Anisotropic superconducting properties of single-crystalline FeSe\textsubscript{0.5}Te\textsubscript{0.5}

M. Bendele,\textsuperscript{1,2} S. Weyeneth,\textsuperscript{1} R. Puzniak,\textsuperscript{3} A. Maisuradze,\textsuperscript{2} E. Pomjakushina,\textsuperscript{4} K. Conder,\textsuperscript{4} V. Pomjakushin,\textsuperscript{5} H. Luetkens,\textsuperscript{2} S. Katrych,\textsuperscript{6} A. Wisniewski,\textsuperscript{3} R. Khasanov,\textsuperscript{2} and H. Keller\textsuperscript{1}

\textsuperscript{1}Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland
\textsuperscript{2}Laboratory for Neutron Scattering, ETHZ & PSI, CH-5232 Villigen PSI, Switzerland
\textsuperscript{3}Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5222 Villigen PSI, Switzerland
\textsuperscript{4}Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5222 Villigen PSI, Switzerland
\textsuperscript{5}Laboratory for Developments and Methods, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
\textsuperscript{6}Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, PL-02-668 Warsaw, Poland

Iron-chalcogenide single crystals with the nominal composition FeSe\textsubscript{0.5}Te\textsubscript{0.5} and a transition temperature of $T_c \approx 14.6$ K were synthesized by the Bridgman method. The structural and anisotropic superconducting properties of those crystals were investigated by means of single crystal X-ray and neutron powder diffraction, SQUID and torque magnetometry, and muon-spin rotation. Room temperature neutron powder diffraction reveals that 95% of the crystal volume is of the same tetragonal structure as PbO. The structure refinement yields a stoichiometry of Fe\textsubscript{1+0.4}Se\textsubscript{0.406}Te\textsubscript{0.594}. Additionally, a minor hexagonal FeSe\textsubscript{2} impurity phase was identified. The magnetic penetration depth $\lambda$ at zero temperature was found to be $\lambda_{ab}(0) = 491(8)$ nm in the $ab$-plane and $\lambda_c(0) = 1320(14)$ nm along the $c$-axis. The zero-temperature value of the superfluid density $\rho_s(0) \propto \lambda^{-2}(0)$ obeys the empirical Uemura relation observed for various unconventional superconductors, including cuprates and iron-pnictides. The temperature dependences of both $\lambda_{ab}$ and $\lambda_c$ are well described by a two-gap $s$+$s$-wave model with the zero-temperature gap values of $\Delta_{ab}(0) = 0.51(3)$ meV and $\Delta_{c}(0) = 2.61(9)$ meV for the small and the large gap, respectively. The magnetic penetration depth anisotropy parameter $\gamma_\lambda(T) = \lambda_c(T)/\lambda_{ab}(T)$ increases with decreasing temperature, in agreement with $\gamma_\lambda(T)$ observed in the iron-pnictide superconductors.

PACS numbers: 74.25.Ha, 74.25.Op, 74.25.Xa, 76.75.+i, 64.05.cp, 61.05.fm

I. INTRODUCTION

Since the discovery of superconductivity in LaFeAsO\textsubscript{1−x}F\textsubscript{x} (Ref. \textsuperscript{[1]}), high transition temperatures $T_c$ up to 56 K were reported for several Fe-based superconductors with La substituted by other lanthanoids (Ln) including e.g., Ce, Pr, Nd, Sm, and Gd.\textsuperscript{[2,3]} Meanwhile, the family of Fe-based superconductors range from LnFeAsO\textsubscript{1−x}F\textsubscript{x} (the so called 1111 family) over A\textsubscript{e}Fe\textsubscript{2}As\textsubscript{2} (122, A\textsubscript{e} = alkaline earth metal)\textsuperscript{[4]} to the more simple LiFeAs (111)\textsuperscript{[5]} and FeCh (11, Ch = chalcogenide)\textsuperscript{[6]} The FeCh system is especially similar to the FeAs-based superconductors, reflecting the ionic nature of the As and chalcogen atoms in these compounds.\textsuperscript{[7]} Recently, two even more complicated families were discovered: the (Fe\textsubscript{2}As\textsubscript{2})(A\textsubscript{e}4M\textsubscript{2}O\textsubscript{6}) (22426, $M$ = transition metal) and the (Fe\textsubscript{2}As\textsubscript{2})(A\textsubscript{e}3M\textsubscript{2}O\textsubscript{5}) (22325) systems.\textsuperscript{[8,9]} If the parent compound is not already superconducting, superconductivity can be induced by charge carrier doping into either the Fe layers or the spacer layers as well as by applying external or internal pressure.\textsuperscript{[10,11]}

Fe-based superconductors share some common properties with high-$T_c$ cuprates such as a layered crystal structure, the presence of competing orders, a low carrier density, a small coherence length, and an unconventional pairing mechanism. On the other hand, there are some differences: The Fe-based superconductors have metallic parent compounds, the anisotropy is in general lower compared to that of the cuprates, and the order parameter symmetry is claimed to be $\pm s$-wave with Fermi-surface nesting playing a major role.\textsuperscript{[12,13]} So, the fundamental question arises whether the mechanisms leading to superconductivity in both families of high-temperature superconductors (HTS) share a common origin.

Among the Fe-based superconductors the "11" system has attracted a lot of attention. The transition temperature $T_c$ of FeSe\textsubscript{1−x} reaches values up to $\approx 37$ K by applying hydrostatic pressure\textsuperscript{[14]} and $\approx 14$ K by partially substituting Se by the isovalent Te or S.\textsuperscript{[15]} In FeSe\textsubscript{2}Te\textsubscript{1−x} the antiferromagnetic order of FeTe is gradually suppressed by increasing $x$, and superconductivity emerges with a maximal $T_c$ at $x \approx 0.5$.\textsuperscript{[16]} Additionally, the "11" system has the simplest crystallographic structure among the Fe-based superconductors consisting of layers with a Fe square planar sheet tetrahedrally coordinated by $As$ and $Se$.\textsuperscript{[17,18]}

In this paper we report on the structural and anisotropic superconducting properties of single crystals with the nominal composition of FeSe\textsubscript{0.5}Te\textsubscript{0.5} that were studied by neutron powder diffraction, SQUID and torque magnetometry as well as muon spin rotation ($\mu$SR). A part of the present results are in agreement with the findings of a recent $\mu$SR study performed on a polycrystalline sample of FeSe\textsubscript{0.5}Te\textsubscript{0.5}.\textsuperscript{[19]}
fit is observed here. In conclusion, the main phase in shows the polished cleaving facet. No orientation mis-
tations and/or different phases are observed. Figure 2b
Distinct domains of different crystallographic orienta-
crystal surface cut perpendicular to the cleaving facet.

microscope. Figure 2a shows a microphotography of the
the surface morphology was examined in a polarized light
signal indicates strong pinning. The low value of the fc
magnitude obtained in the zfc mode reflects a full dia-
characteristic for optimal doping \( x \approx 0.5 \) of FeSe\(_{0.5}\)Te\(_{0.5}\).

II. EXPERIMENTAL DETAILS

A. Single crystal growth

Single crystals with the nominal composition of FeSe\(_{0.5}\)Te\(_{0.5}\) were grown by the Bridgman method, similar to that reported by Sales et al.\(^{22}\) Appropriate amounts of Fe, Se, and Te powders with a minimum purity of 99.99 % were mixed together, pressed into a rod (diameter 7 mm), and than evacuated and sealed in a double-
ampoule for air protection. The ampoule was placed into a vertical furnace with a temperature gradient and annealed at 1200 °C for 4 h. Afterwards the sam-
ple was cooled down with a rate of 4 °C/h to 750 °C, followed by a quick cooling (50 °C/h) to room temperature. The so-obtained crystals were easily cleaved from the as-grown crystal along the \( ab \)-plane (cleaving facet).

Figure 1 presents a low-field measurement of the mag-
netic moment \( m \) as a function of temperature \( T \) in a magnetic field of 1 mT applied parallel to the \( c \)-axis of single-crystal FeSe\(_{0.5}\)Te\(_{0.5}\), recorded in the Meissner state in zero field cooled (zfc) and in field cooled (fc) mode. The onset transition temperature \( T_\text{c} \approx 14.6 \) K (vertical arrow) is characteristic for optimal doping \( x \approx 0.5 \) of FeSe\(_{0.5}\)Te\(_{0.5}\).

The surface of the as-grown crystal was polished, and the surface morphology was examined in a polarized light 
the material is textured with the \( c \)-axis perpendicular to the 
the material is textured with the \( c \)-axis perpendicular to the 
the material is textured with the \( c \)-axis perpendicular to the 

B. Crystal structure

The crystal structure and the phase purity were checked using a single crystal X-ray diffractometer equipped with a charged-coupled device (CCD) detector (Xcalibur PX, Oxford Diffraction, sample-detector distance 60 mm). Crystallites with approximate dimensions of \( 1 \times 1 \times 0.2 \) mm\(^3\) were cleaved from the as-grown crystal for the single crystal X-ray diffraction studies. The single crystal diffractographs are shown in Fig. 2. Two distinct crystallographic phases were identified. The major phase of the crystal exhibits a tetragonal lattice (space group: \( P4/nmm \), lattice parameters: \( a = 3.7980(2) \) Å, \( c = 6.038(1) \) Å). The reconstruction of the reciprocal space sections of the studied plate-like crystals lead to pronounced mosaic spreads with an average mosaicity of the order of about 4°. A small part of the studied crystals with polygonal structure exhibits a hexagonal lattice structure, which is associated with an impurity phase.

Detailed crystal structure investigations were completed by means of neutron powder diffraction (NPD) at the neutron spallation source SINQ at the Paul Scherrer Institute (PSI, Switzerland) using the high resolution powder diffractometer for thermal neutrons HRP\(^{23}\) (neutron wavelength \( \lambda_n = 1.494 \) Å). For these experi-
ments a part of the crystal with the nominal composi-
FeSe$_{0.5}$Te$_{0.5}$ was cleaved, powdered, and loaded into the sample holder in a He-glove box to protect the powder from oxidation. Room temperature NPD experiments revealed that the sample consists mainly of the tetragonal phase (space group $P4_{4}/nmm$) of the PbO type which becomes orthorhomic and superconducting at low temperatures. The results of the Rietveld refinement of the NPD spectra performed with the program FULLPROF are shown in Fig. 4. For the refinement it was assumed that all Fe sites are occupied. Additionally, a preferred orientation was assumed as small plate-like grains are created during the powderization process. The refined stoichiometry is Fe$_{1.045}$Se$_{0.406}$Te$_{0.594}$ (see text for details).

It was shown that in the $\beta$-phase additional excess Fe occupies interstitial lattice sites. However, introduction of interstitial Fe atoms in the refinement of the data did not improve the fit. This suggests the presence of only a very small amount of such defects, in agreement with the model that in isostructural FeSe$_{1-x}$ no interstitial Fe is present. This is in contrast to FeTe where interstitial Fe atoms were detected. The existence of an impurity phase of Fe$_7$Se$_8$ in the studied crystal was confirmed by magnetization measurements. Figure 5 shows the temperature dependence of the magnetic moment measured in zero field cooling (zfc) and field cooling (fc) mode in a magnetic field of 1 T applied parallel to the $c$-axis of the crystal with nominal composition FeSe$_{0.5}$Te$_{0.5}$. The spin-axis transition at 130 K leading to a reduction of magnetization for $H$ parallel to the $c$-axis.

FIG. 4: (color online) Rietveld refinement pattern (red) and difference plot (blue) of the neutron diffraction data for the crystal with the nominal composition of FeSe$_{0.5}$Te$_{0.5}$. The rows of ticks show the Bragg peak positions for the main phase and two impurity phases. The refined stoichiometry of the main tetragonal phase is Fe$_{1.045}$Se$_{0.406}$Te$_{0.594}$ (see text for details).

FIG. 5: (color online) Temperature dependence of the magnetic moment measured in zero field cooling (zfc) and field cooling (fc) mode in a magnetic field of 1 T applied parallel to the $c$-axis of the crystal with nominal composition FeSe$_{0.5}$Te$_{0.5}$. The spin-axis transition at 130 K leading to a reduction of magnetization for $H$ parallel to the $c$-axis.
as observed in the studied sample (Fig. 5).

III. MAGNETIC PROPERTIES

A. Magnetization measurements

The magnetic properties of the crystals were investigated by a commercial Quantum Design 7 T Magnetic Property Measurement System (MPMS) XL SQUID Magnetometer at temperatures ranging from 2 K to 300 K and in magnetic fields from 0 T to 7 T using the Reciprocating Sample Option (RSO). Magnetic torque measurements were performed with a commercial Quantum Design 9 T Physical Property Measurement System (PPMS) equipped with a magnetic torque option.

The magnetization of FeSe$_{0.5}$Te$_{0.5}$ was measured on a crystal with a mass of the order of 200 mg. The Meissner fraction derived from the magnetic moment in the fc mode as compared to the one from zfc is estimated to be $\sim 1\%$ in 1 mT (Fig. 1). This indicates strong vortex pinning in agreement with the weakly field-dependent and pronounced critical current density and with the significant irreversibility in the magnetic torque experiments already present slightly below $T_c$ (as discussed later, Fig. 8). Using Bean’s model,$^{30,31}$ magnetization hysteresis loop measurements allow to estimate the superconducting critical current of the order of $10^7$ A/m$^2$.

The presence of impurity phases is lowering the transport current density as phase separation boundaries prevent to develop a global circulating current. This leads to a relatively low value of the estimated critical current density as compared to those achieved for monocrystalline iron-pnictides.$^{32}$

From temperature-dependent magnetization measurements at various magnetic fields the irreversibility line $H_{irr}(T)$ was deduced by following the temperatures for which the zfc and fc branches of the magnetic moment merge for different fields. The results are presented in Fig. 3 where the inset to the figure illustrates the derivation of $H_{irr}$ in a magnetic field of 5 T parallel to the ab-plane. The data were analyzed using the power-law $(1-T/T_c)^n$ with $n \approx 1.5$, typical for cuprate HTS.$^{33}$ The irreversibility line $H_{irr}$ is located at relatively high magnetic fields. Interestingly, $H_{irr}$ is for $H$ parallel to the ab-plane almost overlapping with the values of the upper critical field $H_{c2}^{ab}$ reported by Fang et al.$^{33}$

The temperature dependence of the lower critical field $H_{c1}$ was studied by following the field $H_{c1}^{ab}$, where the first vortices start to penetrate the sample at its surface, which is directly related to $H_{c1}$. The field dependence of the magnetization was measured at different temperatures for the magnetic field parallel to the ab-plane and parallel to the c-axis of the sample. For a given shape of the investigated crystal the demagnetizing factors $D$ were calculated for the magnetic field applied along all of the crystallographic axis. The deviation of the magnetic induction $B$ as a function of the internal magnetic field $H$ was studied by following the field $H_{c1}^{ab}$, where the first vortices start to penetrate the sample at its surface (Fig. 3). This indicates strong vortex pinning in agreement with the weakly field-dependent and pronounced critical current density $j_\text{c}$ as compared to those achieved for monocrystalline iron-pnictides.$^{33}$

The critical field $H_c^{ab}(0)$ and $H_c^{ab}(2)$ at $T=0$ were measured in magnetic fields up to 5 T parallel to the ab-plane and to the c-axis, respectively. The critical current density $j_\text{c}$ was estimated from $H_c^{ab}(0)$ and $H_c^{ab}(2)$ using the following basic relations$^{33}$

$$H_c^{ab} = \frac{\Phi_0}{8\pi \mu_0 \lambda_{ab} \lambda_c} \ln \left[ \frac{\lambda_{ab} \lambda_c}{\xi_{abc}} \right] + 1,$$

where $\lambda_{ab}$ and $\lambda_c$ are the magnetic penetration depths parallel to the ab-plane and to the c-axis, respectively, $\xi_{abc}$ the corresponding coherence lengths, $\Phi_0$ is the elementary flux quantum, and $\mu_0$ the magnetic constant.

The values of $\xi_{abc}$ were derived from $H_c^{ab}$ and $H_c^{ab}$ measurements.$^{33}$ The following zero temperature values of magnetic penetration depths were obtained: $\lambda_{ab}(0) \approx 460(100)$ nm and $\lambda_c(0) \approx 1100(300)$ nm. These values are in good agreement with the values determined by $\mu$SR discussed below (see Table 1).

In order to quantify the anisotropy of superconducting state parameters, magnetic torque studies were performed close to $T_c$, where irreversibility effects are small. The measurements on small crystals ($\sim 1 \times 1 \times 0.2$ mm$^3$) revealed a major superconducting response, in agreement with the NPD results discussed above. Unfortunately, due to the small amplitude of the superconducting torque

$H_{int} = H_{ext} - DM$ ($H_{ext}$ denotes the external magnetic field) is presented in Fig. 7. The lower critical fields for $H$ parallel to the ab-plane and parallel to the c-axis, respectively, $\xi_{abc}$ and $\xi_c$ the corresponding coherence lengths, $\Phi_0$ is the elementary flux quantum, and $\mu_0$ the magnetic constant. The values of $\xi_{abc}$ and $\xi_c$ were derived from $H_c^{ab}$ and $H_c^{ab}$ measurements.$^{33}$

$H_{ext} = \frac{\Phi_0}{8\pi \mu_0 \lambda_{ab} \lambda_c} \ln \left[ \frac{\lambda_{ab} \lambda_c}{\xi_{abc}} \right] + 1.$
signal in the mixed state close to $T_c$, a relatively strong background component of magnetic origin is contributing significantly to the torque signal. The magnetic background signal in the superconducting state is confirmed by following the torque to temperatures above $T_c$. In order to exclude artefacts in the subsequent analysis, all background components within the superconducting state were subtracted from the torque prior to the analysis (see below). To minimize the influence of pinning the mean reversible torque $\tau_{rev} = [\tau(\theta^+) + \tau(\theta^-)]/2$ was derived from measurements with clockwise and counterclockwise rotating the magnetic field around the sample. The superconducting anisotropy parameter $\gamma = \lambda_c/\lambda_{ab}$ may be extracted from the measured torque $\tau(\theta)$ using the relation:

$$
\tau(\theta) = -\frac{V\Phi_0 H}{16\pi\lambda_{ab}^2} \left( 1 - \frac{\sin(2\theta)}{\gamma^2} \right) \frac{\sin(2\theta)}{\epsilon(\theta)} 
\times \ln \left( \frac{\eta H_{c2}^{lc}}{\epsilon(\theta) H} \right) + A_c \sin(2\theta),
$$

where $V$ is the volume of the crystal, $\lambda_{ab}$ is the in-plane component of the magnetic penetration depth, $H_{c2}^{lc}$ is the upper critical field along the $c$-axis of the crystal, $\eta$ denotes a numerical parameter of the order of unity depending on the structure of the flux-line lattice, $A_c$ is the amplitude of the background torque, and $\epsilon(\theta) = [\cos^2(\theta) + \gamma^{-2}\sin^2(\theta)]^{1/2}$. Since Eq. (3) contains multiple correlated parameters, making a simultaneous fit of all quantities difficult, all $H_{c2}^{lc}$ values were fixed to those reported in Ref. [33] during the fitting procedure by neglecting any influence of the parameter $\eta$. Because the magnetic background contributions tend to influence and alter the fitting parameter $H_{c2}^{lc}$ strongly, the data were fitted by Eq. (3) using the symmetrized expression for the torque $\tau_{symm}(\theta) = \tau(\theta) + \tau(\theta + 90^\circ)$[5]. The result of this analysis is depicted in Fig. 8, yielding an anisotropy parameter $\gamma = 3.1(4)$ in the vicinity of $T_c$.

\section*{B. Muon spin rotation}

Muon spin rotation ($\mu$SR) is a direct and bulk sensitive probe to investigate local magnetic fields in magnetic solids. Nearly 100% spin-polarized positive muons $\mu^+$ are implanted into the sample and stop at interstitial lattice sites, where the muon spins precess around the local magnetic field $B$ with the Larmor frequency $\omega_L = \gamma_{\mu}B$ ($\gamma_{\mu}/2\pi = 135.5$ MHz/T is the muon gyromagnetic ratio). At the stopping site the muon acts as a magnetic micro probe and measures the internal field distribution. Within the muon’s life time of $\tau = 2.2$ $\mu$s it decays into two neutrinos and a positron, which is emitted predominantly along the muon spin polarization at the moment of decay. The direction of the emitted decay positron and the time between the muon implantation and its decay is measured for typically 10$^6$ muons. This way the time evolution of the muon spin polarization $P(t)$ is obtained. Zero-field (ZF) $\mu$SR experiments probe the magnetic state of a material as the muon spins precess only around the internal field without applying an external magnetic field. In transverse field (TF) $\mu$SR experiments the local magnetic field at the muon site in the sample is probed in the presence of an external magnetic field perpendicular to the initial muon spin polarization. TF $\mu$SR is a very powerful tool to investigate the local magnetic field distribution in the vortex state of type II superconductors. A comprehensive review of the application of $\mu$SR to the study of superconductors can be found in
The μSR experiments were carried out at the πM3 beam line at the Swiss Muon Source (SμS) at PSI. ZF and TF μSR experiments were performed in a temperature range from 1.5 K to 20 K. The TF experiments were carried out in two sets of measurements when the external field \( \mu_0 H = 11.8 \) mT was applied either parallel to the crystallographic c-axis or parallel to the ab-plane.

The ZF μSR spectra obtained at 1.6 K and above \( T_c \) show no difference (Fig. 9a). This indicates that the magnetic state of FeSe\(_{0.5}\)Te\(_{0.5}\) below and above \( T_c \) is the same. The solid lines in Fig. 9a correspond to a fit using an exponential decay of the initial muon spin polarization:

\[
A^{ZF}(t) = A_{SC} \cdot e^{-\Lambda t} + A_{bg} \cdot e^{-\Lambda_{bg} t}.
\] (4)

Here \( A_{SC} \) is the asymmetry of the superconducting phase and \( \Lambda \) is the corresponding depolarization rate. The temperature independent background signal \( A_{bg} \), arising from the Fe\(_7\)Se\(_8\) impurity phase was fixed to 6% of the total asymmetry during the fit, corresponding to the results of the NPD refinement. The exponential character of the muon spin depolarization is typical for diluted and randomly distributed magnetic moments, that are static on the muon time scale as shown in Ref. 41.

In the TF geometry muons probe the magnetic field distribution \( P(B) \) in the sample. In the mixed state of a type II superconductor \( P(B) \) is determined by the magnetic penetration depth \( \lambda \) and the coherence length \( \xi \). The \( P(B) \) distributions obtained from the Fourier transform of the μSR time spectra at 1.6 K and above \( T_c \) are shown in Figs. 9b and e. In the normal state a symmetric \( P(B) \) at the position of the applied magnetic field is observed. The broadening of \( P(B) \) in the normal state is due to nuclear and diluted electronic magnetic moments. Below \( T_c \) an additional broadening and an asymmetric line shape \( P(B) \) due to the formation of the flux line lattice (FLL) shows up. The TF μSR time spectra were analyzed by a theoretical polarization function \( A(t) \) by assuming an internal field distribution \( P_{FLL}(B) \) and to account for the FLL disorder by multiplying \( P_{FLL}(B) \) by a Gaussian function

\[
A(t) = A_0 e^{i\phi} e^{-\left(\sigma_k^2 + \sigma_{nm}^2 \right) t^2/2 - \Lambda_{nt} t^2} \int P_{FLL}(B)e^{i\gamma_B B t}dB. \] (5)

Here \( A_0 \) and \( \phi \) are the initial asymmetry and the phase of the muon spin ensemble, respectively, \( \sigma_k \) is a parameter related to the FLL disorder, \( \sigma_{nm} \) is the nuclear moment contribution measured at \( T > T_c \), which is generally temperature independent, and \( \Lambda_n \) is the relaxation rate of the electronic moment contribution, which was obtained from the measurements taken above \( T_c \).

The magnetic field distribution \( P_{FLL}(B) \) for a FLL of an anisotropic superconductor was determined from the spatial variation of the magnetic field \( B(r) \) calculated in an orthogonal frame \( x, y, z \) with \( H \parallel z \) (z

\[
B(r) = \langle B \rangle \sum_G \exp(-iG \cdot r) B_G(\lambda, \xi, b). \] (6)

Here, \( \langle B \rangle \) is the average magnetic field in the superconductor (magnetic induction), \( b = \langle B \rangle / B_{c2} \) the reduced field \( (B_{c2} = \mu_0 H_{c2}) \), and \( r \) the vector coordinate in a plane perpendicular to the applied field. The Fourier components \( B_G \) were obtained within the framework of the Ginzburg-Landau (GL) model for a detailed description of the fitting procedure we refer to Ref. 42. The solid lines in Figs. 9b and e correspond to the fast Fourier transforms of the described fits to the μSR time spectra.

The temperature dependences of \( \lambda_{ab}^{-2} \) and \( \lambda_{c}^{-2} \) extracted from the μSR time spectra using the fitting procedure described above are shown in Fig. 10. These data were analyzed within the framework of the phenomenological \( \alpha \)-model by assuming that \( \lambda^{-2} \) is a linear combi-
nation of two terms
\[
\frac{\lambda^2(T)}{\lambda^2(0)} = w \frac{\lambda^2(T, \Delta^0_S)}{\lambda^2(0, \Delta^0_S)} + (1 - w) \frac{\lambda^2(T, \Delta^0_L)}{\lambda^2(0, \Delta^0_L)}.
\]
(7)

Here, \(\Delta^0_S\) and \(\Delta^0_L\) are the zero-temperature values of the small and the large gap, respectively, and \(w\) (0 \(\leq\) \(w\) \(\leq\) 1) is the weighting factor which measures the relative contribution of the two gaps to \(\lambda^2(T) \div \lambda^2(0)\). For the temperature dependence of \(\lambda^2\) of a London superconductor (\(\lambda \gg \xi\)) with a s-wave gap the following relation can be used:

\[
\frac{\lambda^2(T, \Delta^0_{S(L)})}{\lambda^2(0, \Delta^0_{S(L)})} = 1 + 2 \int_{\Delta(T)}^\infty \frac{\partial f}{\partial E} \frac{E}{\sqrt{E^2 - \Delta^2(T)}} dE.
\]
(8)

Here \(\lambda(0)\) is the zero temperature value of the magnetic penetration depth, \(f(E) = [1 + \exp(E/k_B T)]^{-1}\) is the Fermi function (\(E\) is the excitation energy, \(k_B\) is the Boltzmann constant), and \(\Delta(T) = \Delta(0)\Delta(T/T_c)\) represents the temperature dependence of the gap with \(\Delta(T)/\Delta_c = \tanh(1.82(1.018(T_c/T - 1)^{0.51}))\).23

The temperature dependencies of \(\lambda_{ab}\) and \(\lambda_c\) were determined simultaneously, assuming the same values for the small and large gap (\(\Delta_{S,ab} = \Delta_{S,c}\) and \(\Delta_{L,ab} = \Delta_{L,c}\), but different weighting factors \(w\). The results of this analysis are summarized in Table I. The ratios \(2\Delta_S/k_B T_c = 0.84(4)\) and \(2\Delta_L/k_B T_c = 4.3(1)\) are close to what was reported for isostructural FeSe\textsubscript{1-x}Y\textsubscript{x}. Based on scanning tunneling spectroscopy measurements, Kato \textit{et al.}\textsuperscript{14} reported for FeSe\textsubscript{0.4}Te\textsubscript{0.6} only one s-wave gap \(\Delta \approx 2.3\) meV. This value is quite similar to our result of the large gap \((\Delta_L = 2.61(9)\) meV). However, a single s-wave gap is not sufficient to describe the present \(\muSR\) data. The weighting factors \(w\) are about the same for \(1/\lambda^2_{ab}\) and \(1/\lambda^2_c\). Similar results were already reported for isostructural FeSe\textsubscript{1-x}Y\textsubscript{x}.\textsuperscript{11} Recently, Kim \textit{et al.}\textsuperscript{25} reported on magnetic penetration depth measurements on Fe\textsubscript{1.0}Se\textsubscript{0.37}Te\textsubscript{0.63} by means of a radio-frequency tunnel diode resonator technique. Their value \(\lambda_{ab}(0) \approx 560(20)\) nm is in good agreement with the value reported here (see Table I). Furthermore, they found a clear signature of multi-gap superconductivity with comparable gap values \((\Delta_S \approx 1.2\) meV and \(\Delta_L \approx 2\) meV). In a recent \(\muSR\) study of polycrystalline FeSe\textsubscript{0.5}Te\textsubscript{0.5} the temperature dependence of \(\lambda_{ab}\) was found to be compatible with either a two gap s+is-wave or anisotropic s-wave model with \(\lambda_{ab} = 534(2)\) nm\textsuperscript{23}. For the s+is-wave analysis the following results were obtained: \(\Delta_S(0) = 2.6(1)\) meV, \(\Delta_L(0) = 0.87(6)\) meV, and \(1 - w = 0.70(3)\)\textsuperscript{23} These results are in fair agreement with the present results listed in Table I.

Uemura \textit{et al.}\textsuperscript{24} found an empirical relation between the zero temperature superfluid density \(\rho_s(0) \approx \lambda_{ab}^2(0)\) and \(T_c\) which seems to be generic for various families of cuprate HTS (Uemura plot). This “universal” relation \(T_c(\rho_s)\) has the following features: With increasing carrier doping \(T_c\) initially increases linearly (\(T_c \propto \rho_s(0)\)), then saturates, and finally is suppressed for high carrier doping. It is interesting to check whether the Uemura relation also holds for iron-based superconductors. For this reason \(T_c\) vs. \(\lambda_{ab}^{-2}(0)\) is plotted in Fig. 11 for a selection of various Fe-based superconductors investigated so far.\textsuperscript{13,14,32,131,133,134,135,136,137} For comparison the linear parts of the Uemura relation for hole-doped (dashed line) and electron-doped (dotted line) cuprate HTS are also shown in Fig. 11. Due to the small number of data points available for a particular family of Fe-based superconductors there is no obvious trend visible. However, all data points are located within an area determined by the straight lines representing the hole-doped and electron-doped cuprates. Whereas various of the Fe-based HTS, including FeSe\textsubscript{0.5}Te\textsubscript{0.5} (red star in Fig. 11) investigated here, are located near the hole-doped cuprates in the Uemura plot, the “111” system appears to be close to the

**TABLE I: Summary of the parameters obtained for single-crystal FeSe\textsubscript{0.5}Te\textsubscript{0.5} by means of \(\muSR\) and magnetization measurements. The errors of the \(\muSR\) data are statistical errors and do not take into account any systematical errors that may be present in the data.**

| Parameter | \(\muSR\) | Magnetization |
|-----------|-----------|--------------|
|           | ab-plane | c-axis       | ab-plane | c-axis       |
| \(T_c\) (K) | 14.1(1)  | 14.6(1)      |           |              |
| \(\Delta_S\) (meV) | 0.51(3)  | -            | 0.32(1)  | 0.36(2)      |
| 2\(\Delta_S/k_B T_c\) | 0.84(5)  | -            | 2\(\Delta_L/k_B T_c\) | 4.3(1)      |
| \(\Delta_L\) (meV) | 2.61(9)  | -            | \(w\)     | 0.32(1) 0.36(2) |
| 2\(\Delta_L/k_B T_c\) | 4.3(1)   | -            | \(\lambda_{ab,c}(0)\) (nm) | 491(8) 1320(14) |
| \(H_{c1}\) (mT) | -        | 460(100) 1100(300) |          | 2.0(2) 4.5(3) |
IV. TEMPERATURE DEPENDENT ANISOTROPY PARAMETERS

For a conventional single-band s-wave layered superconductor the anisotropy parameter is defined as:

\[ \gamma = \sqrt{m^*_c/m^*_{ab}} = \lambda_c/\lambda_{ab} = H_{c2}^{\parallel ab}/H_{c2}^{||} = \xi_{ab}/\xi_c. \]  

(9)

Here, \( m^*_c \) and \( m^*_{ab} \) are the effective charge carrier masses related to supercurrents flowing in the \( ab \)-planes and along the \( c \)-axis, respectively. Whereas the cuprates were characterized by a well-defined effective mass anisotropy, the observation of two distinct anisotropy parameters in MgB\(_2\) challenged the understanding of anisotropic superconductors. Various experiments, such as magnetic torque,\(^{37,38}\) tunneling,\(^{39,40}\) point contact and infrared spectroscopy,\(^{41,42}\) as well as the measurements of the specific heat\(^ {43}\) the lower and upper critical field\(^{44,45}\) and the superfluid density\(^ {46,47,48}\) indicate that Fe-based pnictides are multi-gap superconductors having unconventional anisotropic properties,\(^ {49,50}\) similar to MgB\(_2\).\(^ {51,52}\)

The temperature dependence of the magnetic penetration depth anisotropy parameter \( \gamma_\lambda = \lambda_c/\lambda_{ab} \) extracted from the \( \mu SR \) data (see Fig. \ref{fig:12}) is shown in Fig. \ref{fig:12}. Note that \( \gamma_\lambda \) increases with decreasing temperature and saturates at \( \gamma_\lambda \approx 2.6(3) \) at low temperatures. This observation is further supported by the temperature dependence of \( \gamma_\lambda \) determined from the lower critical field measurements presented in Fig. \ref{fig:7}. In this case \( \gamma_\lambda \) is readily obtained from Eqs. \ref{eq:1} and \ref{eq:2}:

\[ \gamma_\lambda = \frac{\lambda_c}{\lambda_{ab}} = \frac{H_{c2}^{||}}{H_{c1}^{\parallel ab}} \left( 1 + \frac{\ln(\gamma_\lambda) + \ln(\gamma_{Hc2})}{2 \ln(\kappa_{ab}) + 1} \right) \]  

(10)

Here, \( \kappa_{ab} = \lambda_{ab}/\xi_{ab} \) denotes the Ginzburg-Landau parameter. In this work \( \kappa_{ab} \) was estimated to be \( \approx 180 \) from present experiments.\(^ {53,54} \) The values of \( \gamma_\lambda \) extracted from the SQUID data using Eq. \ref{eq:10} are also depicted in Fig. \ref{fig:10} and are in fair agreement with those obtained from the \( \mu SR \) data.

The upper critical field anisotropy parameter \( \gamma_{Hc2} = H_{c2}^{\parallel ab}/H_{c2}^{||} = \xi_{ab}/\xi_c \), was studied by Fang \textit{et al.}\(^ {53} \) and Lei \textit{et al.}\(^ {54} \) by resistivity measurements on Fe\(_{1+\text{y}}\)Se\(_{0.4}\)Te\(_{0.6}\) \((y = 0.02 \text{ and } 0.11)\). These data are plotted in Fig. \ref{fig:12} as well. Note that \( \gamma_{Hc2} \) decreases with decreasing temperature. Obviously, the behavior of the two distinct anisotropy parameters \( \gamma_\lambda \) and \( \gamma_{Hc2} \) is not consistent with Eq. \ref{eq:10}. The observed behavior is similar to the one of the two-gap superconductor MgB\(_2\), however, \( \gamma_\lambda \) decreases with decreasing temperature while \( \gamma_{Hc2} \) increases.\(^ {55} \)
Single crystals with a nominal composition of FeSe\(_{0.5}\)Te\(_{0.5}\) were studied by means of muon spin rotation (\(\mu\)SR), SQUID and torque magnetometry, and neutron powder diffraction. At room temperature the crystal shows mainly a tetragonal phase of PbO type that becomes orthorombic and superconducting at low temperatures. The stoichiometry was refined to Fe\(_{0.43}\)Se\(_{0.46}\)Te\(_{0.5}\). The onset transition temperature is \(T_\text{c} = 14.6\) K, and the lower critical field values measured for both crystallographic directions were determined at zero temperature as \(H_{\text{c1}}(0) = 2.0(2)\) mT and \(H_{\text{c2}}(0) = 4.5(3)\) mT.

By means of \(\mu\)SR it was found that for FeSe\(_{0.5}\)Te\(_{0.5}\) the temperature dependence of the magnetic penetration depth for both crystallographic directions is best described by a two gap \(s+\)s-wave model with zero-temperature values of the magnetic penetration depth of \(\lambda_{\text{ab}}(0) = 491(8)\) nm and \(\lambda_{\text{c}}(0) = 1320(14)\) nm, consistent with recent \(\mu\)SR results obtained for a polycrystalline sample.\(^{23}\) This two-gap scenario is in line with the generally accepted view of multi-gap superconductivity in Fe-based HTS. Evtushinsky et al.\(^{23}\) pointed out that most Fe-based HTS exhibit two gaps, a large one with \(2\Delta_2/k_BT_c = 7(2)\) and a small one with \(2(5,1.5)\). The magnitudes of the large and the small gap for FeSe\(_{0.5}\)Te\(_{0.5}\) (\(2\Delta_2/k_BT_c = 0.84(4)\) and \(2\Delta_1/k_BT_c = 4.3(1)\)) are at the lower limit for Fe-based HTS. Moreover, the magnetic penetration depth anisotropy parameter \(\gamma_\lambda\) determined from penetration depth experiments by means of \(\mu\)SR, is within experimental error the same as the one deduced from \(H_{\text{c1}}\) measurements. Both techniques yield a temperature dependent \(\gamma_\lambda\) that increases with decreasing temperature from 1.6 at \(T_c = 14.6\) K to 2.6 at \(T = 1.6\) K. Compared to SmFeAsO\(_8\)F\(_{0.2}\) and NdFeAsO\(_8\)F\(_{0.2}\) superconducting FeSe\(_{0.5}\)Te\(_{0.5}\) is much more isotropic, but quite comparable to the 122 class of Fe-based superconductors.\(^{24}\) This suggests that the direct electronic coupling of the Fe\(_2\)Se\(_2\) layers in the “11” system is similar to the one through the intervening A\(_2\) layers in the “122” class of superconductors, but more effective than the coupling through the LuO layers in the “1111” Fe-based systems. While \(\gamma_\lambda\) increases with decreasing temperature the anisotropy parameter of the upper critical field \(\gamma_{\text{H}_c}\) determined by resistivity measurements decreases.\(^{33,34}\) The observed behavior is similar to that of the two-gap superconductor MgB\(_2\) and other Fe-based superconductors and supports a two-gap scenario also in FeSe\(_{0.5}\)Te\(_{0.5}\).\(^{35}\) Note, however, that for MgB\(_2\) the slopes of \(\gamma_{\lambda}(T)\) and \(\gamma_{\text{H}_c}(T)\) have reversed signs as compared to the Fe-based superconductors. The reason for this difference is still unclear. Furthermore, the value of \(\lambda_{\text{ab}}^{-1}(0)\) for FeSe\(_{0.5}\)Te\(_{0.5}\) extracted from \(\mu\)SR data as well as the values of \(\lambda_{\text{c}}^{-1}(0)\) obtained for various Fe-based superconductors fall on the Uemura plot\(^{39}\) within the limits of hole-doped and electron-doped cuprates.\(^{30}\) This suggests that the pairing mechanism in the Fe-based superconductors is unconventional, as is also the case for the cuprates.

In conclusion, FeSe\(_{0.5}\)Te\(_{0.5}\) shows evidence for two-gap superconductivity, which is reflected in the temperature dependence of \(\lambda^{-2}\) and by the existence of two distinct anisotropy parameters \(\gamma_{\lambda}(T)\) and \(\gamma_{\text{H}_c}(T)\). The two-gap scenario is observed for most Fe-based superconductors, suggesting that this behavior is generic for layered high-temperature superconductors: It is strongly supported by various experiments for Fe-based superconductors (Ref. \(^{75}\) and references therein), it is well established for MgB\(_2\)\(^{30}\) and there is firm evidence for two-gap superconductivity also in the cuprates.\(^{77}\)\(^{80}\) However, it remains to be seen whether superconductivity in these classes of high-temperature superconductors has the same or a similar origin.

VI. ACKNOWLEDGMENTS

The \(\mu\)SR experiments were performed at the Swiss Muon Source, Paul Scherrer Institut, Villigen, Switzerland. This work was partially supported by the Swiss National Science Foundation, the EU Project CoMePhS, the Polish Ministry of Science and Higher Education with the research project No. N N202 4132 33, and by the NCCR Program MaNEP.

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* Electronic address: markus.bendele@physik.uzh.ch

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