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## Research articles

## Magnetotransport properties of FeSe in fields up to 50 T

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## ABSTRACT

A study of the magnetotransport properties of a high-quality FeSe crystal in a wide temperature range and in magnetic fields up to 50 T shows that the main electron-like and hole-like bands have very similar values of carrier density and mobility, indicating good electron-hole symmetry in this compound. In addition to the main two bands, there is also a tiny, highly mobile, electron-like band which is responsible for the non-linear behavior of  $\rho_{xy}(B)$  at low temperatures and some other peculiarities of FeSe. We observe the inversion of the  $\rho_{xx}$  temperature coefficient at a magnetic field higher than about 20 T which is an implicit confirmation of the electron-hole symmetry in the main bands.

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## 1. Introduction

FeSe is a very important and interesting superconducting material with complicated electronic and transport properties [1]. It is a nearly compensated semimetal with low carrier concentration. For the physics of superconductivity, it is a new type of superconducting materials and it is a new playground to test out the existing theories of superconductivity. In particular, the low carrier concentration should have allowed a significant variation of a superconducting transition temperature ( $T_c$ ) under variation of a carrier concentration. Indeed, it is demonstrated that the transition temperature can be substantially varied using a gate electrode [2]. However the pairing mechanism in FeSe and other iron-based superconductors is still being debated, and the reasons, causing a  $T_c$  increase under pressure [3], and for a mono-layer FeSe film on an epitaxial substrate [4], are unclear.

The properties of FeSe, as well as many other iron-based superconductors, cannot be described by the simple two-band model. The first studies of the iron-based superconductors revealed multi-band effects and electron-hole asymmetry in  $\text{Ba}(\text{FeCo})_2\text{As}_2$  [5]. Later, an analysis of the magnetic field dependence of  $\rho_{xy}$  and  $\rho_{xx}$

suggested the presence of the highly mobile electronlike band in  $\text{BaFe}_2\text{As}_2$  [6]. The similar highly mobile band exists in many other iron-based superconductors including FeSe family [7,8] and, apparently, originates from a local region of the Fermi surface. Since the mobilities of the two main bands are several times lower than for the highly mobile band, their properties can be studied separately in a high magnetic field where the conductivity of the highly mobile band is suppressed.

Here we report the magnetotransport properties of the high-quality FeSe crystal measured in a wide temperature range and magnetic fields up to 50 T. The obtained data prove a good symmetry of the main electronlike and holelike bands. A remarkable phenomenon is observed at temperatures below 100 K. All  $\rho_{xx}(B)$  curves, corresponding to different temperatures, cross each other in the region 15–20 T and 0.1–0.15 m $\Omega$ cm. Therefore, a crossover from a metallic-type  $\rho_{xx}(T)$  to a semiconductor-type dependence occurs at a magnetic field higher than 20 T. Such behavior has a simple description within the two-band model which gives another way to extract the parameters of the main bands.

## 2. Experiment

The FeSe crystals were grown using the KCl/AlCl<sub>3</sub> flux technique [9]. The chemical composition of the crystals was studied

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with the energy dispersive microanalysis system. The composition measurements were done at three points for four average size crystals.

Electrical measurements were done on a cleaved rectangular sample with lengths of 1.2 mm, widths 0.6 mm and thicknesses about 0.05 mm. Contacts were made by sputtering of Au/Ti layers through a precisely machined mechanical mask. The current electrodes were 0.1 mm wide lines along small sides of the bar. Potential and Hall  $0.1 \times 0.1 \text{ mm}^2$  electrodes were connected to a sample holder with a 0.025 mm gold wire using H20E silver epoxy.

DC magnetoresistance and Hall effect measurements were done using EDC options of Quantum Design MPMS 7T with Keithley 2400 and Keithley 2182A. Measurements of resistance in pulsed magnetic fields up to 50 T were done in HLD at HZDR, Germany.

### 3. Results and discussion

The temperature dependence of the sample resistance is shown in Fig. 1. The anomaly in  $\rho_{xx}(T)$  around 90 K corresponds to the structural phase transition. The resistivity at 15 K is 22 times lower than at 300 K which indicates a high quality of used crystal. An optical image of the studied crystal is shown in the top inset of Fig. 1. The bottom inset of Fig. 1 shows the temperature dependence of the Hall coefficient  $R_H$ . The Hall coefficient has sign

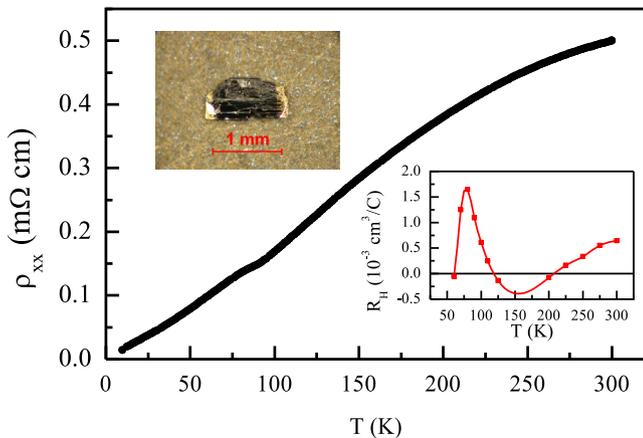


Fig. 1. The temperature dependence of the resistivity  $\rho_{xx}$ . Top inset: the picture of the investigated crystal. Bottom inset: Temperature dependence of the Hall coefficient  $R_H$ .

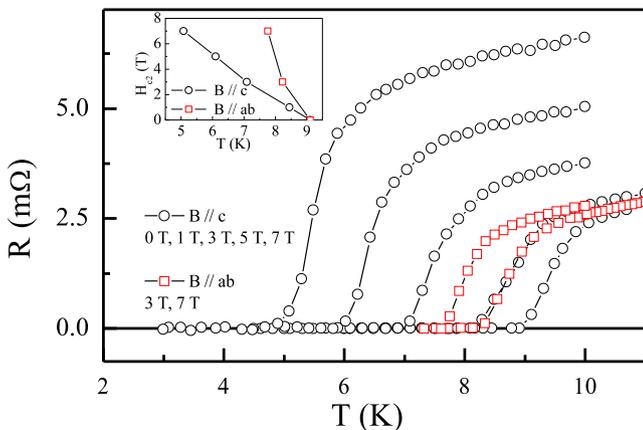


Fig. 2. The temperature dependence of the resistance near a superconducting transition at the various magnetic fields. Inset: Temperature dependence of  $H_{c2}$  critical field for the two field orientations.

reversal points in the presented temperature range which is one of the consequences of a carrier compensation. The low-temperature behavior of  $R_H$  is not plotted because of non-linearity of  $\rho_{xy}(B)$  at low temperatures. The quality of the sample is also confirmed by  $R(T, B)$  measurements near the superconducting transition temperature. Fig. 2 shows  $R(T)$ , measured around the transition, in magnetic fields parallel and perpendicular to the crystal plane. The inset shows the temperature dependencies of the critical fields for these two orientations determined at zero-resistivity points. The ratio of slopes for these dependencies is 3.1–3.4. It is the ratio of coherence lengths for the  $ab$  plane and for the  $c$  axis direction. This value of anisotropy is close to the highest reported for FeSe single crystals which confirms a perfect layered structure of the studied crystal.

The field dependence of the resistivity tensor components within a quasiclassical relaxation-time approximation can be expressed as a sum of  $l$  band terms:

$$\sigma_{xx} = \sum_{i=1}^l \frac{\sigma_i}{(1 + \mu_i^2 B^2)} \quad (1)$$

$$\sigma_{xy} = \sum_{i=1}^l \frac{s_i \sigma_i \mu_i B}{(1 + \mu_i^2 B^2)} \quad (2)$$

$$\sigma_i = en_i \mu_i \quad (3)$$

where  $\sigma_{xx}$  and  $\sigma_{xy}$  are conductivity tensor components,  $i$  is a band index,  $\sigma_i$ ,  $\mu_i$ , and  $n_i$  are absolute values of a band conductivity, a carrier mobility and a concentration correspondingly;  $s_i$  is “–1” for a hole and “+1” for an electron bands. Resistivity tensor components  $\rho_{xx}$  and  $\rho_{xy}$  in a tetragonal crystal are related as follows:

$$\rho_{xx} = \rho_{yy} = \frac{\sigma_{xx}}{(\sigma_{xx}^2 + \sigma_{xy}^2)} \quad (4)$$

$$-\rho_{xy} = \rho_{yx} = \frac{\sigma_{xy}}{(\sigma_{xx}^2 + \sigma_{xy}^2)} \quad (5)$$

For the two-band material, this model gives a linear in  $B$  law for  $\rho_{xy}$  and  $B^2$  for  $\rho_{xx}$  in the limit  $\mu_i B \ll 1$  for both mobilities. For the studied crystal, the measured dependencies  $\rho_{xy}(B)$  and  $MR(B) = (\rho_{xx}(B) - \rho_{xx}(0))/\rho_{xx}(0)$  depending on  $B^2$  are shown in Fig. 3a) and b) respectively. It is clearly seen that the curves corresponding 12 K deviate substantially from a linear dependence. A similar behavior was reported for many iron-based superconductors and can be described within the three-band model by adding to a couple of main electron and hole bands, which have almost the same concentrations and mobilities, the tiny band with appreciably higher mobility [8]. The Table 1 lists the results of the simultaneous fit of  $\sigma_{xy}(B)$  and  $\sigma_{xx}(B)$  data, obtained at 12 K and 30 K, with three-band Eqs. (1)–(3). The ratios  $n_e/n_h$  and  $\mu_e/\mu_h$  at 12 K are 0.84 and 1.12 respectively. Therefore, in a quasiclassical relaxation-time approximation FeSe can be described as having the two main electron and hole bands, with approximately equal values of a concentration and a mobility, and a tiny mobile band with a 3–5% of the total carrier concentration which provide about 10–15% of the total conductivity in zero fields. The relative contribution to the total conductivity of this highly mobile band rapidly decreases with increasing magnetic field. For example, according to the data listed in Table 1, the band  $e_2$  provides 13% of the total conductivity at 12 K in zero fields and only about 2% in 5 T.

Consequently, in high magnetic fields, a two-band semimetal is a good model to describe the FeSe transport properties. It allows giving a simple description for a crossover to a negative temperature coefficient of  $\rho_{xx}$  in high magnetic fields, which is demonstrated in Fig. 4. This figure shows  $\rho_{xx}(B)$  corresponding to

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