Static and Dynamic transport study of β-FeSi$_2$ single crystals

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Abstract

Static transport properties and transient thermoelectric effect (TTE) of β-FeSi$_2$ single crystals, which has received considerable attention as optical and thermoelectric devices, have been measured. The Hall and TTE data clearly showed the existence of multiple conduction carrier. From these results, the tentative band scheme is discussed.

Key words: β-FeSi$_2$; transport properties ; transient thermoelectric effect

1. INTRODUCTION

β-FeSi$_2$ attracts considerable attention as potential constituents in optical and thermoelectric devices. However, its type of semiconductor and physical properties depend on how to prepare samples [1,2]. Band calculations predicted that the strong coupling of the band edge-states to the lattice gives rise to a lowering of the carrier mobility [3]. However, the magneto-transport experiments suggest that there exist not only these carriers but also some other carriers with extremely high mobility [4]. In order to clarify such contradictory, it is necessary to perform the detailed studies related to conduction carrier mechanism.

On the other hand, we have currently applied for various types of conductors using a "transient thermoelectric effect (TTE)" which gives us important information on carrier dynamics in multiple conduction carrier systems [5,6]. In the present work, we performed the static transport, magnetization, and photo-induced TTE measurements for β-FeSi$_2$ single crystals. This paper mainly reports conduction carrier dynamics as a multiple conduction system and discuss tentative band nature and impurity scatterings based on the recent band calculations.

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2. EXPERIMENTAL

β-FeSi$_2$ single crystals were grown by a chemical vapor transport method [7]. Electrical contacts to the needle-like crystals [typically (0.1-0.3)$\times$(0.1-0.3)$\times$(2-5) mm^3] for the static transport and TTE measurements were made using In or gold paste. Transport measurements for β-FeSi$_2$ single crystals were performed along the elongated crystalline direction, and were done in the wide temperature range of 4.2-300 K. The magnetization measurements were carried out using SQUID in the range of 4.2-300 K, and the TTE experiments were performed from 77 to 300 K. The experimental setup and measureing principle of the TTE method have been reported earlier [5,6].

3. RESULTS AND DISCUSSION

The typical temperature dependence of resistivity ρ for β-FeSi$_2$ single crystal is shown in Fig. 1. The resistivity ρ shows a characteristic temperature dependence whose features are divided into three regions. In the Region I above 220 K, ρ increases slightly with decreasing temperature, but in the intermediate Region II ($\sim$90 $< T <$ 220 K) ρ behaves as a "degenerate semi-

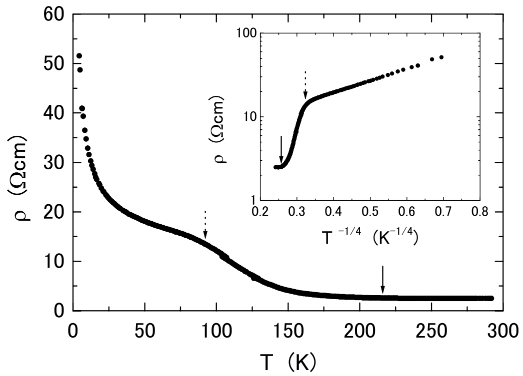

Fig. 1. Temperature dependence of resistivity ρ for β-FeSi$_2$ single crystal. The inset shows the lnρ vs. $(T_0/T)^{1/4}$ plot based on the Mott VRH theory.

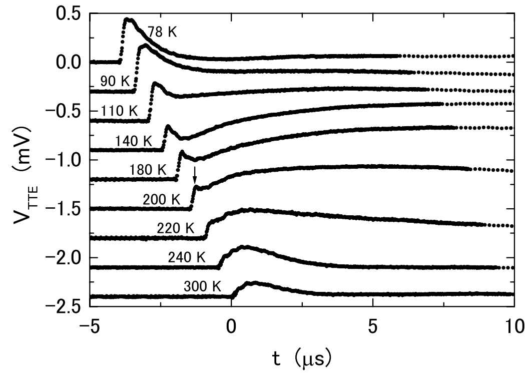

Fig. 2. Typical TTE signals observed in the fast time range of 0-10 μs for β-FeSi$_2$ single crystal.

conductor" whose density of state is finite even at absolute zero temperature. At low temperature below ~90 K (Region III), the ρ-T curve can be well expressed by the three-dimensional Mott-type variable range hopping (VRH) conduction : $\ln\rho \sim (T_0/T)^{1/4}$. It should be mentioned that Regions I and II can be distinguished by an inflection in the ρ-T curve as indicated by the arrow, which suggests an existence of not a crossover but "some phase transition" at 220 K. Such anomaly has been observed for other samples. However, the magnetization data did not show any magnetic ordering in the whole temperature regions. The static magneto-transport data and the negative sign of the static thermoelectric effect at room temperature suggests that the present system in the Region I can be regarded as a single electron system (n-type semiconductor) with the electron concentration of $n = 8\times10^{17}$ cm^{-3} and the low mobility of $\mu = 4$ cm^2/Vs. In the Region II and III, we observed non-linear Hall effect which suggests that the system undergoes multiple carrier system in these temperature regions.

Typical TTE signals in the short time interval of 10 μs, observed in the Region I and II are shown in Fig. 2. In the Region I, the TTE signals are simple; after the pulsed laser is irradiated the positive TTE voltage V_{TTE} is induced within 1 μs and then decays rapidly. Since the present system is the n-type semiconductor with $E_{\mathrm{g}} = 0.8$ eV [8], electron-hole pairs should be excited by the laser light with the photon energy of 1.17 eV, whose carriers are located at the Γ point in the Brillouin zone. The positive TTE voltage induced suggests that the hole mobility is larger than the electron mobility. From the band calculations, on the other hand, the electron and hole effective masses were determined to be of similar magnitude, $0.8m_0$ and $0.85m_0$, respectively. These facts suggests the strong scattering of electrons with non-intentionally doped donors.

The decay process may be due to a "recombination" of the photo-generated electron-hole pairs called as "stage 1", as reported earlier [5]. In the Region II, we have found the interesting results that a very rapid increase becomes visible at 220 K and then shows a peak [see the arrow at 200 K in Fig. 2]. The TTE results obtained in the Region II reveal that the system undergoes from single carrier system to at least two carrier systems at 220 K. The TTE data also suggest that the photo-generated holes (and also electrons) have extremely large mobility compared with those at the Γ point as described above and it supports the reported experimental results [4]. However, the band calculations do not give us that such carriers with extremely light mass exist. One possibility may be that the band structure changed drastically, in which some part in the bands have extremely sharp band edge, due to the phase transition at 220 K. Since the electron density of the present system is very low, any density wave transitions should be ruled out from the possible transition mechanisms. To understand in detail the physical properties of the present system, it is necessary to perform the TTE experiment in the Region III and also low temperature X-ray analysis.

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