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Electrical and thermoelectric properties of the intermetallic $FeGa_3$

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Abstract

The transport properties including electrical resistivity (ρ), thermal conductivity (κ), as well as Seebeck coefficient (S) of intermetallic $FeGa_3$ have been measured as a function of temperature between 10 and 300 K. The electrical resistivity exhibits metallic behavior in the temperature range we investigated. The thermal conductivity is approximately 6 W/m K at room temperature, and is mainly governed by the lattice thermal conductivity. The observed Seebeck coefficient is positive, indicating p-type carriers dominating the thermoelectric transport for $FeGa_3$. In addition, the Fermi level of 0.14 eV measured from the top of valence band was estimated. These observations are in contrast with the reported semiconducting behavior for this compound, presumably attributed to the off-stoichiometric effect on the electronic band structure of $FeGa_3$.

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1. Introduction

Materials with complex band structures have been of considerable interest due to their unusually magnetic and transport properties. Phenomena such as heavy fermion behavior, a Kondo insulating state, and unconventional superconductivity are frequently found in these materials. It has been argued that the effect of hybridization plays an important role for these observations [1–6]. The peculiar features are commonly seen in rare-earth-based compounds, as the localized f electrons of the rare-earth element have the tendency to hybridize with the s and/or p electrons of other elements. Such a hybridization effect may lead to the formation of narrow electronic gaps or pseudogaps at the Fermi level density of states (DOS). For transition-metal-based materials, the relatively dispersive d-electronic wave functions normally have a weaker hybridization effect but form d-bands instead [2]. Hence, it is of particular importance to examine the physical properties on the unconventional transition-metal-based alloys in order to shed light on such a hybridization scenario. For examples, the semiconducting and semimetallic behavior observed previously in $RuGa_2$ and Fe_2VGa, respectively, have been attributed to such hybridization-induced gap and pseudogap at their Fermi level DOS [7,8].

Intermetallic $FeGa_3$ crystallizes in the tetragonal $CoGa_3$-type structure with the space group symmetry $P4_2/mnm$. A recent electronic structure calculation predicted that $FeGa_3$ is also a hybridization-gap semiconductor with a bandgap of about 0.3 eV [9]. Accordingly, the strong hybridization of the Fe-d and Ga-p electrons in this material is responsible for the unusual band feature. To further understand the nature of electronic states in $FeGa_3$, we thus performed the Seebeck coefficient (S) measurement, a sensitive probe of energy relative to the Fermi surface, on the titled compound. Since S is not influenced by intergrain transport, it should reflect more intrinsic properties of the studied material. In addition, we reported the electrical resistivity (ρ) and thermal conductivity (κ) to provide a full investigation of the transport properties of $FeGa_3$.

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2. Experiments and results

The polycrystalline $FeGa_3$ sample studied here was prepared in an induction furnace under partial argon. To promote homogeneity, the resulting ingot was annealed in a vacuum-sealed quartz tube at 800 °C for 2 days; this was followed by furnace cooling. The same preparation technique has been reported in the literature [10]. An X-ray analysis taken with Cu Kα radiation on the powder specimen shows a single phase. All reflection peaks in the diffraction spectra could be indexed according to the expected structure, as demonstrated in Fig. 1. The determined lattice parameters are $a = 0.6251$ and $c = 0.6543$ nm, respectively, consistent with previously reported values [9].

The electrical resistivity was measured during warming process by a standard four-terminal method. The thermal conductivity was carried out in a close-cycle refrigerator over temperatures from 10 to 300 K, using a direct heat-pulse technique. The $FeGa_3$ ingot was cut to a rectangular parallelepiped shape of typical size of 1.5 mm × 1.5 mm × 5.0 mm with one end glued (with thermal epoxy) to a copper block that served as a heat sink, while a calibrated chip resistor as a heat source was glued to the other end. The temperature difference was measured by using an E-type differential thermocouple with junctions thermally attached to two well-separated positions along the longest axis of the sample. The temperature difference was controlled to be less than 1 K to minimize the heat loss through radiation. During measurements the sample space is maintained in a good vacuum (better than 10^{-2} Pa). For the Seebeck coefficient measurements, Seebeck voltages were detected using a pair of thin Cu wire electrically connected to the sample with silver paint at the same positions as the junctions of differential thermocouple. The stray thermal emfs are eliminated by applying long current pulses (∼100 s) to the chip resistor, where the pulses appear in an off-on-off sequence. All experiments were performed during warming with a rate slower than 20 K/h. The reproducibility of κ and S measurements is better than 2%, while the absolute accuracy of κ is approximately 15%, which mainly arises from the error in measuring the geometrical factor of the samples.

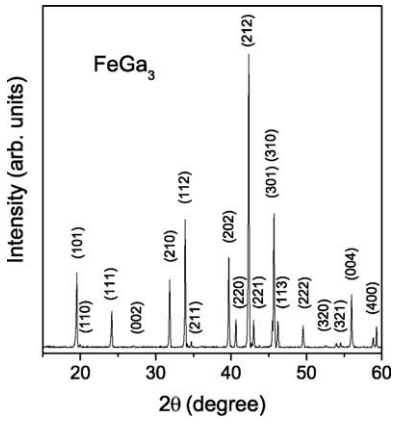

Fig. 1. X-ray diffraction pattern in $FeGa_3$.

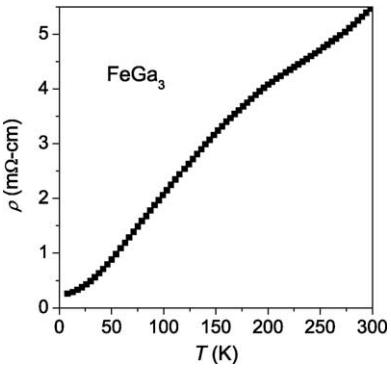

Fig. 2. Electrical resistivity as a function of temperature for $FeGa_3$.

As shown in Fig. 2, the observed ρ of $FeGa_3$ exhibits a metallic character (positive temperature coefficient), in contrast to the semiconducting behavior reported by Haussermann et al. [9]. The rather large ρ values in the entire temperature range we measured may be attributed in part to the grain boundaries. However, the magnitude of measured ρ is similar to those of semimetals such as $FeAl_2$ [11]. Possible reasons for the inconsistency between the reported result and our data will be addressed in Section 3.

The T-dependent thermal conductivity of $FeGa_3$ is displayed in Fig. 3. At low temperatures, κ increases with temperature and a maximum appears at around 40 K. This is a typical feature for the reduction of thermal scattering at lower temperatures. The maximum takes place at the temperature where the phonon mean free path is approximately equal to the crystal site distance. After passing through the maximum, κ drops with increasing temperature. For conventional metals and semimetals, the total thermal conductivity (κ_{tot}) can be expressed as a sum of lattice (κ_L) and electronic (κ_e) terms: $\kappa_{tot} = \kappa_L + \kappa_e$. The electronic contribution can be estimated by means of the Wiedemann–Franz law: $\kappa_e \rho / T = L_0$. Here ρ is the dc electric resistivity and $L_0 = 2.45 \times 10^{-8}\ \mathrm{W\,\Omega\,K^{-2}}$ is the Lorentz number. We thus

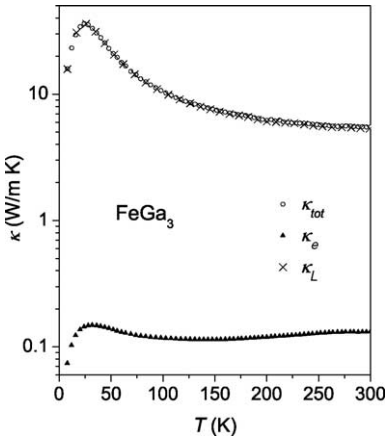

Fig. 3. Temperature dependence of the thermal conductivity in $FeGa_3$.