Transport properties of Heusler Compound Mn$_3$Si under high pressure

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Abstract. The electrical resistivity $\rho$ and the thermopower $S$ of the single crystalline sample of the Heusler compound Mn$_3$Si have been measured in the temperature range between 2 and 300 K under high pressures up to 2.2 GPa. The temperature variations of $\rho$ and $S$ indicate the characteristic features at the Néel temperature $T_N$. An additional anomaly in $S(T)$, related to the 3$Q$ satellites in SDW, is observed at $P<1$ GPa, and it disappears at $P>1$ GPa. The Néel temperature, obtained from $\rho(T)$ and $S(T)$ curves, increases with increasing pressure. The pressure dependences of the residual resistivity and the thermopower at $T=2$ K show the discontinuous changes at $P \approx 1$ GPa, indicating a pressure induced phase transition.

1. Introduction
The Heusler compound of Mn$_3$Si with the DO$_3$-type cubic crystal structure orders antiferromagnetically at the Néel temperature $T_N = 23$ K with incommensurate spin structure of a propagation vector $Q = 0.425G_{111}$, where $G_{111}$ is the reciprocal lattice vector along the [111] direction [1, 2]. The Mn atoms have two crystallographic sites of Mn(I) and Mn(II). The Mn(I) and Mn(II) atoms are surrounded by eight Mn nearest neighbors, and four Mn and four Si nearest neighbors, respectively. Due to this difference of the nearest neighbor atomic configurations, the atoms of Mn(I) and Mn(II) sites have different magnetic moments in magnitude. This crystal structure can be seen as a layered structure stacking the (111) planes in a sequence of planes of Mn(I), Mn(II), and Si atoms, respectively.

From the neutron diffraction measurements, the spin structure in the SDW of Mn$_3$Si has been found to be either a helical or a transversal sinusoidal structures [2, 3, 4]. However, the correct spin structure is not determined yet. The estimated values of magnetic moments of Mn(I) and Mn(II) from the analysis of the fundamental satellites by assuming the helical spin structure are 1.7 $\mu_B$ and 0.2 $\mu_B$, respectively, and for the transversal sinusoidal structure the maximum amplitude of their magnetic moments are 2.4 $\mu_B$ and 0.28 $\mu_B$, respectively [1, 2].

Tomiyoshi et al. have investigated higher harmonics SDW in Mn$_3$Si by the neutron diffraction [2]. At low temperatures below $T_a \approx 8$ K, the third-order harmonics satellites have been observed at the 3$Q$ positions expected by the propagation wave vector $Q$ of the fundamental satellite. The anomalies in the temperature dependence of the specific heat $C$ were
observed at $T_N$ and $T_a$. It was also reported that $T_a$ is independent of an external magnetic field up to 14 T [5].

The results of the band structure calculations for Mn$_3$Si reveal that the large electronic density of states (DOS) due to mainly Mn 3d electrons lies near the Fermi level [6]. Since the electron scattering is sensitive to the electronic state in the vicinity of the Fermi level, the measurements of the transport properties, such as the electrical resistivity and the thermopower, are instructive in investigating the magnetism and the electronic state around the Fermi level. In order to clarify the pressure effect on the magnetic and the transport properties of Mn$_3$Si, we have measured the electrical resistivity $\rho$ and the thermopower $S$ at temperatures from 2 to 300 K under hydrostatic pressures up to 2.2 GPa.

2. Experimental

Single crystalline sample of Mn$_3$Si was prepared by the Bridgeman method from the stoichiometric ratio of the pure constituents of 99.9% Mn and 99.999% Si. The detailed procedure for the sample preparation has been described elsewhere [2]. No impurity phase in the specimen was detected in the powder X-ray diffraction measurement. The measurements of the electrical resistivity $\rho$ and the thermopower $S$ were carried out by the standard four-probe dc method and the differential method with seesaw heating procedure [7], respectively. The piston-cylinder-type high-pressure cell with Daphne 7373 as the pressure transmitting medium was used for the simultaneous measurements of $\rho$ and $S$ at temperatures from 2 to 300 K under hydrostatic pressures up to 2.2 GPa [8]. The electrical current and the heat flow were applied in the same direction of the [111] axis.

3. Results and Discussion

Figure 1 shows the temperature dependences of the electrical resistivity $\rho$ and thermopower $S$ of Mn$_3$Si in the temperature range between 2 and 300 K at ambient pressure. $\rho$ decreases with decreasing temperature, and shows a sharp drop below $T_N$. $S$ also decreases monotonously with decreasing temperature, and shows a characteristic feature at low temperatures below about 50 K, as seen in Fig. 1. $S$ shows upturn below $T \approx 30$ K, having a maximum at $T \approx 17$ K, and
Figure 2. Temperature dependence of the electrical resistivity $\rho$ of Mn$_3$Si under pressures up to 2.2 GPa.

Figure 3. Temperature dependence of the thermopower $S$ of Mn$_3$Si under pressures up to 2.2 GPa. The inset shows an enlarged view of $S(T)$ at low temperatures.

an additional anomaly in the form of a local minimum, as indicated in Fig. 1, was observed at $T_a \approx 7.8$ K, where the 3Q satellites in SDW were confirmed by the neutron diffraction [2]. No distinct change around $T_a$ in $\rho(T)$ curve, however, was detected.

Figure 2 and 3 show the temperature dependences of $\rho$ and $S$ under pressures up to 2.2 GPa, respectively. The temperature variation of $\rho$ under pressure is almost the same as that in ambient pressure in the whole temperature range. $\rho$ decreases with decreasing temperature in the paramagnetic phase, and shows a steep decrease in the antiferromagnetic phase. The residual resistivity $\rho_0$, which is determined as the resistivity at the lowest temperature of 2 K, increases with increasing pressure $P$. The electrical resistivity at higher temperatures above $T_N$ increases with increasing pressure up to $P \approx 1$ GPa, and decreases with further increase of $P$. In the whole pressure range, $S$ shows qualitatively the same temperature dependence at temperatures above $T \approx 50$ K. On the other hand, the low-temperature thermopower shows the large pressure variation, as can be seen in the inset of Fig. 3. The pressure dependences of $T_N$ and $T_a$, obtained from $\rho(T)$ and $S(T)$ curves, are shown in Fig. 4. $T_N$ increases linearly with increasing pressure $P$, $dT_N/dP \approx 3.5$ K/GPa. $T_a$ also increases with increasing $P$ at $P < 1$ GPa, and most likely disappears at the critical pressure $P_c \approx 1$ GPa.

In low temperature limit, the diffusion thermopower $S_d$ for metallic conductor is expressed by the Mott’s formula:

$$S_d = \frac{\pi^2 k_B^2}{3e} T \left( \frac{1}{\sigma} \frac{\partial \sigma}{\partial \varepsilon} \right).$$

Here, $k_B$ is the Boltzmann’s constant, $e$ is the electronic charge and $\sigma$ is the energy dependent electrical conductivity [9]. This formula predicts a linear temperature dependence for $S$ at the low temperature region. As shown in the inset of Fig. 3, no linear temperature variations of $S(T)$ in Mn$_3$Si, however, are observed at low temperatures, indicating a large contribution of the magnetic scattering of conduction electrons to the low temperature transport properties. Then, we use the thermopower at $T = 4$ K, $S_{4K}$, instead of the temperature gradient of thermopower $S/T$, to investigate the effect of pressure on $S$. In Fig. 5, we show the pressure dependences of
Figure 4. Pressure dependences of $T_N$ and $T_a$ of Mn$_3$Si. The symbols of the circles and triangles are obtained from $\rho(T)$ and $S(T)$, respectively.

Figure 5. Pressure dependences of the thermopower at $T = 4$ K, $S_{4K}$, and the residual resistivity $\rho_0$.

$S_{4K}$ and the residual resistivity $\rho_0$ by the closed and open symbols, respectively. As seen in Fig. 5, both $S_{4K}$ and $\rho_0$ show the discontinuous changes at $P_c \approx 1$ GPa, where an anomaly in $S(T)$ related to the 3Q satellites in SDW disappears. The sign of $S_{4K}$ is positive for $P < 1$ GPa and is negative for $P > 1$ GPa. The variation of $\rho_0$ also indicate a discontinuous change around $P_c$. These behaviors imply that the electronic state around the Fermi level is modified by applying pressure, namely a pressure induced phase transition takes place.

In summary, the electrical resistivity and the thermopower have been measured at temperatures from 2 to 300 K under hydrostatic pressures up to 2.2 GPa. The Néel temperature $T_N$, obtained from $\rho(T)$ and $S(T)$ curves, increases linearly with increasing pressure $P$, $dT_N/dP \approx 3.5$ K/GPa. An additional anomaly in $S(T)$ related to the 3Q satellites in SDW is confirmed at $P < 1$ GPa, and it most likely disappears at $P_c \approx 1$ GPa. The pressure dependence of the residual resistivity and the thermopower at $T = 4$ K show the discontinuous changes at $P_c \approx 1$ GPa, indicating a pressure induced phase transition.

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