Magnetotransport properties and Seebeck effect in the superconductor $FeSe_{0.5}Te_{0.5}$

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Abstract. We carried out measurements of the electrical resistivity, magnetoresistance, Hall resistivity and Seebeck effect in a highly oriented sample of the Fe-based $FeSe_{0.5}Te_{0.5}$superconductor. Complementary structural and magnetic characterizations were also performed. Our sample do not show long-range magnetic order down to 4.2 K. Superconductivity occurs with critical temperature $T_c \simeq 15$ K. In the normal phase, the resistivity versus temperature behavior mimics that of a Kondo-lattice system. The magnetoresistance, Hall coefficient and Seebeck coefficient show sign reversals. These results are discussed with basis on the combined effects from two-band conduction and weak magnetic fluctuations. Effects from superconducting fluctuations are also observed near T_c.

Keywords: Fe-based superconductors; magneto-transport properties; Seebeck coefficient
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1. Introduction

The discovery of the Fe-based superconductors [1] attracted considerable interest since most of the compounds having high Fe content present strong magnetic properties rather than superconductivity. Moreover, the Fe-based superconductors have some similarities with the high-T_c cuprates, mostly concerning the strong planar anisotropy, doping allowance and the occurrence of spin fluctuations. In the cuprates, these magnetic excitations lead to the pseudogap phenomenon [2]. In non-doped Fe-based parent compounds, enhanced spin fluctuations lead to spin density wave (SDW) ordering [3]. In general, doping either with donors or acceptors disrupts this long-range magnetic ordering, so that a superconducting ground state may emerge [3,4]. In many cases, however, coexistence between magnetism and superconductivity has been reported [5].

In the present communication, we report on magneto-transport and Seebeck thermal transport experiments on a highly oriented sample of $FeSe_{0.5}Te_{0.5}$. This compound does not order magnetically [6]. However, our results on resistivity, longitudinal magnetoresistance, Hall resistivity and Seebeck coefficient as functions of the temperature consistently show effects from spin fluctuations. In particular, the Hall and Seebeck coefficients reveal an energy scale for these fluctuations that we interpret as related with the pseudogap phenomenon.

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2. Experimental

Highly c-axis oriented samples with nominal composition $FeSe_{0.5}Te_{0.5}$ were prepared using the self-flux method [7]. The obtained samples were characterized by x-ray diffraction and scanning electron microscopy. Both techniques confirm the highly textured microstructure of the samples, where large grains having 50 μm thickness are staked perpendicularly to the c-axis of the PbO-type tetragonal structure. Auxiliary magnetization measurements were performed in several applied fields as functions of the temperature. A weak Pauli-type susceptibility is observed above $T_c^{(mag)}$= 15.1 K, where the onset of a strong diamagnetic contribution to the magnetization is located. The resistivity, magnetoresistance and Hall effect experiments were performed on one of the samples using a conventional Physical Properties Measuring System (PPMS)@manufactured by Quantum Design, Inc. Magnetic fields up to 9 T were applied in the orientation parallel to c-axis. The measurements of the thermoelectric Seebeck effect were carried out with a cryogen-free PPMS@.

3. Results

The inset in Fig. 1 shows resistivity measurements as a function of the temperature for a typical sample of $FeSe_{0.5}Te_{0.5}$. At high temperatures, the resistivity $\rho(T)$ is semiconducting-like, then goes through a broad maximum centered around 150 K before decreasing strongly in temperatures below 100 K, approximately. The superconducting transition given by the maximum of $d\rho/dT$ is T_c =14.5 K. The overall behavior of $\rho(T)$ reminds that of a Kondo-lattice system, where coherent scattering by Kondo resonances produces a strong resistivity decrease in temperatures below the crossover between the single-impurity and the coherent regimes.

The magneto resistance is small and approximately linear with the field in the whole normal phase, except near T_c, where the suppression of superconducting fluctuations produces strong positive magnetoresistance. Figure 1 shows the amplitude of the magnetoresistance measured at H = 9 T as a function of the temperature. Results are normalized with respect to the resistivity at zero applied field. The magnetoresistance is positive at high temperatures, changes sign to negative at $T \sim 240$ K, then changes back to positive below $T \sim 50$ K.

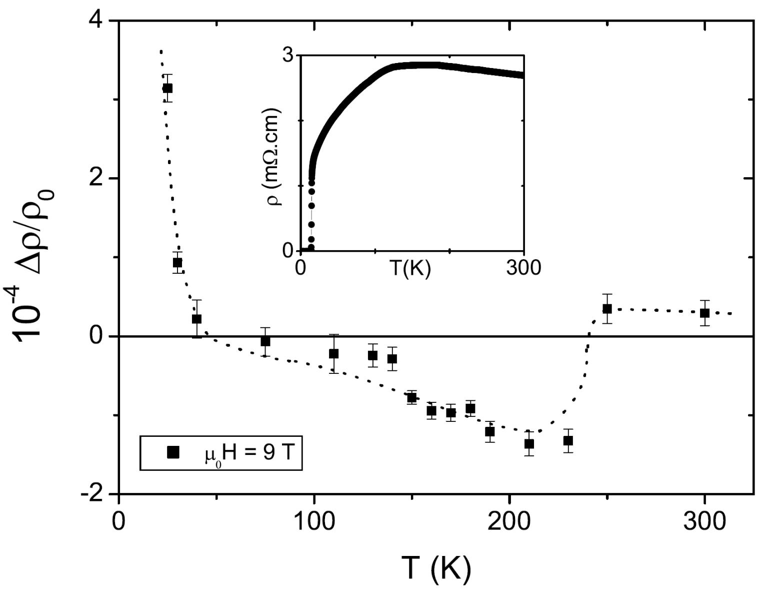

Figure 1. Intensity of the magnetoresistance, $[\rho(H) - \rho(0)]/\rho(0)$, measured at H = 9 T as a function of temperature for $FeSe_{0.5}Te_{0.5}$. The dotted line is a guide for the eyes. The inset shows resistivity versus temperature results for the same sample.

The Hall coefficient, defined as $R_H = \rho_{xy}/B$, where ρ_{xy} is the Hall resistivity and B is the magnetic induction, is plotted in Fig. 2 as a function of the temperature. Three sign reversals are observed. As for the magnetoresistance, at high temperatures R_H is positive. Decreasing the temperature, $R_H(T)$ becomes negative at T ~240 K, then changes back to positive around T ~50 K. The Hall coefficient shows a sharp maximum just above T_c. Then, upon further decreasing the temperature R_H abruptly reverses sign once more and goes through a sharp negative peak before becoming zero in the superconducting phase. Excepting for this low temperature feature, results in Fig. 2 are qualitatively similar to results previously reported for thin film samples of $FeSe_{0.5}Te_{0.5}$ [8].

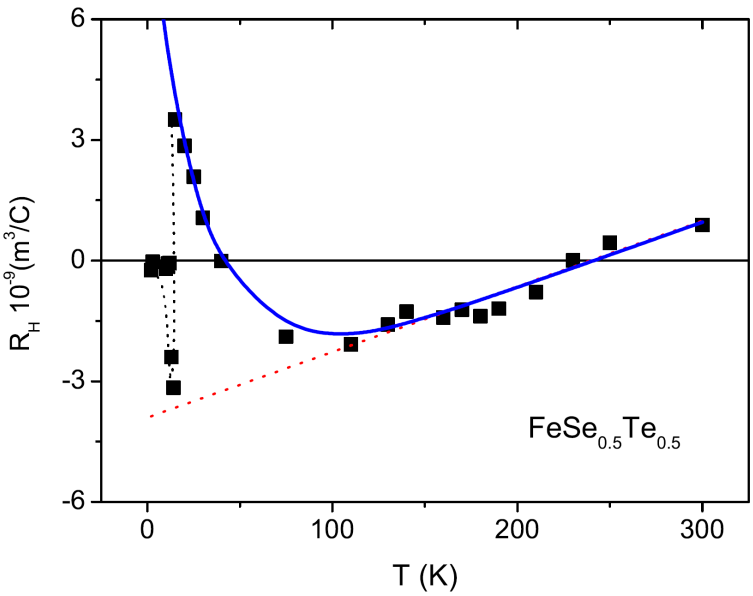

Figure 2. Hall coefficient for $FeSe_{0.5}Te_{0.5}$as a function of the temperature. The solid line is a fit based on Eq. (1). The dotted line represents the term linear in temperature in Eq. (1).

Figure 3 shows the Seebeck coefficient, defined as $S = E/\nabla T$, where E is the electrical field, as a function of the temperature for the studied system. This thermoelectric property also presents a sign reversal. In high temperatures, $S(T)$ is small and positive. Upon decreasing the temperature, S changes sign at T ~160 K, reaches a negative maximum with significant amplitude at T ~20 K , then decreases steeply to zero at T_c.

4. Discussion

The results in Figs. 1-3 strongly suggest that the electrical magneto-transport properties and the electronic contribution to thermal transport in $FeSe_{0.5}Te_{0.5}$ may be described by mechanisms combining two-current conduction with magnetic and superconducting fluctuations. The conduction by electron-like and hole-like carriers is expected with basis on the known band structure for the Fe-based superconductors [9]. Near room temperature, the conduction is dominated by the hole's mobility, as obtained from the positive R_H. Since the magnetoresistance is also positive in this region, one deduces that the Lorentz force mechanism is the most important in high temperatures. When the temperature is decreased below T ~240 K, both the Hall coefficient and the magnetoresistance become negative. This means that the suppression of spin disorder is appreciable in the intermediate and low temperature regimes. In the same temperature regions $\rho(T)$ goes through a maximum before strongly decreasing with negative curvature when temperature approaches T_c from above. We propose that spin resonances

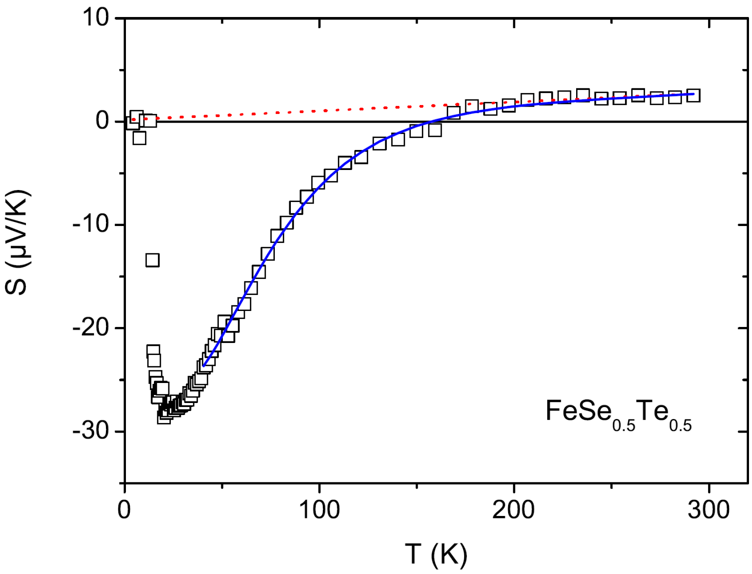

Figure 3. Seebeck coefficient versus temperature for $FeSe_{0.5}Te_{0.5}$. The continuous line correspond to a fit with Eq. (2). The dotted line is the extrapolation of the linearly T-dependent high temperature behavior.

start to built up localized magnetic momenta in the Fe sites in the intermediate temperature range. These resonances scatter carriers coherently in the low temperature regime leading to a significant drop in resistivity, as much as in Kondo-lattice systems. The same magnetic fluctuation term influences the Hall resistivity. Indeed, as shown in Fig. 2, we could describe the Hall coefficient phenomenologically as

$$R_H = a\,(T - T^*) + b\,e^{-\frac{T}{\Delta}}, \tag{1}$$

where a = 1.6 10^{-11}m^3/C·K , b = 1.3 10^{-8}m^{-3}/C, T^*= 240 K, and Δ = 32 K. We interpret the first term in Eq. (1) as resulting from the interplay between Lorentz-force-driven hole and electron mobilities [10]. The second term in Eq. (1) accounts for the fast decay of spin correlations with increasing temperature [11] or, alternatively, to progressive localization of holes in the Fe sites when the temperature is decreased. These processes are related to the coherent scattering observed in the resistivity experiment at low temperatures. The exponential term in Eq. (1) leads to a sign reversal in $R_H(T)$, from negative to positive, at T ∼50 K. Near the superconducting transition, the sign reversal and deep minimum observed in R_H have been reported to occur in other superconductors [12]. The almost coincident values of the intensity of this peak and the extrapolation of the normal contribution to R_H (see Fig. 1) suggest that this controversial feature of the Hall effect might be related to remaining electron-like quasiparticles just below T_c in the case of $FeSe_{0.5}Te_{0.5}$.

The Seebeck coefficient shown in Fig. 3 may be fitted to the expression

$$S = cT + gT\,e^{-\frac{T}{\Delta}}, \tag{2}$$

where c = 8.6 $10^{-3}\mu$V/K^2, g = 2.48 μV/K^{2}and Δ = 32 K. The value for Δ is identical, within the experimental uncertainties, to the one obtained from the fit of $R_H(T)$ to Eq. (1). Using the nearly-free-electron model [10], one may show that $S \propto T\,R_H$. In view of Eq. (2), this result is consistent with the assumption that both the Hall and Seebeck effects in $FeSe_{0.5}Te_{0.5}$are related to the same damped spin fluctuations in the temperature range where $\rho(T)$ exhibits a behavior seemly consistent with the scattering of carriers by localized magnetic resonances. The cutoff energy Δ leading to the suppression of the magnetic excitations at high temperatures might be reminiscent of the pseudogap phenomenon, mostly studied in the cuprates context [2] but also expected to be relevant in the Fe-based superconductors [13].

5. Conclusions

Measurements of the electrical resistivity, magnetoresistance, Hall effect and Seebeck effect in melt-textured samples of $FeSe_{0.5}Te_{0.5}$ indicate that two-band conduction must be taken into consideration to describe the electronic transport in this material. The obtained results also show that scattering due to correlated spin fluctuations play an important role in the electrical and thermal transport properties of this Fe-based superconductor, mostly in the temperature range between $T_c$and room temperature. In particular, the observed exponential temperature dependence of both Hall and Seebeck coefficients consistently furnishes the characteristic energy scale related to the damping of these magnetic excitations. Tentatively, we propose that the relevant spin excitations in $FeSe_{0.5}Te_{0.5}$ are short-range spin density waves, having extension larger than the electron mean-free-path and life-time longer than the relaxation time of the normal electronic transport in the studied compound. Close to the critical temperature, effects from superconducting fluctuations are observed in all studied properties.

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