Electronic transport properties of the semimetallic heavy fermion YbBiPt

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The electronic transport properties of YbBiPt are examined in the temperature range 4–325 K to gain insight into the electronic structure of this compound. The magnitude of the strongly magnetic-field-dependent Hall effect is consistent with a semimetallic electronic structure. The data place an upper limit on the carrier concentration of 6×10^{20} holes/cm^3. The thermoelectric power (TEP) is dominated by a large phonon-drag peak below 100 K, while above 200 K the TEP is dominated by a large linear-in-temperature contribution. The temperature-dependent resistivity manifests very little indication of a magnetic scattering contribution. These characteristics indicate the YbBiPt is a low-carrier concentration semimetal. It appears that this low-carrier conducting state is closely tied to the massively renormalized electronic state evident in this compound below 1 K. [S0163-1829(97)01138-7]

I. INTRODUCTION

YbBiPt stands out within the rare-earth intermetallic series *R*BiPt in that it displays both a metallic resistivity and a huge low-temperature Sommerfeld coefficient γ that exceeds 8 J/mol K^2.[1–4] This γ value corresponds to a Kondo temperature of roughly $T_K=1$ K. Out of this strongly renormalized state YbBiPt undergoes magnetic order at $T_c=0.4$ K. Muon-spin-resonance measurements detect an ordered moment of only $0.1\mu_B$,[5] while resistivity measurements show that YbBiPt becomes anisotropic below T_c.[6] These results suggest that a spin-density-wave transition occurs at T_c, and that this transition partially gaps the Fermi surface.[6–8] Inelastic neutron-scattering measurements[9,10] indicate that a Γ_8 quartet is separated from a very narrow Γ_7 ground state by 1 meV (10 K). The width of the ground-state doublet corresponds to a Kondo temperature of roughly 2 K, consistent with the observed low-temperature Sommerfeld coefficient.[11]

It has been assumed that this massive electronic state comes about due to two features inherent in YbBiPt.[1] First, the fcc structure of this compound produces frustrated Ruderman-Kittel-Kasuya-Yosida interactions such that magnetic order cannot circumvent Kondo interactions. Second, it appears that YbBiPt may be a low-carrier concentration metal given that the other members of the *R*BiPt series are small-gap semiconductors.[2] A low-carrier concentration presumably produces a small Kondo temperature, while the crystal structure ensures that local moment ordering cannot preempt the Kondo effect.

We examine the normal-state electronic transport properties of YbBiPt to test the assumption that this is a low-carrier compound. The magnetic-field and temperature dependences exhibited by the Hall effect R_H, thermoelectric power (TEP), and resistivity ρ indicate that YbBiPt exhibits all the hallmarks of a semimetal: a small carrier concentration ($\sim10^{20}$ cm^3), a strongly field-dependent Hall coefficient, anomalously large diffusion, and phonon-drag contributions to the TEP, and carrier mobilities that are at least two orders-of-magnitude larger than those exhibited in other heavy fermion systems. These results support the view[1] that the extremely renormalized electronic state in YbBiPt stems from a low-carrier count.

II. EXPERIMENTAL RESULTS

Single-crystal samples of YbBiPt were grown from a bismuth-rich flux.[12] X-ray[1] and neutron-diffraction[13] measurements indicate that YbBiPt is face-centered cubic ($a=6.60$ Å), crystallizing in the half-Heusler MgAgAs structure. The resistivity was measured by using a conventional four-probe dc technique. The thermoelectric power was measured by suspending a single crystal between two electrically isolated copper posts across which a variable temperature gradient is applied.[14] The absolute TEP was measured relative to copper. The experimental configuration employed a maximum relative temperature gradient ($\Delta T/T$) of roughly 0.5%. This gradient was determined with a 25.4-μm diameter chromel-constantan reference thermocouple. The Hall effect was measured using a five-contact method[15] wherein a 200 Hz ac current source and three current contacts are used to null the zero magnetic field ($H=0$) misalignment voltage. The Hall effect specimen was thinned to 25 μm to maximize the transverse Hall voltage. All transport measurements were carried out on samples from a single growth batch, and in all cases electrical connections were made with a silver conductive paint.

The temperature-dependent resistivity of YbBiPt is depicted in Fig. 1. The resistivity is relatively large (~400 $\mu\Omega$ cm at room temperature) and monotonically decreases with decreasing temperature. A small shoulder is evident in $\rho(T)$ centered near 30 K. In general, however, $\rho(T)$ does not show the influence of Kondo scattering since there is no temperature range where $d\rho/dT<0$ as is frequently observed in heavy electron systems.[16] The resistivity of LuBiPt, a nonmagnetic analog to YbBiPt, is greater than that of YbBiPt at all temperatures. This precludes the standard subtractive method of separating magnetic and nonmagnetic resistivity contributions in YbBiPt.

The thermoelectric power S of YbBiPt (Fig. 2) is positive at all temperatures. This suggests that holes are the pre-

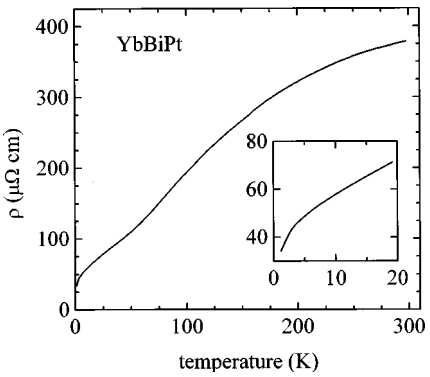

FIG. 1. Temperature-dependent resistivity of YbBiPt from 1.2 to 300 K. The inset depicts $\rho(T)$ in the temperature range 1.2 to 20 K.

dominant carrier in this compound. The most prominent feature in the TEP is the broad peak centered at 65 K. There is also a small shoulder located at 20 K. Above 200 K, S varies linearly with temperature. The overall magnitude of the TEP is roughly a factor of 10 larger than that exhibited by conventional wide-band metals; the TEP is instead suggestive of a narrow-band or reduced-carrier count system.

The temperature-dependent Hall effect of YbBiPt is pictured in Fig. 3. R_H is positive at all temperatures and fields. This is consistent with the positive sign of S, and conclusively demonstrates that holelike carriers dominate the electronic transport in YbBiPt. The low-field ($H=1$ kOe) Hall coefficient is only weakly temperature dependent, and is roughly 10^{-8} m^3/C. This value is 10^2-10^3 times bigger than that found in conventional metals.[17] $10-10^2$ times bigger than that of heavy electron compounds,[18,19] and nearly equal to that of the elemental semimetal antimony.[20] R_H is essentially field independent for $H\leqslant 100$ kOe above 100 K. Below 100 K, R_H becomes increasingly H dependent as the temperature decreases. This field dependence is highlighted in Fig. 4 at the temperatures 4, 12, 50, and 100 K and in fields to 100 kOe. At 4 K, R_H is nearly constant below $H_{\rm con}^{4\,\rm K}\approx 10$ kOe, rises with increasing applied field in the range 20–60 kOe, and begins to saturate near $H_{\rm sat}^{4\,\rm K}\approx 80$ kOe. The data at 12, 50, and 100 K indicate that the characteristic fields $H_{\rm con}$ and $H_{\rm sat}$ rise with increasing temperature. By 12 K, $H_{\rm sat}$ has moved above 100 kOe, while R_H is essentially T

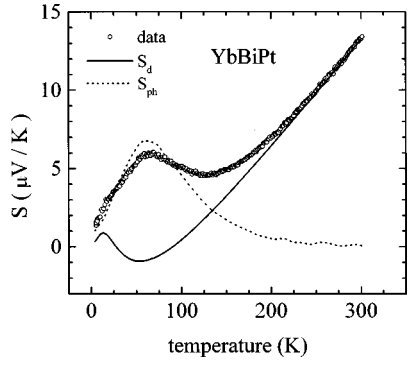

FIG. 2. Temperature-dependent thermoelectric power of YbBiPt from 4 to 300 K (open circles). The solid line depicts the calculated diffusion TEP (see text) while the dashed line shows the resulting phonon-drag TEP component.

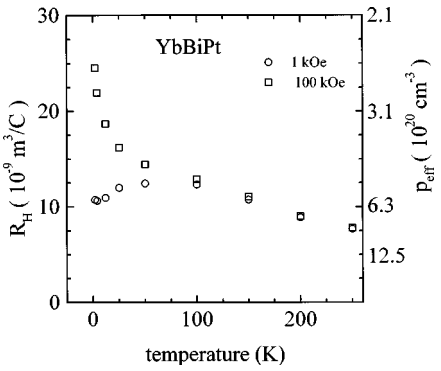

FIG. 3. Temperature-dependent Hall coefficient of YbBiPt from 2 to 250 K in 1 kOe (open circles) and 100 kOe (open squares). The effective hole concentration $p_{\rm eff}$ is plotted on the right axis.

independent at 100 K (i.e., $H_{\rm con}^{100\,\rm K}>100$ kOe).

III. DISCUSSION

A semimetal's electronic structure is characterized by an electronlike band and a holelike band that barely overlap at the Fermi energy. The bands form small ellipsoidal electron and hole pockets with nearly equivalent, temperature-independent carrier concentrations that are much less than that of a conventional wide-band metal. The electronic transport properties of such a system is a weighted average of the transport due to both bands. In general, one band exhibits a significantly lower effective mass, and, hence, a higher mobility than does the other band. This high-mobility band will, therefore, dominate the transport properties. The presence of two bands with low-carrier concentrations is reflected in the resistivity, Hall effect, and thermoelectric power, and easily distinguishes a semimetal from a conventional wide-band metal. In the discussion to follow, the electronic transport properties of YbBiPt are analyzed semiquantitatively and are shown to be fully consistent with a semimetallic description.

The field and temperature dependences exhibited by the Hall effect of YbBiPt are characteristic of a semimetal. In contrast, conventional metals display essentially no temperature or field dependence in R_H. To describe R_H for a semimetal, a two-band model is required; with an electron concentration n, a hole concentration p, and electron and hole mobility's of μ_e and μ_h, the Hall coefficient is given by[21]

$$R_H=\frac{1}{e}\,\frac{p\mu_h^2-n\mu_e^2+\mu_e^2\mu_h^2(p-n)H^2}{(n\mu e+p\mu_h)^2+\mu_e^2\mu_h^2(p-n)^2H^2}, \qquad (1)$$

where e is the electron's charge. While this model misses many details required to fully describe the Hall effect of a semimetal (the electron and hole pockets are usually anisotropic and require six orthogonal mobility parameters to describe the two bands), it can be employed to interpret qualitatively the H and T dependence evident in the data shown in Figs. 3 and 4. Equation (1) indicates that the characteristic fields $H_{\rm con}$ and $H_{\rm sat}$ will vary as $(\mu_e\mu_h)^{-1}$. With mobilities dominated by electron-phonon interactions, $\mu\propto 1/T$. Hence,

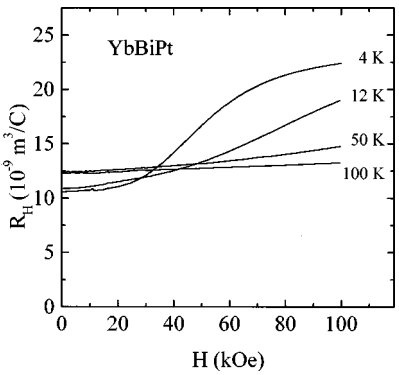

FIG. 4. Magnetic-field-dependent Hall coefficient of YbBiPt in fields to 100 kOe at 4, 12, 50, and 100 K.

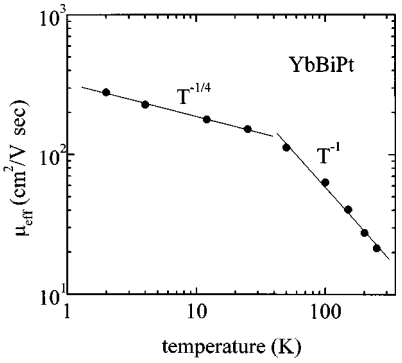

FIG. 5. Temperature-dependent one-band effective mobility μ_{eff} of YbBiPt. The solid lines indicate the power-law dependences of μ_{eff} in the low ($T \leqslant 30$ K) and high-temperature regimes.

Eq. (1) predicts that H_{con} and H_{sat} should rise with increasing temperature; this is precisely the H and T dependence displayed in Fig. 4.

To move beyond this qualitative description, a more vigorous model is required that accounts for the ellipsoidal nature of the carrier pockets. A description of this nature is beyond the scope of this paper. Although not as precise, a one-band model can usually describe a semimetal because one band typically dominates the transport due to mobility/mass effects. With a dominate-band model the transport is described by an effective mobility μ_{eff} and hole concentration p_{eff} (so chosen for YbBiPt since R_H and S are positive). The Hall coefficient becomes

$$R_H = \frac{1}{e p_{\text{eff}}}. \tag{2}$$

This simple approach works surprisingly well for bismuth and antimony. In both cases reliance on Eq. (2) predicts carrier concentrations that are less than the actual values by only a factor of 2–5, while μ_{eff} differs from the actual value for the dominate band by less than a factor of 2.[20,22] The dominant-band approach, therefore, provides an estimate of these key parameters that should be off by significantly less than an order-of-magnitude. The errors produced by this method are such as to overestimate the carrier concentration. Hence, compounds will be even more semimetallic than indicated by the dominant-band description.

With these caveats in mind, p_{eff} for YbBiPt is noted on the right axis in Fig. 3. The hole concentration of $\sim 6 \times 10^{20}$ cm^{-3} (corresponding to 0.04 carriers per formula unit) is 100 times less than copper, comparable to that of arsenic or graphite, and ten times bigger than that of antimony. This suggests that YbBiPt is a semimetal with a modest carrier number. The T-dependent, low-field ($H = 1$ kOe) effective mobility $\mu_{\text{eff}} = R_H/\rho$ is portrayed in Fig. 5. In keeping with the low-carrier concentration of YbBiPt, the effective mobility is one to two orders of magnitude larger than that of large carrier concentration heavy fermion compounds. Above 40 K the effective temperature dependence of $\mu_{\text{eff}} \propto T^{-1}$ indicates that electron-phonon interactions dominate carrier scattering. Below 40 K the effective mobility varies as $T^{-1/4}$, this unusual temperature dependence is not easily explained. R_H becomes field dependent in this range, suggesting that the anomalous μ_{eff} T-dependence signals a breakdown in the dominate-band approach. While this breakdown may occur due to the influence of multiband effects below ~ 40 K, it may also arise from crystalline electric field (CEF) or Kondo scattering effects.

An alternative description of the Hall effect in YbBiPt is provided by that of the anomalous skew-scattering Hall contribution. Skew scattering is the predominant source of a transverse Hall voltage in most heavy fermion systems. In this description the Hall coefficient becomes[19]

$$R_H = R_0 + \xi g \frac{\mu_B}{k_B} \frac{\chi(T)}{C} \rho_m(T), \tag{3}$$

where R_0 is the conventional Hall term, $g = 8/7$ for Yb,[23] μ_B is the Bohr magneton, k_B is Boltzmann's constant, $\chi(T)$ is the T-dependent magnetic susceptibility, C is the susceptibility's Curie constant, and $\rho_m(T)$ is the resistivity contribution due to magnetic (Kondo) scattering. ξ is a scattering constant that characterizes the strength of the skew scattering; values greater than 0.1 are physically unrealistic. Equation (3) has been employed to successfully describe $R_H(T)$ in a wide variety of heavy electron systems.[19,24] In those cases, R_H is considerably smaller than that exhibited by YbBiPt. As a result, the poor-quality fits that result from describing R_H for YbBiPt with Eq. (3) require unphysically large values of ξ ($\xi \approx 1$). Hence, any skew contribution to the Hall effect of YbBiPt is overwhelmed by the carrier term R_0. That is, the Hall effect of YbBiPt is characteristic of a low-carrier concentration semimetal and not of a conventional metal with a skew-scattering dominated R_H.

As with the Hall effect, the temperature dependence and overall magnitude of the TEP will reflect the underlying electronic structure. The thermal carrier diffusion that produces the TEP effect stems from two sources: a conventional electron-diffusion term (S_d), and a phonon-drag term S_{ph} that stems from carriers interacting with diffusing phonons. The large peak in S evident in the data presented in Fig. 2 is characteristic of the phonon-drag effect, while the T-linear dependence above 200 K is indicative of diffusion thermoelectric power. A semiphenomenological model[25] that can estimate the diffusion TEP for heavy fermion compounds can be used to test this description. The model accounts for both CEF and Kondo scattering contributions to S_d. The phenomenological description produces a diffusion TEP given by[25]

$$S_d = -a\left[S_d^{(1)} + \frac{1}{6\pi^3 N_0 J} S_d^{(2)}\right] + \alpha T, \quad (4)$$

where $S_d^{(1)}$ is a Kondo scattering term, $S_d^{(2)}$ stems from inelastic spin-flip carrier scattering between CEF levels, and a conventional T-linear TEP contribution is accounted for by the term on the right. The signs of both fitting constants α and a are determined by the sign of the dominant carriers, while N_0 is the density of states at the fermi energy E_F, and $J<0$ is the exchange interaction parameter. Both $S_d^{(1)}$ and $S_d^{(2)}$ are calculated via integrals involving the dynamic susceptibility $\mathrm{Im}\chi(\omega)$. This model has been employed successfully to describe the TEP of a number of Kondo systems.[26]

The diffusion TEP of YbBiPt can be calculated with the model presented above by using the inelastic neutron-scattering (INS) measurements of Robinson *et al.*[10] These INS measurements indicate that YbBiPt has a single excitation at $\delta = 5.7$ meV (~ 66 K). The diffusion TEP determined from the model appears as a solid line in Fig. 2; the fitting parameters used are $T_K = 1$ K, $\alpha = 0.07\ \mu\mathrm{V/K^2}$, and $N_0 J = -0.12$. A small peak in S_d occurs at $0.3\delta(\sim 20\ \mathrm{K})$. This corresponds well with the shoulderlike feature evident in the experimental data at this temperature. A further glimpse at the electronic structure is provided by the fitting value α. This parameter is related to the Fermi energy by

$$\alpha = \frac{k_B^2}{e}\frac{\pi^2}{3}\frac{1}{E_F}. \quad (5)$$

The Fermi energy determined from the α fitting value is $E_F = 0.35$ eV, which is considerably smaller than that determined from the TEP of wide-band metals. Lastly, the estimates of E_F and $N_0 J$ derived from the TEP fit provide an independent determination of the Kondo energy scale via the expression $k_B T_K = E_F \exp(-1/N_0|J|)$. The value for T_K so determined (≈ 1 K) is equivalent to that calculated from γ, indicating that the TEP fit depicted in Fig. 2 is fully consistent with the low-T specific heat of YbBiPt.

The difference between the experimental TEP data and the calculated S_d should be the phonon-drag contribution S_{ph}; this difference is denoted by the dashed line in Fig. 2. This remnant term displays the proper temperature dependence expected for the phonon-drag TEP, indicating that this TEP analysis is self-consistent. Assuming a Debye temperature for YbBiPt of $\Theta_D \approx 300$ K, the peak in S_{ph} at $T_{\mathrm{peak}} = 60$ K is consistent with the general expectation $T_{\mathrm{peak}} = \Theta_D/5$. The magnitude of S_{ph} at T_{peak} is roughly a factor of 6 larger than that observed in conventional metals.[27] Theoretically, S_{ph} varies inversely with carrier concentration,[27] indicating again that the carrier count in YbBiPt is well below that of a conventional metal.

The low-carrier count in YbBiPt appears to influence a number of other physical properties of this compound. The Kondo scattering contribution to the resistivity ρ_m scales as N_0,[28,29] and produces a peak at $T_p \sim 0.3\delta$.[29] The modest size of the CEF-derived feature in ρ at this temperature (roughly 20 to 30 K) indicates that magnetic scattering has a minor influence on the resistivity of YbBiPt, instead, the resistivity is dominated by the semimetallic nature of this compound. Similarly, both the Kondo energy scale [$T_K \sim \exp(-1/N_0|J|)$] and the magnetic ordering energy scale ($T_N \sim N_0 J^2$) are quite low, in part, due to the low density of states at the Fermi energy.

IV. CONCLUSIONS

The electronic transport properties of YbBiPt indicate that this compound is a semimetal. From the Hall effect a one-band approximation gives an upper limit carrier concentration estimate of 6×10^{20} holes/cm^3 and a mobility dominated by electron-phonon scattering. The TEP displays a anomalously large phonon-drag peak and a large T-linear contribution that are both consistent with a low-carrier concentration. This low-carrier count also dominates the resistivity and reduces any magnetic contribution to $\rho(T)$. These results indicate that the original conjecture by Fisk *et al.*,[1] that the highly renormalized state of YbBiPt is a manifestation of a semimetallic electron structure, was correct.

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