Anomalous Diamagnetism of YbPb₃ Compound: Pressure Effects


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The effect of a uniform pressure on the magnetic susceptibility was measured for YbPb₃ compound, wherein a degeneracy point of the energy bands is located just below the Fermi level and responsible for the anomalous diamagnetism. Theoretical analysis of the experimental data has revealed that a pronounced increase of diamagnetism with pressure is governed by closing the degeneracy point towards the Fermi energy

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1. Introduction

The detailed calculations of the band structure in isostructural and isovalent AuCu₃-type compounds CaSn₃, CaPb₃, YbSn₃, and YbPb₃ (where Yb atoms are divalent) [1, 2] revealed a degeneracy point of the energy bands $E_d$ in the vicinity of

![Fig. 1. Experimental (○) and theoretical (solid line) magnetic susceptibility of YbPb₃ [1] (a) and its pressure dependence at 78 and 300 K (b).](243)
the Fermi level $E_F$. According to the existing theory of the orbital susceptibility for degenerated bands [3, 4] this peculiarity gives rise to an anomalous diamagnetism with a distinctive temperature dependence, which was observed experimentally in these systems (see e.g. [1, 5]). The real magnitude of the effect is strongly governed by the parameter $\xi = E_F - E_d$, being a giant at $E_F = E_d$, $T = 0$ K. In YbPb$_3$ compound $E_F$ is so close to $E_d$ that the anomalous diamagnetism dominates in its magnetic susceptibility [1, 2] (see Fig. 1a). Here we report results of a study of the pressure effect on magnetic susceptibility and electronic structure of YbPb$_3$ to gain a better insight into the nature of the anomalous magnetism in this and similar $RM_3$ compounds.

2. Results and discussion

The YbPb$_3$ sample was grown by a similar to [6] method in the form of druse involving a few single crystals of 1–3 mm in size immersed in an excess of Pb with total mass of about 0.7 g. The measurements of susceptibility $\chi$ were carried out under helium gas pressure up to 2 kbar at fixed temperatures 78 and 300 K by using the pendulum-type magnetometer placed into a non-magnetic pressure cell [7]. The relative errors did not exceed 0.2%. Experimental dependences $\chi(P)$ (Fig. 1b) show a linear increase of diamagnetism with pressure. The corresponding pressure derivatives of susceptibility are listed in Table.

<table>
<thead>
<tr>
<th>$T$ (K)</th>
<th>$\chi_0$</th>
<th>$\chi_{\text{meas}}$</th>
<th>$d\chi_{\text{meas}}/dP$</th>
<th>$d\chi_0/dP$</th>
<th>$d\chi_{\text{theor}}/dP$</th>
</tr>
</thead>
<tbody>
<tr>
<td>78</td>
<td>$-1.542$</td>
<td>$-1.062$</td>
<td>$-8.5 \pm 1.5$</td>
<td>$-11.1 \pm 2$</td>
<td>$-13.3$</td>
</tr>
<tr>
<td>300</td>
<td>$-0.715$</td>
<td>$-0.526$</td>
<td>$-3.4 \pm 1$</td>
<td>$-4.4 \pm 1.5$</td>
<td>$-3.3$</td>
</tr>
</tbody>
</table>

It should be noted that our values of the magnetic susceptibility at ambient pressure somewhat differ from the data of [1] for the YbPb$_3$ single crystal of high quality (see Table). That is obviously due to the presence in our sample, of the free Pb foreign phase and a small amount of Yb$_2$O$_3$ impurity, which contribute the temperature independent weak diamagnetism of Pb and the Curie–Weiss paramagnetism [5] of Yb$^{3+}$ ions. From analysis of the difference in $\chi$ at two temperatures from Table the weight contents of Pb and Yb$_2$O$_3$ were estimated to be about 23% and 1%, respectively. Despite the relatively large content of the free Pb in the sample, its contribution to the measured pressure effect is negligible because of
a mainly ionic nature of Pb diamagnetism. As to the paramagnetism of Yb$_2$O$_3$, its pressure dependence, arisen from the volume effect on the paramagnetic Curie temperature $\theta$ ($\approx -3$ K [5]), appears to be well below the experimental error bars. Hence the evaluations of the pressure derivative for the intrinsic susceptibility of YbPb$_3$ from the measured effect (Table) include only corrections for the weight content of the YbPb$_3$ compound in the sample.

As it has been established earlier [1, 2], the dominant contribution to the magnetic susceptibility $\chi$ ($\equiv \chi_0$) of YbPb$_3$ is the orbital diamagnetism $\chi_d$ of degenerated bands. Within two-band approximation of the spectrum in the vicinity of the critical point $E_d$ (Fig. 2a) $\chi_d$ can be calculated by [2]

$$\chi_d = A \int_{0}^{\xi_0} \frac{d\xi}{\varepsilon} \left[ \frac{1}{1 + \exp \left( \frac{-\varepsilon - \xi}{T} \right)} - \frac{1}{1 + \exp \left( \frac{\varepsilon - \xi}{T} \right)} \right].$$

(1)

Here $A$ is ab initio calculated scaling coefficient, $\xi_0$ — so-called cutoff parameter, and $\xi = E_F - E_d$. By including in (1) the effect of electron scattering on defects of the lattice in terms of the effective temperature $T_{sc}$ added to the real $T$, the best fit of (1) to the experimental $\chi(T)$ data [1] has been obtained with $\xi \approx 0.7$ mRy and $T_{sc} \approx 50$ K [2]. Since the $\chi_d$ magnitude is mainly determined by the $\xi$ value, the pressure effect on $\chi$ is assumed to be governed by the pressure dependence of $\xi(P)$ and can be described as

$$\frac{d\chi}{dP} \approx \frac{d\chi_d}{dP} \approx \frac{\partial \chi_d}{\partial \xi} \frac{d\xi}{dP}.$$  

(2)

Fig. 2. (a): Calculated band structure of YbPb$_3$ along the XR direction of the Brillouin zone (see insert) in the vicinity of the Fermi level $E_F = 0$ [2]. (b) Volume dependence of the relative position of $E_F$ and degeneracy point $E_d$. The data for the equilibrium unit-cell volume at ambient pressure are marked by arrow.

The ab initio full potential linear muffin-tin orbital (FP-LMTO) band structure calculations for YbPb$_3$ (see [2] for details) are carried out for a number of the lattice parameters close to the experimental value. This has allowed us to determine the volume dependence of $\xi$ (Fig. 2b) and the corresponding pressure derivative $d\xi/dP \approx -23$ mRy/Mbar, by using the calculated value of the bulk
modulus \( B = 0.53 \) Mbar. By substitution of this \( \frac{d\xi}{dP} \) value into (2), together with the value of \( \frac{\partial \chi_{\varphi}}{\partial \xi} \) evaluated within (1) with the above-mentioned set of \( \xi \) and \( T_{sc} \) data, the obtained estimates for the pressure effect of \( \frac{d\chi}{dP} \) appeared to be in good agreement with the experimental results (see Table).

3. Summary

In summary, the experimental and theoretical studies of the pressure effect on \( \chi \) in YbPb\(_3\) have revealed that the pronounced increase of the anomalous diamagnetism with pressure is caused by decreasing the energy separation between \( E_F \) and the degeneracy point \( E_d \). The initial \( E_F \) position has been unambiguously determined to be above \( E_d \) energy. The obtained estimate of \( \frac{d\xi}{dP} \approx -23 \) mRy/Mbar together with the best fit initial value of \( \xi \approx 0.7 \) mRy from [2] allow to expect a topological electronic phase transition in YbPb\(_3\) at \( P \approx 30 \) kbar, which is accompanied by closing the small electron “pockets” at the XR line of the Brillouin zone and a peak of the anomalous diamagnetism.

References