Magnetic-field induced band-structure change in CeBiPt

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We report on a field-induced change of the electronic band structure of CeBiPt as evidenced by electrical-transport measurements in pulsed magnetic fields. Above \( \sim 25 \) T, the charge-carrier concentration increases nearly 30% with a concomitant disappearance of the Shubnikov-de Haas signal. These features are intimately related to the Ce 4f electrons since for the non-4f compound LaBiPt the Fermi surface remains unaffected. Electronic band-structure calculations point to a 4f-polarization-induced change of the Fermi-surface topology.

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The influence of magnetic fields on the electronic band structure of metals is usually minute and may, therefore, in most cases be disregarded because of the different relevant energy scales of the itinerant electrons in conventional metals and of the applied magnetic fields: the typical Fermi energy is of the order of \( eV \) compared to a Zeeman energy of \( \sim 6 \) meV at 50 T. However, the situation may change considerably in case the relevant energy scales of the electronic system are strongly reduced.

Prominent examples for field-induced changes of the Fermi surface are, e.g., strongly correlated metals close to a “quantum critical point” \( 1 \). Usually, the criticality results from magnetic interactions leading to field-induced modifications of the magnetic ground state \( 2, 3 \). For some materials different Fermi surfaces could be detected above and below a metamagnetic phase transition \( 2, 4, 5 \). In the paramagnetic state of a metal, however, a direct influence of an external magnetic field on the electronic band structure is usually not expected.

Here, we provide evidence for a rather sudden field-induced increase of the charge-carrier concentration connected with a Fermi-surface change in the semimetal CeBiPt. This remarkable phenomenon is absent in the non-4f sister compound LaBiPt. Both compounds belong to the intermetallic series \( RBiPt \) (\( R \) = rare-earth metal) that shows a rich diversity of ground states depending on \( R \). Explicitly, YbBiPt is a “super”-heavy-fermion metal \( 6 \), NdBiPt is a small-gap semiconductor \( 6 \), LaBiPt is a superconductor with critical temperature \( T_c \) \( = 0.9 \) K, and CeBiPt is a commensurate antiferromagnet with an ordering temperature of \( T_N \) \( = 1.1 \) K \( 8, 9 \).

In the following we present high-field investigations of the magnetization and of the electrical-transport properties of LaBiPt and CeBiPt in the paramagnetic metallic state. Both compounds are semimetals with very low charge-carrier concentrations and correspondingly small Fermi surfaces \( 2 \). The electronic properties of LaBiPt can consistently be described by standard Fermi-liquid theory. The observed magnetic quantum oscillations \( 2, 10 \) agree very well with band-structure calculations \( 11 \). The picture changes considerably for the isostructural semimetal CeBiPt. Above \( \sim 10 \) K and below \( \sim 20 \) T, the electronic properties follow conventional Fermi-liquid theory as in LaBiPt. Towards lower temperatures, however, the Fermi surface changes, i.e., for certain field orientations the Shubnikov-de Haas (SdH) frequency increases by almost a factor of two between 10 and 0.4 K \( 6 \). Another unusual feature is found in pulsed-field experiments. Above about 25 T the SdH signal vanishes and, instead, the magnetoresistance increases considerably (Fig. \( \text{D} \)) hinting at a field-induced Fermi-surface modification \( 10 \). This feature is not related to the quantum limit since at 25 T still about five Landau levels (of both spin orientations) are occupied.

The single crystals of CeBiPt and LaBiPt were grown at Hiroshima University by use of the Bridgman technique. Details of the crystal growth have been reported elsewhere \( 1 \). The electrical-transport and magnetization measurements were performed at the High Magnetic Field Laboratory Dresden (HLD) in pulsed fields up to about 50 T at temperatures above \( T = 1.8 \) K by use of a \( ^4 \)He gas-flow cryostat. For the transport measurements six 40 \( \mu \)m gold wires were attached to the samples with graphite paste. AC currents up to 1 mA with frequencies between 10 and 50 kHz were applied for about 80 ms just before and during the field pulse. The reliability of the data was checked for different currents and frequencies. Uncertainties of the geometry factors result in error bars of about 20% in the absolute resistivity. The samples were tightly fixed to the sample holder with IMI7031 varnish. Since small misalignments of the contacts are unavoidable the longitudinal and transverse
oscillating behavior of $\Delta$ ambiguity determining signal disappears. We should note that there is some am-
biguity either the completely symmetric (longitudinal) and antisymmetric (transverse) signals.

The overall agreement between pulsed-field and static-field data is very good (Fig. 1) [9]. The initial decrease of the resistivity, $\rho$, reflects most probably antiferromagnetic fluctuations above $T_N$ in the paramagnetic state as evident from its absence at 20 K [10]. Then, up to about 25 T, the oscillations caused by the SdH effect appear. Towards higher fields, however, instead of exhibiting further maxima and minima, $\rho$ just increases monotonically.

The inset in Fig. 1 shows the expected SdH signal (dashed curve) in comparison to the experimental data. For the theory curve we used the well-known SdH formulas (see [13] for details) with parameters $F = 48$ T for the SdH frequency, $m_c = 0.24 m_e$ for the effective mass, and $T_D = 2.7$ K for the Dingle temperature, in good agreement with the static-field data [9]. For the experimental signal we plotted $\Delta \rho = (\rho - \rho_b)/\rho_b$, with $\rho_b$ the steady background resistivity shown by the dashed line in Fig. 1. It is evident that above 25 T the oscillating signal disappears. We should note that there is some ambiguity determining $\rho_b$. However, in order to recover an oscillating behavior of $\Delta \rho$ above 25 T a highly artificial oscillatory background would have to be assumed.

In previous experiments, it was shown that the resistance increase can be followed up to 60 T and that the SdH oscillations vanish independent of sample orientation in field [10]. This contrasts with the temperature-dependent change of the Fermi surface that occurs only for fields aligned within about 15 deg along the main cubic-lattice axes [9].

In order to investigate the high-field behavior of CeBiPt in more detail, we measured the Hall effect. Indeed, as the most important result of this study, Hall-effect measurements in pulsed fields reveal a clear change of slope of the Hall signal at this field range (Fig. 2). This effect was found to be temperature independent between 1.8 and 10 K. Matching the field where the strong increase of the longitudinal resistance sets in, the average Hall coefficient, $R_H = \rho_{xy}/B$, decreases by about 28% (difference in the slopes of the two dashed lines in Fig. 2). The fit to the low-field ($B \lesssim 22$ T) Hall data results in a hole-like charge-carrier concentration of $n_{h}^{low} = (R_H e)^{-1} = 7.2(3) \times 10^{17}$ cm$^{-3}$ whereas at high fields ($B \gtrsim 38$ T) it increases to $n_{h}^{high} = 9.2(3) \times 10^{17}$ cm$^{-3}$. The low-field value agrees well with the result of static-field measurements ($n_{h}^{low} = 7.7 \times 10^{17}$ cm$^{-3}$ [9]) in view of the experimental error caused mainly by the sample-geometry uncertainties.

It is this field-induced increase of the charge-carrier concentration that is unique for the present paramagnetic metal. Earlier band-structure calculations resulted in two small hole-like Fermi surfaces at the Brillouin-zone center and even smaller electron-like Fermi surfaces surrounding them [9]. Assuming a simple single-band picture, the low-field (below 25 T) SdH results are in line with these calculations, although the smallness of the electron pockets prohibits an experimental verification by our SdH measurements. From theory it is not clear how this band structure is modified above 25 T. A detailed analysis of the high-field Fermi-surface topology from our data is excluded due to the lack of any detectable SdH signal at these fields. The increasing number of hole-like charge carriers would lead to a small increase (by about 18%) of the SdH frequency.

The temperature-dependent Fermi-surface change was found only for CeBiPt, but not for the homologous non-
4$f$ compound LaBiPt. It was, therefore, straightforward to check for any unusual field-induced phenomena in LaBiPt. As shown in Fig. 3 for this metal neither the longitudinal resistance nor the Hall effect reveal any unusual slope change. The SdH signal increases – except for small SdH traces – linearly with magnetic field without any unusual field-induced phenomena.

As an alternative scenario, the external field dependence of the band structure was checked. Though the Fermi surfaces are tiny, the direct Zeeman splitting of the band states is probably too small to explain the effect. Field-induced 4$f$ polarization, however, produces an exchange field on the Ce 5$d$ states that may yield field splittings of $\sim 0.1$ eV at 50 T. The experimental data clearly fall below the expected $M$.

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open-core approach), intra-atomic exchange interaction splits the Ce-5d bands close to the center of the Brillouin zone [Fig. 4(b-d)]. The nominal Fermi level (integer number of valence electrons) is taken as reference for exact stoichiometry. The work at Dresden was supported by the DFG through SFB 463 and the BMBF (FKZ 035C5 DRE). The work at Hiroshima was supported by a grant for the International Joint Research Project NEDO and the COE Research (13E2002) in a Grant-in-Aid from the Ministry of Education, Culture, Sports, Science, and Technology of Japan. The work at Karlsruhe was supported by the DFG through SFB 195.

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FIG. 4: LSDA bands of CeBiPt close to the Brillouin-zone center along the symmetry lines $\Delta$ [from (0 1 0) to (0 0 0)] and $\Lambda$ [from (0 0 0) to (0.067 0.067 0.067)]. The nominal $E_F$ is at zero energy, the shifted Fermi level that yields the correct Fermi-surface area is indicated at $-20$ meV by the dotted line. (a) shows the non-magnetic case with unpolarized 4f shell; In (b), (c), and (d), the 4f spin moment is fixed to be 0.2$\mu_B$, 0.5$\mu_B$, and 1.0$\mu_B$, respectively.

In conclusion, we have presented evidence for a drastic change of the electronic band structure of CeBiPt at $\sim 25$ T. Above this field the SdH oscillations vanish and the hole-like charge-carrier concentration increases by about 28%. The absence of these features in LaBiPt clearly reflects the relevance of the 4f states to exchange interaction with the polarized 4f states is a possible explanation. This mechanism would yield a magnetic-field driven metal-insulator transition for exact stoichiometry.