ELECTRONIC STRUCTURE OF Y AND Lu BOROCARBIDES DETERMINED BY DE HAAS – VAN ALPHEN EXPERIMENTS

K. WINZER, K. KRUG

I. Physikalisches Institut der Universität Göttingen
Bunsenstr. 9, D-37073 Göttingen, Germany

Abstract

The Fermi surfaces of the nonmagnetic borocarbide superconductors YNi$_2$B$_2$C and LuNi$_2$B$_2$C were studied by the de Haas – van Alphen (dHvA) effect. Several branches of dHvA frequencies were observed in the normal state for $B \parallel c$ on single crystals of both systems. The observed dHvA frequencies and their angular dependencies are very similar indicating the same topology of the corresponding parts of the Fermi surfaces. Together with the effective cyclotron masses $m_e$ and the Fermi velocities $v_F$, the results were discussed in the context of electronic band structure calculations. In both systems magnetoquantum oscillations were also observed in the superconducting state below the upper critical field $B_C$. The additional damping of the dHvA oscillations in the vortex state strongly depends on the extremal orbit taken into consideration.

1. Introduction

The series of nickel based borocarbides RNi$_2$B$_2$C (R = rare earth elements) have attracted continuous interest due to the coexistence of superconductivity with relatively high transition temperatures and magnetism in the compounds with magnetic rare earth elements [1,2]. The crystal structure is known to be a filled variant of the body-centred-tetragonal ThCr$_2$Si$_2$ type [3]. This structure is essentially a stack of infinite R-C sheets and Ni$_2$B$_2$ layers arranged in an alternating sequence along the c-axis. The short B-C bonds provide contact between the R-C planes and the Ni$_2$B$_2$-layers; they are responsible for the good conductivity along the c-axis. Electronic band-structure calculations for YNi$_2$B$_2$C [4,5] and LuNi$_2$B$_2$C [6-10] revealed a three-dimensional band structure despite the layered structure with rather complicated band components near the Fermi level $E_F$ with mainly Ni 3d character. Very detailed insight into the electronic structure can be gained from de Haas-van Alphen measurements. DHvA oscillations not only probe the Fermi surface topology but also probe the many-body properties of the material through the field and temperature dependence of the dHvA amplitudes. Thus, not only the cross sections of the extremal orbits and their angular dependence, but also the effective masses and the Fermi velocities of different parts of the Fermi surface can

be obtained from dHvA measurements. The aim of this paper is to compare the existing experimental data for YNi$_2$B$_2$C and LuNi$_2$B$_2$C with each other and with results from band structure calculations. Unfortunately, there are much more dHvA data available for YNi$_2$B$_2$C than for LuNi$_2$B$_2$C, while on the other hand there are only two band structure calculations published for YNi$_2$B$_2$C [4,5] but five for LuNi$_2$B$_2$C [6-10].

2. Experimental results

2.1. MEASUREMENTS ON YNi$_2$B$_2$C

The first results on YNi$_2$B$_2$C single crystals obtained with the field modulation technique in magnetic fields up to 12 T were published by Heinecke et al. [11]. For $B \parallel c$ two dHvA frequencies $F_a = 0.499$ kT and $F_\beta = 6.933$ kT were observed, which correspond to 1.5% and 21.0% of the cross section area $(2\pi / a)^2$ of the Brillouin zone (BZ). From the temperature dependence of the amplitudes the cyclotron masses were calculated to be $m_{c\alpha} = 0.34 m_o$ and $m_{c\beta} = 1.24 m_o$, respectively. The calculated Fermi velocities $v_F = \sqrt{2heF / m_c}$ of the both orbits are nearly the same $v_{F_a} \equiv v_{F_\beta} = 4.2 \cdot 10^5$ m/s. Both dHvA frequencies could be observed above and below the upper critical field $B_{c2}$ without an additional damping in the superconducting state. Terashima et al. [12] have reported on an additional frequency $F_\gamma = 11.700$ kT for $B \parallel c$ and two other fundamental frequencies $F_\delta$ and $F_\epsilon$ at field directions away from the [001] direction in the (010) plane. The most extensive dHvA study were performed by Nguyen et al. [13] in the field range 19 T $\leq B \leq 23$ T at the Grenoble High Magnetic Field Laboratory. The angular dependence of the dHvA branches in the (1 $\bar{1}$ 0) plane obtained at $T = 0.4$ K is given in figure 1a. In addition to the above mentioned frequencies, two further branches $F_{\eta_{1/2}}$ and $F_\kappa$ were observed. The branches $F_{\eta_{1/2}}$ show a strong angular dependence and are degenerated for $B \parallel c$ with $F_{\eta}(0) = 5.818$ kT. The corresponding cyclotron mass $m_{c\eta} = 3.7 \cdot m_o$ is relatively large which explains the fact that the frequency $F_\eta$ is unobservable in magnetic fields of about 12 T. The additional branch $F_\kappa$ occurs only for $\Theta > 10^\circ$ and increases for larger values of $\Theta$. An extrapolation to $B \parallel c$ leads to a frequency $F_\kappa(0) \equiv 8.6$ kT. In addition to the branch with the highest dHvA frequency $F_\gamma(0) = 11.70$ kT observed by Terashima [11] there is a slightly smaller frequency $F_{\eta_1}(0) = 11.19$ kT with a weak angular dependence.

2.2. MEASUREMENTS ON LuNi$_2$B$_2$C

The first results on LuNi$_2$B$_2$C were obtained on a c-axis orientated powder sample in pulsed fields up to $B = 38$ T and $T = 1.4$ K by Tokunaga et al. [14]. For $B \parallel c$ they observed one dHvA frequency $F_a = 0.288$ kT which correspond to 0.84% of the cross section area of the BZ. From measurements on LuNi$_2$B$_2$C single crystals we obtained