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Electronic band structure of the borocarbide superconductor LuNi$_2$B$_2$C

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Abstract. We present de Haas-van Alphen (dHvA) measurements of the nonmagnetic rare-earth borocarbide superconductor LuNi$_2$B$_2$C which have been performed by using a torque cantilever for temperatures down to 0.45 K and in magnetic fields up to 32.5 T. We mapped the dHvA oscillations of a high-quality single crystal by rotating between all three principal crystallographic axes [100], [001], and [110]. This set of data gives a complete overview of the electronic band structure of LuNi$_2$B$_2$C. A comparison with band-structure calculations allowed us to assign the dHvA frequencies to individual bands. Overall positions and band dispersions resemble those observed in the isostructural compound YNi$_2$B$_2$C, which is another nonmagnetic member in the family of the borocarbide superconductors.

1. Introduction

Soon after the discovery of the quaternary borocarbides [1, 2] specific-heat experiments in magnetic fields indicated the possibility of a complex non-s-wave order parameter [3]. These results triggered the interest of experimentalist and theorists alike in the nonmagnetic (Y,Lu)Ni$_2$B$_2$C borocarbides. (Y,Lu)Ni$_2$B$_2$C crystallize in a tetragonal lattice, where B–C containing layers are stacked alternating with (Y,Lu)–Ni-layers along the c-direction [2]. Measurement of the specific heat, $C$, in magnetic fields $B$ on YNi$_2$B$_2$C showed a sizeable contribution $C(B) \propto \sqrt{B}$ [4]. One possible explanation for this result is the admixture of a higher order $g$-wave components to the conventional $s$-wave order parameter leading to an $s + g$-wave order parameter [5, 6]. Subsequent thermal-conductivity, $\kappa$, measurements in YNi$_2$B$_2$C with the heat flow along the [001]-axis in an applied magnetic field $B$ which was rotated through the plane perpendicular to the [001]-direction, showed a fourfold symmetry with maxima of $\kappa$ along the [100] and [010] directions [7]. Results of angular-dependent specific-heat measurements in (Y,Lu)Ni$_2$B$_2$C also made by rotating $B$ in the plane perpendicular to the [001]-direction led to a similar conclusion [8]. Both these findings were interpreted in favor of a $d$-wave symmetry with line nodes of the superconducting order parameter for YNi$_2$B$_2$C [7].

However, band-structure calculations on (Y,Lu)Ni$_2$B$_2$C show a rather complicated Fermi surface consisting of three different bands [9, 10, 11, 12, 15]. These results are in
principle calling for a multi-band analysis with a strongly anisotropic Fermi surface for the superconducting properties [16]. An effective two-band model can describe rather well the peculiar curvatures in the temperature and magnetic-field dependence of the upper critical field \( B_{c2}(T,B) \) of (Y,Lu)Ni\(_2\)B\(_2\)C as determined from magnetic susceptibility and electrical resistivity measurements [16]. These findings point to the importance of multi-band effects for the superconducting properties of (Y,Lu)Ni\(_2\)B\(_2\)C [16] and could suggest a different origin for the observed angle dependence of the thermal conductivity [7] and specific heat [8] in a magnetic field.

A clear picture of the band-structure along with the effective masses in the different bands may play a crucial role in understanding the superconducting properties of (Y,Lu)Ni\(_2\)B\(_2\)C. We thus have measured the angle-dependent de Haas–van Alphen (dHvA) oscillations of LuNi\(_2\)B\(_2\)C up to 32.5 T.

2. Experimental
The single crystals used in this study were grown from NiB\(_2\) flux [17]. On this same sample we observed dHvA signals in the superconducting state down to fields as low as \( B / B_{c2} \approx 0.4 \), indicating a high degree of crystallographic perfection [18]. The dHvA signal was measured with a torque capacitance magnetometer using a \(^3\)He insert in magnetic fields up to 33 T at the High Field Magnet Laboratory Nijmegen. The insert allowed rotation around one axis, thus for recording dHvA signals for rotations in steps of about 9° between all the three principal crystallographic axes [100], [001], and [110], the sample was mounted in three different orientations.

3. Results and Discussion
Figure 1 shows typical torque data for a magnetic field \( B \) rotated by \( \Theta_{001} = 9^\circ \) from [100] towards [001] in the (001)-plane. For fields below the upper critical field \( B_{c2} \) we observe a large “peak effect” [19] in the field range between 7 and 9 T, which is most probably associated with
the vortex lattice [20]. Magnetic quantum oscillations can be resolved after the subtraction of a smooth background from the torque signal. The non-oscillating background was approximated by fitting a low-order polynomial over a restricted field range between 20 and 32.5 T. The inset of Figure 1 shows the Fourier spectra obtained via fast Fourier transformation in the same field range. For this direction we can clearly distinguish seven characteristic frequencies belonging to five extremal orbits of the Fermi surface and two higher harmonics. For this specific orientation of the sample the frequencies are $F_a = 520$ T, $F_b = 780$ T, $F_c = 1300$ T, $F_n = 1508$ T, and $F_g = 5512$ T.

Figure 2 shows the angular dependence of the dHvA frequencies of LuNi$_2$B$_2$C. The overall angular dependence is qualitatively very similar to the one reported for YNi$_2$B$_2$C [13, 14]. Also, first results for the effective masses of the various bands of LuNi$_2$B$_2$C give comparable values to those of YNi$_2$B$_2$C [13, 14]. In the following we thus compare our data with band-structure calculation for YNi$_2$B$_2$C for which orientation-dependent dHvA frequencies were computed [15]. This calculation shows Fermi surfaces made up from three different bands consisting of multiple disjoints pockets [15]. The simplest band has an approximately spherical Fermi surface in the center of the Brillouin zone at the so-called $\Gamma$-point whose dHvA frequency we denote with $F_a$ [15]. Another band consists of an approximately cubic Fermi surface which is also centered at the $\Gamma$-point associated with $F_n$, and four flat “cushions” centered at the edges of the Brillouin zone with the flat side perpendicular to the [001]-direction giving rise to $F_c$ [15]. All the other frequencies, $F_a$, $F_b$, $F_c$, $F_d$, $F_e$, $F_f$, and $F_g$ are associated with the most complicated piece of the Fermi surface, which is multiply connected [15].

With the additional knowledge of the effective masses of the various bands, one can speculate that it would become possible to calculate the superconducting properties including the anisotropy of the superconducting gap. As the non-magnetic borocarbides might be an a multiband superconductor [16] analogous to the multiband superconductor MgB$_2$ [21]. From understanding how the individual bands contribute to the superconductivity one might be able to explain why the dHvA oscillations in (Y,Lu)Ni$_2$B$_2$C can be observed down to fields as low as $B/B_{c2} \approx 0.4$ [22, 23, 24, 18].
4. Conclusion and Outlook
We measured dHvA oscillations in the nonmagnetic borocarbide LuNi$_2$B$_2$C by rotating the field between all major crystallographic directions. Our experimental results closely resemble those calculated for YNi$_2$B$_2$C [15]. In combination with band-structure calculations, these results will help to establish a full understanding of the band structure of the multiband superconductor LuNi$_2$B$_2$C. This might allow to find an answer the pertinent questions in the nonmagnetic borocarbides on the origin of the angular dependence of the thermal conductivity [7] and specific heat [8] in a magnetic field, as well as on the origin of the persistence of the quantum oscillations deep into the superconducting state [18, 25].

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