 < \frac{T}{T_c} \leqslant 0.98 \qquad (1)$$

and the late saturation at low T provided the ratio of these velocities is large $v = v_{F1}/v_{F2} \approx 5$ [6]. This PC is measured by the critical exponent α which is maximal $\sim$0.35–0.45 in the clean limit [7]. Similarly $\alpha \approx 0.4$–0.5, has been reported for the electron doped $Nd_{1.85}Ce_{0.15}CuO_4$ [8] as well as for underdoped hole cuprates. For the cuprates such a PC has been frequently interpreted in terms of bose condensation or various bose-fermion scenarios [8]. To illustrate the effect of a reasonable v_F-anisotropy, we show the shape and v-dependencies of $H_{c2}(T)$ in Fig. 1. The inspection of recent ARPES (angle resolved photoemission) data

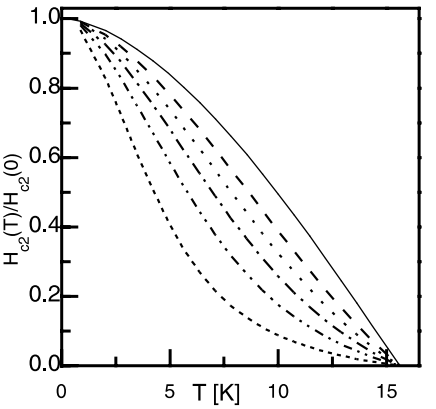

Fig. 1. Upper critical field within a two-band model with different Fermi velocity ratios $v =$ 1, 3.2, 4.5, 6.3, 10 and 20 from top to bottom.

[9] reveals an anisotropy of a factor of 2 for the dressed v_F in (π,π) and $(0,\pi)$ directions, respectively. Since the interaction in the (π,π) direction is expected to be stronger, one might arrive at a sizable anisotropy the bare v_F comparable to the RTBC[N] case. In contrast for optimally hole doped cuprates the PC vanishes. This is in accord with recent ARPES data of hole doped Bi cuprates which point to weak anistropy and this way to a standard shape of $H_{c2}(T)$ within the framework of Eliashberg-(BCS) approach irrespective on mechanism and symmetry of the order parameter [10]. The stronger decrease of H_{c2} compared with T_c by replacing the nonmagnetic Y partially by Tb (see Fig. 2) suggests that in terms of our two-band model the slow electrons are stronger affected by the pair weakening exchange coupling to the Tb local moments. In cuprates the coupling to magnetic ions in the charge reservoir can be neglected.

3. Disorder effects

The unusual PC and $H_{c2}(T)$ of high quality pure single crystals in the clean limit can be well explained within the effective two-band model [6]. Using the parameter set given in Ref. [6] supplemented with increasing impurity scattering rates $\gamma = \gamma_{ab} = \gamma_b = 2\gamma_a = 2\gamma_{ba}$, the *suppression* of $B_{c2}(T)$ and of α can be reproduced (Figs. 3–5). With the

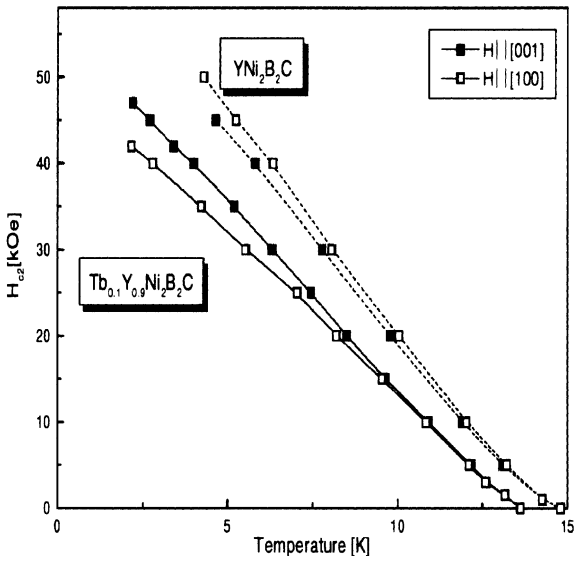

Fig. 2. Upper critical field H_{c2} vs. temperature T for partial substitution of Y by magnetic Tb.

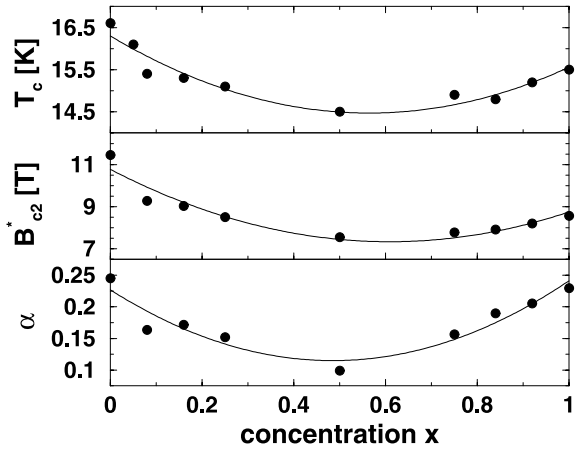

Fig. 3. Composition dependence of T_c (a) the extrapolated upper critical field H^*_{c2} at $T = 0$ (b) and its curvature exponent α for $Y_xLu_{1-x}C(NiB)_2$.

above aim the thermodynamic properties of polycrystalline $Y_xLu_{1-x}C(NiB)_2$ and $YC(Ni_{1-y}Pt_yB)_2$ systems have been investigated as a function of x and y (Figs. 3 and 5). The critical temperature T_c and H_{c2} are somewhat suppressed from both end values of x. Several peculiarities of the clean limit as well as the sublinear H-dependence of c_p in the mixed state

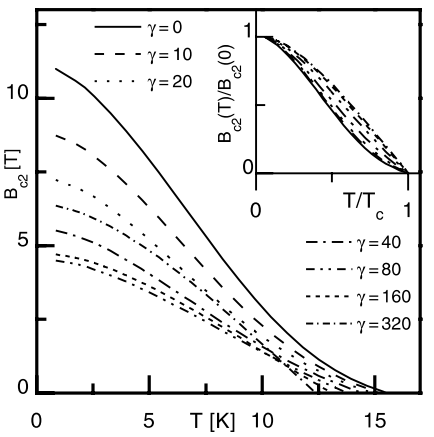

Fig. 4. Upper critical field H_{c2} vs. temperature T within the two-band model for various degrees of disorder given by the impurity scattering rate γ (in cm^{-1}). Inset: the same in relative units.

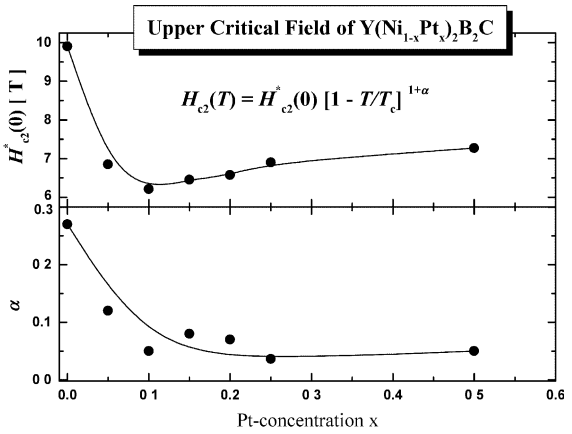

Fig. 5. Composition dependence of the extrapolated upper critical field H^*_{c2} at $T = 0$ and its curvature exponent α.

$$c_p \propto TH^{1-\beta}, \tag{2}$$

are at first weakened by the disorder but are yet clearly visible for all x and y at variance to the statement $\beta(y = 0.2) = 0$ [5]. A much stronger initial decrease occurs for the partial replacement at T-sites compared with that at R-sites: Sharp minima of $H_{c2}(0)$ and the critical exponent $\beta = 0.18$ occur near $y = 0.2$. Approaching $y = 0.5$; α remains small ≈ 0.05. Only for very strong disorder in the network the quasidirty limit is reached. Here H_{c2} increases with disorder. Hence, the increase of

β for $y > 0.2$ cannot be ascribed to a return to the clean limit. Alternatively the vortex–vortex interaction could be enhanced. A third group of electrons related to the ridge-pillow FS might be responsible for this unexpected behaviour (see below). Thus in general, there is no simple relation between α and β. For our samples, including also single crystals, $\alpha \leqslant 0.45$ holds and it provides a more sensitive measure of the disorder than $\beta \leqslant 0.67$ does. Anyhow, this β value corresponds to the best of our knowledge to the strongest sublinear behaviour observed for any superconductor so far.

4. Isotope effects: evidence for el–ph coupling?

Traditionally the isotope effect for T_c

$$\alpha_M = -\frac{M\,\Delta T_c}{T_c\,\Delta M} \approx -\frac{\mathrm{d}\ln T_c}{\mathrm{d}\ln M}, \tag{3}$$

where M is the mass of an atom involved in the lattice vibrations, is regarded as evidence for phonon mediated superconductivity. The same happened at the early days with cuprates where the firstly discovered underdoped and low-T_c systems exhibit substantial oxygen IE. However, later on it became clear that the optimally doped cuprates with the highest T_c values exhibit the *smallest* oxygen related α_O's which may be even negative. Then, despite of many other possible explanations like anharmonicity, van Hove singularity, etc. a nonphonon origin of IE proposed by several authors [12,13] is of interest. For RTBC[N] the only IE reported so far is the B one for $LuC(NiB)_2$ and $YC(NiB)_2$ [15,14]. Considering the experimental boron values $\alpha_B = 0.11 \pm 0.05$ and $\alpha_B = 0.21 \pm 0.07$ for $LuC(NiB)_2$ and $YC(NiB)_2$ respectively, the question arises: why is α_B for these two closely related superconductors so different? This is difficult to understand in terms of ordinary phononic IE. In addition, adopting $\hbar\omega_B = 106$ meV and a substantial α_B for $YC(NiB)_2$ within such a standard scenario leads to weak coupling which contradicts the large jump $\Delta c_p/\gamma T_c$ and the $\lambda > 1$ estimated in Ref. [11]. So we shall suppose that the boron IE is of *nonphononic* origin and the B vibration affects mainly the charge state of the TB network, i.e. changing the charge density n similar as it has been proposed for the apical oxygen in the cuprates [12,16].

$$T_c = 2T_{cm}(1 - n/n_m)n/n_m, \tag{4}$$

where T_{cm} is the optimal critical temperature which is achieved at the optimal charge carrier density n_m. Then the IE reads

$$\alpha_M = \pm\beta_M T_{cm}\sqrt{1 - T_c/T_{cm}}/T_c, \tag{5}$$

where $\beta_M = -(m/n_m)\mathrm{d}n/\mathrm{d}M$ is the isotope mass coefficient of the condensate density. α_M vanishes for optimal doping and large normal IE can be explained for underdoped cuprates. Within in such a scenario the higher T_c value of $LuC(NiB)_2$ compared with $YC(NiB)_2$ suggests just the closeness of the former to the optimally doped regime which might be achieved in $YC(PdB)_2$ where only a small $\alpha_B \approx 0$ would be expected (see Fig. 6). On the contrary, we predict larger α_B-values for the

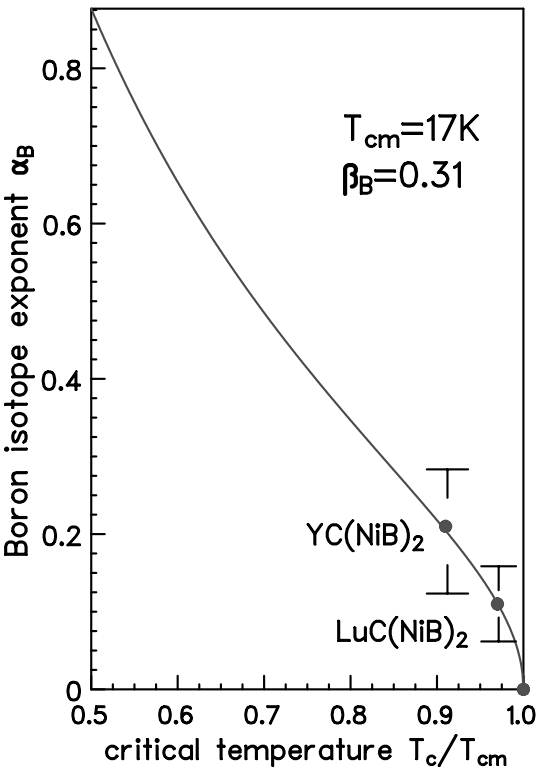

Fig. 6. The boron isotope exponent α_B vs. T_c in units of the maximal (optimal) critical temperature T_{cm} for the model given by Eqs. (3)–(5).

two-layer compounds Lu(Y)CNiB compared with the single-layer Lu(Y)C(NiB)$_2$ which are already nearly optimally doped.

5. Discussion

The analysis of $H_{c2}(T)$ revealed the presence of a strongly coupled group of slow electrons and intermediately or weakly fast electrons. Considering the calculated distributions of v_F for the prototypical best studied borocarbide YC(NIB)$_2$ one has formally two options to assign this group to small parts on the large Fermi surface (FS) (Fig. 7) with nesting properties or to the FS formed by pillows with with crosswise ridges (Fig. 8). Since in the nonsuperconducting LaC(NiB)$_2$ on one hand there are neither nesting, nor slow electrons at the large FS (see Fig. 9) but a somewhat broadened ridge like feature survives at the second part of the FS (see Fig. 10), we conclude that the part of

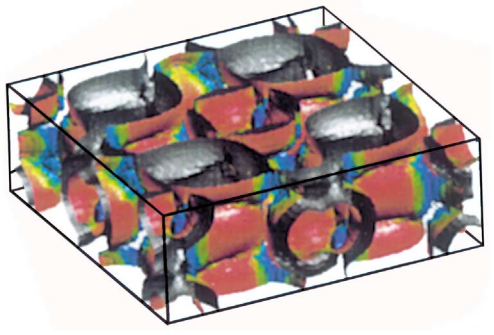

Fig. 7. The calculated large FS with the distribution of Fermi velocities in atomic units (see the colour ridge at the bottom, (blue = slow; red = fast)) for the superconducting YC(NiB)$_2$ (see Fig. 8).

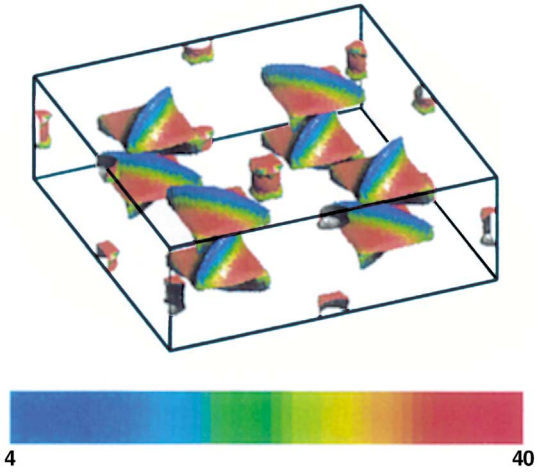

Fig. 8. The same as in Fig. 7 for the pillow-ridge FS for the superconducting YC(NiB)$_2$. Velocities in units of 1.14×10^6 cm/s. For the sake of optimum colour contrast, a small group of electrons which exhibit velocities outside the shown interval were set formally to the bound values.

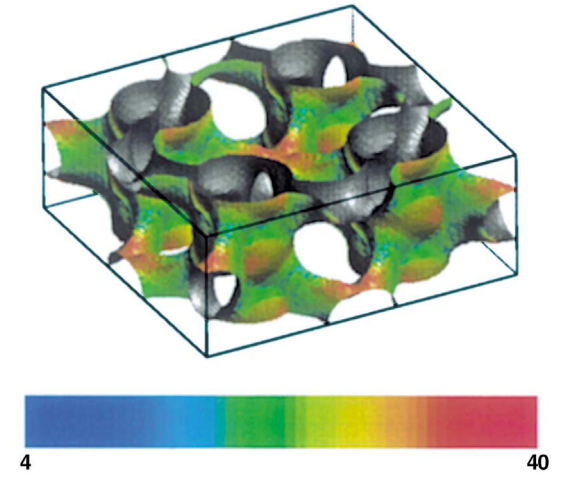

Fig. 9. The same as in Fig. 7 for the large FS for the nonsuperconducting LaC(NiB)$_2$.

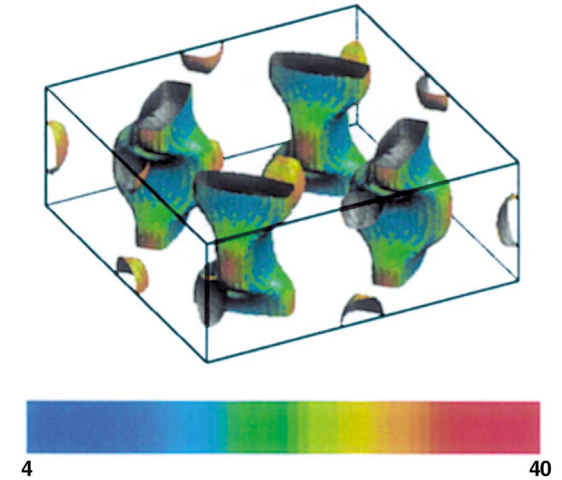

Fig. 10. The same as in Figs. 7 and 8 for the ridge FS of the nonsuperconducting LaC(NiB)$_2$. Velocities in units of 1.04×10^6 cm/s.

electrons important for the superconductivity should be related to the large FS with a special role of the nested parts. On the contrary the ridge FS might be only weakly coupled both internally as well as with the electrons on large FS or not superconducting at all. Such a group of electrons especially, if the fast electrons of the pillow are yet present, is expected hardly to affect the upper critical field. This assignment is supported by the larger contribution of Y $4d_{(x,y)z}$ or R $5d_{(x,y)z}$ states to the nested parts of the large FS compared with the ridge FS and the stronger depression of H_{c2} by magnetic R ions discussed above. These strongly interacting electrons are also responsible for the phonon softening and sharpening in the superconducting state [17] being this way a counter part of the hot spots and the resonance mode, respectively, in the case of cuprates.

From the point of view of correlations RTBC[N] and cuprate superconductors are rather different. In the former there are several bands crossing E_F, they are essentially three dimensional, the onsite Coulomb repulsion at the T-site is smaller than in T-oxides. In addition, borocarbides can be viewed as strongly doped electron systems. Thus the quasiparticles in the normal state are well defined in accord with de Haas van Alphen data (the corresponding information for cuprates is not available). There is a growing amount of experimental data pointing to a significant group of unpaired electrons which manifest themselves as nodes or points of unconventional order parameters. Noteworthy, various properties in the normal state can be described with high accuracy by the LDA [18] in contrast to cuprates.

To summarize, the combined study of RTBC[N] including LDA band structure analysis, multiband Eliashberg calculations and controlled disorder introduced by isoelectronic substitutions at the R-site (relatively weak disorder) compared with those at the T-site (strong disorder) provide a powerful tool suitable for the microscopic understanding of complex metals.

Acknowledgements

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