Resistivity and thermopower of CaB_6 single crystal

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Abstract

The resistivity ρ and thermopower S of CaB_6 single crystal have been measured at temperatures from 2 K to 1100 K in magnetic fields up to 15 T. Temperature dependence of ρ is expressed as $[\rho(T) - \rho(0)] \propto \exp\left[-(T^*/T)^{1/2}\right]$ for $T \leq$90 K and 1.7-th power of T for 90 K$\leq T \leq$1100 K, where ρ_0=232 $\mu\Omega$ cm. The magnitude of ρ and S are very large suggesting thin concentrration of carriers. The temperature dependence of them suggests the conduction is metallic type. ρ and S can be fitted on the basis of free electron model and obtained the Fermi level is situated near the bottom of an electron band with small electron pocket. The experimental and fitting results appear this compound is semi-metallic. It was observed no scattering anomalies in temperature dependence of ρ and also no sudden change of the Fermi surface accompanied with magnetic transition in it of S above 400 K where it might be considered to have ferromagnetic transition.

Key words: semi-metal; resistivity; thermopower; magnetism

1. Introduction

Many interests have been focused on the compound system of CaB_6 whether the ferromagnetism exists or not, as it was reported that weak ferromagnetism with high ordering temperature over 600 K even if no magnetic elements are included in the compounds [1]. As theoretical calculations and also experimental results of electric structure [2,3] suggested that CaB_6 is in a subtle state whether it is semi-metal or semiconductor, it is also interested to elucidate the electronic structure of CaB_6, however a special conclusion was not established yet. A single crystal of CaB_6 was obtained by XeFZ methods and transport properties of thermopower and resistivity on this crystal have been measured. It is estimated from the results that this compound is semi-metal with single electron bands.

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2. Result and Discussion

The resistivity ρ and thermopower S of CaB_6 single crystal have been measured at temperatures from 2 K to 1100 K in magnetic fields up to 15 T. At first, the resistivity and thermopower at high temperature region are depicted in Fig. 1. It can be seen that the temperature dependence of resistivity exhibits no scattering anomaly over the experimental temperature range and that thermopower shows also no remarkable Fermi surface change at a certain temperature. No evidence of magnetic ordering is observed in the transport properties.

Figure 2 shows thermopower and resistivity at low temperature region. The residual resistivity is 232 $\mu\Omega$ cm, very high compared to usual metals suggesting the band structure is semi-metal. The temperature dependence of ρ is expressed as follows:

$$[\rho(T) - \rho(0)] \propto \exp\left[-(T^*/T)^{1/2}\right] \text{ for } T \leq 90 \text{ K}$$

and,

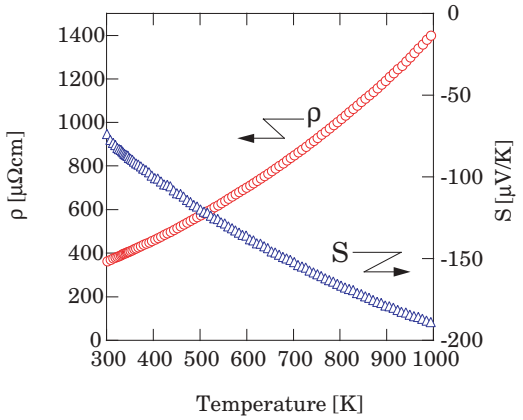

Fig. 1. The resistivity and thermopower at high temperature region from 300 K to 1000 K.

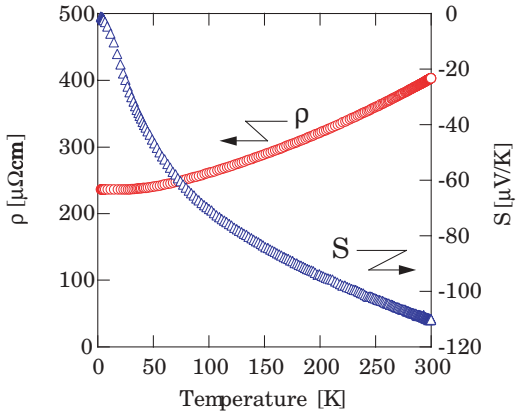

Fig. 2. The resistivity and thermopower at low temperature region from 2 K to 300 K.

$$[\rho(T) - \rho(0)] \propto T^{1.69} \text{ for 90 K} \leq \text{T} \leq \text{1100 K}.$$

Thermopower is negative for all the temperatures and the temperature dependence is simple. The absolute values are very large at room temperature. It is suggested that carriers are electrons in a positive energy derivatives of DOS and that a very small number of carriers in the electron pocket. Qualitative fitting calculation for the resistivity and thermopower has been carried out. The assumption is as follows: Modified free electron model is applied. Chemical potential is determined from reservation of carrier number. The spectral conductivity can be divided in energy dependent part and temperature dependent part as follows: $\omega(\epsilon, T)$=$\omega(\epsilon)\omega(T)$. The phonon resistivity is proportional to T and $\omega(\epsilon)$=ϵ^n, here in the case of complete free electron, $n = 1$.

$$\sigma(T) = \int \omega(\epsilon, T)(-\frac{\partial f^0}{\partial \epsilon})d\epsilon \qquad (1)$$

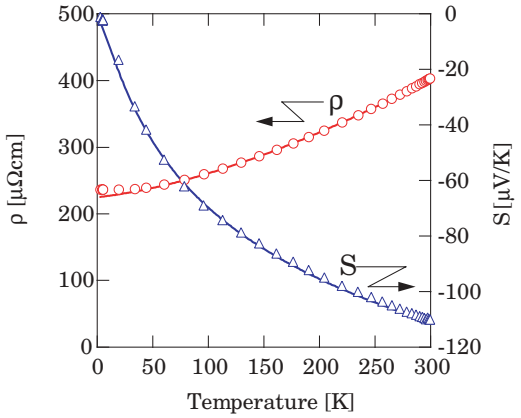

Fig. 3. The fitting results for resistivity and thermopower. Open circles: experimental results of the resistivity, open triangular: experimental results of the thermopower, lines: calculated results.

$$S(T) = \frac{-1}{eT}\frac{\int \omega(\epsilon, T)(\epsilon - \mu)(-\frac{\partial f^0}{\partial \epsilon})d\epsilon}{\sigma(T)} \qquad (2)$$

The results are shown in Fig. 3. The theoretical curves are coincide very well with the experimental results of the resistivity and the thermopower, here fitting parameter of Fermi level ϵ_F =85 K, and $n = 0.8$, close to the free electron value. The results suggest the band structure of this compound is semi-metal as expected. Magnetic fields up to 15T have almost no effect for the resistivity and the thermopower. Thus experimental results suggest that the compound of CaB_6 is semi-metal with a single electron pocket. High resolution ARPES on the same ingot of single crystal [4] reveals that the Fermi surface of this compound is composed of a small electron pocket at X point of Brillouin zone and complete coincide with our results. It also supports a low concentration electron gas model assuming single carrier type [5], however, evidence of ferromagnetism is not observed in this experiments.

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