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Superconductivity in clean and disordered nonmagnetic borocarbides

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The effect of weak substitutional disorder in the rare-earth intermediate layer in between the NiB-networks upon various thermodynamic properties in the superconducting state of $Y_xLu_{1-x}C(NiB)_2$ is investigated theoretically as well as experimentally. The suppression of the upper critical field and its positive curvature near T_c are shown to be a highly sensitive measure of small amounts of disorder even at the rare-earth site.
Keywords: Transition metal borocarbides, Electronic structure, Disorder, Superconductivity

1. INTRODUCTION

The anomalous disorder dependence of several thermodynamic properties in the superconducting state, e.g. $B_{c2}(T)$, $c_p(B)$ and to less extent also T_c in contrast to B_{c1} and normal state resistivity seems to be a generic feature of rare-earth transition metal borocarbides (nitrides) (RTBC(N)). In the electronic sense RTBC(N) can be divided into two subsystems: the $(TB)_2$-$C(2p_z)$ network and the remaining R-$C(2p_{x,y})$ layer. Since the position of the Fermi Energy E_F within the sharply peaked density of states (DOS) is strongly affected by nonisoelectronic substitutions, the isoelectronic substitutions at the R-site can be considered as a convenient tool to study the effect of disorder with tiny shift of E_F.

2. EXPERIMENT

With the above aim the thermodynamic properties of polycrystalline mixed $Y_xLu_{1-x}C(NiB)_2$ systems have been investigated as a function of x (Fig. 1). The critical temperature T_c and the upper critical field B_{c2} are somewhat suppressed from both end values of x. The largest suppression is near $x \approx 0.5$ to 0.6. This is in sharp contrast to the predictions of a phenomenological analysis [1] where for an optimal Ni-Ni distance realized in our samples near $x = 0.6$ [2], a maximum of $T_c \approx$17 K has been predicted. In addition, several peculiarities such as the positive curvature of $B_{c2}(T)$ near T_c

$$B_{c2}(T) = B^*_{c2}\left(1-\frac{T}{T_c}\right)^{1+\alpha}, 0.3 < \frac{T}{T_c} \leq 0.98 \quad (1)$$

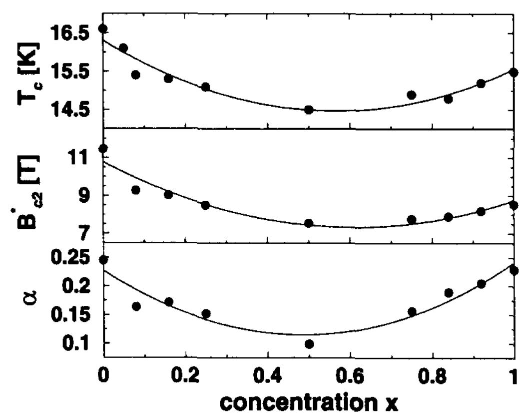

Figure 1. Composition dependence of the critical temperature (a) the extrapolated upper critical field B^*_{c2} at zero temperature (b) and its exponent α measuring the positive curvature near T_c (c).

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as well as the nonlinear field dependence of the electronic specific heat c_p in the mixed state

$$c_p \propto TB^{1-\beta}, \quad (2)$$

are weakened by the disorder but are yet clearly visible for all x in contrast to the case of a 20 % substitution for Ni by Pt [3] where $\alpha=\beta=0$. For our samples, including also single crystals, $\alpha \leq 0.45$ holds and it provides a more sensitive measure of the disorder than $\beta \leq 0.67$ does.

3. THEORY AND DISCUSSION

The unusual positive curvature and the absolute value of the upper critical field of high quality pure single crystals can be well explained within the effective two-band model[4]. Using the parameter set given in Ref. 4 supplemented with an 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 (Fig. 2). Comparing the calculated $N(0)$ values with the measured Sommerfeld constants $\gamma_s \propto N(0)(1+\lambda)$, we arrive at total electron-phonon coupling constants λ=1.05 and 1.1 for x=1 and x =0, respectively.

Our band structure calculations performed in the coherent potential approximation for the mixed $Y_xLu_{1-x}C(NiB)_2$ systems at the experimental values of the lattice constants [2] predict only a weak dependence of the total DOS upon x. The calculated maximal relative suppression of $N(0)$ near x=0.6 is about 1.5%. Admitting an additional suppression of $N(0)$ of the same order due to local lattice distortions caused by the different ionic radii, the experimentally found [5] suppression of the Sommerfeld constant $\gamma_S(x) \propto T_c(x)$ can be reproduced only, if a sizeable ($\sim$ 10%) suppression of the coupling constant $\lambda(x)$ is assumed. We attribute this effect to indirect disorder effects such as hardening of the soft phonon frequencies near 4 and 7 meV which are closely related to the nested parts of the Fermi surface [6]. The anomalous suppression of H_{c2} in the quasi-clean limit with increasing disorder can be explained by a combination of direct and indirect effects.

To summarize, isoelectronic substitutions at the R-site cause relatively weak disorder effects compared with those at the T-site. The anomalous disorder effects near the clean limit can be described within the effective two-band model.

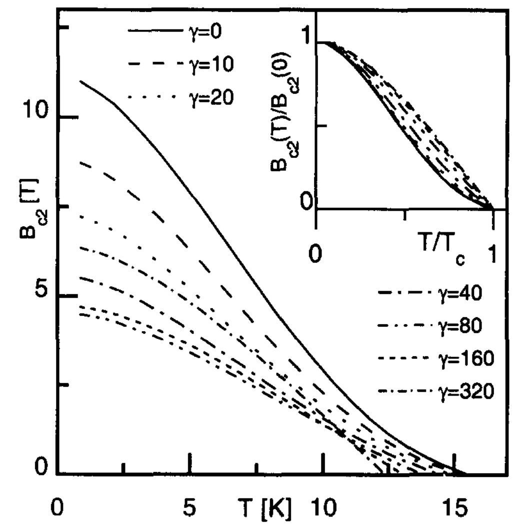

Figure 2. Upper critical field B_{c2} vs. temperature T within the two-band model for various degrees of disorder given by the impurity scattering rate γ (in cm^{-1}). Inset: the same in relative units.

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