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Magnetothermoelectric effects in $Fe_{1+d}Te_{1-x}Se_x$

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ABSTRACT

We report resistivity as well as the Hall, Seebeck and Nernst coefficients data for $Fe_{1+d}Te_{1-x}Se_x$ single crystals with $x = 0$, 0.38, and 0.40. In the parent compound $Fe_{1.04}Te$ we observe at $T_N = 61$ K a sudden change of all quantities studied, which can be described to the Fermi surface reconstruction due to onset of the antiferromagnetic order. Two very closely doped samples: $Fe_{1.01}Te_{0.62}Se_{0.38}$ (Se38) and $Fe_{1.01}Te_{0.60}Se_{0.40}$ (Se40) are superconductors with $T_c = 13.4$ K and 13.9 K, respectively. There are no evident magnetic transitions in either Se38 or Se40. Properties of these two single crystals are almost identical at high temperatures, but start to diverge below $T \approx 80$ K. Perhaps we see the onset of scattering that might be a related to changes in short range magnetic correlations caused by selenium doping.

1. Introduction

The discovery of the simplest iron-based superconductor, the chalcogenide $Fe_{1+d}Te_{1-x}Se_x$ [1,2], gives hope for understanding the pairing mechanism in the entire family of new Fe-based materials. Yet soon it become apparent that the ground state of the parent compounds of the iron–chalcogenide and iron–pnictides were magnetic phases of a different nature. Namely, the antiferromagnetic (AFM) spin-density-wave (SDW) order observed in the "1111" [3,4] and "122" families [5,6] seems to be absent from "11" Fe-chalcogenides, despite these compounds have similar electronic band structure [7]. The in-plane magnetic wave vector of the AFM order in the $Fe_{1+d}Te$ parent compound has been identified to be $(\pi,0)$ [7,8], whereas SDW in iron pnictides forms with the nesting vector (π,π) [9]. This discrepancy raised a question whether superconductivity in "11" has the same origin as in other iron-based families [7]. Nonetheless, the recent inelastic neutron scattering measurements shows that (π,π) spin correlations, which are common for iron-pnictides [10,11] and copper-based superconductors [12,13], develops in $Fe_{1+d}Te_{1-x}Se_x$ upon selenium doping [14,15].

In this paper we take a closer look at the region of the phase diagram of $Fe_{1+d}Te_{1-x}Se_x$, where the (π,π) spin fluctuations are expected to overwhelm $(\pi,0)$ ones. To this end we study transport properties of parent iron chalcogenide $Fe_{1.04}Te$ as well as two selenium doped superconductors: $Fe_{1.01}Te_{0.62}Se_{0.38}$ (Se38) and $Fe_{1.01}Te_{0.62}Se_{0.40}$ (Se40). The results show rather sudden change of the low temperature behavior, which may be related to moving (upon Se-doping) from region of coexistence of (π,π) and $(\pi,0)$ fluctuations, to the region of domination of (π,π) fluctuations. In such a case it is likely that different types of spin fluctuations interact with different conducting bands.

2. Material and methods

Single crystals of $Fe_{1.01}Te_{0.6}Se_{0.4}$ and $Fe_{1.04}Te$ nominal compositions were grown using a modified Bridgeman method. The respective amounts of Fe, Se and Te powders of a minimum purity of 99.99% were mixed and pressed into a rod of 7 mm diameter and placed into evacuated sealed quartz ampoule. This ampoule was sealed into a second quartz ampoule. The rod was first melted and homogenized at 1200 °C for 4 h, cooled in a temperature gradient at a rate 4 °C/h down to 750 °C followed by 50 °C/h cooling [16]. For this study we cut out one single crystal from the $Fe_{1.04}Te$ rod and two single crystals from different places of the $Fe_{1.01}Te_{0.6}Se_{0.4}$ rod. The chemical compositions of these two Se-doped crystals were determined by the energy dispersive X-ray (EDX) analysis, and they turned out to differ slightly in Se-content ($x = 0.38$ and 0.40). The data were collected in four independent places for both samples and the noticed variation in composition (a difference between the highest and lowest reading) was smaller than one percent for every element.

The resistivity was measured using the four-probe technique with 25 μm gold wires attached to the sample with two component silver epoxy (EPO-TEK H20E). For the Hall coefficient measurement, the sample was mounted on a rotatable probe and continuously turned by 180° (face down and up) in a magnetic field (B) of 12.5 T to effectively reverse the field anti-symmetrical signal. During the thermoelectric power and Nernst coefficient measurements, the sample was clamped between two phosphor

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bronze blocks, which had two Cernox thermometers and resistive heaters attached to them. The temperature runs were performed in magnetic fields from −12.5 to +12.5 T in order to extract the field voltage components that were odd and even in B.

3. Results

The $Fe_{1+d}Te$ parent compound is known to have the first-order magneto-structural transition around $T_N \approx 60$ K [17]. This transition strongly affects all transport coefficients studied here, as shown in Fig. 1. The step-like change in the temperature dependences of the electrical resistivity (ρ), as well as Hall (R_H) coefficient at T_N was suggested to occur due to reconstruction of the Fermi surface due to formation of the antiferromagnetic order [18]. It seems that this reconstruction can be related to formation of spin stripes, which are expected to produce a maximum (or minimum) in the Nernst signal at $T \approx 1/3T_N$ [19]. In fact, such a minimum is observed in $\nu(T)$ of $Fe_{1.04}Te$ at $T = 25$ K.

As reported previously, there is practically no detectable influence of the magnetic field up to $B = 12.5$ T on the resistivity [18], thermoelectric power [20] and Hall coefficient [18]. The Nernst effect appears to be no exception here. The magnetic field dependence of the Nernst signal ($N(B)$) shows no deviation from linearity in the temperature and magnetic field studied (see inset in Fig. 1b). A lack of response of the transport properties to the magnetic field in $Fe_{1.04}Te$ suggests strong magnetic coupling, which is characterized by the in-plane wave-vector $(\pi,0)$ [7,8]. Nonetheless, the antiferromagnetic $(\pi,0)$ order in $Fe_{1+d}Te_{1-x}$ can be suppressed by substitution of tellurium with selenium [16]. Moreover, such a substitution introduces (π,π) fluctuations that seem to be directly related to formation of the superconductivity [14,15], whereas $(\pi,0)$ fluctuations were attributed to low temperature weak charge carrier localization effects [15].

In order to study these phenomena we measured two very closely substituted single crystals: $Fe_{1.01}Te_{0.62}Se_{0.38}$ (Se38) and $Fe_{1.01}Te_{0.60}Se_{0.40}$ (Se40). The critical temperatures of these samples, defined as the maximum in $d\rho/dT$, are similar: $T_c = 13.4$ K for Se38 and $T_c = 13.9$ K for Se40. The resistivity of Se38, shown in Fig. 2a, rises below $T_{loc} \approx 40$ K, which can be a result of the aforementioned charge carrier localization. The presented in Fig. 2a $R_H(T)$ of the same sample rises with decreasing T for the entire temperature range studied, but this trend becomes steeper below T_{loc}. The behavior of the $\rho(T)$ and $R_H(T)$ below T_{loc} might be related, since in the simple one-band picture: $\rho \propto n^{-1}$ as well as $R_H \propto n^{-1}$ (n is the charge carrier concentration). The field dependence of the Hall coefficient observed below T_{loc} could be understand within the same picture. Namely, if the observed localization is due to the onset of the short range AF correlations, the magnetic field will decrease this effect by quenching fluctuations. As discussed later, this may be better seen in Hall effect than in the resistivity in a case of a multiband conductor, and $Fe_{1+d}Te_{1-x}Se_x$ is known to have a complex electronic band structure [9].

Fig. 2b presents the resistivity and Hall coefficient for the second doped crystal: Se40. The high temperature dependence of both coefficients are very similar to those for Se38, but their low temperature parts differ obviously for these closely doped samples. Namely, there is no sign of localization in $\rho(T)$, and $R_H(T)$ start to decreases below $T \approx 40$ K. The B-dependence of R_H is weaker in

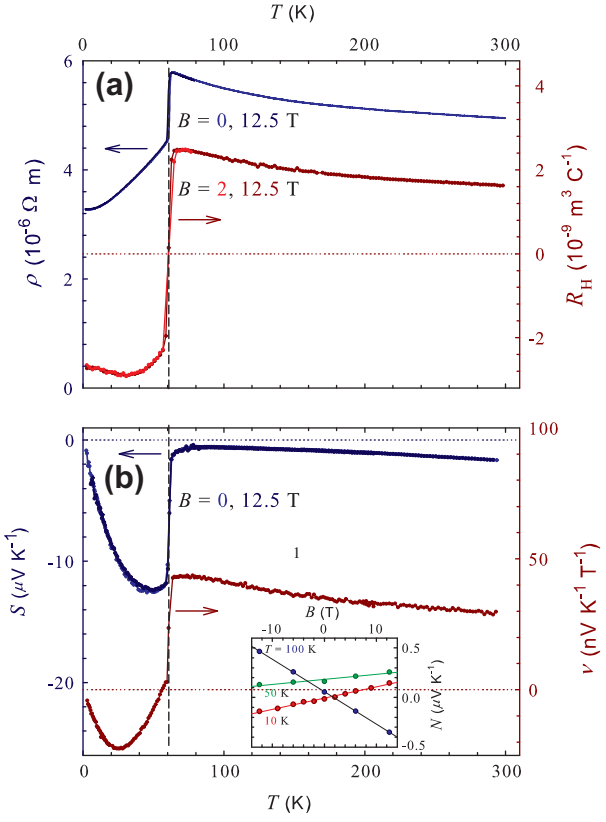

Fig. 1. The temperature dependences of the resistivity and Hall effect (upper panel a) as well as the Seebeck and Nernst effects (bottom panel b) of the $Fe_{1.04}Te$ single crystal. The dashed line marks the structural/magnetic transition at $T_N = 61$ K. Figure presents data taken for the maximal magnetic field of $B = 12.5$ T (dark lines) as well for smaller (or absent) fields (light lines), but the difference is insignificant. The inset in panel b shows field dependence of the Nernst signal, which also does not show deviation from linearity.

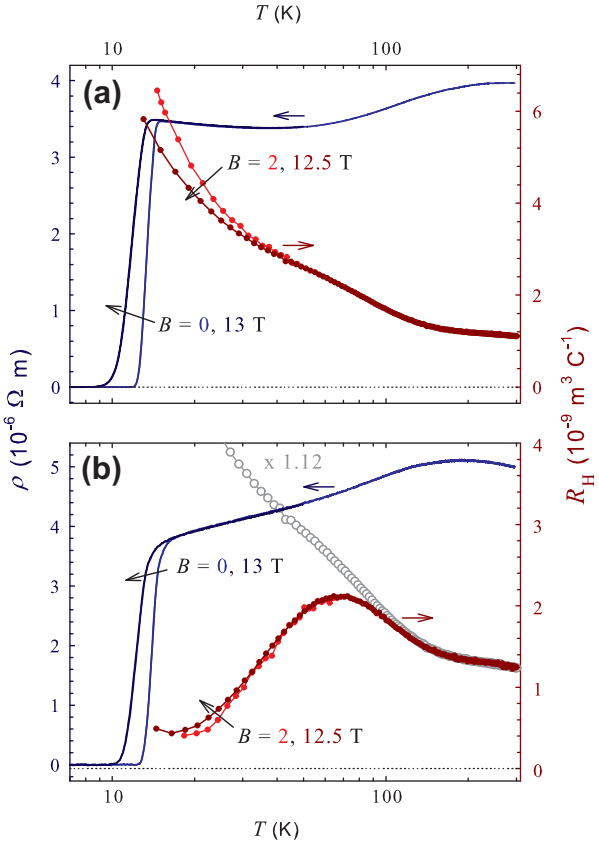

Fig. 2. The temperature dependences of the resistivity and Hall coefficient of the $Fe_{1.01}Te_{0.62}Se_{0.38}$ (panel a) and $Fe_{1.01}Te_{0.60}Se_{0.40}$ (panel b) single crystals. The gray open points in the panel b depict $R_H(T)$ for Se38 normalized to the room temperature value of $R_H(T)$ for Se40.