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Anomalous Diamagnetism of $YbPb_3$ Compound: Pressure Effects

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The effect of a uniform pressure on the magnetic susceptibility was measured for $YbPb_3$ 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 $AuCu_3$-type compounds $CaSn_3$, $CaPb_3$, $YbSn_3$, and $YbPb_3$ (where Yb atoms are divalent) [1, 2] revealed a degeneracy point of the energy bands E_d in the vicinity of

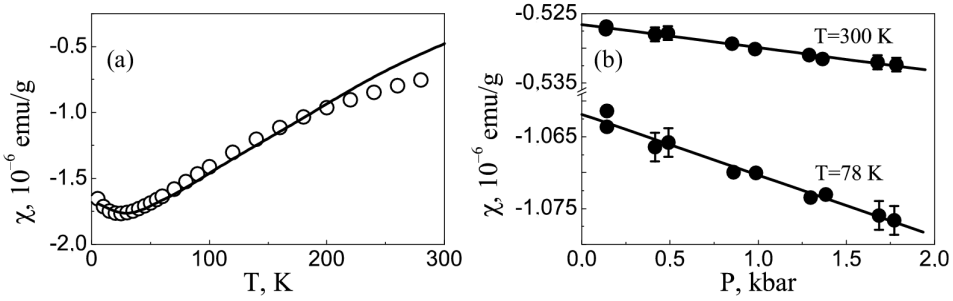

Fig. 1. Experimental (○) and theoretical (solid line) magnetic susceptibility of $YbPb_3$ [1] (a) and its pressure dependence at 78 and 300 K (b).

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 $\xi = E_{\mathrm{F}} - E_{\mathrm{d}}$, being a giant at $E_{\mathrm{F}} = E_{\mathrm{d}}$, $T = 0$ 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_3compounds.

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 χ 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

Magnetic characteristics of $YbPb_3$ compound: χ_0 is intrinsic susceptibility according to work [1], χ_{meas} and $\mathrm{d}\chi_{\mathrm{meas}}/\mathrm{d}P$ measured values of the sample susceptibility and its pressure derivative, $\mathrm{d}\chi_0/\mathrm{d}P$ pressure derivative of the intrinsic susceptibility, and $\mathrm{d}\chi_{\mathrm{theor}}/\mathrm{d}P$ calculated pressure effect.

T	χ_0	χ_{meas}	$\mathrm{d}\chi_{\mathrm{meas}}/\mathrm{d}P$	$\mathrm{d}\chi_0/\mathrm{d}P$	$\mathrm{d}\chi_{\mathrm{theor}}/\mathrm{d}P$
K	10^{-6} emu/g		10^{-6} (emu/g)/Mbar		
78	-1.542	-1.062	-8.5 ± 1.5	-11.1 ± 2	-13.3
300	-0.715	-0.526	-3.4 ± 1	-4.4 ± 1.5	-3.3

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_2O_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 χ at two temperatures from Table the weight contents of Pb and Yb_2O_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_2O_3, its pressure dependence, arisen from the volume effect on the paramagnetic Curie temperature θ (≈ -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 χ ($\equiv \chi_0$) of $YbPb_3$ is the orbital diamagnetism $\chi_{\rm d}$ of degenerated bands.Within two-band approximation of the spectrum in the vicinity of the critical point $E_{\rm d}$ (Fig. 2a) $\chi_{\rm d}$ can be calculated by [2]

$$\chi_{\rm d} = A \int_0^{\xi_0} \frac{{\rm d}\varepsilon}{\varepsilon} \left[\frac{1}{1+\exp\left(\frac{-\varepsilon-\xi}{T}\right)} - \frac{1}{1+\exp\left(\frac{\varepsilon-\xi}{T}\right)} \right]. \tag{1}$$

Here A is *ab initio* calculated scaling coefficient, ξ_0 — so-called cutoff parameter, and $\xi = E_{\rm F} - E_{\rm d}$. By including in (1) the effect of electron scattering on defects of the lattice in terms of the effective temperature $T_{\rm sc}$ added to the real T, the best fit of (1) to the experimental $\chi(T)$ data [1] has been obtained with $\xi \simeq 0.7$ mRy and $T_{\rm sc} \simeq 50$ K [2]. Since the $\chi_{\rm d}$ magnitude is mainly determined by the ξ value, the pressure effect on χ is assumed to be governed by the pressure dependence of $\xi(P)$ and can be described as

$$\frac{{\rm d}\chi}{{\rm d}P} \simeq \frac{{\rm d}\chi_{\rm d}}{{\rm d}P} \simeq \frac{\partial\chi_{\rm d}}{\partial\xi}\frac{{\rm d}\xi}{{\rm d}P}. \tag{2}$$

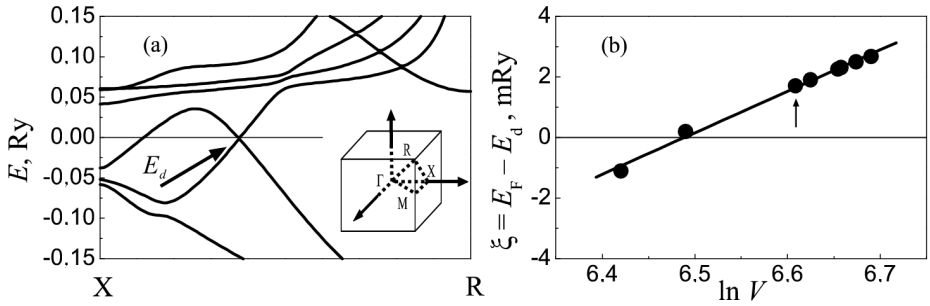

Fig. 2. (a): Calculated band structure of $YbPb_3$ along the XR direction of the Brillouin zone (see insert) in the vicinity of the Fermi level $E_{\rm F} = 0$ [2]. (b) Volume dependence of the relative position of $E_{\rm F}$ and degeneracy point $E_{\rm d}$. The data for the equilibrium unit-cell volume 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 ξ (Fig. 2b) and the corresponding pressure derivative ${\rm d}\xi/{\rm d}P \simeq -23$ mRy/Mbar, by using the calculated value of the bulk

modulus $B = 0.53$ Mbar. By substitution of this $\mathrm{d}\xi/\mathrm{d}P$ value into (2), together with the value of $\partial\chi_{\mathrm{d}}/\partial\xi$ evaluated within (1) with the above-mentioned set of ξ and T_{sc} data, the obtained estimates for the pressure effect of $\mathrm{d}\chi/\mathrm{d}P$ 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 χ 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 $\mathrm{d}\xi/\mathrm{d}P \simeq -23$ mRy/Mbar together with the best fit initial value of $\xi \simeq 0.7$ 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.

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