

SUPERCONDUCTIVITY, INCLUDING HIGH-TEMPERATURE SUPERCONDUCTIVITY

Interrelation of superconductivity and magnetism in $\text{FeSe}_{1-x}\text{Te}_x$ compounds. Pressure effects

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The effect of isotropic pressures P up to 5 kbar on the superconducting transition temperature T_c of the $\text{FeSe}_{1-x}\text{Te}_x$ system ($x = 0, 0.85, 0.88, 0.90$) is studied. For the first time, a change in the sign of the effect of pressure on T_c on going from FeSe to the tellurium-rich alloys is observed. This makes it possible to specify more precisely the form of the dependence of the pressure derivative dT_c/dP on composition in this system. This dependence is compared with first principles calculations of the electron structure and magnetism of FeSe, FeTe, and $\text{FeSe}_{0.5}\text{Te}_{0.5}$ as functions of pressure, as well as with our earlier experimental data on the effect of pressure on the magnetic susceptibility of the normal state in FeSe and FeTe. This comparison is indicative of a competitive interrelationship between superconductivity and magnetism in tellurium rich $\text{FeSe}_{1-x}\text{Te}_x$ compounds. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4890990>]

1. Introduction

Most systems in the recently discovered class of iron-containing high-temperature superconductors (HTSC) are characterized by a correlation between the development of superconductivity in the system and the suppression of a magnetically ordered state with doping or application of isotropic pressure.^{1–4} In this regard, there is a widespread opinion to the effect that spin fluctuations play an important role in the formation of Cooper pairs.^{5–7} Nevertheless, it has been shown⁸ that for many compounds in this series the experimental values of the superconducting transition temperature are satisfactorily described by an electron-phonon coupling mechanism. The close interrelation between magnetism and superconductivity is why further study of the magnetic and superconducting properties and of their evolution with varying composition, pressure, etc., is important for understanding the mechanism of HTSC in this new class of compounds. One of the representatives of this class, the iron chalcogenides $\text{FeSe}_{1-x}\text{Te}_x$, has the simplest crystal structure and this favors the experimental and theoretical study of its properties.

The superconducting properties of $\text{FeSe}_{1-x}\text{Te}_x$ are characterized by a nonmonotonic dependence of the transition

temperature T_c on composition; there is a significant rise from $T_c \approx 8$ K for $x = 0$ to a maximum of ~ 15 K for $x \sim 0.5$, with a subsequent drop to 0 K near $x \sim 0.9$.⁹ In addition, in FeSe there is a large increase in T_c up to 35–37 K for pressures of $P = 70$ –80 kbar.^{10,11} Similar behavior of T_c with pressure has been observed in $\text{FeSe}_{0.5}\text{Te}_{0.5}$.^{12,13} With further increases in x in the $\text{FeSe}_{1-x}\text{Te}_x$ system, the positive pressure effect tends to decrease and apparently even changes sign, as observed in the related tellurium-rich alloy $\text{FeS}_{0.2}\text{Te}_{0.8}$.⁹ This apparent change in the sign of the pressure effect on T_c with increasing Te content also probably explains the unsuccessful attempts to observe superconductivity in FeTe at pressures up to 190 kbar.^{14,15}

The magnetic properties of the $\text{FeSe}_{1-x}\text{Te}_x$ system have been studied repeatedly,^{16–24} but data on the magnetic susceptibility of the normal state are incomplete and quantitatively contradictory. This is both because of the different quality of the samples and because of the presence of admixtures of iron and its secondary magnetic phases in the samples, which substantially mask the intrinsic magnetic susceptibility and require careful accounting.²² The best experimental data indicate that as Se is replaced by Te, the susceptibility of the compounds increases monotonically, approaching a value that is an order of magnitude higher in

FeTe than in FeSe. Furthermore, FeTe becomes magnetically unstable and antiferromagnetic ordering is observed in it at temperatures of roughly 70 K.¹⁷

It should be noted that the largest increase in the magnetic susceptibility of the normal state, $\chi(x)$, with increasing x has been observed in compounds that are rich in Te, where, in turn, $T_c(x)$ falls off rapidly, with FeTe no longer being a superconductor under normal conditions. This suggests that the interrelation of magnetism and superconductivity is of a competitive nature, at least for this range of compositions. For further study of this interrelationship in the $\text{FeSe}_{1-x}\text{Te}_x$ family, an examination of the correlation of superconductivity and magnetism at high pressures is undoubtedly of some interest. Therefore, in this paper we investigate the effect of hydrostatic pressure on the superconducting transition temperature in the tellurium-rich compounds. The experimental data are compared with data on the pressure dependence of the magnetic susceptibility in the base compounds FeSe²⁵ and FeTe^{14,26} supplemented by the calculated dependence of the electronic structure and magnetic susceptibility of $\text{FeSe}_{0.5}\text{Te}_{0.5}$.

2. Experimental details and results

Single crystal samples of the superconductor $\text{FeSe}_{0.96}$ (subsequently FeSe) were grown over a period of 50 days by a method described in Ref. 27 in evacuated fused silica cells filled with a molten mixture of AlCl_3/KCl with a constant temperature gradient. The temperature of the hot end of the cell, which contains a batch with the initial composition, was 427 °C and the colder end, where the crystals grew, was kept at roughly 380 °C. A series of tellurium enriched superconducting single crystals of $\text{Fe}_{1+\delta}\text{Se}_{1-x}\text{Te}_x$ ($\delta \sim 0.05$; $x = 0.85, 0.88, \text{ and } 0.90$) was synthesized in similar fashion. Here a mixture of the salts KCl/NaCl was used and the temperatures of the hot and cold ends of the cell were kept at 750 and approximately 700 °C, respectively. The synthesis process lasted 20–25 days. The grown single crystal slabs had typical sizes of $(1\text{--}3) \times (1\text{--}3) \times (0.2\text{--}0.3)$ mm. The tetragonal $P4/nmm$ crystal structure of the samples was determined at room temperature by x-ray diffraction and their composition was checked by x-ray fluorescence analysis (Cameca SX-100) with an accuracy no worse than 2% in the determination of the ratio of the components (for details of the certification of the samples see Refs. 24 and 27).

The magnetic properties were studied using a SQUID magnetometer (Quantum Design MPMS-XL6) equipped with a miniature high pressure chamber of the cylinder-piston type (similar to that used in Ref. 28) made of nonmagnetic CuBe alloy and with inner and outer diameters of 1.6 and 5 mm, respectively. PES-2 polyethylsiloxane fluid was used as the pressure transmission medium (freezing temperature 164 K). The pressure at low temperatures was determined from the known pressure dependence of the superconducting transition temperature of a pure tin sample²⁹ located inside the chamber near the sample being measured. The corresponding error was no more than 0.2 kbar.

Figure 1 shows the temperature dependences $M(T)$ of the magnetic moment for FeSe at different pressures measured with cooling of the sample in zero magnetic field (ZFC, zero field cooling) followed by heating in a field of

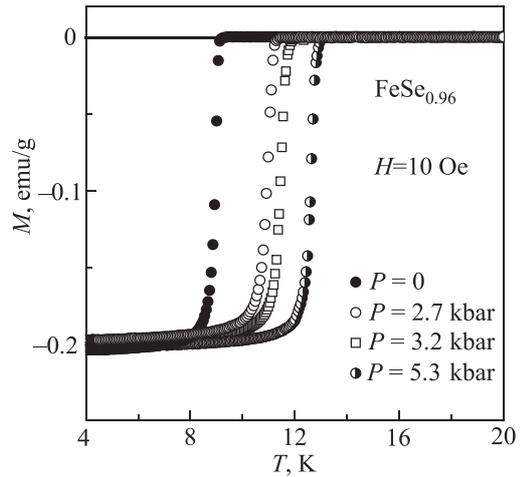


FIG. 1. Temperature dependences of the magnetic moment of FeSe measured in a magnetic field of $H = 10$ Oe at different pressures.

$H = 10$ Oe. The resulting pressure dependence of the superconducting transition temperature T_c , defined here and in the following by its onset, is shown in Fig. 2. Within the experimental errors and in the pressure range used here, this curve is close to linear and can be used to determine the pressure derivative dT_c/dP .

Figure 3 shows the $M(T)$ curves measured in the ZFC regime at different pressures for tellurium enriched $\text{FeSe}_{1-x}\text{Te}_x$ compounds. These curves reveal a distinctly negative pressure effect on the superconducting transition temperature. The experimental values of T_c and its derivative with respect to pressure for all the alloys studied here are listed in Table 1. These data show that the scale of the pressure effect in the tellurium enriched $\text{FeSe}_{1-x}\text{Te}_x$ alloys is comparable to that for FeSe, but has an opposite sign.

3. Calculating the electronic structure and paramagnetic susceptibility of $\text{FeSe}_{0.5}\text{Te}_{0.5}$

The electronic structure of the compound $\text{FeSe}_{0.5}\text{Te}_{0.5}$ was calculated using the LMTO method with the full potential (FP-LMTO, version RSP^{30,31}). The exchange-correlation potential is taken into account through the local

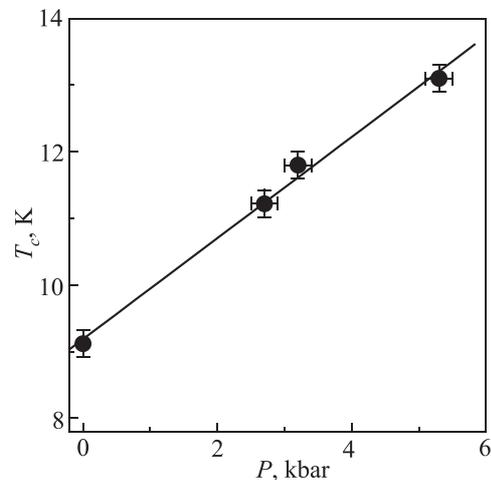


FIG. 2. Superconducting transition temperature as a function of pressure for FeSe.

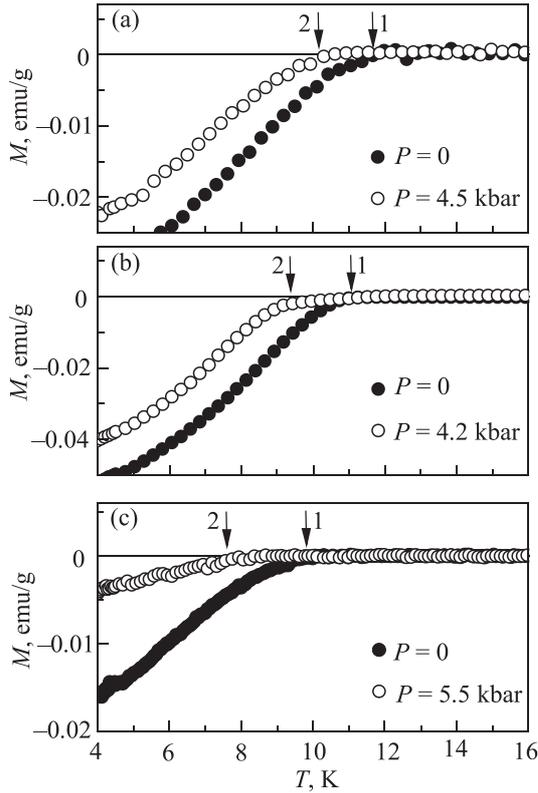


FIG. 3. Temperature dependences of the magnetic moment of the compounds $\text{FeSe}_{1-x}\text{Te}_x$ with $x=0.85$ (a), 0.88 (b), and 0.9 (c) in a field of $H=10\text{Oe}$ at two pressures. The arrows 1 and 2 indicate T_c for zero pressure and the finite pressure, respectively.

electron density approximation (LDA)³² of the density functional theory (DFT). The calculations were done for a $2 \times 2 \times 1$ supercell constructed by twofold translation of the unit cell of the ordered tetragonal phase of the compounds FeSe and FeTe along the crystallographic [100] and [010] directions using the experimental values of the lattice parameters of $\text{FeSe}_{0.5}\text{Te}_{0.5}$.^{33–35} Figure 4 shows the calculated electron density of states $N(E)$ of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ in the paramagnetic phase. Here the Fermi level E_F is located in a segment of the $N(E)$ curve that is close in shape to a local plateau and is determined primarily by the d -states of iron. This feature of the position of E_F assumes a weak temperature dependence of the spin susceptibility in $\text{FeSe}_{0.5}\text{Te}_{0.5}$, in agreement with the available experimental data for this compound.

We have also calculated the electronic structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ in the paramagnetic phase in an external magnetic field \mathbf{B} . The influence of the field was taken into account self consistently³¹ through the local spin density approximation (LSDA) by including the Zeeman operator

TABLE 1. The superconducting transition temperature T_c and its derivative dT_c/dP for $\text{FeSe}_{1-x}\text{Te}_x$ alloys.

Composition	T_c , K	dT_c/dP , 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

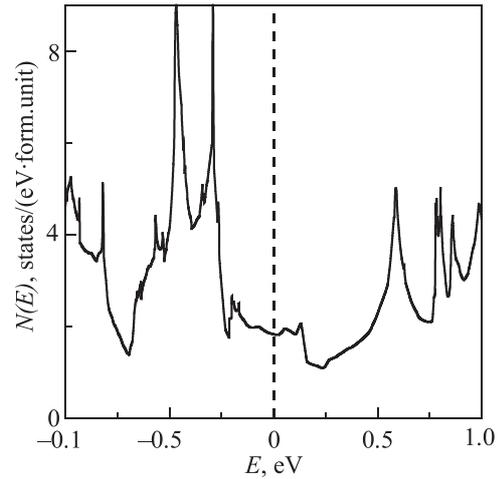


FIG. 4. The electron density of states $N(E)$ of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ near the Fermi level ($E=0$), which is indicated by a vertical line.

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

in the FP-LMTO hamiltonian, where $\hat{\mathbf{s}}$ is the spin operator and $\hat{\mathbf{l}}$ is the orbital angular momentum operator. The induced spin and orbital angular momenta calculated for an external field $B=10\text{T}$ made it possible to obtain the corresponding components of the magnetic susceptibility tensor, χ_{spin} and χ_{orb} , by differentiation with respect to the induced magnetizations.

These calculations of the electronic structure and magnetic susceptibility show that the dominant contribution to the susceptibility of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ is the exchange-enhanced spin paramagnetism χ_{spin} . In the Stoner model this contribution can be written in the form $\chi_{\text{spin}} = S\mu_B^2 N(E_F)$, where S is the Stoner factor, $N(E_F)$ is the density of states at the Fermi level, and μ_B is the Bohr magneton. Using the calculated values of the spin magnetic susceptibility of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ based on data on the spin moment, $\chi_{\text{spin}} = 0.6 \times 10^{-3} \text{emu/mol}$, and the density of states at the Fermi level, $N(E_F) = 1.85 \text{eV}^{-1}$, we obtain an estimate for the Stoner factor: $S=10$. Note that the above calculated value of χ_{spin} is in satisfactory agreement with the experimental magnetic susceptibility of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ in the normal state.^{16,23} This confirms the predominance of the spin contribution to the magnetism of this compound; this appears to be typical of the entire $\text{FeSe}_{1-x}\text{Te}_x$ family as a whole.^{23,25,26}

Using experimental data³⁵ on the variation in the lattice parameters of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ subjected to isotropic pressure, here we calculate the pressure dependence of the electron density of states at the Fermi level. At low pressures (0–10 kbar) we find that $N(E_F)$ increases with the pressure derivative $d \ln N(E_F)/dp \simeq 1 \text{Mbar}^{-1}$. We note that this behavior of $N(E_F)$ correlates with the increase in the superconducting transition temperature with pressure in $\text{FeSe}_{0.5}\text{Te}_{0.5}$.

We have also used the method for calculating the magnetic susceptibility described above to study its dependence on the isotropic pressure in the $\text{FeSe}_{0.5}\text{Te}_{0.5}$ system. By direct calculation of the magnetic moment induced by an external field, we obtain a value of the pressure derivative of the magnetic susceptibility, $d \ln \chi/dp \simeq 13 \text{Mbar}^{-1}$, that is

close to the analogous values for FeSe and FeTe (see Table 2).

In order to clarify the mechanism for the rapid rise in the magnetic susceptibility of FeSe_{0.5}Te_{0.5} under pressure, we have analyzed the effect of the unit cell volume V and the internal structure parameter Z (which determines the relative height of the chalcogenide atoms above the plane of the iron atoms) on the susceptibility. The corresponding pressure effect on χ can be written in the form

$$\frac{d \ln \chi}{dP} = \frac{\partial \ln \chi}{\partial \ln V} \frac{d \ln V}{dP} + \frac{\partial \ln \chi}{\partial Z} \frac{dZ}{dP}. \quad (2)$$

The method of small variations in the cell volume V and structural parameter Z near their experimental values was used to calculate the following partial derivatives of the paramagnetic susceptibility of FeSe_{0.5}Te_{0.5}: $\partial \ln \chi / \partial \ln V \simeq 10$ and $\partial \ln \chi / \partial Z \simeq 90$. Together with the experimental values of the compressibility $d \ln V / dP \simeq -3.1 \text{ Mbar}^{-1}$ and the derivative of Z with respect to pressure, $d \ln Z / dP \simeq 49 \text{ Mbar}^{-1}$, derived from the data of Ref. 35, these results (according to Eq. (2)) determine the corresponding contributions to the combined pressure effect: $(\partial \ln \chi / \partial \ln V) (d \ln V / dP) \simeq -31 \text{ Mbar}^{-1}$ and $(\partial \ln \chi / \partial Z) (dZ / dP) \simeq +44 \text{ Mbar}^{-1}$. These estimates suggest that the large positive pressure effect on the susceptibility of FeSe_{0.5}Te_{0.5} calculated here is determined by a dominant positive effect owing to the high sensitivity of the susceptibility to the internal structure parameter Z and to the way it varies with pressure.

4. Discussion of results

The experimental values of the superconducting transition temperature for the compounds studied here are in reasonable agreement with published data (see Fig. 5(a)).

The most studied compositions ($x \geq 0.4$) are characterized by a sharp drop in T_c with increasing x for $x \geq 0.7$ and the complete disappearance of superconductivity as $x \rightarrow 1$. In this range of compositions there is a sharp rise in the magnetic susceptibility of the normal state (Fig. 5(b)). The strictly opposite tendencies in the behavior of the superconductivity and the magnetism with composition in FeSe_{1-x}Te_x systems indicate that the interrelationship of these phenomena is of a competitive nature, at least in the tellurium enriched compounds.

We now consider the evolution of the superconducting and magnetic properties of the family of FeSe_{1-x}Te_x compounds subjected to isotropic pressure. Figure 6(a) is a plot

TABLE 2. The derivative of the magnetic susceptibility with respect to pressure, $d \ln \chi / dP$, for compounds in the family FeSe_{1-x}Te_x (the experimental temperature is given in brackets; the computed results correspond to $T = 0 \text{ K}$). The data for FeTe refer to the paramagnetic state.

Compound	$d \ln \chi / dP, \text{ Mbar}^{-1}$	
	Experiment	Theory
FeSe	$10 \pm 3 (78 \text{ K})^a; \sim 9 (20 \text{ K})^b$	$\simeq 8^a$
FeSe _{0.5} Te _{0.5}	...	$\simeq 13$
FeTe	$23 \pm 1.5 (78 \text{ K})^c; 21 (78 \text{ K})^d$	$\simeq 20^c$

Note: ^afrom Ref. 25; ^bfrom NMR (Knight shift) data (Ref. 39); ^cfrom Ref. 26; ^dfrom the magnetization measurements of Ref. 14.

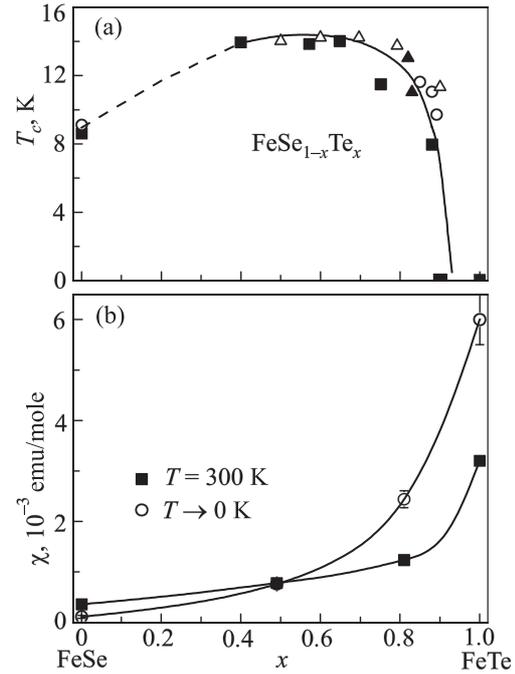


FIG. 5. (a) Superconducting transition temperature (■—, ⁹△—, ²⁰▲—, ³⁶○— this paper) and (b) magnetic susceptibility in the normal state for $T \rightarrow 0 \text{ K}$ and $T = 300 \text{ K}$ (Ref. 23) for FeSe_{1-x}Te_x compounds as functions of Te content.

of the experimentally measured derivative of the superconducting transition temperature with respect to pressure that includes our results along with published data. These data describe a monotonic reduction in the effect of pressure on T_c as Se is replaced by Te and a change in its sign $x \sim 0.8$. The value of $dT_c/dP = -0.25 \text{ K/kbar}$ for the related

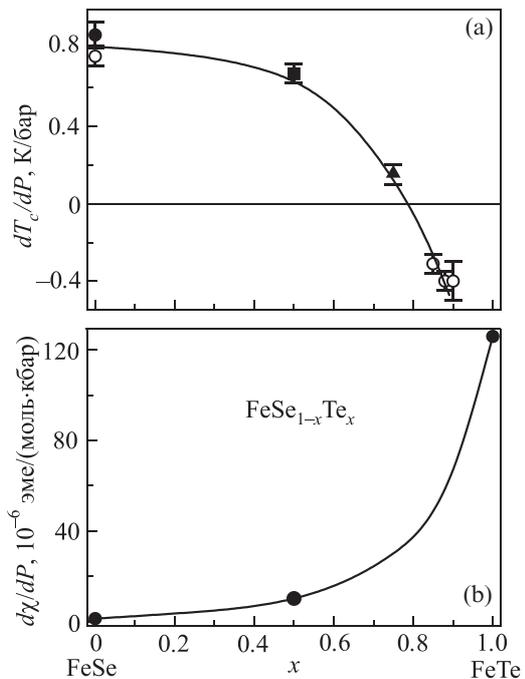


FIG. 6. (a) The derivative dT_c/dP as a function of composition for FeSe_{1-x}Te_x compounds (○— this paper, ●—, ³⁷■—, ¹³▲—³⁸). (b) The derivative of the magnetic susceptibility in the normal state as a function of composition (see text for details).

compound $\text{FeSe}_{0.2}\text{Te}_{0.8}$ (Ref. 9) is essentially in agreement with the curve plotted here.

As opposed to the change in sign of the effect of pressure on T_c as a function of composition (Fig. 6(a)), the magnetic susceptibility of the normal state of the $\text{FeSe}(\text{Te})$ family is characterized by a substantial rise with pressure for the entire system as a whole. This conclusion follows from the available experimental data and theoretical estimates for the base compounds FeSe ²⁵ and FeTe ,^{14,26} together with our calculations of the pressure dependence of the magnetic susceptibility of $\text{FeSe}_{0.5}\text{Te}_{0.5}$.

The values of the derivative of the susceptibility, $d\chi/dP$, for the $\text{FeSe}(\text{Te})$ system given in Table 2 show that this effect is not only an order of magnitude greater than the typical amount in exchange-enhanced band paramagnets,³¹ but also has an opposite *positive* sign. This suggests the unusual possibility of a transition of a metallic system into a ferromagnetic state at experimentally attainable pressures. This applies particularly to the compound FeTe , where the magnitude of this effect is greatest. An analysis²⁶ of the temperature dependence of the susceptibility of FeTe in the paramagnetic region in terms of the Curie-Weiss law yielded values for the paramagnetic Curie temperature and its derivative with respect to pressure of $\Theta \simeq -240\text{ K}$ and $d\Theta/dP \sim 7\text{ K/kbar}$. A corresponding rough estimate of the critical pressure at which ferromagnetism appears gives approximately 35 kbar. This is in reasonable agreement with the first observation⁴⁰ of a ferromagnetic state in FeTe at pressures $P \geq 20\text{ kbar}$.

For clarity in comparing the observed pressure effects on the superconducting transition temperature (Fig. 6(a)) and the analogous effects on the magnetic susceptibility, the solid circles in Fig. 6(b) indicate the derivative $d\chi/dP \equiv \chi d \ln \chi / dP$ of the susceptibility with respect to pressure for FeSe , $\text{FeSe}_{0.5}\text{Te}_{0.5}$, and FeTe . These were estimated using the corresponding values of $\chi(T \rightarrow 0\text{ K})$ from Ref. 23 (Fig. 5(b)) and the averaged values of $d \ln \chi / dP$ from Table 2. The composition plots of Fig. 6 show that the effects of pressure on the magnetic and superconducting properties of the system $\text{FeSe}_{1-x}\text{Te}_x$ are strictly opposite. This fact, along with similar trends in the composition dependence of the magnetic susceptibility and T_c in the normal state (Fig. 5), indicates that the interrelationship of magnetism and superconductivity in this system is competitive in character. This shows up most strongly in the tellurium enriched region.

5. Conclusion

In this paper, we report for the first time a negative effect of pressure on the superconducting transition temperature for tellurium enriched compounds of the $\text{FeSe}_{1-x}\text{Te}_x$ family. The data obtained here have made it possible to determine the general behavior of the magnitude of the pressure effect on T_c as a function of composition which decreases with increasing x and changes sign at $x \sim 0.8$.

Another feature of this system is an anomalously large positive pressure effect on the magnetic susceptibility of the normal state over the entire range of compositions; the magnitude of this effect increases as selenium is replaced by tellurium. Our calculations of the magnitude of this effect

for $\text{FeSe}_{0.5}\text{Te}_{0.5}$ and similar calculations done previously for FeSe and FeTe show that the large positive pressure effect on the susceptibility of $\text{FeSe}_{1-x}\text{Te}_x$ is determined by a dominant positive contribution owing to the high sensitivity of the susceptibility to the internal structure factor Z and its variation with pressure. The effect is largest in FeTe and is the source of the ferromagnetic state observed in it at high pressures.

Finally, the opposing tendencies in the behavior of the superconducting transition temperature and the magnetic susceptibility of the normal state that depend on composition and pressure suggest that the interrelation between superconductivity and magnetism is competitive in the iron chalcogenides $\text{FeSe}_{1-x}\text{Te}_x$ examined here. This fact is important and should be kept in mind in further studies of the possible contributions of magnetic excitations to the mechanism of superconductivity in this system.

This paper is devoted to the 100-anniversary of the birth of Academician A. A. Galkin, the founder of the Donetsk Institute of Physics and Technology of the National Academy of Sciences of Ukraine and the Donetsk school of high pressure physics and solid state spectroscopy.

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- ¹M. D. Lumsden and A. D. Christianson, *J. Phys.: Condens. Matter* **22**, 203203 (2010).
- ²C. W. Chu and B. Lorenz, *Physica C* **469**, 385 (2009).
- ³J. Paglione and R. L. Greene, *Nat. Phys.* **6**, 645 (2010).
- ⁴J. Wen, G. Xu, G. Gu, J. M. Tranquada, and R. J. Birgeneau, *Rep. Prog. Phys.* **74**, 124503 (2011).
- ⁵I. I. Mazin, *Nature* **464**, 183 (2010).
- ⁶P. J. Hirschfeld, M. M. Korshunov, and I. I. Mazin, *Rep. Prog. Phys.* **74**, 124508 (2011).
- ⁷Y. Kohama, Y. Kamihara, M. Hirano, H. Kawaji, T. Atake, and H. Hosono, *Phys. Rev. B* **78**, 020512(R) (2008).
- ⁸M. V. Sadovskii, E. Z. Kuchinskii, and I. A. Nekrasov, *J. Magn. Magn. Mater.* **324**, 3481 (2012).
- ⁹Y. Mizuguchi and Y. Takano, *J. Phys. Soc. Jpn.* **79**, 102001 (2010).
- ¹⁰D. Braithwaite, B. Salce, G. Lapertot, F. Bourdarot, C. Marin, D. Aoki, and M. Hanfland, *J. Phys.: Condens. Matter* **21**, 232202 (2009).
- ¹¹S. Medvedev, T. M. McQueen, I. A. Troyan, T. Palasyuk, M. I. Erements, R. J. Cava, S. Naghavi, F. Casper, V. Ksenofontov, G. Wortmann, and C. Felser, *Nature Mater.* **8**, 630 (2009).
- ¹²K. Horigane, N. Takeshita, C.-H. Lee, H. Hiraka, and K. Yamada, *J. Phys. Soc. Jpn.* **78**, 063705 (2009).
- ¹³J. Pietosa, D. J. Gawryluk, R. Puzniak, A. Wisniewski, J. Fink-Finowicki, M. Kozłowski, and M. Berkowski, *J. Phys.: Condens. Matter* **24**, 265701 (2012).
- ¹⁴H. Okada, H. Takahashi, Y. Mizuguchi, Y. Takano, and H. Takahashi, *J. Phys. Soc. Jpn.* **78**, 083709 (2009).
- ¹⁵H. Takahashi, H. Okada, H. Takahashi, Y. Mizuguchi, and Y. Takano, *J. Phys.: Conf. Ser.* **200**, 012196 (2010).
- ¹⁶B. C. Sales, A. S. Sefat, M. A. McGuire, R. Y. Jin, D. Mandrus, and Y. Mozharivskiy, *Phys. Rev. B* **79**, 094521 (2009).
- ¹⁷G. F. Chen, Z. G. Chen, J. Dong, W. Z. Hu, G. Li, X. D. Zhang, P. Zheng, J. L. Luo, and N. L. Wang, *Phys. Rev. B* **79**, 140509 (2009).
- ¹⁸R. Vienneis, E. Giannini, D. van der Marel, and R. Eerný, *J. Solid State Chem.* **183**, 769 (2010).
- ¹⁹J. Yang, M. Matsui, M. Kawa, H. Ohta, C. Michioka, C. Dong, H. Wang, H. Yuan, M. Fang, and K. Yoshimura, *J. Phys. Soc. Jpn.* **79**, 074704 (2010).

- ²⁰T. Noji, T. Suzuki, H. Abe, T. Adachi, M. Kato, and Y. Koike, *J. Phys. Soc. Jpn.* **79**, 084711 (2010).
- ²¹Y. Liu, R. K. Kremer, and C. T. Lin, *Supercond. Sci. Technol.* **24**, 035012 (2011).
- ²²A. V. Fedorchenko, G. E. Grechnev, V. A. Desnenko, A. S. Panfilov, S. L. Gnatchenko, V. V. Tsurkan, J. Deisenhofer, H.-A. Krug von Nidda, A. Loidl, D. A. Chareev, O. S. Volkova, and A. N. Vasiliev, *Fiz. Nizk. Temp.* **37**, 100 (2011). [*Low Temp. Phys.* **37**, 83 (2011)].
- ²³G. E. Grechnev, A. S. Panfilov, A. V. Fedorchenko, V. A. Desnenko, S. L. Gnatchenko, V. Tsurkan, J. Deisenhofer, A. Loidl, D. A. Chareev, O. S. Volkova, and A. N. Vasiliev, *J. Magn. Magn. Mater.* **324**, 3460 (2012).
- ²⁴Y. A. Ovchenkov, D. A. Chareev, E. S. Kozlyakova, O. S. Volkova, and A. N. Vasiliev, *Physica C* **489**, 32 (2013).
- ²⁵G. E. Grechnev, A. S. Panfilov, V. A. Desnenko, A. V. Fedorchenko, S. L. Gnatchenko, D. A. Chareev, O. S. Volkova, and A. N. Vasiliev, *J. Phys.: Condens. Matter* **25**, 046004 (2013).
- ²⁶A. V. Fedorchenko, G. E. Grechnev, V. A. Desnenko, A. S. Panfilov, S. L. Gnatchenko, V. Tsurkan, J. Deisenhofer, A. Loidl, O. S. Volkova, and A. N. Vasiliev, *J. Phys.: Condens. Matter* **23**, 325701 (2011).
- ²⁷D. Chareev, E. Osadchii, T. Kuzmicheva, J.-Y. Lin, S. Kuzmichev, O. Volkova, and A. Vasiliev, *Cryst. Eng. Comm.* **15**, 1989 (2013).
- ²⁸M. Baran, V. Dyakonov, L. Gladczuk, G. Levchenko, S. Piechota, and H. Szymczak, *Physica C* **241**, 383 (1995).
- ²⁹L. D. Jennings and C. A. Swenson, *Phys. Rev.* **112**, 31 (1958).
- ³⁰J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, and A. Grechnev, *Full-Potential Electronic Structure Method. Energy and Force Calculations With Density Functional and Dynamical Mean Field Theory*, Springer Series in Solid-State Sciences Vol. 167 (Springer Verlag, Berlin, 2010), p. 200.
- ³¹G. E. Grechnev, *Fiz. Nizk. Temp.* **35**, 812 (2009), [*Low Temp. Phys.* **35**, 638 (2009)].
- ³²U. von Barth and L. Hedin, *J. Phys. C: Solid State Phys.* **5**, 1629 (1972).
- ³³G. Tsoi, A. K. Stemshorn, Y. K. Vohra, P. M. Wu, F. C. Hsu, Y. L. Huang, M. K. Wu, K. W. Yeh, and S. T. Weir, *J. Phys.: Condens. Matter* **21**, 232201 (2009).
- ³⁴V. Tsurkan, J. Deisenhofer, A. Günther, Ch. Kant, M. Klemm, H.-A. Krug von Nidda, F. Schrettle, and A. Loidl, *Eur. Phys. J. B* **79**, 289 (2011).
- ³⁵P. S. Malavi, S. Karmakar, N. N. Patel, and S. M. Sharma, e-print [arXiv:1308.3367\[cond-mat.mtrl-sci\]](https://arxiv.org/abs/1308.3367).
- ³⁶Y. Koshika, T. Usui, S. Adachi, T. Watanabe, K. Sakano, S. Simayi, and M. Yoshizawa, *J. Phys. Soc. Jpn.* **82**, 023703 (2013).
- ³⁷M. Bendele, A. Ichsanow, Yu. Pashkevich, L. Keller, Th. Strässle, A. Gusev, E. Pomjakushina, K. Conder, R. Khasanov, and H. Keller, *Phys. Rev. B* **85**, 064517 (2012).
- ³⁸Y. Mizuguchi, F. Tomioka, K. Deguchi, S. Tsuda, T. Yamaguchi, and Y. Takano, *Physica C* **470**, S353 (2010).
- ³⁹T. Imai, K. Ahilan, F. L. Ning, T. M. McQueen, and R. J. Cava, *Phys. Rev. Lett.* **102**, 177005 (2009).
- ⁴⁰M. Bendele, A. Maisuradze, B. Roessli, S. N. Gvasaliya, E. Pomjakushina, S. Weyeneth, K. Conder, H. Keller, and R. Khasanov, *Phys. Rev. B* **87**, 060409 (2013).

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