Thermodynamic phase diagram of Fe(Se$_{0.5}$Te$_{0.5}$) single crystals up to 28 Tesla

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We report on specific heat ($C_p$), transport, Hall probe and penetration depth measurements performed on Fe(Se$_{0.5}$Te$_{0.5}$) single crystals ($T_c \sim 14$ K). The thermodynamic upper critical field $H_{c2}$ has been deduced from $C_p$ measurements up to 28 T for both $H \parallel c$ and $H \parallel ab$, and compared to the lines deduced from transport measurements (up to 55 T in pulsed magnetic fields). We show that this thermodynamic $H_{c2}$ line presents a very strong downward curvature for $T \rightarrow T_c$ which is not visible in transport measurements. This temperature dependence associated to an upward curvature of the field dependence of the Sommerfeld coefficient confirm that $H_{c2}$ is limited by paramagnetic effects. Surprisingly this paramagnetic limit is visible here up to $T/T_c \sim 0.99$ (for $H \parallel ab$) which is the consequence of a very small value of the coherence length $\xi(0) \sim 4 \AA$ (and $\xi_{ab}(0) \sim 15 \AA$), confirming the strong renormalisation of the effective mass (as compared to DMFT calculations) previously observed in ARPES measurements [Phys. Rev. Lett. 104, 097002 (2010)]. $H_{c1}$ measurements lead to $\lambda_{ab}(0) = 430 \pm 50$ nm and $\lambda_{c}(0) = 1600 \pm 200$ nm and the corresponding anisotropy is approximatively temperature independent ($\sim 4$), being close to the anisotropy of $H_{c2}$ for $T \rightarrow T_c$. The temperature dependence of both $\lambda (\propto T^2)$ and the electronic contribution to the specific heat confirm the non conventional coupling mechanism in this system.

I. INTRODUCTION

The discovery of superconductivity up to 55K in iron-based systems [1] has generated tremendous interest. Among those, iron selenium (FeSe$_{1-x}$) [2] has been reported to be superconducting with a critical temperature of 8 K at ambient pressure, rising to 34-37 K under 7-15 GPa [3]. On the other hand, the substitution of tellurium on the selenium site in Fe$_{1-x}$(Te$_x$)Se$_2$ increases $T_c$ to a maximum on the order of 14-15 K at ambient pressure [4,5] (for $x \sim 0.5$). This binary compound is very interesting as it shares the most salient characteristics of iron based systems (square-planar lattice of Fe with tetrahedral coordination) but has the simplest crystallographic structure among Fe-based superconductors (no charge reservoir, so-called 11-structure). Moreover, even though the endpoint Fe$_{1.5}$Te [7] compound displays antiferromagnetic ordering, a magnetic resonance similar to that observed in other parent compounds (with a (1/2, 1/2) nesting vector connecting the $\Gamma$ and $M$ points of the Fermi surface) is recovered for intermediate Te contents [8,9] suggesting a common mechanism for superconductivity in all iron based superconductors. However, in contrast to iron pnictides which show weak to moderate correlations, recent ARPES measurements suggested the existence of very large mass renormalization factors (up to $\sim 20$ as compared to DMFT calculations) [10] indicating that Fe(Se,Te) is a strongly correlated metal differing significantly from iron pnictides.

In order to shed light on superconductivity in these systems, it is of fundamental importance to obtain a precise determination of both upper and lower critical fields and their anisotropy. Up to now $H_{c2}$ has mainly been deduced from transport measurements [11-13], and more recently by specific heat up to 14 T [14]. As in other pnictides (see [15] and references therein), high $H_{c2}(0)$ values have been reported but, in the case of Fe(Te$_x$Se$_{1-x}$), strong deviations from the standard Werthamer-Helfand-Hohenberg model for $H_{c2}(T)$ have been reported. Those deviations have been associated to paramagnetic limitations (so-called Pauli limit) [11-13]. However, in presence of strong thermal fluctuations (see discussion below), the determination of $H_{c2}$ from transport measurement becomes very hazardous and a thorough analysis was hence lacking of an unambiguous determination of $H_{c2}$ from specific heat measurements.

We show that the $H_{c2}$ lines actually display a very strong downwards curvature close to $T_c$ corresponding to $\mu_0 dH_{c2}/dT$ values rising up to $\sim 12$ T/K for $H \parallel c$ and even $\sim 45$ T/K for $H \parallel ab$. This strong curvature, not visible in transport data, shows that $H_{c2}$ remains limited by paramagnetic effects up to temperatures very close to $T_c$ (up to $T/T_c \sim 0.99$ for $H \parallel ab$). The corresponding Pauli field $H_{p}$ is slightly anisotropic ($H_{p}^{ab}/H_{p}^{c} \sim 0.8$) whereas the orbital limit ($H_{o}(0)$) presents a much stronger anisotropy $H_{o}(0)^{ab}/H_{o}(0)^{c} \sim 3-4$. The huge $\mu_0 H_{o}(0)$ values ($\sim 130 \pm 20$ T for $H \parallel c$ and $\sim 400 \pm 50$ T for $H \parallel ab$) correspond to very small coherence length values ($\xi_{ab}(0) \sim 15 \pm 1 \AA$ and $\xi_{c}(0) \sim 4 \pm 1 \AA$) confirming the large value of the effective mass previously observed by ARPES [10] and hence supporting the presence of strong electronic correlations in this system.

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havior, attributed to a clear signature of multigap superconductivity. We present here detailed first penetration field measurements performed with Hall sensor arrays in a variety of single crystals showing very different aspect ratios. We hence obtained $\mu_0 H_{c1}(0) = 78 \pm 5$ G and $\mu_0 H_{c2}^{ab}(0) = 23 \pm 3$ G. The $H_{c1}$ lines clearly flatten off at low temperature but do not show the pronounced deep previously obtained in Tunnel Diode Oscillator (TDO) measurements \[18\]. Our TDO measurements however lead to a similar deep which is probably due to an overestimation of the absolute $\Delta \lambda(T)$ value related to spurious edge effects. Finally, we obtained a temperature independent $\Gamma_{H_{c1}} = H_{c1}^{||}/H_{c1}^{ab}$ values $\sim 3.3 \pm 0.5$ which corresponds to $\Gamma_\lambda = \lambda_c/\lambda_{ab} \sim 4.0 \pm 0.8$ (see below), being close to the $\gamma_{H_{c1}}$ value obtained for $T \to T_c$ (i.e. $\sim H_0^{ab}/H_0^{ab}$).

Finally, we confirm that $\lambda \propto T^2$ in both crystallographic directions and show that the temperature dependence of $C_p$ strongly deviates from the standard BCS weak coupling behavior confirming the non conventional coupling mechanism of this system. However, the amplitude of the specific heat jump is much larger than those previously reported in other Fe(Se,Te) samples and hence does not follow the $\Delta C_p$ vs $T_c^3$ scaling law reported in iron based systems \[19, 20\].

II. SAMPLE PREPARATION AND EXPERIMENTS

We present here specific heat, transport, Hall probe and Tunnel Diode Oscillator (penetration depth) measurements performed in Fe$_{1+\delta}$(Se$_{0.5}$Te$_{0.5}$) single crystals grown by two different techniques. Samples A have been grown using the sealed quartz tube method. The samples were prepared from very pure iron and tellurium pieces and selenium shots in a 1:0.5:0.5 ratio, loaded together in a quartz tube which has been sealed under vacuum. The elements were heated slowly (100˚C/h) at 500˚C for 10 h, then melted at 1000˚C for 20h, cooled slowly down to 350˚C at 5˚C/h, and finally cooled faster by switching off the furnace. Single crystals were extracted mechanically from the resulting ball, the crystals being easy cleaved perpendicular to their c crystallographic axis. The refined lattice parameters of the Fe$_{1+\delta}$(Se$_{0.5}$Te$_{0.5}$) tetragonal main phase, a = 3.7992(7) Å and c = 6.033(2) Å, are in agreement with the literature \[4, 17\]. The real composition of the crystals checked by x-ray energy dispersive micro-analysis using a scanning electron microscope was found to be Fe$_{1.05(2)}$(Te$_{0.55(2)}$Se$_{0.45(2)}$). The temperature dependence of the resistivity shows a metallic behavior at low temperature as expected for this low level ($\delta = 0.05$) of interstitial iron \[21\].

Samples of batch B were grown with the Bridgman technique using a double wall quartz ampoule. The inside tube had a tapered bottom with a 30° angle and an open top. The inside wall of the outer ampoule was carbon coated to achieve the lowest possible oxygen par-

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**FIG. 1:** AC specific heat measurements $C_p/T^2$ as a function of $T$ of a Fe(Se$_{0.5}$Te$_{0.5}$) single crystal (sample A4) for $\mu_0 H = 0$, 8, 12, 16, 20, 24 and 28 T (from right to left) for $H||ab$ (A) and $H||c$ (B). The data have been renormalized taking $C_p(T = 20K) = 3.8 J/molK$. The $H_{c2}$ line is deduced from the midpoint of the specific heat jump after subtraction of a smooth polynomial background. (C) : Specific heat from relaxation data $(H||c)$ for the indicated magnetic fields (sample A5). Inset: temperature dependence of the electronic contribution to the specific heat $C_e = C_p - \beta T^3 - \delta T^5$ (solid symbols) where the phonon contribution $(\beta T^3 + \delta T^5)$ has been subtracted from the normal state data (see thin line in Fig 1C). The BCS behavior for $2\delta/kT_c = 3.5$ (solid line) and $2\Delta/kT_c = 5$ (dotted line) are displayed for comparison.
H (T)
H (T)
H (T)
µ
µ
µ
0
0
0
H
been measured after applying a magnetic field
rem
rem
local DC field (\(B_\omega\) Oe (\([\sim 210\,\text{Hz}])
induction as the sample is exposed to an ac field
×
up to 9T.

sweeping the field back to zero. In the Meissner state, no
vortices penetrate the sample and \(B_{\text{rem}}\) remains
equal to zero up to \(H_a = H_f\) (the first penetration field). A
finite remanent field is then obtained for field amplitudes
larger than \(H_f\) as vortices remain pinned in the sample.

Finally, the London magnetic penetration depth in the
Meissner state, \(\lambda\), has been measured on the same
samples with a LC oscillating circuit (14MHz) driven by a
Tunnel Diode (TDO). The samples have been glued at the bottom of a sapphire rod which were introduced in a coil of inductance $L$. The variation of the penetration depth induce a change in $L$ and hence a shift of the resonant frequency $\delta f(T) = f(T) - f(T_{\text{min}})$. $\delta f(T)$, renormalised to the frequency shift corresponding to the extraction of the sample from the coil $\Delta f_0$ is then equal to the magnetic susceptibility. At low temperatures (typically for $T \leq 12K$), $\lambda < d$ ($d$ being the lowest dimension of the sample, here the thickness), and we have $\frac{\delta f(T)}{\Delta f_0} = \frac{1}{R}$ where $\lambda$ is an effective penetration depth depending on the field orientation and $R$ an effective dimension of the sample. When the magnetic field is applied along the c-axis, only the in-plane supercurrents are probed and $\tilde{\lambda} = \lambda_{ab}$, whereas $\lambda = \lambda_{ab} + \frac{d}{w}\lambda_c$ for $H/ab$ ($w$ being the width of the sample). The effective dimension $\tilde{R}$ is calculated following [22].

III. UPPER CRITICAL FIELD

Fig.1 displays typical AC measurements for both $H||c$ and $H||ab$ (sample A4). As shown, a well defined specific heat jump is obtained at $T_c$ for $H = 0$ ($\sim 20\%$ of the total $C_p$) and this peak progressively shifts towards lower temperature as the magnetic field is increased (here up to 28 T). The $H_{c2}$ line has been deduced from the midpoint of the $C_p/T$ anomaly after subtraction of a smooth polynomial background from the raw data. As shown in Fig.2A, the corresponding $H_{c2}$ lines present a very strong downward curvature for $T \rightarrow T_c$ which was not revealed by previous transport measurements (the same behavior is observed in all measured samples, see for instance Fig.2B and Fig.3A for a comparison between samples A4 and B1). Note that a very similar curvature has been reported recently from [25].

Such a curvature is a strong indication for paramagnetic effects and we have hence fitted the experimental data using a weak coupling BCS clean limit model including both orbital and Pauli limitations [23]. This model only requires two fitting parameters (plus $T_c$) : the initial slope $dH_{c2}/dT|_{T=T_c}$ and the zero temperature Pauli limit $H_p$. The results are shown in Fig.3A for sample A4 and B1. As shown, very good fits can be obtained in both samples using very similar fitting parameters : $\mu_0 dH_{c2}/dT|_{T=T_c} \sim 38 \pm 3$ T/K and $\sim 13 \pm 2$ T/K for $H||ab$ and $H||c$ respectively and $\mu_0 H_p \sim 45 \pm 2$ T and $\sim 54 \pm 4$ T/K for $H||ab$ and $H||c$, respectively.

As previously observed in layered systems (see [24] and discussion in [25]) $H_{c2||ab}$ is actually very close to a $(1 - T/T_c)^{1/2}$ law. Strikingly, this simple behaviour is valid up to $T/T_c \sim 0.99$ in our system (see Fig.3B). Such a dependence can be directly inferred from a Ginzburg-Landau (GL) expansion which leads to [25]:

$$\left(\frac{H}{H_p}\right)^2 + \frac{H}{H_o} = 1 - \frac{T}{T_c}$$

(1)

(where $H_o$ is the orbital field) i.e. $H_{c2} \sim H_p(1 - t)^{0.5}$ for $H >> H_p^2/H_o$. A fit to Eq.(1) (solid line in Fig.3B) leads
to $\mu_0 H_o^{ab} \sim 65$ T and $\mu_0 H_o^{ab} \sim 75$ T, $\mu_0 H_o^{ab} \sim 650$ T and $\mu_0 H_o^{ab} \sim 170$ T (sample A4) \cite{24}. We hence have $\mu_0 H_o^{ab}/H_o \sim 6$ T for $H || ab$, field which is reached for $T/T_c \sim 0.99$. Fe(Se,Te) is thus a rare example of superconductor for which the upper critical field is dominated by paramagnetic effects almost the totality of the phase diagram (for $H || ab$). A shown in Fig.3B, a linear dependence is recovered very close to $T_c$ with $\mu_0 dH_o^{ab}/dT \approx 45$ T/K and $\mu_0 dH_o \parallel c/dT \approx 12$ T/K, in good agreement with a values deduced from the BCS fitting procedure \cite{27}.

Those extremely high $H_o$ values are related to very small values of the coherence lengths $\xi_{ab} = \Phi_0/2\pi [0.7 \times \mu_0 H_o] \sim 15 \pm 1$A and $\xi_c = \xi_{ab} \times (H_o^{ab}/H_o || ab) \sim 4 \pm 1$A which confirm the very strong renormalization of the Fermi velocity observed in ARPES measurements \cite{10} (see also theoretical calculations in \cite{28}). Indeed, one gets $v_{F,ab} = \pi \Delta \xi_{ab}/\hbar \sim 1.4 \times 10^4$ m/s ($\Delta$ being the superconducting gap $\sim 2$ meV \cite{29} \cite{30}) i.e. $hv_{F,ab} \sim 0.09$ eVÅ in perfect agreement with ARPES data which also led to $h v_{F,ab} \sim 0.09$ eVÅ for the $\alpha_3$ hole pocket centered on the $\Gamma$ point [note that the $H_{c2}$ line will be dominated by the band having the larger critical field i.e. the lower Fermi velocity]. Our measurements do hence confirm the strong correlation effects previously suggested by ARPES measurements \cite{10}.

An estimate of the paramagnetic field in the weak coupling limit is given by the Clogston-Chandrasekhar formula : $\mu_0 H_p = 2\Delta/\sqrt{2g\mu_B} \sim 26$ T in our sample (taking $g = 2$) i.e. well below the experimental suggesting that $g \sim 1.0 - 1.2$. However, it is important to note that $H_p$ may be increased by strong coupling effects \cite{31} and a fit to the data can be obtained introducing an electron-phonon coupling constant $\lambda \sim 0.6 - 0.7$ and $g \sim 2$ (still having an anisotropy on the order of 1.2 between the two main crystallographic axis). Even if it is difficult to conclude on the exact value of $g$, our data clearly indicate a small anisotropy of this coefficient ($\sim 1.2$) supporting the possibility of a crossing of the $H_{c2}$ lines at low temperature. Note that this anisotropy is much lower than the one inferred from transport measurements ($\sim 4 \cite{13}$) confirming that the large apparent anisotropy of $g$ deduced from those measurements is an artifact, probably related to the anisotropy of flux dynamics (see discussion on the irreversibility line below). The anisotropy of the upper critical field is then strongly temperature dependent rising from $H_{c2}^{ab}/H_{c2}^{ab} \sim H_{c2}^{ab}/H_{c2}^{ab} \sim 0.8$ for $T \rightarrow 0$, reflecting the small anisotropy of the g factor, to $H_{c2}^{ab}/H_{c2}^{ab} \sim H_{o}^{ab}/H_{o}^{ab} \sim 3.5 - 4$ close to $T_c$, reflecting the anisotropy of the coherence lengths (see Fig.7).

**IV. IRREVERSIBILITY LINE**

The small $\xi$ values associated to large $\lambda$ values ($\lambda_{ab}(0) \sim 430$ nm (see below and \cite{17}) lead to strong fluctuation effects hindering any direct determination of $H_{c2}$ from either transport of susceptibility measurements. These fluctuations can be quantified by the Ginzburg-Landau number $G_i = (k_B T_c/\epsilon_0 \xi_c)^2/\epsilon_0$ where $\epsilon_0 = (\Phi_0/4\pi \lambda_{ab})^2$ is the line tension of the vortex matter. One hence obtains $\epsilon_0 \xi_c \sim 40$ K (as a comparison $\epsilon_0 \xi_c \sim 200$K in cuprates) and $G_i \sim 10^{-2}$ which is very similar to the value obtained in YBa$_2$Cu$_3$O$_{7-\delta}$ or NdAs$_2$Fe(O$_{1-\delta}$F$_\delta$) (so called 1111-phase, see \cite{32} and references therein) clearly showing that thermal fluctuations are very strong in this system.

To emphasize this point, we have reported in Fig.2, the temperatures corresponding to both $R \rightarrow 0$ and $R/R_N = 0.5$ deduced from transport measurements up to 9T for sample A4 (see also Fig.4) and even up to 50T for sample B1 (see \cite{13}) ($R_N$ being the normal state resistance). As shown, none of those lines present the strong

![FIG. 4: Transport and AC transmittivity measurements as a function of $T$ for the indicated magnetic fields ($H || c$) in Fe(Se$_{0.5}$Te$_{0.5}$) single crystals. In the inset: comparison between transport and specific heat data for $\mu_0 H = 0$ and 6 T ($|| c$) emphasizing that the midpoint of the specific heat anomaly does not correspond to any characteristic temperature in $R(T)$ for $H \neq 0$.](image)
downward curvature obtained in $C_p$ measurements. On the contrary, the $R/R_N = 0$ lines vary almost linearly with $T$ with $d\mu_0 H /dT \sim 11$ T/K and $\sim 5$ T/K for $H || ab$ and $H || c$, respectively in agreement with previous measurements \[11\] \[12\]. However, as pointed above, these lines do not correspond to any thermodynamic criterion and discussions of the corresponding lines should hence be taken with great caution. Moreover whereas the midpoint of the specific heat coincides with the $R = 0$ temperature for $H = 0$ in sample A4, this midpoint rather lies close to the $R/R_N = 0.5$ point in sample B1 clearly showing that neither of those two transport criteria can be associated with the $H_{c2}$ line.

Similarly, as previously observed in high temperature cuprates and 1111-pnictides \[32\], the onset of the diamagnetic response ($T_H \to 0$) also lies well below the the $H_{c2}$ line. (see Fig.2A and Fig.4). Indeed, this onset is related to the irreversibility line above which the system is unable to screen the applied AC field due to the free motion of vortices. This irreversibility line is then expected to lie close to the $R = 0$ line. As shown in Fig.4 the onset of diamagnetism actually differs slightly from the onset of resistivity. This difference is much probably related to different voltage-current criteria (the magnetic screening corresponds to much smaller electric fields but requires higher currents) but both lines present the positive curvature characteristic of the onset of irreversible processes. Note that, as expected for vortex melting (for a review see \[33\]), the irreversibility line (here defined as the onset of $T_H$) varies as : $H_{c2} \propto (1 - T/T_c)\alpha$ with $\alpha \sim 2$ (see Fig.3B). A similar curvature has also been reported by Bendele \textit{et al.} \[17\] for the irreversibility field deduced from magnetization measurements.

\section{V. LOWER CRITICAL FIELD}

The first penetration field has been measured on a series of Fe(Se$_{0.5}$Te$_{0.5}$) samples with very different aspect ratios (see Table 1). To avoid spurious effects associated to strong pinning preventing the vortex diffusion to the center of the sample \[34\] $H_f$ has also been measured on several locations of the same sample. The inset of Fig.5 displays typical examples on sample A3' (2 positions) and A3". In samples with rectangular cross sections, flux lines partially penetrate into the sample through the sharp corners even for $H_a < H_f$ but remain ”pinned” at the sample equator. The magnetization at $H_a = H_f$ is then larger than $H_{c1}$ and the standard "elliptical" correction for $H_{c1} (= H_f/(1 - N))$ where $N$ is the demagnetization factor) can not be used anymore. Following \[35\], in presence of geometrical barriers, $H_f$ is related to $H_{c1}$ through :

$$H_{c1} \approx \frac{H_f}{\tanh(\sqrt{\alpha d/w})} \quad (2)$$

where $\alpha$ varies from 0.36 in strips to 0.67 in disks ($d$ and $w$ being the thickness and width of the sample, respectively. To reduce the uncertainty associated with the $\alpha$ value as well as the $d/w$ ratio in real samples of irregular shape, five different samples with different aspect ratios have been measured (see Table 1). Sample A3' has been cut out of sample A3 and finally A3" out of A3' in order to directly check the influence of the aspect ratio on $H_f$. The corresponding $H_f$ values are reported in the inset of Fig.7 together with the theoretical predictions from Eq.(2) taking $\mu_0 H_{c1}^{ab} = 78$ G (the predictions for an standard "elliptical" correction are also displayed for comparison).

The lower critical fields ($\mu_0 H_{c1}^c, \mu_0 H_{c1}^{ab}$) are then related to the penetration depth ($\lambda_c, \lambda_{ab}$) through :

$$\mu_0 H_{c1}^c = \frac{\Phi_0}{4\pi\lambda_{ab}^c} \left( \text{Ln}(\kappa) + c(\kappa) \right) \quad (3)$$

$$\mu_0 H_{c1}^{ab} = \frac{\Phi_0}{4\pi\lambda_{ab}\lambda_c} \left( \text{Ln}(\kappa^*) + c(\kappa^*) \right) \quad (4)$$

where $\kappa = \lambda_{ab}/\xi_{ab}$, $\kappa^* = \lambda_c/\xi_{ab}$ and $c(\kappa)$ is a $\kappa$ dependent function tending towards $\sim 0.5$ for large $\kappa$ values. Taking $\mu_0 H_{c1}^c(0) = 7.0 \times \mu_0 H_a \sim 130$T, and $H_{c1}^{ab} = 78 \pm 5$ G one gets $\lambda_{ab}(0) \sim 430\pm 50$ nm, which is in fair agreement with muons relaxation data \[17\] \[30\]. This very large $\lambda$ value confirms the general trend previously inferred in iron pnictides (see for instance \[17\] and references therein) pointing towards a linear increase of $T_c$ vs $1/\lambda_{ab}^2$ as ini-
dependence of the superfluid density \( \rho \) one hence obtains \( H \parallel \lambda \) et al. partially proposed in cuprates by Uemura et al. [36] and displayed as the thick solid line.

As described in sec.II, \( \lambda_c \) and \( \lambda_{ab} \) were deduced from the frequency shift in TDO measurements (sample \( A^\prime \), Table 1). Inset : temperature dependence of the superfluid density \( \rho_s^{TDO}(T)/\rho_s^{TDO}(0) = 1/(1 + \lambda_{ab}(T)/\lambda_{ab}(0))^2 \) taking \( \lambda_{ab}(0) = 430 \text{ nm} \) and \( R = 14 \mu \text{m} \) (solid symbols) (i.e. following [22], see corresponding \( \Delta\lambda_{ab}(T) \) values on the main panel) or \( R = 70 \mu \text{m} \) (open symbols). The average \( H_{c1}(T)/H_{c1}(0) \) curve (see Fig.5) is displayed as the thick solid line.

\( \gamma(0) \) obtained for all samples). The TDO data then require the introduction of the value of \( \lambda_{ab}(0) \) to convert the \( \Delta\lambda(T) \) data into \( \rho_s^{TDO}(T)/\rho_s^{TDO}(0) = 1/(1 + \lambda_{ab}(T)/\lambda_{ab}(0))^2 \). Introducing \( \lambda_{ab}(0) \sim 430 \text{ nm} \) and taking \( R \sim 14 \mu \text{m} \) (from [22]), \( \rho_s^{TDO}(T) \) shows a change of curvature around 5K, very similar to the one previously reported in [18] (see inset of Fig.6). A similar discrepancy has already been observed in MgC\( \text{N}_3 \) and interpreted as a reduction of the critical temperature at the surface of the sample due to a modification of the carbon stoechiometry [35]. However, such an explanation is not expected to hold here as single crystals were extracted mechanically from the bulk.

It is important to note that the temperature dependence of the superfluid density is very sensitive to the absolute value of \( \Delta \lambda \) and, although very similar to the one reported by Kim et al. [18], the amplitude of \( \Delta\lambda_{ab}/T^2 \sim 40 \text{ A/K}^2 \) observed in our samples is much larger than the one reported recently by Sarafin et al. [13] (~ 10 A/K^2). Similar discrepancies in the absolute amplitude of \( \Delta \lambda \) have also been reported in other pnic-rides [39] and have been attributed to complications from rough edges which may lead to an overestimation of \( \Delta \lambda \). Dividing the absolute \( \Delta\lambda_{ab} \) by a factor ~ 5 (i.e. taking \( R = 70 \mu \text{m} \) for \( H \parallel c \) instead of 14 (\( \mu \text{m} \)) actually leads to a very good agreement between TDO and \( H_{c1} \) data (see Fig.6) hence indicating that this value has probably been overestimated due to an underestimation of the effective dimension \( R \) in presence of rough edges.

Very similar temperature dependences of \( H_{c1} \) were obtained in both directions (see Fig.5) leading to a (almost) temperature independent anisotropy of \( H_{c1} : \Gamma_{H_{c1}} \sim 3.4 \pm 0.5 \) and hence \( \Gamma_{H_{c1}} = \lambda_c/\lambda_{ab} = [H_{c1}^c/H_{c1}^p]^0 \times ([\ln(\kappa^c) + c(\kappa))/([\ln(\kappa^c) + c(\kappa))]] \sim \Gamma_{H_{c1}} \times 1.2 \sim 4.1 \pm 0.8 \) (see Fig.7). This value is hence very close to the one obtained for \( H_{c2} \) close to \( T_c \) as \( \Gamma_{H_{c2}}(T \to T_c) \sim \Gamma_{H_{c1}} \simeq \xi_b/\xi_c \) (see Fig.7). Similarly, very similar temperature dependences have been observed for \( \Delta\lambda_c \) and \( \Delta\lambda_{ab} \) (with \( \Delta\lambda_c \sim 5 \times \Delta\lambda_{ab} \) up to \( T \to T_c \)), again suggesting a weak temperature dependence of this anisotropy. Finally, this value is also close to the one obtained for the irreversibility field deduced from the onset of dihmagentic screening.

VI. FINAL DISCUSSION

The value of the normal state Sommerfeld coefficient (\( \gamma_N \)) in Fe(Se,Te) compounds remains debated as values ranging from ~ 23 mJ/molK^2 [40] to ~ 39 mJ/molK^2 [4] have been obtained. For non superconducting samples, it has even been shown recently [41] that \( \gamma_N \) rises rapidly for \( x \leq 0.1 \) reaching ~ 55 mJ/molK^2 for \( 0.1 \leq x \leq 0.3 \). Even though our maximum field (28 T) is too low to fully destroy superconductivity down to 0 K hence hindering any precise determination of \( \gamma_N \), it is worth noting that a \( \gamma_N \) value on the order of ~ 39 mJ/molK^2 is incompatible with the entropy conservation rule in our sample. A reasonable fit to the data (solid line in Fig.1C) assuming that \( C_p/T = \gamma_N + \beta T^2 + \delta T^4 \) for \( 20 > T > 12 \) K...
and \( \mu_0 H = 28 \, T \) leads to \( \gamma_N = 23 \pm 3 \, \text{mJ/molK}^2 \) in good agreement with the value obtained by by Tsurkan et al. [10]. This \( \gamma_N \) value is also in fair agreement with the one deduced from ARPES measurements (\( \sim 30 \, \text{mJ/molK}^2 \) [10]). Similarly, the Debye temperature (\( \Theta_D \sim 143 \, \text{K} \)) is in reasonable agreement with the one previously reported in both Fe(Se\(_{0.67}\)Te\(_{0.33}\)) (\( \Theta_D \sim 174 \, \text{K} \)) and Fe\(_{1.05}\)Te (\( \Theta_D \sim 141 \, \text{K} \) [22]).

The electronic contribution to the specific heat (\( C_v/T = C_p/T - \beta T^2 - \delta T^4 \)) is then displayed in the inset of Fig.1 together with the theoretical prediction for a single gap BCS superconductor in the weak coupling limit (i.e. taking \( 2\Delta/kT_c \sim 3.5 \), thin solid line). As shown, this standard behavior largely overestimates the experimental data at low temperature suggesting the presence of a much larger gap. A reasonable agreement to the data is obtained assuming that \( 2\Delta/kT_c \sim 5 \) (dotted line). However, even though some indication for the presence of a large gap were obtained by fitting either \( \mu SR \) or optical conductivity [43] data, the corresponding gap value (\( \sim 3 \, \text{meV} \)) is much larger than the value obtained by spectroscopy (\( \sim 1.8 - 2 \, \text{meV} \) [23, 50]). Moreover, those former measurements also suggest the presence of a much smaller gap which is not present in our specific heat measurements.

Some evidence for nodes (or for deep gap minima) in Fe(Se\(_{0.5}\)Te\(_{0.5}\)) has been suggested by four fold oscillations in the low temperature specific heat for \( H || c \) [45]. However, despite the high resolution of our AC technique and the very good quality of our samples (the specific heat jump at \( T_c \) is slightly larger than in [45]) we did not observe these oscillations in our samples (i.e \( \Delta C_p(\theta)/C_p < 10^{-3} \)). Nodes are also expected to show up in the field dependence of the Sommerfeld coefficient (\( \gamma(H) \)) which is then expected to vary as \( H^\alpha \) with \( \alpha < 1 \) (\( \alpha = 0.5 \) for the so-called Volovik effect for d-wave pairing with line nodes whereas \( \alpha \sim 1 \) for classical single gap BCS systems). We have hence extrapolated the \( C_v(H)/T \) data to zero using either a BCS formula (see discussion above, \( C_v/T - \gamma(H) \propto exp(-\Delta(H)/kT) \) in our temperature range) or a phenomenological second order polynomial fit. Both procedure led to a concave curvature for \( \gamma(H) \) with \( \alpha \sim 1.5 \pm 0.3 \) for \( H || c \) and \( \alpha \sim 2.2 \pm 0.6 \) for \( H || ab \). This concave behavior can be attributed to the effect of Pauli paramagnetism on the vortex cores [46] (see [37, 38] for experimental data in heavy fermions) hence clearly supporting the importance of these effects in Fe(Se\(_{0.5}\)Te\(_{0.5}\)).

Finally note that it has been suggested that \( \Delta C_p/T_c \) could be proportional to \( T_c^2 \) in iron pnictides [19, 20] due to strong pair breaking effects [49] with \( \Delta C_p/T_c^2 \sim 0.06 \, \text{mJ/molK}^4 \). One hence would expect an anomaly \( \Delta C_p/T_c \sim 12 \, \text{mJ/molK}^2 \) at \( T_c \) in our system which is clearly lower than the experimental value \( \sim 40 \pm 5 \, \text{mJ/molK}^2 \). Similarly, it has been suggested that the initial slope of the \( H_{c2} \) line could scale as \( \mu_0 dH_{c2}/dT \sim 0.2 \times T_c \) (T/K) but, again, this scaling does not hold in our sample for which \( \mu_0 dH_{c2}/dT \sim 12 \, \text{T/K} \). Finally note that the temperature dependence of the superfluid density (see discussion above) supports the \( \Delta \lambda_{ab}/T^2 \sim 10A/\text{K}^2 \) value obtained by Serafin et al. [14] which is also much smaller than the one suggested from the scaling of [50]: \( \Delta \lambda_{ab}/T^2 \sim 8.8 \times 10^4/T_0^2 \sim 32A/\text{K}^2 \).

VII. CONCLUSION

In summary,

(i) Precise determinations of the \( H_{c2} \) lines from \( C_p \) measurements led to a very strong downward curvature, similar to that observed in layered systems.

(ii) The temperature dependence of the upper critical field and the field dependence of the Sommerfeld coefficient both indicate that \( H_{c2} \) is limited by strong paramagnetic effects with \( \mu_0 H_{c2} \sim 45 \pm 2 \, \text{T} \) and \( \sim 54 \pm 4 \, \text{T} \) for \( H || ab \) and \( H || c \), respectively.

(iii) The very small value of the coherence length \( \xi_{ab}(0) \sim 15A \) confirms the strong renormalisation of the effective mass (compared to DMFT calculations) previously observed in ARPES measurements [10] and associated strong electron correlation effects. \( \gamma_N \) is estimated...
to $\sim 23\pm 3$ mJ/molK$^2$ in fair agreement with the ARPES value.

(iv) The anisotropy of the orbital critical field is estimated to be on the order of 4 hence leading to a $\xi_c(0)$ value smaller than the c lattice parameter.

(v) Neither the temperature dependence of $\lambda$ nor that of the electronic contribution to the specific heat follow the weak coupling BCS model (an BCS dependence with $\Delta/kT_c \sim 5$ remains possible) but no evidence for nodes in the gap is obtained from the field dependence of the Sommerfeld coefficient. We did not observe the fourfold oscillations of the low temperature specific heat previously obtained by Zeng et al. [45].

(vi) The amplitude of the specific heat jump $\Delta C_p/T_c \sim 40 \pm 5$ mJ/molK$^2$ is much larger than that previously observed in Fe(Se,Te) and does not follow the $\Delta C_p/T_c^3$ inferred in iron pnictides. Similarly neither the slope of the $H_{c2}$ line nor the absolute value of $\Delta\lambda(T)$ obey the scaling laws previously proposed for iron pnictides [49, 50].

(vii) $\lambda_{ab}(0) = 430 \pm 50$ nm and $\lambda_c(0) = 1600 \pm 200$ nm, confirming the very small superfluid density previously observed in iron pnictides. The corresponding anisotropy is almost temperature independent with $\Gamma_{ab} \sim \Gamma_{H_{c2}}(T \to T_c) = \gamma_c$. (viii) These large $\lambda$ values associated to small $\xi$ values lead to a very small condensation energy $\epsilon_0\xi_c \sim 40$K and hence to large fluctuation effects hindering any determination of $H_{c2}$ from either transport or susceptibility measurements. A detailed analysis of the influence of these fluctuations on the specific heat anomaly will be presented elsewhere.

(ix) The strong upward curvature of the irreversibility line (defined as the onset of diamagnetic screening) : $H_{irr} \sim (1 - T/T_c)^2$ strongly suggests the existence of a vortex liquid in this system.

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