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Electronic structure and anisotropic superconductivity in diborides and borocarbides

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Abstract

We compare calculated Fermi surface sheet (FSS) areas F and masses of MgB_2 and ZrB_2 with dHvA data. Deviations in F in MgB_2 can be removed by a small mutual shift of σ- and π bands. The dHvA masses lead to orbit averaged el–ph coupling constants $\bar{\lambda}_\sigma \approx 1.03$ and $\bar{\lambda}_\pi \approx 0.32$, while for ZrB_2 only $\bar{\lambda} < 0.1$ holds. The anisotropy of the Fermi velocities and the orbital character of various FSS of rare earth (R) transition metal (T) borocarbides RT_2B_2C, their relationship to the H_{c2}-anisotropy, and the coexistence of magnetism and superconductivity are discussed.

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Although MgB_2 and borocarbides appear to be well described as Fermi liquids based on the band structure described in the local density approximation (LDA), only recently detailed comparisons with de Haas van Alphen (dHvA) [1] and angle resolved photoemission spectroscopy (ARPES) data [2] became possible. In the mean time exotic scenarios have been proposed [3,4]. Lacking/low-T_c superconductivity in other diborides should be explained too [5–7]. With this aim we compare first normale state properties of MgB_2 with nonsuperconducting ZrB_2. As a basic property of a clean limit type-II superconductor the upper critical field $H_{c2}(T)$ provides insight into the relationship of electronic structure, e.g. by the Fermi velocities $\mathbf{v}_F$, and superconductivity.

A marked out-of-plane (OPA, $\gamma_H(T) = H_{c2}^{ab}/H_{c2}^{c} > 1$) and no in-plane (IPA) H_{c2}-anisotropies have been reported for MgB_2 whereas Y(Lu)Ni_2B_2C exhibit weak (∼10%) OPA and IPA as well. A sizable *reversed* OPA ($\gamma_H < 1$ up to 0.5) at low T in related (nearly)magnetic systems with Y, Lu (sometimes partially) replaced by rare earths elements R has been ascribed to crystal field effects (CFE) [8]. Here, we address the questions: How is $\gamma_H \leqslant 1/\gamma_v$ related to the $\mathbf{v}_F$-anisotropy (defined as $\gamma_v = \sqrt{2}v_z/\sqrt{v_x^2 + v_y^2}$) averaged on disjoint Fermi surface sheets (FSS)? What is their specific role in the coexistence of superconductivity and magnetism?

We have performed relativistic and scalar relativistic (pseudo-core for 4f electrons where necessary) band structure calculations for most diborides and borocarbides using the FPLO code [5,9–11]. To ensure high precision and consistency of the calculations, we have applied for diborides also the FLAPW method as implemented in the WIEN97 code which has produced equivalent results. ARPES was the first check to probe the LDA electronic structure of MgB_2 [2]. The inspection of the data revealed some unexpected features which could not be ascribed to bulk states. Applying the layered KKR, we were able to resolve assignment problems in terms of surface states [12]. Let us turn to the FSS areas F and electronic masses of MgB_2 (see Table 1). Basically, we find good agreement for the F similarly as Ref. [13]. However, at variance with Ref. [13], the remaining deviations between our LDA and dHvA F can be removed by a slight downshift $\delta\epsilon \sim 100$ meV of the

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Table 1
LDA parameters of MgB_2 compared to dHvA data[1], (F in kT)

Orbit	F_{calc}	F_{exp}	m_b	$\lvert m^*\rvert$	$\lambda = \lvert m^*\rvert/\lvert m_b\rvert - 1$
σ_Γ^S	0.78 (0.79)	0.551	−0.25	0.548	1.19
σ_Γ^L	1.65 (1.67)	1.18	−0.57	1.2	1.11
π_Γ	34.5		1.87		
σ_A^S	1.83 (1.81)	1.534	−0.31	0.61	0.97
σ_A^L	3.45 (3.46)	2.971	−0.64	1.18	0.84
π_A	30.6		−0.93		
π_M	0.45	0.576	−0.25	0.31	0.26
π_L	3.03	2.705	0.32	0.439	0.37

The FPLO values, using 16221 k points in the irreducible BZ; values in parentheses—FLAPW using the GGA exchange-correlation; band masses in m_e. Orbit notation see Ref. [11].

σ-bands relative to the π-bands. Its microscopic reason (beyond the LDA) is still unclear. Several scenarios such as weak polaronic corrections generic for multiband systems with markedly different el–ph interaction in various bands and high-frequency phonons ω_{ph} involved [5]: $\delta\epsilon \propto (\lambda_\sigma - \lambda_\pi)\hbar\omega_{ph}$ or electron–electron self-energy effects will be considered elsewhere. Here, we note only that the search of B isotope effects for the F might be helpful to distinguish between them. Turning to ZrB_2, we note that the agreement between dHvA and LDA is even better than in MgB_2. The value of the orbit averaged el–ph coupling constant $\lambda \leqslant 0.1$ is in accord with the FS averaged λ from specific heat [6], point-contact measurements [7], and the lack of superconductivity.

All considered RTBC exhibit a complex FS with up to five sheets. The largest FSS shows small nested parts, most pronounced for RTBC with T = Ni with a partial weight of about 5% of the total density of states (DOS) at E_F. These slow electrons with strong electron–phonon interaction prove to cause the H_{c2}-pecularities in $Y(Lu)Ni_2B_2C$. To a first approximation their main contribution to $H_{c2}(0)$ and their interplay with FSS's of weakly interacting fast electrons in determining the upward curvature near T_c have been explained using a two-band model [14]. The $\mathbf{v_F}$-anisotropy of the nested parts on the large FSS is huge $1/\gamma_v \approx 10$. It dominates the value of γ_H for nonmagnetic RTBC. For isolated nesting electrons we would arrive at a huge γ_H like in MgB_2. But the net effect is reduced by the admixture of opposite contributions from other FSS with $\gamma_v > 1$. The orbital analysis of states near E_F shows that these nested parts of the large FSS contain marked admixtures of R 5d states whereas the central, second-largest, FSS inside the lemon-like features is formed almost only by Ni $3d_{x^2-y^2}$ and $3d_{xy}$ derived states. This FSS (called pillow-like in [15]) contributes about 70% to the total DOS $N(0)$. In view of the missing correlation between T_c-values and the calculated DOS, we conclude that these electrons play a minor role in the superconductivity of nonmagnetic RTBC. But for magnetic RTBC that pillow FSS is least affected by the magnetic moments of R elements since the magnetism is transferred from the R 4f states to the conducting electrons via the local polarization of the R 5d states. Thus the pillow FSS derived electrons are of main interest for the coexistence of magnetism and superconductivity. Naturally, the significant opposite $\mathbf{v_F}$-anisotropy $\gamma_v \sim 2$–2.4 is comparable with the reversed value $\gamma_H \approx 0.5$ observed for $Y_{0.8}Tb_{0.2}Ni_2B_2C$ and RNi_2B_2C, where R = Ho, Dy, Er. Further improvements should result taking into account the ignored CFE [8] which are relevant for R = Tm, Gd with an enhanced normal γ_H-value.

To summarize, the nice description of the LDA FSCS of MgB_2 and ZrB_2 as well as the ARPES data for MgB_2 emphasizes our quite reasonable understanding of diborides. Most of them differ from MgB_2 mainly by lacking σ-derived holes with strong el–ph interaction. Thus, our study yields strong support for multiband Eliashberg models [16] (possibly with small many-body corrections). H_{c2} is governed mainly by the Fermi velocity anisotropy. Less space is left for exotic scenarios [3].

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