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The energy gap of the compound $FeSe_{0.5}Te_{0.5}$ determined by specific heat and Point Contact Spectroscopy

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ABSTRACT

The superconductor $FeSe_{0.5}Te_{0.5}$ was studied with Point Contact spectroscopy and specific heat in polycrystalline samples. The transition temperature determined by magnetic measurement was $T_C = 14.5$ K. The size of the energy gap measured by junctions is $\Delta = 1.9$ meV, whereas the gap determined by the specific heat measurements was $\Delta = 2.3$ meV. The gap evolution with temperature follows BCS, the ratio $2\Delta/K_BT_C$ has values between $2.88 \leq 2\Delta/K_BT_C \leq 3.04$. The compound was grown by solid state synthesis in quartz ampoules under vacuum at 950 °C. Crystal structure was characterized by X-ray diffraction. The superconducting properties were characterized by magnetization, resistivity and specific heat. This superconductor shows an isotropic energy gap as observed with the fitting of the specific heat at low temperature.

1. Introduction

The new superconducting materials FeSe are interesting because they may give guides to elucidate the superconducting mechanism of other similar members with Fe and to others of the FeAs family. FeSe compound is one of the simplest Fe-based superconductors with a transition temperature $T_C \simeq 8$ K. It has crystalline structure type anti-PbO and space group P4/nmm [1–3].

Compounds in these families have different transition temperatures, some with higher transition temperatures as the basic FeSe [2,4–7]. Recently many study have been performed on these compounds [2,5,7–9] some with transition temperatures as high as $T_C = 40$ K.

In those compounds the magnetism of Fe may play a relevant role which still is not totally understood for the superconducting behavior.

In this work we report a study of the superconductivity in Fe–Se–Te performed in polycrystalline samples. The study was mainly directed to observe and analyze the behavior of the energy gap and to determine the symmetry of the pairing wave function. In general for the determination of the energy gap, two tools are well appropriate: Point Contact Spectroscopy (PCS) and Tunnel junctions. We used in this study one of those spectroscopic techniques. The junctions were formed with the superconducting compound with stoichiometry $FeSe_{0.5}Te_{0.5}$ and a normal metal. The sample has a high transition temperature of about $T_C = 14.5$ K, as determined by magnetic-temperature measurements. Our studies show the size of the energy gap, the ratio $2\Delta/K_BT_C$, and the evolution with temperature of the gap. In addition, specific heat measurements indicated an isotropic energy gap with *s* symmetry and the superconducting gap follows the BCS theory. The junctions were characterized with the BTK model [10]. With this model we can describe the type of junctions; i.e. PCS or tunnel, using the dimensionless barrier strength parameter *Z* given by the theory. Depending on this parameter the junctions may be considered as a tunnel or a metallic contact (PCS).

2. Experimental details

2.1. Compound and junctions characteristics

The superconducting samples were prepared by solid state reaction in evacuated quartz tubes with powder and purities: Fe 99.9%, Se 99.9%, and Te 99.99%. The nominal proportion was 1.01:0.5:0.05, the powders were mixed pressed and sintered at 950 °C for 3 days, finally annealed at 400–500 °C in a period of one day. R-X diffraction patterns gave the crystalline structure as reported by [9,11–17].

The study was performed with junctions that behave as metallic point contacts PCS. The junctions were prepared with the superconductor and a thin wire of tungsten plated gold W(Au) which has a diameter of 5 μm, the stoichiometry of the superconductor was $FeSe_{0.5}Te_{0.5}$. For the fabrication of the PCS the wire

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was diagonally clipped as the procedure used in tips for use in scanning tunneling microscopy and carefully pressed into the superconducting sample. This cut allows us to obtain very sharp tips with very small diameters about or less than 1 μm [18]. Oxford varnish was used to glue the sample to a glass support. The estimated area of the junctions was ~ 1 μm^2, as observed in an optical microscopy. The determined parameters with the BTK model gave values for the Z parameter from 3.4 to 6 [10]. This was one of the main considerations to determine the type of junction.

At the initial measurements several try outs were performed until reproducible data and stable characteristics were obtained. Results presented in this work are the most reproducible for all the junctions.

Many junctions, more than 25 PCS's were prepared. The characteristics displayed in Figs. 4 and 5 were the most reproducible. The characteristics were measured from 1.7 to 25 K. Results show the size of the energy gap, the gap evolution with temperature, and ratio $2\,\Delta/K_BT_C$. The compound characteristics were determined by resistivity, ρ–T, specific heat, C_P–T, and magnetization, M–T, according to transport and magnetic measurements the transition temperature was T_C=14.5 K, as shown by other researchers [6,7,11,12].

The superconducting characteristics were determined in a Quantum Design MPMS system, the amount of superconducting phase was estimated by Zero Field Cooling (ZFC) and Field Cooling (FC) measurements with 10 Oe. The proportion of superconducting material was ~ 70%, compared with pure Pb with the same mass as the sample. Transport characteristic was determined in a Quantum Design PPMS system, Fig. 1 displays the resistivity versus temperature for the selected sample. Main panel shows the resistivity ρ–T close to the transition temperature and the inset presents the overall behavior to high temperature. In Fig. 2 we display the magnetic characteristics of the three different compositions. The sample with the composition $FeSe_{0.5}Te_{0.5}$ was used for determination of the spectroscopic characteristics because it has the maximum proportion of superconducting material.

The isotropic characteristics of the energy gap were determined by thermal characterization measuring the specific heat capacity. The main panel in Fig. 3 displays the observed characteristic close to the transition temperature. The specific heat measurements, C_P–T, were performed with a thermal relaxation method using a Quantum Design PPMS apparatus. The C_P values were corrected by subtracting the addenda of the sample support and grease used to glue the sample to the support. Thermal measurements show similar overall characteristics as determined by Sales and Awana. The Debye temperature was Θ_D = 171–174 K [9,13]. At low temperature specific heat measurements may give indications related to the type of superconducting pairing [19]. Our observations at low temperature show a decrease that fit quite well to an exponential decay, as $C_P = C_0 + Ae^{(-\Delta/K_BT)}$. Two different parameters for the fitting were used as shown in the main panel of Fig. 3, C_0 and A are parameters to adjust the background level of the specific heat curve at low temperature, whereas Δ = 2.3 meV. The important result is that the superconducting compound is isotropic with a single gap and *s−wave* symmetry, the size of the energy gap is similar to that determined by the PCS, and the transition temperature was about T = 13.3 ± 0.03 K. However, it is important to mention that determination of the energy gap with specific heat measurements is not as precise as tunneling or PCS measurements, nevertheless, specific heat may give clear information about features of multi-gap or single gap characteristics.

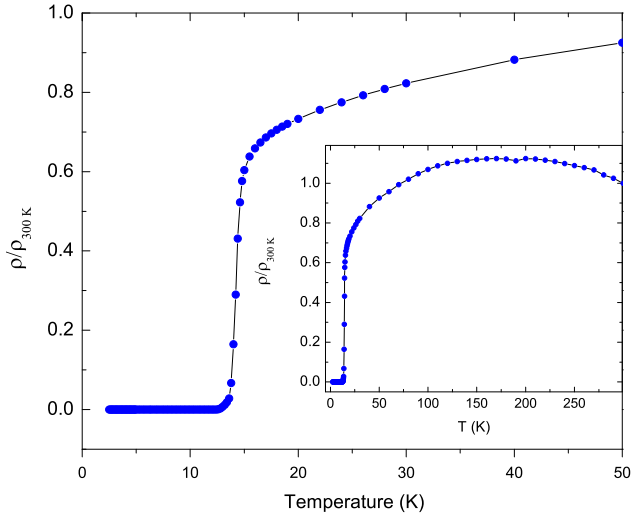

Fig. 1. (Color online) Resistivity–temperature characteristic of the superconducting compound $FeSe_{0.5}Te_{0.5}$. Main panel displays the temperature interval close to the transition temperature, T_C=14.5 K. The inset shows the overall characteristics.

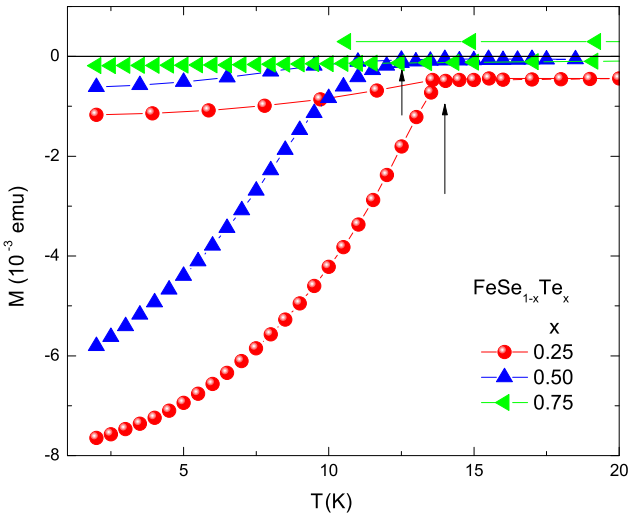

Fig. 2. (Color online) Magnetization measurements of three different compounds with different stoichiometries. The compound $FeSe_{0.5}Te_{0.5}$ was selected for the study. This shows the maximum proportion of superconducting material. The panel displays the M–T measurements in the temperature interval close to the transition temperature in ZFC and FC modes in order to determinate the amount of superconducting material. The transition temperature was T_C=14.5 K.

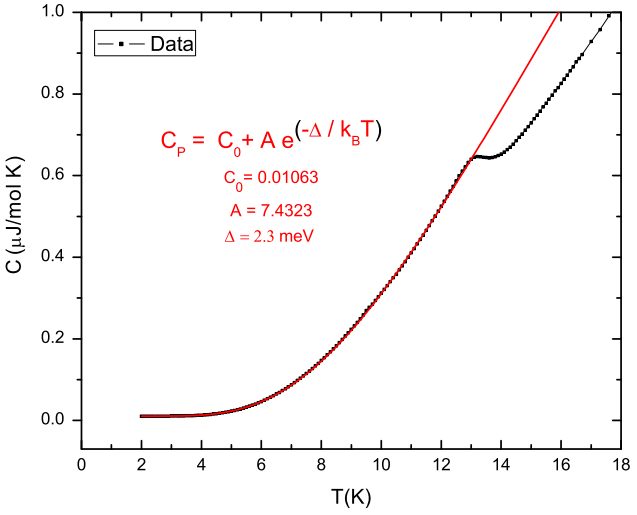

Fig. 3. (Color online) Specific heat of the superconducting compound $FeSe_{0.5}Te_{0.5}$. Main panel displays the fitting of C_P experimental data to the function $C_P = C_0 + Ae^{(-\Delta/K_BT)}$, from 14 to 2 K (red line). According to the specific heat measurements the transition temperature is about T_C=13.3 ± 0.03 K.

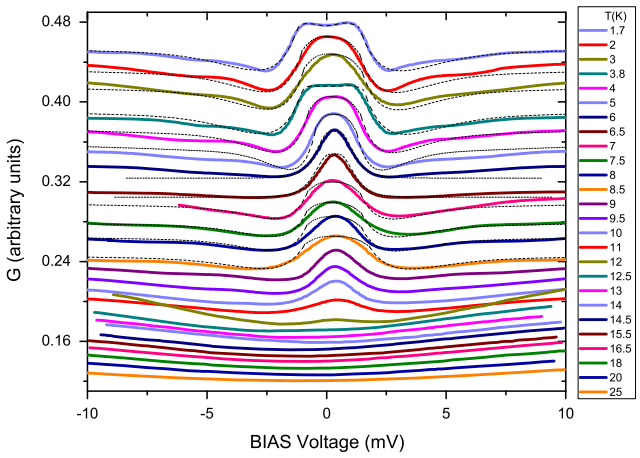

Fig. 4. (Color online) Differential conductance of a contact formed with a W(Au) wire tip and the compound $FeSe_{0.5}Te_{0.5}$. Figure shows the differential conductance at different temperatures in the region close to the features of the energy gap. All curves were displaced vertically by a small amount of the differential conductance for a better view of the general behavior. Values extracted with the BTK model give $Z=3.42$, and $\Delta=1.9$ meV. The fitting Z were taken into the same context as to the BTK model. This was performed for data taken from 1.7 to 8.5 K as shown in figure with black pointed lines. The fitting is clearly seen in Fig. 5 plotted in one curve of the normalized differential conductance at a temperature of $T=1.7$ K.

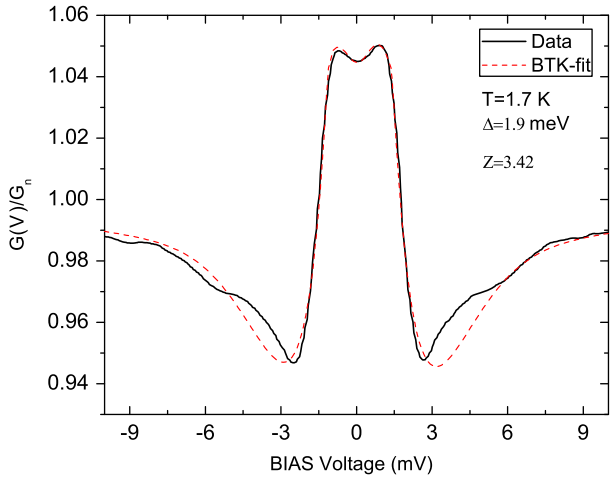

Fig. 5. (Color online) Normalized differential conductance for the PCS data of Fig. 4. The figure displays data measured at $T=1.7$ K (black lines). Parameters determined with the BTK model (dotted red line) give values for the energy gap, $\Delta=1.9$ meV, $Z=3.42$, and ratio $2\Delta/K_BT_C$, as $2.88 \leq 2\Delta/K_BT_C \leq 3.04$.

For the point contact measurements the differential resistance dV/dI as a function of the bias voltage V for all junctions was measured with the standard techniques: AC Lock-in amplifier and bridge [20,21]. A Quantum Design MPMS system was used as a cryostat. The junctions were measured in the temperatures range from 1.7 to 25 K. PCS's were close to the ballistic regime according to the electronic parameters of the compound and to the values of the differential resistance (at zero bias voltage) and Z parameter. In Figs. 4 and 5 we show the overall characteristics of the PCS's. Fig. 4 displays the general behavior of the differential conductance versus bias voltage at different temperatures measured from 1.7 to 25 K. In this set of measurements the BTK model fits well to the experimental data at low temperatures from 1.7 to about 7.5 K. With this result, it was possible to extract values for Z, which were $Z=3.42$, and energy gap $\Delta=1.9$ meV. The Z parameter used in this study has the same meaning as mentioned in the BTK theory; this measures the barrier strength at the interface. As one example for the resulting fitting Fig. 5 shows the extracted parameters. In Fig. 6 we

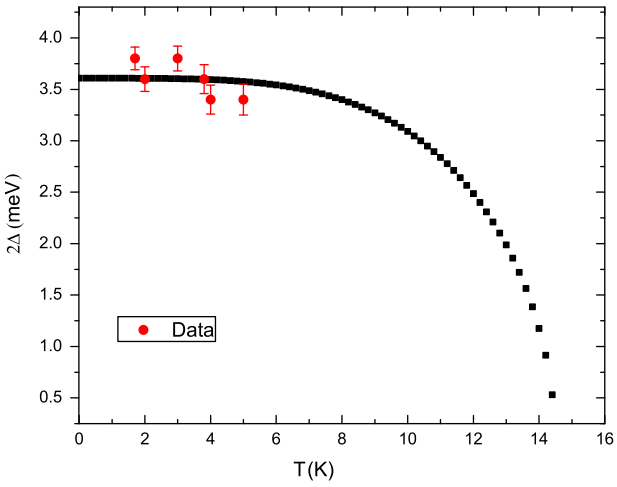

Fig. 6. (Color online) Evolution of the energy gap with temperature obtained from curves of the differential conductance of the PCS's data shown in Fig. 4 (red dots), fitted with BTK model. Black squares are the BCS theory. The fit was performed only in the low temperature range as explained in the main text.

show the evolution of the gap with temperature plotted in terms of Δ–T. The experimental data was plotted only at low temperature region, data at higher temperatures was difficult to fit as mentioned in the description of Fig. 4. The characterization of the work regime of the PCS's was estimated with Wexler's interpolation formula [22]; we substituted the mean free electronic path estimated as $l \simeq 100$ Å using the Drude model and according to the resistivity measurements [23], the resistivity $\rho \sim 40$ μΩ cm measured at 2 K and the resistance of the junction measured at zero bias voltage. The obtained radius values were between 320 Å and 3700 Å, which indicate that some contacts are in the diffuse regime, and others in the ballistic limit, only PCS's in the ballistic regime, or close to it were used to determined the spectroscopic features [24–26].

No broadening parameter was used for the determination of the spectroscopic characteristics as the one introduced by Dynes et al. [27].

3. Results, discussion and conclusions

Junctions with different characteristics behaving as PCS were used to investigate the nature of the superconducting state in a $FeSe_{0.5}Te_{0.5}$ compound. PCS and tunneling are tools well appropriated to study electronic processes occurring close to the Fermi surface, as the energy gap and the evolution with temperature and ratio $2\Delta/K_BT_C$. Our measurements with specific heat give us information about the pairing and symmetry state of the compound, and information about the characteristics of the order parameter. Our analyses indicate the characteristics of the pairing symmetry; according to the experimental data, this superconducting compound behaves as a full *s−wave* BCS superconductor. A single feature of the gap that was observed in thermal measurements corroborated the shape of the decreasing of the specific heat below T_C. An exponential decay of the specific heat with temperature was observed. It shows a good fitting to an exponential rate of decrease, indicating that a single gap exists. The decreasing of C_p–T below the transition is quite similar to the observations by Dong et al. [19] in $FeSe_x$. In our work the C_P–T curve can be well fitted to the exponential function without signs of a multi-gap system.

It is important to mention that Li et al. [28] reported the evidence of nodes in a compound with a similar stoichiometry as in this work. The observation of the gap features by Li et al. shown

a wave pairing different from *s−wave*, that could be *p* or *d*. However, the multigap feature determined by Li et al. was measured close to a vortex state and the information could be distorted with the real features. Lastly, other important probes appropriated to determine types of Cooper pairs was using ARPES. With this technique as observed by Miao et al. found that at the composition $FeTe_{0.55}Se_{0.45}$, which is quite similar to our shown only an isotropic single energy gap [29].

Our conclusions of this work are that this superconductor behaves as a *s−wave* symmetry with a clear evolution of the energy gap with temperature of the BCS type. The values for the size of the energy gap with the PCS junctions gave $\Delta = 1.9$ meV, whereas with specific heat measurements the energy gap determined was $2\Delta = 2.3$ meV. Other important parameter of this compound is the ratio $\Delta/K_BT_C = 2.96 \pm 0.05$, accordingly, this superconducting material is in weak coupling limit.

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