Interplay of superconductivity and magnetism in $FeSe_{1-x}Te_x$ compounds. Pressure effects.

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The influence of uniform pressures P up to 5 kbar on the superconducting transition temperature T_c was studied for the $FeSe_{1-x}Te_x$ (x = 0, 0.85, 0.88 and 0.9) system. For the first time, we observed a change in sign of the pressure effect on T_c when going from FeSe to tellurium rich alloys. This has allowed to specify the pressure derivative dT_c/dP for the system as a function of composition. The observed dependence was compared with results of the *ab initio* calculations of electronic structure and magnetism of FeSe, FeTe and $FeSe_{0.5}Te_{0.5}$, and also with our recent experimental data on pressure effects on magnetic susceptibilities of FeSe and FeTe compounds in the normal state. This comparison demonstrates a competing interplay between superconductivity and magnetism in tellurium rich $FeSe_{1-x}Te_x$ compounds.

Keywords: Fe-based superconductors, $FeSe_{1-x}Te_x$, electronic structure, magnetic susceptibility, pressure effects

I. INTRODUCTION

For the most families of recently discovered class of the Fe-based high-temperature superconductors (HTSC) the emergence of superconductivity with doping or under uniform pressure is accompanied by suppression of the magnetic ordering [1–4]. It is widely believed then that spin fluctuations play an important role in formation of the Cooper pairs [5–7]. Nevertheless, as shown e.g. in Ref. [8], for many Fe-based HTSCs the experimental values of superconducting transition temperatures are well described in the framework of the electron-phonon mechanism of pairing. The close interrelation of magnetism and superconductivity determines the importance of further studying of magnetic and superconducting properties and their evolution under variations of composition, pressure, etc. for understanding HTSC mechanism in the considered new class of iron compounds. One of representatives of this class is the system of $FeSe_{1-x}Te_x$ chalcogenides, which possesses the simplest crystal structure among iron-based superconductors, that favors to experimental and theoretical studying the effects of chemical substitution and high pressures on its properties.

Superconducting properties of $FeSe_{1-x}Te_x$ are characterized by nonmonotonic dependence of transition temperatures T_c on composition. There is a noticeable growth from $T_c \simeq 8$ K for $x = 0$ to the maximum value ~ 15 K at $x \simeq 0.5$ with the subsequent falling to 0 K near $x \sim 0.9$ (see, for example, Ref. [9] and references therein). Also, in FeSe compound the extremely large rise of T_c up to $35 \div 37$ K takes place with pressure $P \sim$70–80 kbar [10, 11]. The similar behavior of T_c under pressure was also observed in $FeSe_{0.5}Te_{0.5}$ compound [12, 13]. With further increase of x in $FeSe_{1-x}Te_x$ a tendency to reduction of the positive pressure effect is expected with even probable change of its sign, as it was observed in the related tellurium rich $FeS_{0.2}Te_{0.8}$ alloy [9]. This alleged change in sign of the pressure effect on T_c in $FeSe_{1-x}Te_x$ under substitution of Te for Se could also explain the reason of unsuccessful attempts to observe superconductivity in FeTe under pressures up to 190 kbar [14, 15].

Magnetic properties of $FeSe_{1-x}Te_x$ system were investigated in a number of works [16–24], however, data on the magnetic susceptibility in the normal state remain incomplete and quantitatively inconsistent. This is caused not only by a different quality of the samples used, but also by the existence in them of impurities of iron and its secondary magnetic phases which considerably mask their intrinsic magnetic susceptibility and must be carefully taken into account [22]. The most adequate experimental data indicate that the susceptibility of $FeSe_{1-x}Te_x$ compounds increases gradually with

Te content, being in FeTe about one order of magnitude lager then that of FeSe. Moreover, FeTe compound becomes magnetically unstable, and the antiferromagnetic ordering has been observed at temperatures about 70 K (see e.g. Ref. [17]).

It should be noted that the largest rise of magnetic susceptibility in the normal state, $\chi(x)$, with increase of x is observed in tellurium rich compounds, where, in turn, the $T_c(x)$ dependence falls steeply down and FeTe compound is not superconductor under ambient conditions. This allows to assume a competing interplay between magnetism and superconductivity, at least for this range of compositions. In order to shed more light on the relationship between magnetic and superconducting properties in $FeSe_{1-x}Te_x$ system, it is very important to study evolution of these properties under high pressure. For this purpose in the present work we investigated the influence of hydrostatic pressure on the superconducting transition temperature, mainly in tellurium rich FeTe(Se) compounds. The obtained experimental results were compared with available data on behavior of magnetic susceptibility under pressure for the basic compounds FeSe [25] and FeTe [14, 26], also supplemented by calculated pressure dependencies of electronic structure and magnetic susceptibility for $FeSe_{0.5}Te_{0.5}$ compound.

II. EXPERIMENTAL DETAILS AND RESULTS

The single crystals of $FeSe_{0.96}$ superconductor (hereinafter referred to as FeSe) were grown during 50 days in evacuated quartz ampoules using the $AlCl_3$/KCl flux technique with a constant temperature gradient along the ampoule length [27]. Temperature of the hot end of the ampoule was kept at 427°C, when its more cold end was at about 380°C. A similar method was employed for the synthesis of tellurium-rich single crystals of $Fe_{1+\delta}Se_{1-x}Te_x$ superconductors ($\delta \sim 0.05$, $x = 0.85$, 0.88 and 0.90). In this case we used the KCl/NaCl salt mixture and temperatures of the hot and cold ends of the ampoule were 750°C and about 700°C, respectively. The duration of the synthesis was 20-25 days. Typical dimensions of the produced plate-like single crystals were $(1-3) \times (1-3) \times (0.2-0.3)$ mm^3. Their tetragonal $P4/nmm$ structure was demonstrated at room temperature by an x-ray diffraction technique. The crystals composition was determined using energy dispersive X-ray spectroscopy, performed on a CAMECA SX100 (15 keV) analytical scanning electron microscope, with an accuracy of the components ratio not worse than 2% (for details, see [24, 27]).

The measurements of magnetic properties were performed using a SQUID magnetometer (MPMS-XL5 Quantum Design) equipped with a miniature high-pressure cell of a piston-cylinder type (similar to that described in Ref. [28]). The cell was made of non-magnetic CuBe alloy with the inside and outside diameters of 1.6 mm and 5 mm, respectively. Polyethylsiloxane liquid PES-3 was used as a hydrostatic pressure-transmitting medium. The value of pressure at low temperatures was determined according to the known pressure dependence of the superconducting transition temperature for a sample of pure tin [29], located inside the cell close to the measured sample. The corresponding error did not exceed 0.2 kbar.

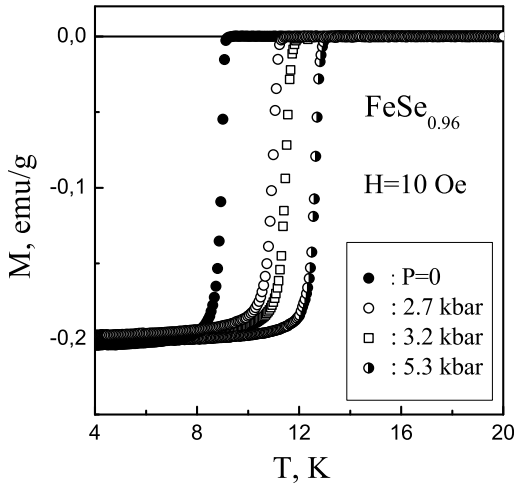

Figure 1: Temperature dependence of the magnetic moment of FeSe, measured in magnetic field $H = 10$ Oe at different pressures.

Fig. 1 shows the temperature dependencies of magnetic moment $M(T)$ for FeSe at different values of pressure, which were measured under cooling of the sample in zero magnetic field (ZFC) followed by its heating in the field $H = 10$ Oe. Resulted from Fig. 1 pressure dependence of the superconducting transition temperature T_c, determined from here on by the onset of the transition, is given in Fig. 2. Within the experimental errors and the operating range of pressure, this dependence appeared to be close to linear that allows to evaluate the pressure derivative dT_c/dP.

The $M(T)$ dependencies for tellurium-rich $FeSe_{1-x}Te_x$ compounds were measured at different pressures in ZFC regime, and are shown in Fig. 3. They demonstrate clearly defined negative pressure effect on the superconducting transition temperature. Experimental values of T_c and its pressure derivative for all investigated samples are listed in Table I. As is evident from the presented data, the pressure effects on T_c in the tellurium rich $FeSe_{1-x}Te_x$ compounds are comparable in magnitude with that for FeSe but have opposite negative sign.

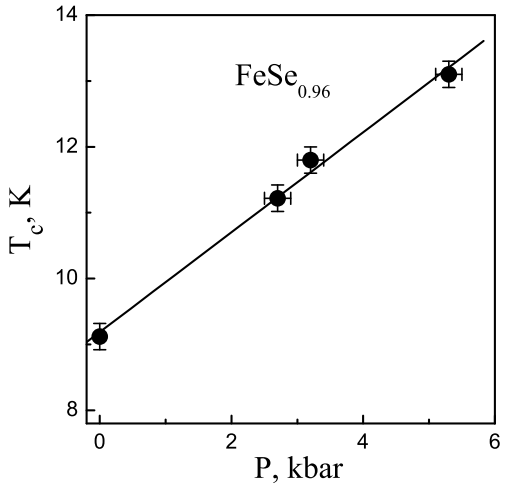

Figure 2: Pressure dependence of the superconducting transition temperature for FeSe.

Table I: Superconducting transition temperature T_c and its pressure derivative $\mathrm{d}T_c/\mathrm{d}P$ for $FeSe_{1-x}Te_x$ compounds.

Composition	T_c (K)	$\mathrm{d}T_c/\mathrm{d}P$ (K/kbar)
x= 0	9.12	0.78 ± 0.05
x= 0.85	11.62	-0.31 ± 0.05
x= 0.88	11.05	-0.40 ± 0.05
x= 0.90	9.71	-0.40 ± 0.1

III. CALCULATIONS OF ELECTRONIC STRUCTURE AND MAGNETIC SUSCEPTIBILITY OF $FESE_{0.5}TE_{0.5}$ COMPOUND

For calculations of electronic structure of $FeSe_{0.5}Te_{0.5}$ compound we employed the relativistic full potential LMTO method (FP-LMTO, RSPt implementation [30, 31]). The exchange-correlation potential was treated within the local density approximation (LDA [32]) of the density functional theory (DFT). The calculations were carried out for a supercell $2 \times 2 \times 1$, constructed by double translations of the unit cell for the ordered tetragonal phase of FeSe and FeTe along the crystallographic [100] and [010] directions, by using experimental values of crystal lattice parameters for $FeSe_{0.5}Te_{0.5}$ from Refs. [33–35]). The calculated density of electronic states (DOS) $N(E)$ of the paramagnetic $FeSe_{0.5}Te_{0.5}$ compound is presented in Fig. 4. The Fermi level E_F is situated in the region of a local flat plateau of $N(E)$, where the main contribution to DOS comes from the d-states of iron. Such position of E_F implies a weak temperature dependence of the spin susceptibility in $FeSe_{0.5}Te_{0.5}$, which is consistent with available experimental data for this compound [16, 22, 23].

To evaluate the paramagnetic susceptibility of

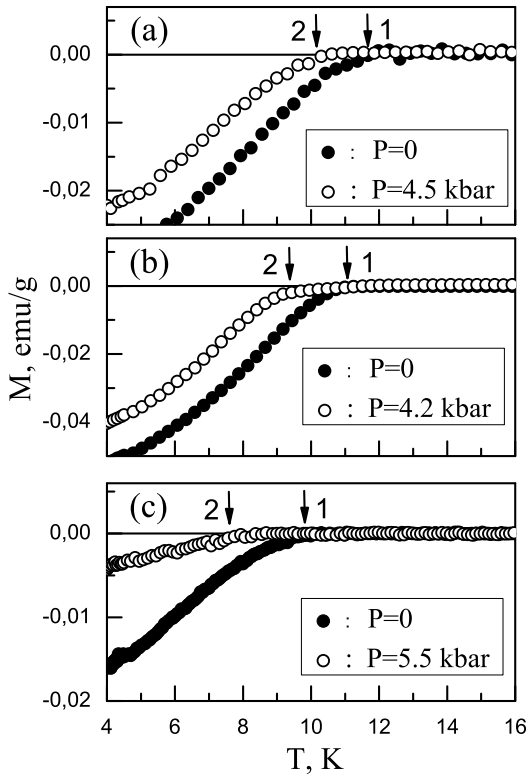

Figure 3: Temperature dependencies of the magnetic moment measured in $H = 10$ Oe at two values of pressure for tellurium-rich $FeSe_{1-x}Te_x$ compounds: (a) - $x = 0.85$, (b) - $x - 0,88$, (c) - $x = 0.9$. Arrows 1 and 2 denote T_c at zero and finite values of pressure, respectively.

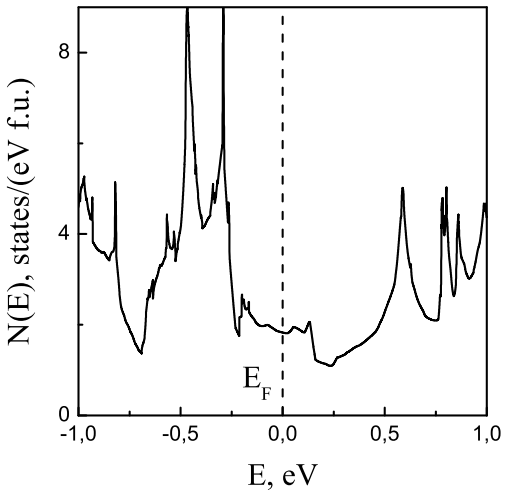

Figure 4: Density of electronic states $N(E)$ of $FeSe_{0.5}Te_{0.5}$ compound. The Fermi level position at 0 eV is marked by a vertical line.

$FeSe_{0.5}Te_{0.5}$ compound, the FP-LMTO calculations of field-induced spin and orbital (Van Vleck) magnetic moments were carried out with the approach described in Ref. [31] within the local spin density approximation (LSDA) of DFT. The relativistic effects, including spin-orbit coupling, were incorporated, and the effect of an external magnetic field **B** was taken into account self-consistently by means of the Zeeman term:

$$\mathcal{H}_Z = \mu_B \mathbf{B} \cdot (2\hat{\mathbf{s}} + \hat{\mathbf{l}}), \quad (1)$$

Here μ_B is the Bohr magneton, $\hat{\mathbf{s}}$ and $\hat{\mathbf{l}}$ are the spin and orbital angular momentum operators, respectively. The ratio of the field-induced magnetizations to the field strength ($\mathbf{B} = 10$ T) provided corresponding spin and orbital components of magnetic susceptibilities, $\chi_{\rm spin}$ and $\chi_{\rm orb}$, respectively.

According to results of the calculations, the exchange-enhanced spin paramagnetism $\chi_{\rm spin}$ appears to be the main contribution to magnetic susceptibility of $FeSe_{0.5}Te_{0.5}$ compound. Within the Stoner model, this contribution can be presented as: $\chi_{\rm spin} = S\mu_{\rm B}^2 N(E_{\rm F})$, where S is the Stoner factor, $N(E_{\rm F})$ DOS at the Fermi level, $\mu_{\rm B}$ the Bohr magneton. Using the calculated values of spin magnetic susceptibility of $FeSe_{0.5}Te_{0.5}$ compound, $\chi_{\rm spin} \simeq 0.6 \times 10^{-3}$ emu/mol, and DOS at the Fermi level, $N(E_{\rm F}) \simeq 1.85$ eV^{-1}, we have obtained the estimation of the Stoner factor: $S \simeq 10$. It should be noted that the above listed calculated value of $\chi_{\rm spin}$ is in agreement with the experimental magnetic susceptibility of $FeSe_{0.5}Te_{0.5}$ compound in the normal state (see Refs. [16, 23]). This confirms the dominating role of the spin contribution to magnetism of $FeSe_{0.5}Te_{0.5}$ compound, that is, apparently, characteristic for the whole $FeSe_{1-x}Te_x$ system [23, 25, 26].

By using the experimental data of Ref. [35] on evaluation of the lattice parameters of $FeSe_{0.5}Te_{0.5}$ under uniform compression, we calculated the behavior of density of electronic states at the Fermi level. For the region of small pressures (0÷10 kbar) we established the growth of $N(E_{\rm F})$ with the rate of $\mathrm{d}\ln N(E_{\rm F})/\mathrm{d}P \simeq 1$ Mbar^{-1}. We should note that such behavior of $N(E_{\rm F})$ correlates with increase of the superconducting transition temperature in $FeSe_{0.5}Te_{0.5}$ under pressure [12, 13].

Within the considered above method of calculation of magnetic susceptibility, we also investigated the dependence of χ in $FeSe_{0.5}Te_{0.5}$ compound on the uniform pressure. By direct calculations of the field-induced magnetic moments, we have obtained the value of pressure derivative of paramagnetic susceptibility, $\mathrm{d}\ln\chi/\mathrm{d}P \simeq 13$ Mbar^{-1}, which appeared to be close to the corresponding values in FeSe and FeTe (see Tab. II). In order to clarify the mechanism of the strong increase of magnetic susceptibility in $FeSe_{0.5}Te_{0.5}$ under pressure, we calculated value of χ as a function of the unit cell volume V and the internal structural parameter Z, which determines the relative height of chalcogen atoms over the plane of iron atoms. Then the corresponding pressure effect on χ can be presented as follows:

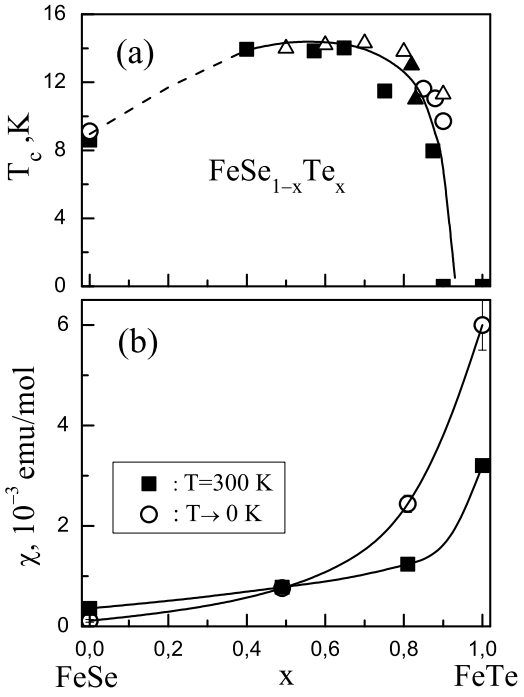

Figure 5: Concentration dependencies of (a) superconducting transition temperature (from Refs: ■ – [9], △ – [20], ▲ – [36], ○ – present work) and (b) magnetic susceptibility in the normal state for $T \to 0$ K and $T = 300$ K (from Ref. [23]) on Te content x in $FeSe_{1-x}Te_x$ compounds.

$$\frac{\mathrm{d}\ln\chi}{\mathrm{d}P} = \frac{\partial\ln\chi}{\partial\ln V} \times \frac{\mathrm{d}\ln V}{\mathrm{d}P} + \frac{\partial\ln\chi}{\partial Z} \times \frac{\mathrm{d}Z}{\mathrm{d}P}. \quad (2)$$

By small variations of the cell volume V and the structural parameter Z near their experimental values, the following partial derivatives of paramagnetic susceptibility for $FeSe_{0.5}Te_{0.5}$ were calculated to be $\partial\ln\chi/\partial\ln V \simeq 10$ and $\partial\ln\chi/\partial Z \simeq 90$. The necessary values for the compressibility of $FeSe_{0.5}Te_{0.5}$, $\mathrm{d}\ln V/\mathrm{d}P = -3.1$ Mbar^{-1}, and behavior of parameter Z under pressure, $\mathrm{d}Z/\mathrm{d}P \simeq 0.49$ Mbar^{-1}, were taken from Ref. [35]. By substituting the values of these parameters in Eq. (2) we have found that the calculated in this work large positive pressure effect on χ in $FeSe_{0.5}Te_{0.5}$ is related to the strong sensitivity of susceptibility to the parameter Z and its change under pressure, that determines the dominant positive contribution.

IV. DISCUSSION

Experimental values of superconducting transition temperatures for the investigated in this work compounds are in agreement with the literature data (see Fig. 5a). The most studied range of compositions ($x \geq 0.4$) is characterized by the sharp reduction of T_c with increasing x

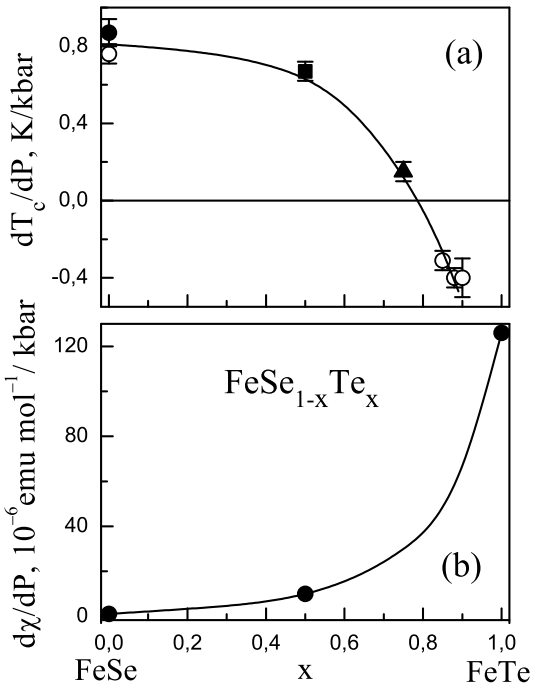

Figure 6: (a): The values of $\mathrm{d}T_c/\mathrm{d}P$ derivative depending on Te composition x in $FeSe_{1-x}Te_x$ compounds (○ – this work; ● – [37]; ■ – [13]; ▲ – [38]. (b): dependence of the pressure derivative of magnetic susceptibility in the normal state on Te composition x (see more details in the text).

at $x \geq 0.7$, and the total disappearance of superconductivity for $x \to 1$. In the same range of compositions the strong growth of magnetic susceptibility in the normal state was observed (Fig. 5b). The obtained strictly opposite tendencies in composition dependencies of superconductivity and magnetism in $FeSe_{1-x}Te_x$ system allow to assume that interrelation of these phenomena has competing character, at least for the tellurium rich compounds.

Let us consider now the evolution of superconducting and magnetic properties of $FeSe_{1-x}Te_x$ compounds under uniform pressure. Experimental values for pressure derivatives of the superconducting transition temperature are given in Fig. 6a, which include the known published data and the results of this work. Apparently, the available data describe the monotonous reduction of the pressure effect in T_c in process of selenium substitution with tellurium, and the change of its sign at $x \sim 0.8$. This trend is also consistent with the value of $\mathrm{d}T_c/\mathrm{d}P \simeq -0.25$ K/kbar for the related $FeS_{0.2}Te_{0.8}$ compound [9].

Unlike the pressure effect on T_c, which changes its sign as a function of composition (Fig. 6a), the magnetic susceptibility of FeSe(Te) system in the normal state is characterized by substantial growth under pressure for the whole system. This conclusion follows from available experimental data and theoretical estimates for the basic FeSe [25] and FeTe [14, 26] compounds, together with the

Table II: Pressure derivatives of the magnetic susceptibility, $\mathrm{d}\ln\chi/\mathrm{d}P$, for $FeSe_{1-x}Te_x$ compounds. Experimental temperatures are specified in brackets, results of calculations correspond to $T = 0$ K. The data for FeTe are referred to the paramagnetic state.

Compound	$\mathrm{d}\ln\chi/\mathrm{d}P$, Mbar^{-1}	
	Experiment	Theory
FeSe	10 ± 3 (78 K)[a]	$\simeq 8$[a]
	~ 9 (20 K) [b]	
$FeSe_{0.5}Te_{0.5}$	–	$\simeq 13$
FeTe	23 ± 1.5 (78 K) [c]	~ 20 [c]
	$\simeq 21$ (78 K) [d]	

[a]– from Ref. [25], [b]– from NMR data of Ref. [39], [c]– from Ref. [26], [d]– from magnetization data of Ref. [14].

results of present calculations for pressure dependence of magnetic susceptibility in $FeSe_{0.5}Te_{0.5}$ compound.

As can be seen from the values of pressure derivative of susceptibility, $\mathrm{d}\ln\chi/\mathrm{d}P$, given in Table II, for considered FeSe(Te) system the pressure effect not only much exceeds its typical value in the exchange-enhanced itinerant paramagnets [31], but also has the opposite *positive* sign. This implies an unusual for metallic system possibility of transition to the ferromagnetic state under the influence of experimentally achievable pressures. This is particularly the case of FeTe compound where the pressure effect is the largest. In Ref. [26] from the analysis of temperature dependence of susceptibility for FeTe in the paramagnetic region within the Curie-Weiss law, the values of the paramagnetic Curie temperature and its pressure derivative were evaluated to be $\Theta \simeq -240$ K and $\mathrm{d}\Theta/\mathrm{d}P \sim 7$ K/kbar. Corresponding to them rough estimate of the critical pressure for ferromagnetic transition amounts to 35 kbar. This is in reasonable agreement with results of Ref. [40], where the ferromagnetic state was observed in FeTe for the first time under pressures of $P \geq 20$ kbar.

For convenient comparison of the observed pressure effects in superconducting transition temperatures (Fig. 6a) with pressure effects in magnetic susceptibility, the values of pressure derivatives of susceptibility, $\mathrm{d}\chi/\mathrm{d}P \equiv \chi \times \mathrm{d}\ln\chi/\mathrm{d}P$, are presented in Fig. 6b for FeSe, $FeSe_{0.5}Te_{0.5}$ and FeTe. To evaluate these derivatives we used the corresponding values of $\chi(T \to 0$ K) from Ref. [23] (Fig. 5b) and the average values of $\mathrm{d}\ln\chi/\mathrm{d}P$ from Table II. As can be seen in Fig. 6, the presented composition dependencies of pressure effects in magnetic and superconducting properties of $FeSe_{1-x}Te_x$ system are strictly opposite to one another. This fact, along with similar trends in behavior of magnetic susceptibility and T_c as function of composition at ambient pressure (Fig. 5), specifies on antagonistic interrelation of magnetism and superconductivity in $FeSe_{1-x}Te_x$ system, which is most pronounced in the tellurium rich com-

pounds.

Conclusions

In this work the negative pressure effect on the superconducting transition temperature of tellurium rich $FeSe_{1-x}Te_x$ compounds was observed for the first time. The obtained data allowed to establish an overall picture of the composition dependence for the pressure effect on T_c, which monotonously decreases with growth of x and changes its sign at $x \sim 0.8$.

Another feature of $FeSe_{1-x}Te_x$ compounds is anomalously large and positive pressure effect on magnetic susceptibility in the normal state for all compositions, which grows with substitution of tellurium for selenium. As appears from the present calculations of the pressure effect on χ for $FeSe_{0.5}Te_{0.5}$ and the earlier similar calculations for FeSe and FeTe, the large positive pressure effect on susceptibility in $FeSe_{1-x}Te_x$ compounds is determined by the dominating positive contribution caused by the strong sensitivity of paramagnetic susceptibility to internal structural parameter Z and its change under pressure. It should be noted that the largest pressure effect on χ appears in FeTe compound, and that is a source of the observed its ferromagnetic state at high pressures [40].

Finally, the revealed here opposite trends in composition and pressure dependencies of superconducting transition temperature and magnetic susceptibility in the normal state indicate to antagonistic interrelation between superconductivity and magnetism in $FeSe_{1-x}Te_x$ chalcogenides. This tendency obviously has to be taken into account in further studies of possible role of magnetic excitations in the mechanism of superconductivity in Fe-based HTSCs.

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