Multiband effect in elastoresistance of Fe(Se,Te)

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Abstract – We have investigated the elastoresistance of two FeSe$_{1-x}$Te$_x$ ($x \approx 0.4–0.5$) compounds that have a close chemical composition but differ significantly in electronic properties. The first compound has a negative temperature coefficient of resistance and does not show any phase transitions other than a superconducting one. The elastoresistance of this compound approximately follows the $1/T$ law which is a special case of the Curie-Weiss law, which is usually observed for Fe(Se,S) with metallic conductivity. The second compound has a metallic type of conductivity and, in addition to the superconducting transition, there is also a phase transition at a temperature of about 30 K. The elastoresistance of the second compound is sign-reversing and can be approximated with the sum of two Curie-Weiss–type terms with opposite signs and different critical temperatures. We attribute this behavior to the competition of contributions to the elastoresistance from different band valleys. These competing contributions may appear since the composition of our compound is close to the critical point at which the low-temperature ground state in the 11 series of iron-based superconductors changes from electronic nematic order to magnetic order.

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Introduction. – The elastoresistance coefficient is the ratio of the relative change in the sample resistance $\Delta R/R_0$ during elongation of the sample, along or transverse to the current flow direction, to the value of elongation $\Delta L/L_0$. This ratio $(\Delta R/R_0)/(\Delta L/L_0)$ is also called “the strain coefficient of electrical resistivity” or “the gauge factor”.

Among iron-based superconductors, many compounds exhibit unusually high values of the elastoresistance coefficient. This interesting phenomenon is being actively studied now since the reasons for the large elastoresistance effect can be associated with the mechanism of superconducting pairing in this family of superconductors [1–3].

In the semiclassical approximation, the contribution to a conductivity from the $i$-th group of carriers $\sigma_i$ is determined by the concentration of carriers $n_i$, the effective mass of carriers $m_i^*$, and the scattering time $\tau_i$:

$$\sigma_i = \frac{e^2 n_i \tau_i}{m_i^*}$$

The elastoresistance of many ordinary metals and alloys is reasonably well explained [4] under the assumption that the effective mass does not change during deformation and the density of states and scattering time change only due to a change in volume. In this approach, changes in concentration and scattering time provide roughly equal contributions to the strain coefficient of resistivity which are of the order of unity.

For silicon, the gauge factor can reach values of the order of a hundred. In semiconductor materials, the change in the value of resistivity during deformation is primarily due to the redistribution of carriers between the valleys with different anisotropy [5]. In other words, it is due to...
changes in the concentrations \( n_i \) of the valleys. The change in the anisotropy of one of the valleys is also an important factor for silicon [6]. The temperature dependence of the elastoresistance of semiconductors normally takes the form of a Curie law \( 1/T \) due to the influence of temperature on the distribution of carriers over the splitting energy states.

In semimetals, the elastoresistance can also be large. For bismuth, for example, this value is of the order of ten. Recently, values of the order of a hundred have been reported for the elastoresistance of one of the transition metal dichalcogenides [7].

In the case of iron-based superconductors, the magnitude of the elastoresistance can reach up to several hundreds. The temperature dependence of the elastoresistance is often of the Curie-Weiss type with diverging behavior at the points of structural or magnetic transitions, which suggest the electronic origin of the corresponding transitions [1]. The important question so far remains open: which of the properties of the electronic subsystem causes this divergence? In the quasiclassical variables of eq. (1) this can be either the thermodynamic properties of the carriers \(-m_i^* n_i\) or the scattering time \(\tau_i\) (“fluctuation scenario”). The “fluctuation scenario” is of interest since it implies a significant role of nematic fluctuations, which may also be important for understanding the mechanism of superconducting pairing in iron-based superconductors [1].

However, the “band scenario” is in good agreement with some recent experimental results. For example, the sign of resistance anisotropy in the ordered state of BaFe\(_2\)As\(_2\) compounds correlates with the type of doping [8]. This behavior is completely analogous to the relationship between the sign of the gauge factor and the type of doping in semiconductors. In the 11 series of iron-based superconductors, the change in the sign of the elastoresistance, apparently, also occurs simultaneously with a change in the sign of the major carriers [9,10].

The noticeable effect of strain on the electronic structure in FeSe was directly observed experimentally [11]. It is also well known that the band structure in FeSe\(_{1-x}\)Te\(_x\) changes significantly during the nematic transition [12] and the effective mass of carriers in the nematic phase is anisotropic for some valleys. Thus, the band contribution to elastoresistance certainly exists.

In general, the components of the mass tensor and the relaxation time tensor enter the Boltzmann equation as pairwise products of the relaxation time and the reciprocal mass. Therefore, within the framework of the semiclassical approximation, the separation of the contribution of these quantities to transport properties is ambiguous. Nevertheless, the question of the sources of the record values of elastoresistance is as important as the question “what drives nematic order in iron-based superconductors?” [13].

To study the relationship between the elastoresistance and other electronic properties, we investigated the properties of two FeSe\(_{1-x}\)Te\(_x\) compounds with close \( x \) but with the opposite signs of the temperature coefficient of resistivity. In our opinion, the results obtained indicate a close relationship between the elastoresistance and band properties. In particular, a competition of contributions from different valleys leads to the temperature dependence of the elastoresistance with a change in sign found in one of the compounds studied.

**Experiment.** – There were selected two compositions from a rather large number of studied batches of the FeSe\(_{1-x}\)Te\(_x\) series for \( x \approx 0.4-0.5 \), as having a maximum difference in transport properties, presumably corresponding to the boundary values of the deviation of the stoichiometry of iron. The range of \( x \) is chosen because of the transition from bad to good metal occurring nearby, and samples with almost the same values of \( x \) can have different signs of the temperature coefficient of resistance. It is also worth noting that in this range the conditions for a topological nontrivial state are fulfilled [14].

Single crystals of Fe\(_{1+\Delta}\)Se\(_{0.5}\)Te\(_{0.5}\) and Fe\(_{1+\delta}\)Se\(_{0.5}\)Te\(_{0.5}\) were grown by recrystallization in the halides flux technique with a constant temperature gradient in a quartz ampoule. A driving force of the recrystallization process is the temperature gradient. The mixture of Fe, Se, and Te powders was dissolved in molten salts at the hot end of an ampoule and transferred to the cold one where crystallization occurs. The difference between temperatures of hot and cold ends of the ampoule was about 50–100 K. See refs. [15,16] for more details of this technique.

Sample Fe\(_{1+\Delta}\)Se\(_{0.5}\)Te\(_{0.5}\) was synthesized in CsCl/KCl/AlCl\(_3\) flux, the temperature of the hot end of the ampoule was 655 °C and the temperature of the cold end was 575 °C. Sample Fe\(_{1+\delta}\)Se\(_{0.5}\)Te\(_{0.5}\) was synthesized in the AICl\(_3\)/NaCl/KCl flux and the temperature mode was 585 °C at the hot end and 495 °C at the cold end. Both syntheses were carried out for about 75 days.

The chemical composition of crystals was studied using an INCA Energy 450 energy dispersive microanalysis system installed in a TESCAN Vega II XMU scanning electron microscope (accelerating voltage 20 kV, probe current 0.4 nA). The experimentally determined chemical composition values were Fe\(_{1.02}\)Se\(_{0.49}\)Te\(_{0.51}\) and Fe\(_{0.98}\)Se\(_{0.5}\)Te\(_{0.04}\) for the batches designated as Fe\(_{1+\Delta}\)Se\(_{0.5}\)Te\(_{0.5}\) and Fe\(_{1+\delta}\)Se\(_{0.5}\)Te\(_{0.04}\), respectively.

Contact pads for electrical measurements were made by magnetron sputtering of Au/Ti layers using a mechanical mask. DC transport measurements were done using QD PPMS and EDC option of MPMS-7T with Keithley 2400 and Keithley 2192. Elastoresitivity was measured similarly to the method described in ref. [1] using AC transport option of a Quantum Design PPMS system equipped with a multifunctional insert. During measurements, the sample was glued to a commercial piezoelectric transducer in such an orientation that the current flow direction coincides with the strain direction. The sample elongation was measured by a strain gauge located on the other side of the piezoelectric device.
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Results. – The temperature dependences of the resistivity of the studied compositions are shown in fig. 1. In the log-log plot, the experimental data are almost linear in a wide temperature range. For Fe$_{1+\Delta}$Se$_{0.5}$Te$_{0.5}$ the slope is about $-0.2$, which is close to the Mott law and apparently reflects the hopping nature of the conductivity in the studied composition. This is in agreement with the supposed increased excess of iron. The critical temperature for this composition is close to 14 K. One should notice that a negative value of the temperature coefficient is almost standard for compositions with 50% tellurium and was observed by many authors [17].

It is known that slight variations in the synthesis of compounds of the 11 series can lead to rather noticeable changes in the transport properties of grown crystals [18]. It was also found that the transport properties noticeably change with various heat treatments that remove non-stoichiometric iron [19].

For our Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$ the slope of $R(T)$ in log-log plots is about 0.3. This is closer to the metallic behavior observed in FeSe$_{1-x}$S$_x$ [20,21], although an activation component is also present in the resistance of the FeSe at high temperatures [22].

In general, the temperature dependence of the resistivity of Fe$_{1+\Delta}$Se$_{0.6}$Te$_{0.4}$ agrees very well with the recently published data for Fe$_{1+\delta}$Se$_{1-x}$Te$_x$ compositions [23], including an anomaly in resistance at a temperature of about 30 K, presumably caused by a magnetic transition.

The temperature dependences of the Hall coefficients of the Hall coefficients of the compositions studied are shown in fig. 2. This plot also indicates a significant difference in the electronic properties of the samples. For Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$ the dependence is again similar to the case of metallic FeSe$_{1-x}$S$_x$ where the Hall coefficient has a change of sign caused by the competition of electronic and hole components. For Fe$_{1+\Delta}$Se$_{0.5}$Te$_{0.5}$ $R_H$ is positive at all temperatures. It is known that removing the excess of iron by heat treatment in FeSe$_{1-x}$Te$_x$ also causes a change in the dependences of the Hall coefficient from being always positive to sign-reversing [24]. Thus, the substantial difference in the transport properties of the studied compounds with similar composition can be explained by variations in the non-stoichiometry of iron. The excess non-stoichiometric iron in Fe$_{1+\delta}$Se$_{0.5}$Te$_{0.5}$ dopes this composition and increases the degree of disorder.

The difference in the electronic transport properties of our compounds also manifests itself in elastoresistance (see fig. 3). Elastoresistance of Fe$_{1+\Delta}$Se$_{0.5}$Te$_{0.5}$ slowly increases with the decreasing temperature down to about

Fig. 1: Log-log plot of the temperature dependence of resistivity for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$ and Fe$_{1+\Delta}$Se$_{0.5}$Te$_{0.5}$ above 15 K. For reference, two dashed lines with a slope of $-0.2$ and $0.3$ are shown. Upper inset: temperature dependence of resistivity below 15 K. Lower inset: temperature dependence of resistivity for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$

Fig. 2: Temperature dependence of the Hall coefficient for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$ and Fe$_{1+\Delta}$Se$_{0.5}$Te$_{0.5}$. Inset: temperature dependence of the Hall coefficient for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$

Fig. 3: Temperature dependence of the longitudinal elastoresistance ($\Delta R/R$/$\Delta L/L$) (strain is along the direction of the current flow) for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$ (closed circles) and Fe$_{1+\Delta}$Se$_{0.5}$Te$_{0.5}$ (open circles). The dotted curves represent a Curie-Weiss–type dependence and the sum of two Curie-Weiss terms with different parameters: $870/T + 2$ for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.5}$ data and $9000/(T - 3700)/(T - 30) + 2$ for Fe$_{1+\delta}$Se$_{0.6}$Te$_{0.4}$ data. Inset: the relative change of resistance ($\Delta R/R$) as a function of elongation ($\Delta L/L$) at several temperatures.
During deformation, the elastoresistance also increases with decreasing temperature, which means that the absolute value of the change in resistance,

\[ d\rho \propto e^2 \nu \times \frac{d}{T} \left( \sum_j \frac{1}{\tau_j} \right) \]  

where \( \tau_j \) is a scattering time for the j-th scattering mechanism, and \( \tau_{nf} \) refers to scattering by nematic fluctuations.

In the "band scenario" of elastoresistance, the experimental data can be easily explained since eq. (3) establishes that \( d\rho \) changes proportionally to the resistance.

In fig. 4, in addition to the \( \Delta R/(\Delta L/L) \) data for \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \) and \( \text{Fe}_{1+\delta}\text{Se}_{0.5}\text{Te}_{0.5} \), the values calculated as a product of \( \Delta R_l/(\Delta L/L) \times (R_2/R_1) \) are plotted, where an index value of 1 means composition \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \) and 2 means composition \( \text{Fe}_{1+\delta}\text{Se}_{0.5}\text{Te}_{0.5} \). According to eq. (3), these values should match the values of \( \Delta R/(\Delta L/L) \) for \( \text{Fe}_{1+\delta}\text{Se}_{0.5}\text{Te}_{0.5} \). In the region of intermediate temperatures, the correspondence is rather good. The deviation at lower temperatures can be explained by the proximity of the phase transition in \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \).

A change in the sign of elastoresistance at a temperature above the structural transition can also be an argument in favor of the "band scenario" since it can reflect the competition of contributions from different valleys. As can be seen from fig. 3, the temperature dependence of the elastoresistance of the sample \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \) is satisfactorily described by the sum of two Curie-Weiss-type contributions with different signs.

In fig. 4, the temperature dependence of the elastoresistance of the sample \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \) is satisfactorily described by the sum of two Curie-Weiss-type contributions with different signs and different critical temperatures.

In the presented fit, we used the temperature of the magnetic transition and zero as values of the Weiss constant. The accuracy of the determination of the Weiss constants from the experimental dependence is not high. For example, it is possible to achieve a completely satisfactory result for a pair of Weiss constants of 20 and 30 K. Nevertheless, the difference in critical temperatures is a key feature since it provides a change of sign. In the band model of elastoresistance, different values of critical temperatures for different valleys are a completely clear assumption, since they can represent a local characteristic of the valley.

It was shown that if there is a direct connection between the band splitting and the order parameter of a phase transition, then the elastoresistance will experience an anomaly at the phase transition point described by the Curie-Weiss law [1]. Otherwise, the anomaly of the elastoresistance is not expected and the temperature dependence will take the usual form of the Curie law 1/T.

For \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \), the temperature dependence of the elastoresistance, as already noted above, is well described as the sum of the 1/T term and the Curie-Weiss term with the critical temperature of the magnetic transition.

To our knowledge, in all previously studied compounds of iron-based superconductors, the elastoresistance did not change the sign above the phase transition point, and one critical temperature of this type was sufficient to describe its temperature dependence. The appearance of the second term in \( \text{Fe}_{1+\delta}\text{Se}_{0.6}\text{Te}_{0.4} \) is unusual.

We suppose that the explanation of the two competing terms may be related to the proximity of the studied composition to the boundary between magnetic and nematic...
ground state. Accordingly, the experimentally discovered competition of two contributions to the elastoresistance may indicate the presence of pockets with magnetic and nematic electronic instability at the same time. Different signs may mean that these are contributions from electron and hole valleys since signs can change due to a change in the type of bonding/antibonding states between the top and bottom of the electronic band.

For the sum of two terms of the Curie-Weiss type to change sign at temperatures above critical temperatures, three conditions must be met: 1) different signs of the terms; 2) different values of the Weiss constants in terms; 3) the term with a smaller value of the Weiss constant must have a larger amplitude, which means a larger Curie constant module value in this term.

The latter condition is not simple. If these Curie-Weiss terms were related to ferromagnetic ordering, then condition 3) could be fulfilled only with different exchange constants. We assume that the competition between the orbital and magnetic ground states can provide different coupling constants between the order parameter and the resistance anisotropy in different pockets of the Fermi surface, which can help fulfill condition 3).

The reason for the change in the ground state upon the substitution of tellurium for selenium in Fe(Se,Te) series in our opinion can be connected with a gradual change in the relative positions of \( xy \) and \((xz, yz)\) levels in the \( t_{2g} \) set of orbitals.

**Conclusion.** – The study of elastoresistance of two close compositions FeSe\(_{1-x}\)Te\(_x\) with substantially different electronic properties revealed two important features. First, a change in the type of conductivity of the compositions does not change the type of temperature dependence of elastoresistance. Second, the sign-reversal temperature dependence of the elastoresistance is observed, which is explained by the existence of two competing contributions with different critical temperatures.

Both detected phenomena have a simple explanation in the framework of the band model of elastoresistance. Thus, the record values of the elastoresistance along with the record values in the absorption of ultrasound [25] and the record increase of the superconducting temperature [26] can be attributed to the features of the band structure of iron-based superconductors.

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