Transport properties and the anisotropy of $Ba_{1-x}K_xFe_2As_2$ single crystals in normal and superconducting states

V. N. Zverev$^\dagger$, A. V. Korobenko$^\dagger$, G. L. Sun$^\dagger$, D. L. Sun$^\dagger$, C. T. Lin$^\dagger$, A. V. Boris$^\Delta$2)

$^\dagger$Institute of Solid State Physics RAS, 142432 Chernogolovka, Moscow region, Russia

$^\dagger$Moscow Institute of Physics and Technology, Dolgoprudny, Moscow region, Russia

$^\Delta$Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

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The transport and superconducting properties of $Ba_{1-x}K_xFe_2As_2$ single crystals with $T_c \approx 31\,K$ were studied. Both in-plane and out-of-plane resistivity was measured by a modified Montgomery method. The in-plane resistivity is almost the same for all studied samples, unlike the out-of-plane resistivity, which differs considerably. We have found that the resistivity anisotropy $\gamma = \rho_c/\rho_{ab}$ is almost independent of temperature and lies in the range 10 -- 30 for the studied samples. This indicates the extrinsic nature of high out-of-plane resistivity, which may be due to the presence of flat defects along Fe-As layers in the samples. This statement is supported by comparatively small effective mass anisotropy, obtained from the upper critical field measurements, and from the observation of the so-called “Friedel transition”, which indicates the existence of some disorder in the samples in the c-direction.

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After the discovery of high-temperature superconductivity in the iron arsenides [1, 2], both experimental and theoretical activity was directed toward the study of the band structure, transport properties and the pairing symmetry in the superconducting state. Despite intensive studies, there is still controversy regarding many important physical issues concerning the properties of these new materials, in particular, anisotropy, which is a highly important parameter. High anisotropy was expected on the basis of band structure calculations [3, 4] and was supported by the experiments in non-superconducting BaFe$_2$As$_2$ [5], SrFe$_2$As$_2$ [6] and superconducting electron-doped BaFe$_{2-x}$Co$_x$As$_2$ [7], where the out-of-plane $\rho_c$ to in-plane $\rho_{ab}$ resistivity ratio $\gamma = \rho_c/\rho_{ab}$ was found to be about 100, within the range of previously reported values of 21 [6] and 150 [5]. Recently, the resistivity anisotropy of samples of pristine AF$e_2$As$_2$ (A=Ca, Sr, Ba) [8] and Co-substituted BaFe$_2$As$_2$ [9] was measured using the Montgomery method, and the ratio $\rho_c/\rho_{ab}$ proved to be well below 10. This result is in agreement with the measurements of the upper critical field $H_{c2}(0)$ anisotropy [9], taking into account that this anisotropy has to be equal to about $\gamma^\dagger$. The reason for a discrepancy between $\rho_c/\rho_{ab}$ values obtained by different groups is still unclear. One must take into account that the anisotropy measurements are often complicated and can contain considerable error when as-grown samples are very thin, making the out-of-plane component difficult to measure.

In this paper we have studied the transport properties and the anisotropy of hole-doped superconducting $Ba_{1-x}K_xFe_2As_2$ single crystals with $T_c \approx 31\,K$, which, unlike to the parent compounds, do not have the anomalies in $\rho(T)$ dependence due to the structural phase transition. Recent studies have demonstrated that the slightly underdoped $Ba_{1-x}K_xFe_2As_2$ samples microscopically preserve the tetragonal symmetry down to the lowest temperatures while showing a phase-separated magnetic order below about $\sim 70\,K$ [10, 11].

Single crystals of $Ba_{1-x}K_xFe_2As_2$ were grown using Sn as flux in a zirconia crucible sealed in a quartz ampoule filled with Ar. A mixture of Ba, K, Fe, As, and Sn in a weight ratio of $(Ba_{1-x}K_xFe_2As_2)$:Sn = 1:85 was heated in a box furnace up to 850°C and kept constant for 2 -- 4 hours to soak the sample in a homogeneous melt. An extra of K with 30 wt% was added into the mixtures to compensate the loss from high melting temperature. A cooling rate of 3°C/h was then applied to decrease the temperature to 550°C, and the grown crystals were then decanted from the flux. The growth method, the crystal structure and composition characterization have previously been described in detail in Ref. [12]. Samples grown at the same conditions have been extensively

$^1$e-mail: zverev@issp.ac.ru

$^2$Department of Physics, Loughborough University, Loughborough, LE11 3TU, United Kingdom.
studied using muon-spin rotation [10] and angle-resolved photoemission spectroscopy [13, 14].

Sample resistance was measured using a four-probe technique by a lock-in detector at 20 Hz alternating current in the temperature range of 300–4.2 K. We have tested four samples obtained in the course of one synthesis. For three of these samples, both in-plane and out-of-plane resistivity tensor components were measured using a modified Montgomery method [15]. This method takes into account the real contact positions on the sample surface (see Fig.1) unlike the traditional Montgomery method [16], for which the contacts have to be placed on the corners of rectangular plate. The samples were plates of about 0.60×0.30×0.15 mm characteristic sizes. Two contacts were applied with conducting silver paste to each of two opposite sample surfaces oriented along the (ab) plane. In the experiment, we were able to measure either \(R_{||} = V_{12}/J_{34}\) or \(R_{\perp} = V_{24}/J_{13}\) when the current \(J\) was run mainly parallel or perpendicular to the (ab) plane, respectively (Fig.1). From \(R_{||}\) and \(R_{\perp}\) values the resistivities \(\rho_c\) and \(\rho_{ab}\) were calculated. The accuracy of the calculated resistivity values is about 30%, determined mainly by the non-ideal shape of the samples. The control measurements were carried out on the thin (about 0.03 mm) sample using standard four-probe technique. In this experiment the in-plane resistivity tensor component was obtained directly from the sample resistance. On the same sample, the Hall measurements and the measurements of the upper critical field were also carried out. According to Hall measurements, our samples have p-type conductivity with carrier concentration of about \(2 \cdot 10^{21} \text{cm}^{-3}\).

Typical \(R_{||}(T)\) and \(R_{\perp}(T)\) dependences are shown in Fig.1. The results of resistivity measurements \(\rho_{ab}(T)\) for all samples are summarized in Fig.2. The curves \(\rho_{ab}(T)\) are convex, with a tendency to saturate at high temperature that is consistent with the results of the previous reports for hole-doped \(\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2\) [2, 5], whereas \(\rho_{ab}(T)\) of electron-doped \(\text{BaFe}_{2-x}\text{Co}_x\text{As}_2\) reveals a roughly linear behavior [9]. The saturation could be brought for the proximity to the so-called Ioffe-Regel limit. At \(T \approx 30 \text{ K}\) the mean free path value of \(l \sim 3 \cdot 10^{-7} \text{ cm}\) for our samples is considerably greater than the lattice parameters (\(a = 3.9 \cdot 10^{-8} \text{ cm}, c = 1.3 \cdot 10^{-7} \text{ cm}\) [2]), but \(l\) decreases when the temperature increases, and near the room temperature these values may become comparable. Alternatively, the saturation could be explained in the framework of a two-band model [17]. In the case of two bands with different parameters, the conductivity of one band can "shunt" the conductivity of another, leading to the saturation of the total resistance at high temperature. This scenario can also explain the qualitative difference in the shape of \(\rho_{ab}(T)\) between electron-and hole-doped systems by an acute difference in their electronic structure [18].

The resistivity anisotropy \(\rho_c/\rho_{ab}\), which is almost independent of temperature, is presented in the insert to Fig.2. We would like to emphasize that the in-plane resistivity values for all studied samples proved similar to each other for both Montgomery and four-probe measurements, unlike the out-of-plane resistivity values. One can see that the \(\rho_c/\rho_{ab}\) values differ considerably for three studied samples and the difference is much greater than the experimental error. In contrast to the DC measurements, the anisotropy ratio extrapolated from our recent far-infrared conductivity measurements is lower by a factor of 2–3 even for the highly conductive sample #3 (lowest curve in the inset to Fig.2). This result demonstrates that, unlike \(\rho_{ab}\), which is almost the same
for all of our samples, $\rho_c$ values differ considerably, probably owing to an extrinsic source. This phenomenon is well known for the layered systems (e.g. graphite, layered semiconductors) in which the out-of-plane conductivity is limited by the presence of flat defects.

The superconducting transition temperature $T_c$, determined from $R_c(T)$ at the midpoint between 10% and 90% transition level, lies within the interval $29.5 - 30.5$ K for our samples. Interestingly, the $T_c$ value proved to be slightly dependent on the current orientation. This effect is demonstrated in Fig.3. As seen from the Figure, the $T_c$ value for $J \parallel c$ is about 1 K smaller than that for $J \parallel (ab)$. This result does not depend on the current value and, hence, has nothing to do with the electron system overheating, which may take place because of the difference in the power dissipation between longitudinal and transversal geometries. The same but more pronounced effect was observed earlier in layered high-$T_c$ superconductors [19, 20]. A possible physical reason for the different $T_c$ values obtained from longitudinal and transversal resistance measurements is a layer decoupling transition, the so-called "Friedel transition" [21], which occurs for a disordered layer array [22].

The influence of the magnetic field on the superconducting transition for $H \parallel c$ is shown in Fig.4. One can see that the transition shifts to low-temperature region without considerable broadening. For $H \parallel (ab)$ the behavior is similar, but the effect of magnetic field is weaker.

The temperature dependence of the upper critical field $H_{c2}(T)$, obtained from these data, is shown in Fig.5. The slopes $\mu_0 dH_{c2}/dT$ for $H \parallel (ab)$ and $H \parallel c$ near $T_c$ are equal to $-12$ T/K and $-5.0$ T/K, respectively. Using the Werthammer-Helfand-Hohenberg formula [23]:

$$H_{c2}(0) = -0.69 \frac{dH_{c2}}{dT} \bigg|_{T_c},$$

one obtains $\mu_0 H_{c2}^{ab}(0) = 248$ T and $\mu_0 H_{c2}^{c}(0) = 105.6$ T for $T_c = 30$ K and the critical field anisotropy 2.4. This last value gives the effective mass anisotropy of about 5.8. We realize that the effective masses in the anisotropic Ginzburg-Landau model are not the same as the actual masses, which describe the normal state transport properties. Nevertheless, the fact that the resistivity anisotropy is considerably greater than that obtained from the critical field measurements support our statement about the extrinsic origin of the out-of-plane resistivity.

In conclusion, we have measured the anisotropy of transport and superconducting properties of
Ba$_{1-x}$K$_x$Fe$_2$As$_2$ single crystals. We have found that the in-plane resistivity for all studied samples, obtained over the course of one synthesis, is almost the same for all studied samples, unlike the out-of-plane resistivity, which differs considerably. This probably indicates the presence of flat defects parallel to Fe-As layers in the samples. This statement is supported by the comparatively small effective mass anisotropy, obtained from the upper critical field measurements and from the observation of the so-called "Friedel transition", which indicates on the existence of some disorder in c-direction.

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