Effect of pressure on thermopower and electrical resistivity of YbMn$_2$Ge$_2$

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Abstract. The thermopower $S$ and electrical resistivity $\rho$ of YbMn$_2$Ge$_2$ were measured under pressures up to 2 GPa in the temperature range from 1.5 to 300 K. The magnetic transition temperature increases with increasing pressure, having maximum at $P_c \approx 1.3$ GPa, and decreases with increasing pressure above $P > 1.3$ GPa. The temperature dependences of $S$ and $\rho$ change their features at critical pressure $P_c \approx 1.3$ GPa, where reported that the mean Yb valence value changes from +2.4 to +2.8 at room-temperature. The pressure dependences of $S$ and $\rho$ at 4.2 and 300 K show the abrupt changes at the critical pressure, which indicate the changes of the electronic state near the Fermi level and the magnetic structure of Mn 3d electron.

1. Introduction

The intermetallic compound of YbMn$_2$Ge$_2$ crystallizes in the ThCr$_2$Si$_2$-type body-centered tetragonal structure. YbMn$_2$Ge$_2$ is an antiferromagnet (AFM-I phase) with the Neel temperature of $T_{N1} \approx 510$ K, where the Mn magnetic moments order in a planar antiferromagnetic structure and an additional magnetic transition at $T_{N2} \approx 185$ K of AFM-II phase. There is no evidence of a magnetic ordering of the Yb sublattice at temperatures down to 1.5 K. It was reported that the Yb ion in this compound is in a mixed valence state between divalent and trivalent [1, 2]. The competing behavior between AFM-I and AFM-II states and the pressure induced magnetic phase transition associated with a change of Yb ionic state at $P \approx 1.25$ GPa were revealed by the measurements of the magnetic susceptibility, XANES and X-ray diffraction under high pressures [3, 4, 5]. It is considered that the instability of Yb ion states has an important role for the magnetic structure of Mn sublattice. The results of the band structure calculations for YbMn$_2$Ge$_2$ indicate that the large density of states (DOS) caused mainly by the Mn 3d electrons lies near the Fermi level [6], which means that the transport properties in YbMn$_2$Ge$_2$ are strongly correlated with the state of Mn 3d electrons. Thus the measurements of the transport properties such as thermopower $S$ and electrical resistivity $\rho$ are instructive in investigating the magnetic state of Mn 3d electrons. However, as far as we know, few studies on the transport properties of YbMn$_2$Ge$_2$ under pressure have been performed. In this paper we present the experimental results on the thermopower $S$ and electrical resistivity $\rho$ of YbMn$_2$Ge$_2$ measured under hydrostatic pressures up to 2 GPa.
2. Experimental Procedure
A single-crystalline sample of YbMn$_2$Ge$_2$ prepared by an In flux method was used for the present study. The measurements of $S$ and $\rho$ were carried out by using the differential method with a seesaw heating procedure [7] and the standard four-probe dc method, respectively. $S$ and $\rho$ were measured simultaneously at temperatures from 1.5 to 300 K. A clamp-type piston cylinder pressure cell was used for the measurements of $S$ and $\rho$ under pressures up to 2 GPa. The directions of the current and the temperature gradient were made perpendicular to the $c$-axis.

3. Results and Discussion
The temperature dependences of $S$ and $\rho$ of YbMn$_2$Ge$_2$, under various pressures at the temperature range between 1.5 K and 300 K, are shown in Fig. 1. With decreasing temperature, Both $\rho(T)$ and $S(T)$ at ambient pressure show a kink around 165 K, indicated by arrows in Fig. 1, which correspond to the lower magnetic transition temperature of $T_{N2}$ [2, 3]. The temperature dependences of $S$ and $\rho$ change their features at the critical pressure $P_c \approx 1.3$ GPa. The temperature dependence of $\rho$ at 2 GPa is consistent with the data in the literature [8]. There is no clear evidence of the magnetic phase transition in $\rho(T)$ at $P > 1.3$ GPa, while $S(T)$ shows the characteristic feature accompanied by the magnetic phase transition in entire pressure range. The magnetic phase transition temperatures $T_{N2}^{R}$ and $T_{N2}^{S}$ are determined as the temperatures where the temperature derivatives of electrical resistivity $d\rho/dT$ and thermopower $dS/dT$ take maxima, respectively. The obtained magnetic phase transition temperatures $T_{N2}^{R}(\triangle)$ and $T_{N2}^{S}(\times)$ are shown in Fig. 2. The pressure dependence of the upper magnetic ordering temperature $T_{N1}$ reported in the earlier study [3] is also presented. As shown in Fig. 2, $T_{N2}^{R}(\triangle)$ and $T_{N2}^{S}(\times)$ are in good agreement with the results in Ref. [3].

The upper panel of Fig. 3 shows the pressure dependences of $S$ and $\rho$ at 300 K. The abrupt decreases in $S$ and $\rho$ are observed at the critical pressure, $P_c \approx 1.3$ GPa, of the magnetic phase...
transition from AFM-I to AFM-III, which corresponds to the change of the mean value of Yb valence from +2.4 to +2.8. The lower panel of Fig. 3 depicts the pressure dependences of $S$ and $\rho$ at 4.2 K. $S$ and $\rho$ indicate the similar behaviors as that at 300 K; Both $S$ and $\rho$ show the abrupt changes at the phase boundary between AFM-I and AFM-III and between AFM-II and AFM-IV \cite{4}, which indicate that the pressure-induced magnetic phase transitions at $P \approx P_c$ are of the first order.

The temperature dependence of $\rho$ at $P \lesssim 1.3$ GPa can be represented as $\rho - \rho_0 = AT^2$ in the temperature region up to 15 K, which implies the significant development of the spin wave in the phase AFM-II. However, the $T^2$ dependence of $\rho$ does not observed in the AFM-IV phase ($P > 1.3$ GPa) even at lowest temperatures. On the other hand, the diffusion thermopower $S_d$ of metal at low temperatures is expressed by the Mott’s formula:

$$S_d = \frac{\pi^2 k_B^2}{3 e} T \frac{1}{\sigma} \frac{\partial \sigma}{\partial \epsilon} \bigg|_{\epsilon = \epsilon_F} .$$

Here, $k_B$ is the Boltzmann’s constant, $e$ is the electronic charge and $\sigma$ is the energy dependent electrical conductivity. This formula predicts a linear temperature dependence for $S$ at low temperatures. In the case of YbMn$_2$Ge$_2$, no linear dependence is observed at low temperatures. Additionally, $T^3$ dependence owing to the phonon drag effect is not observed in $S(T)$ at low temperature region. As mentioned above, in the phase of AFM-II, the electron scattering due to the spin wave has a dominant role for $\rho$ at low temperatures. Therefore, the drag effect of the spin wave on $S(T)$ at low temperatures should be taken into account. We assume that the temperature dependence of thermopower due to the magnon drag $S_m$ is expressed

Figure 3. Pressure dependences of $S$ (●) and $\rho$ (▲) at 300 K (upper panel) and at 4.2 K (lower panel). The vertical dashed lines indicate the critical pressure $P_c$. The dotted lines are guides for the eye.

Figure 4. Pressure dependences of the coefficients of $a$ (●) and $b$ (▲), in eq. (2). The vertical dashed line indicates the critical pressure $P_c$. The dotted lines are guides for the eye.
as $S_m = bT^{3/2}$ [9]. At low temperatures of $T \lesssim 10$ K, the total thermopower $S(T)$ is represented as

$$S(T) = S_d + S_m = aT + bT^{3/2}. \quad (2)$$

The obtained values of the temperature coefficients of $a$ and $b$ show the discontinuous changes at $P \approx P_c$, as shown in Fig. 4.

The existence of the large DOS of Mn 3d electrons $N_d$ near the Fermi level allows us to assume that the diffusion thermopower $S_d$ is expressed as

$$S_d = \frac{\pi^2 k_B^2 T}{3e} \left[ \frac{1}{N_d} \frac{\partial N_d}{\partial \varepsilon} \right]_{\varepsilon = \varepsilon_F},$$

by adopting the Mott’s s-d scattering model for the conductivity $\sigma$ in eq. (1) [9]. It indicates that $S$ is very sensitive to the electronic state near the Fermi level. From the results mentioned above, it is considerable that the pressure variations of the coefficients of $a$ and $b$ at $P \approx P_c$ shown in Fig. 4 are correspond to the discontinuous change of DOS near the Fermi level and the change of the magnetic structure of Mn 3d electrons.

In summary, thermopower $S$ and electrical resistivity $\rho$ of YbMn$_2$Ge$_2$ have been measured under hydrostatic pressures up to 2 GPa at temperatures from 1.5 K to 300 K. The electron scattering due to the spin wave has a dominant role for the low temperature transport properties in the phase AFM-II. The temperature dependences of $S$ and $\rho$ change their feature at $P \approx 1.3$ GPa. The pressure dependences of $S$ and $\rho$ at 4.2 K and 300 K show the abrupt changes at the critical pressure $P \approx 1.3$ GPa, indicating the change of the electronic state near the Fermi level, which corresponds to the valence transition of Yb.

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