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MAGNETIC IMPURITIES IN THE BOROCARBIDE YNi_2B_2C

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Measurements of the specific heat and the magnetization on the quaternary borocarbides RNi$_2$B$_2$C (R = Gd, Er, and Ho) show that the critical temperature T_c scales roughly with the DeGennes factor $(g_J-1)^2J(J+1)$. In GdNi$_2$B$_2$C superconductivity is suppressed by magnetic pair-breaking, whereas in the systems $Y_{1-x}Er_xNi_2B_2C$ and $Y_{1-x}Ho_xNi_2B_2C$ superconductivity and magnetism coexist within the whole range of $0 \leq x \leq 1$. For RNi$_2$B$_2$C with R = Er, Ho and Dy one can show that the coherence length $\xi(0)$ is larger than the lattice parameters of the system, so that the magnetic ions act on the Cooper pairs. Measurements on (Y,R)Ni$_2$B$_2$C show that the variation of the specific heat jump $\Delta C(T_c)$ vs. T_c roughly scales with the Abrikosov–Gor'kov theory for highly diluted systems [1]. Due to these features of the (Y,R)Ni$_2$B$_2$C system, and the fact that it can be very well described by the Eliashberg theory [2], calculations were done to test whether the systems with R = Er, Ho, Dy, Gd and Yb can simply be described by YNi$_2$B$_2$C including magnetic impurities. The calculations show that the model works well for $x \ll 1$.
Key words: borocarbides, magnetic impurities, Eliashberg, phase transition.

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The rare-earth nickel borocarbides RNi$_2$B$_2$C received much attention in the last years due to their very interesting superconducting and magnetic properties. The compounds with the nonmagnetic rare-earth atoms Lu or Y show conventional electon-phonon superconductivity with a relatively high superconducting transition temperature between 15 K and 16 K. These nonmagnetic borocarbides can be very well described by theoretical calculations based on Eliashberg theory [2]. With heavy rare-earth ions R like Dy, Ho, Er or Tm, coexistence of superconductivity and magnetism is observed. The interesting interplay of superconductivity and magnetism in the pseudoquaternary system (Y,R)Ni$_2$B$_2$C (R = Gd, Tb, Dy, Ho, Er and Tm) was investigated by various expermiments [3].

In this paper, we investigate if it is possible to describe the superconducting and thermodynamic properties of the (Y,R)Ni$_2$B$_2$C system by using YNi$_2$B$_2$C as a base system and adding paramagnetic impurities instead of the heavy rare-earth ions within the scope of Elishberg theory. It was already shown that the thermodynamic and superconducting properties of LuNi$_2$B$_2$C and YNi$_2$B$_2$C can be very well described by this approach [2]. Furthermore, the values of T_c from the experiments roughly scale with the Abrikosov–Gor'kov pair-breaking theory [1] which provides a simple relation for T_c as a function of the magnetic impurity concentration $\ln(T_{c0}/T_c) = \Phi(\rho T_{c0}/(2T_c)+1/2)+\Phi(1/2)$; where Φ is the digamma function, T_c and T_{c0} are the transition temperatures in the presence and absence of the magnetic impurities, respectively, and ρ is the pair-breaking parameter.

The first step of our analysis was to calculate T_{c0}/T_c as a function of the paramagnetic impurity content in YNi$_2$B$_2$C. The $\alpha^2(\omega)F(\omega)$ spectrum of the borocarbides, where $\alpha^2(\omega)$ is the electron-phonon coupling function and $F(\omega)$ is the phonon density of states, is shown in Fig. 1. We have used the phonon density of states of Gompf *et al.* [5] for YNi$_2$B$_2$C and weighed it with two decreasing functions of ω: $\alpha^2(\omega)=\omega^{-s}$, with $s=1/2, 1$ as was done by Junod [6] with the A15 compounds. Calculations for clean YNi$_2$B$_2$C within Eliashberg theory using the spectrum with $s=1/2$ showed that this spectum is sufficient for describing the thermodynamic properties and upper critical field of this compound [2]. All other characteristic parameters used in the calculations are listed in Table 1.

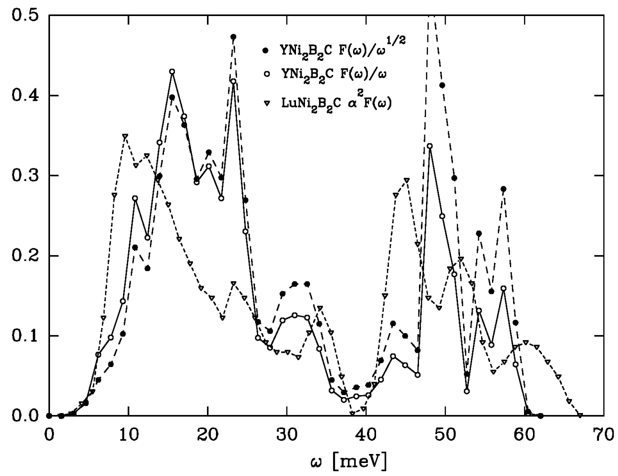

Fig. 1. Electon-phonon spectral functions $\alpha^2(\omega)F(\omega)$ for YNi$_2$B$_2$C obtained from neutron scattering data of Gompf *et al.* [5]. The spectrum of LuNi$_2$B$_2$C was calculated by W. Weber of Universität Dortmund [4] and is shown for comparison.

In order to compare the thermodynamic properites resulting from our analysis with the experimental data, which are functions of T_c/T_{c0}, we have to find a way to map the impurity potential t_- to the impurity concentration x. This is done by calculating the behaviuor of T_c/T_{c0} as a function of t_- and using the experimental data, which are T_c/T_{c0} *vs.* x plots, to obtain the relation t_- *vs.* x for each compound. The numerical results for T_c/T_{c0} *vs.* the paramagnetic impurity potential t_- are shown in Fig. 2 (top). From this figure one can observe that the critical energy of the paramagnetic impurities is $t_{-,\mathrm{crit}} = 0.4761\,\mathrm{meV}$. To correlate these results to the experimental data obtained from specific heat and susceptibility measurements (Fig. 2, bottom left), we used the relation for the magnetic scattering potential t_- as a function of the concentration x:

$$t_-(x) = xS(S+1)N(0)\int |V(\Omega)|^2 d\Omega\,, \qquad (1)$$

where S is the spin, $N(0)$ the density of states, and the $V(\Omega)$ is the scattering potential as a function of the scattering angle Ω. If we set $I(N,V) = N(0)\int |V(\Omega)|^2 d\Omega$, then $t_-/x = S(S+1)I(N,V)$. For small x one can assume that this expression is a constant for a given element. This assumption still holds for the $Y_{1-x}R_xNi_2B_2C$ series because even for $x = 1$, where Y is fully replaced with a magnetic ion, only 1/6 th of the unit cell is paramagnetic. Later in this work we will show that this is only valid for small x.

T_{c0}	λ	γ	atoms	μ^*	$\langle b^2\rangle$	$\langle a^2\rangle$
15.445 K	1.2	0.0029 J/g at K^2	$9.17474\cdot 10^{22}/\mathrm{cm}^{-3}$	0.112101	0.29	0.03

Table 1. Characteristic of parameters of YNi_2B_2C used in the calculations for this work. T_{c0} is the critical temperature, λ the electron-phonon coupling parameter, γ the Sommerfeld constant obtained from specific heat measurements, μ^* the Coulomb pseudo-potential, $\langle b^2\rangle$ the anisotropy parameter of the Fermi velocity, and $\langle a^2\rangle$ the electron-phonon coupling anisotropy parameter.

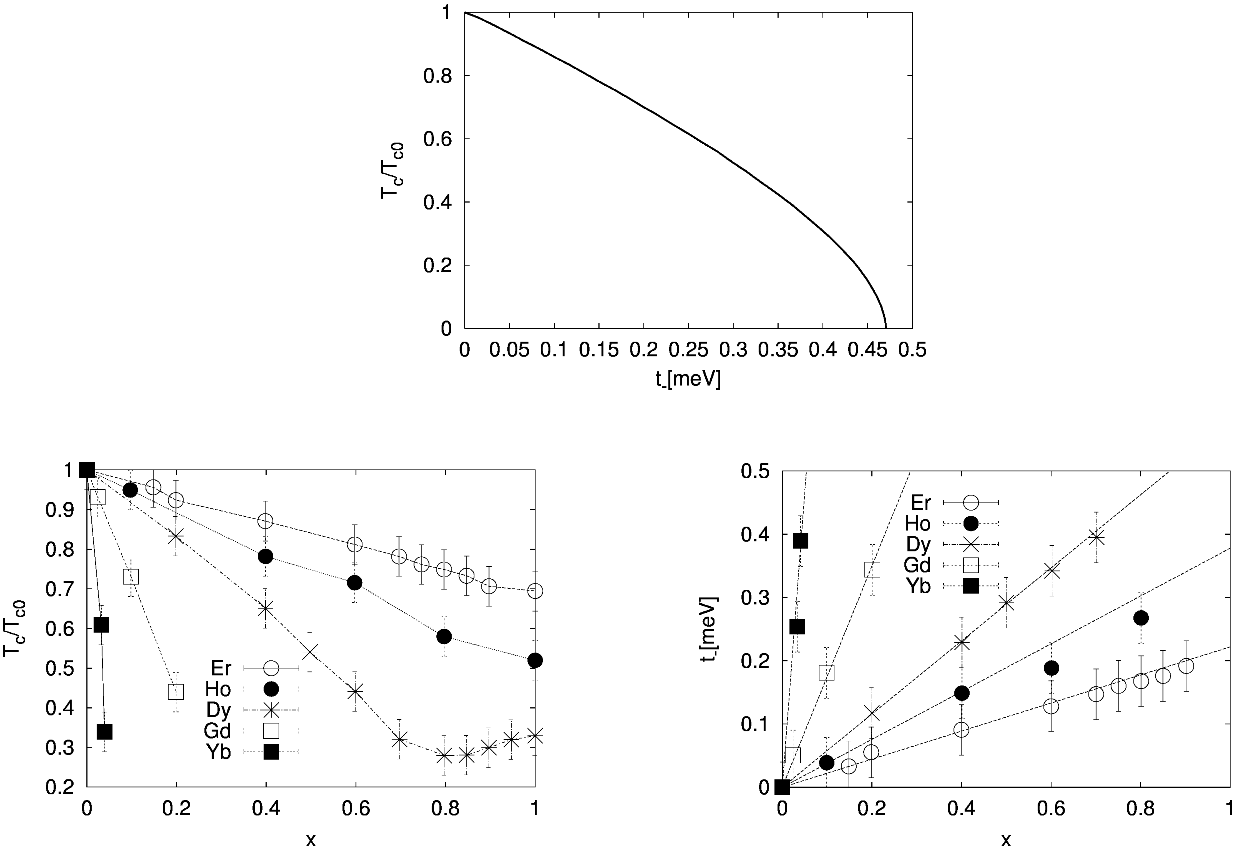

Fig. 2. Numerical results for T_c/T_{c0} *vs.* t_- (top) and experimental data on T_c/T_{c0} *vs.* x (bottom left) for $Y_{1-x}R_xNi_2B_2C$, where R is the rare-earth element as labeled. From these two diagrams the t_- versus x relation is obtained (bottom right).

Fig. 2 (bottom right) shows the combined data from the numerical results and the experimental data in a t_- *vs.* x diagram. The dotted lines are linear fits $t_- = k*x$ of the given data points, which are based on the assumption that t_-/x is constant for small x. With the results for k and the critical impurity potential $t_{-,\mathrm{crit}}$ one can calculate the critical concentrations x_{crit} for each element, and the results are shown in Table 2. These are the main results from our calculations. The x_{crit} values are only higher than 1 for Er and Ho, which shows that for the other compounds superconductivity breaks down before full substitution of Y by the magnetic ions. This further means that the only fully substituted compounds which can be described by Eliashberg theory with YNi_2B_2C as base compound are $ErNi_2B_2C$ and $HoNi_2B_2C$. With these results we are now able to describe the thermodynamic properties as functions of T_c/T_{c0}.

	Er	Ho	Dy	Gd	Yb
t_-/x	0.220	0.378	0.578	1.746	9.294
x_{crit}	2.17	1.26	0.81	0.27	0.05

Table 2. Critical concentrations x_{crit} and fitted values for t_-/x for $Y_{1-x}R_xNi_2B_2C$.

The thermodynamic critical field $H_c(T)$ is calculated from the free energy difference between the normal and superconducting states by using the relation

$$H_c(T) = \sqrt{\frac{2}{\mu_0}\left(F_n(T) - F_s(T)\right)},$$

where $F_n(T)$ is the free energy in the normal state and $F_s(T)$ is the corresponding one in the superconducting state. The calculations of $H_c(T)$ were done without taking the electron-phonon coupling anisotropy parameter $\langle a^2\rangle$ into account (Fig. 3), as it was shown that the anisotropy does not play an important role in describing the thermodynamic properties of YNi_2B_2C [2]. The upper critical field $H_{c2}(T)$, however, is sensitive to changes in $\langle a^2\rangle$ and therefore can not be described with the Werthamer equation $H_{c2}(0) \approx 0.7T_cH'_{c2}(T_c)$ [7] because it does not take both anisotropy parameters $\langle a^2\rangle$ and the anisotropy parameter of the Fermi velocity $\langle b^2\rangle$, which play an important role in describing the upper critical field of YNi_2B_2C, into account. Calculations show that the upper critical field close to T_c and for $H_{c2}(0)$ can not be described without using $\langle a^2\rangle$ and $\langle b^2\rangle$ [2]. With the anisotropy parameters from Table 1 we get the results for $H_{c2}(T)$ as shown in Fig. 3.

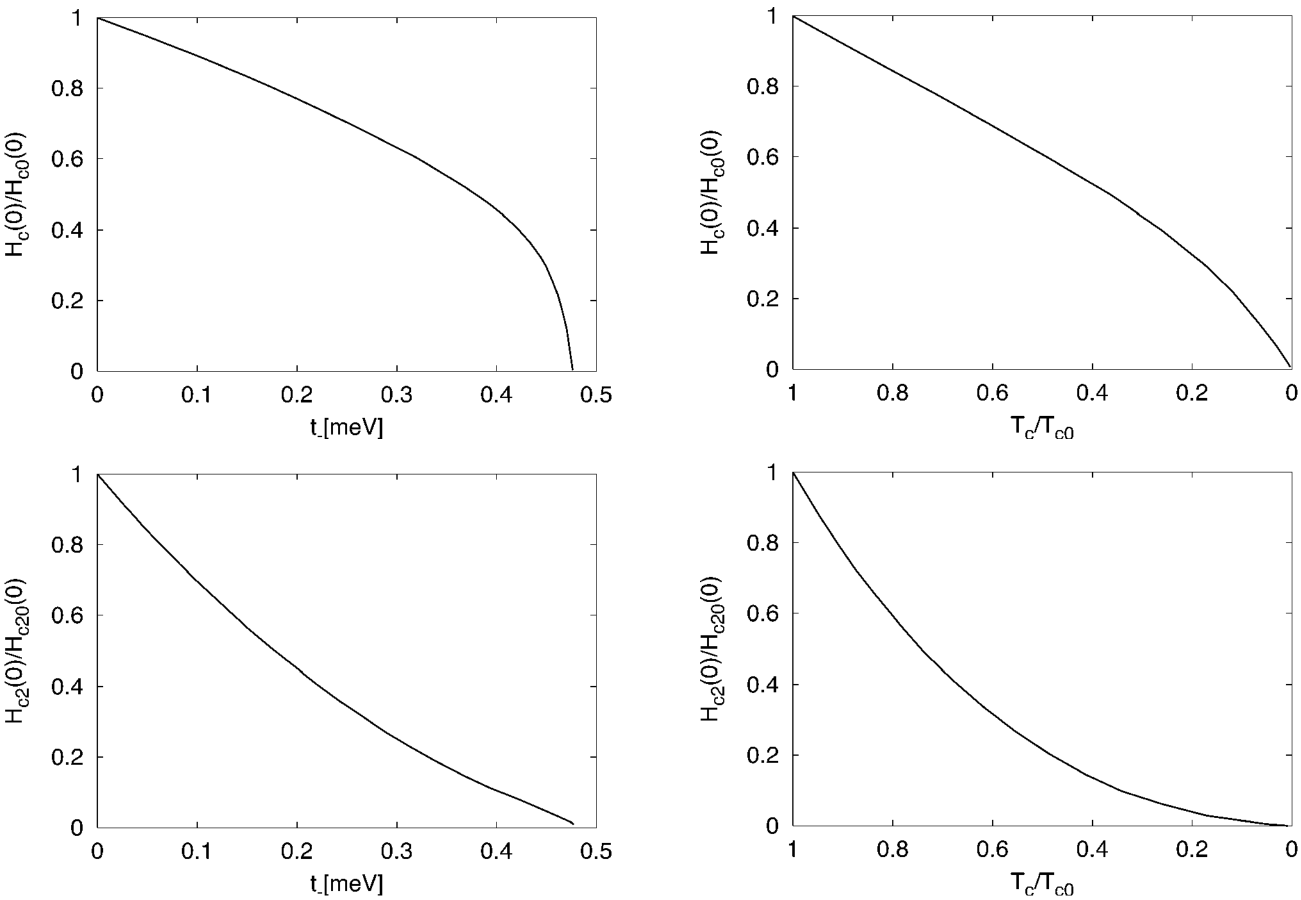

Fig. 3. The thermodynamic critical field $H_c(T)$ and the upper critical field $H_{c2}(T)$ versus T_c/T_{c0} and t_-.

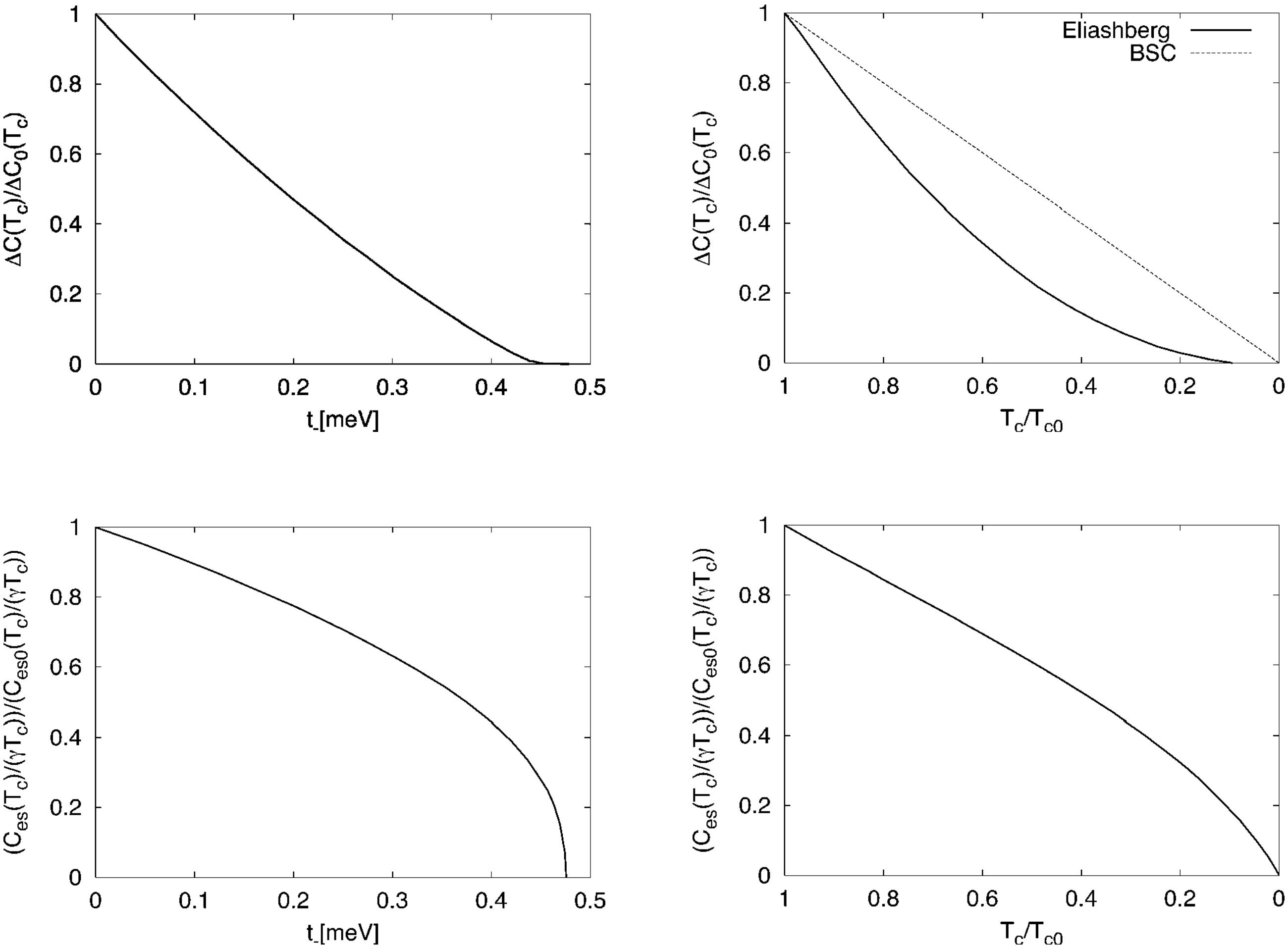

Fig. 4. Calculated jump of the specific heat ΔC and the electronic specific heat contribution C_{es} for YNi_2B_2C with paramagnetic impurities.

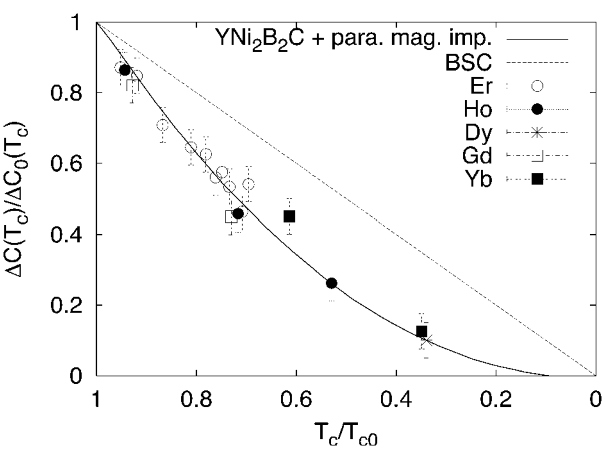

Fig. 5. Variation of the specific heat jump ΔC versus the normalized transition temperature T_c/T_{c0} for $Y_{1-x}R_xNi_2B_2C$, where R is the rare-earth atom as labeled. The solid line are the numerical results of this work. The straight line shows the BCS relation where γ is constant.

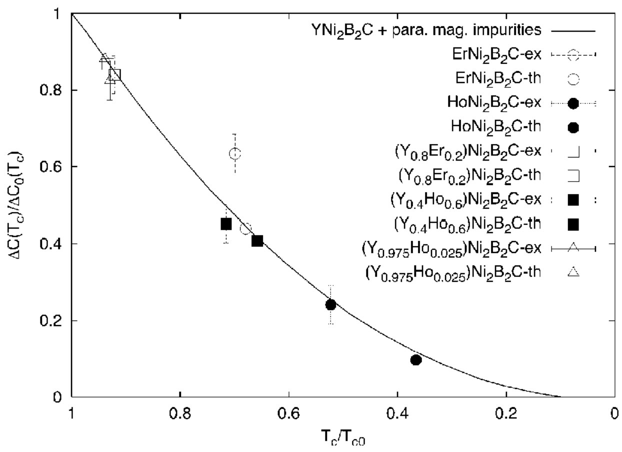

Fig. 6. Detailed comparision of the experimental and theoretical values for ΔC.

	experiment	calculated	error
	T_c[K]	T_c[K]	f[%]
YNi_2B_2C	15.445	15.445	0
$ErNi_2B_2C$	10.8	10.5	−2.8
$HoNi_2B_2C$	8.1	5.7	−30
	$H_c(0)$[mT]	$H_c(0)$[mT]	
YNi_2B_2C	268	269	0.6
$ErNi_2B_2C$	180	201	12
$HoNi_2B_2C$	110	134	22
	$H_{c2}(0)$[mT]	$H_{c2}(0)$[mT]	
YNi_2B_2C	7.9	8.0	1.2
$ErNi_2B_2C$	1.8	3.3	83
$HoNi_2B_2C$	0.85	1.0	17
	$\Delta C(T_c)$[mJ/mol·K]	$\Delta C(T_c)$[mJ/mol·K]	
YNi_2B_2C	572	569	−0.5
$ErNi_2B_2C$	360	249	−30
$HoNi_2B_2C$	140	56	−60

Table 3. Comparison of various experimental and calculated critical values of RNi$_2$B$_2$C.

In our further analysis we calculated the numerical results for the specific heat, the thermodynamic critical field $H_c(T)$ and the upper critical field $H_{c2}(T)$ of YNi_2B_2C with paramagnetic impurities t_-. Fig. 4 shows the electronic specific heat $C_{es}(T_c)$ and the specific heat jump $\Delta C(T_c)/\Delta C_0(T_c)$ versus t_- and T_c/T_{c0}. In Fig. 5 the numerical results are compared to the experimental data. One can see that the numerical results fit the experimental data quite well for $1 < x < 0.7$. The data for $YbNi_2B_2C$ and $DyNi_2B_2C$ do not agree with our calculations due to the fact that the critical concentration with $x = 1$ cannot be reached with our model as was discussed above (see Table 2). In Table 3 the experimental and numerical data are shown together with the relative error, which shows the deviation between the numerical and experimental results in %. For YNi_2B_2C the results are very good as expected. The numerical values for H_c, H_{c2} and ΔC for Er and Ho compounds deviate drastically from the experimental results. This means that even though the agreement between the experimental data and numerical results in Fig. 5 is very good, we can not simply describe $ErNi_2B_2C$ and $HoNi_2B_2C$ in the scope of Eliashberg theory using YNi_2B_2C as base compound and adding paramagnetic impurities corresponding to $x = 1$. To clarify the situation the experimental and theoretical values for ΔC are compared to each in Fig. 6. It shows that, for small amounts of x ($T_c/T_{c0} \gg 0.8$, $x = 0.2$ for Er, and $x = 0.025$ for Gd) in $Y_{1-x}R_xNi_2B_2C$, the experimental and theoretical values agree very well. For these values of x the impurity concentration is below 3%. As a conclusion one can say that it is possible to describe the properties of $Y_{1-x}R_xNi_2B_2C$ with R = Er, Ho, Dy, Gd and Yb for small values of x by using YNi_2B_2C as base compound with paramagnetic impurities within Eliashberg theory.

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МАГНЕТНІ ДОМІШКИ В БОРОКАРБІДІ $\mathbf{YNi_2B_2C}$

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Вимірювання питомої теплоємности та намагнічености в чотирикомпонентних борокарбідах $R\mathrm{Ni_2B_2C}$ (R = Gd, Er і Ho) показують, що критична температура T_c наближено масштабується із фактором Де Жена $(g_J-1)^2J(J+1)$. У $\mathrm{GdNi_2B_2C}$ надпровідність зникає через магнетне розщеплення пар, тоді як у системах $\mathrm{Y_{1-x}Er_xNi_2B_2C}$ та $\mathrm{Y_{1-x}Ho_xNi_2B_2C}$ надпровідність і магнетизм співіснують на цілому проміжку $0 \leq x \leq 1$. Для $R\mathrm{Ni_2B_2C}$ із R = Er, Ho і Dy можна показати, що кореляційна довжина $\xi(0)$ є більшою від параметра ґратки системи, так що магнетні йони впливають на куперівські пари. Вимірювання над $(\mathrm{Y},R)\mathrm{Ni_2B_2C}$ показують, що зміна стрибка теплоємности $\Delta C(T_c)$ щодо T_c підлягає приблизному степеневому співвідношенню відповідно до теорії Абрикосова-Ґорькова для систем із великим розведенням [1]. Згідно з указаними властивостями системи $(\mathrm{Y},R)\mathrm{Ni_2B_2C}$ та тим фактом, що її можна добре описати теорією Еліашберґа, були проведені обчислення, аби протестувати, чи системи з R = Er, Ho, Dy, Gd і Yb можуть просто описуватися $\mathrm{YNi_2B_2C}$ із магнетними домішками. Обчислення показують, що модель добре працює при $x \ll 1$.