SrPt$_3$P: two-band single-gap superconductor

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The magnetic penetration depth ($\lambda$) as a function of applied magnetic field and temperature in SrPt$_3$P ($T_c \simeq 8.4$ K) was studied by means of muon-spin rotation ($\mu$SR). The dependence of $\lambda^{-2}$ on temperature suggests the existence of a single $s$–wave energy gap with the zero-temperature value $\Delta = 1.58(2)$ meV. At the same time $\lambda$ was found to be strongly field dependent which is the characteristic feature of the nodal gap and/or multi-gap systems. The multi-gap nature of the superconducting state is further confirmed by observation of an upward curvature of the upper critical field. This apparent contradiction would be resolved with SrPt$_3$P being a two-band superconductor with equal gaps but different coherence lengths within the two Fermi surface sheets.

After the discovery of first Fe-based superconductors enormous efforts were made in order to improve their superconducting properties. The intensive search lead to discovery series of new Fe-based materials (see e.g. Ref. $^1$ for review and references therein) and related compounds such as BaNi$_2$As$_2$ $^2$, SrNi$_2$As$_2$ $^3$, SrPt$_2$As$_2$ $^4$, SrPtAs $^5$, without Fe and relatively low superconducting transition temperatures $T_c$’s.

Recently, Takayama et al. $^6$ reported the synthesis of a new family of ternary platinum phosphide superconductors with the chemical formula APT$_3$P (A = Sr, Ca, and La) and $T_c$’s of 8.4, 6.6 and 1.5 K, respectively. Theoretical studies on the pairing mechanism in these new compounds achieved partially contradicting results $^7$, $^8$. The authors of Ref. $^7$ performed first-principles calculations and proposed that superconductivity is caused by the proximity to a dynamical charge-density wave instability, and that a strong spin-orbit coupling leads to exotic pairing in at least LaPt$_3$P. In contrast, the first principal calculations and Migdal-Eliashberg analysis performed by Subedi et al. $^8$ suggest conventional phonon mediated superconductivity. Also experimentally seemingly contradicting results were obtained. Based on the observation of nonlinear temperature behavior of the Hall resistivity, the authors of Ref. $^6$ suggest multi-band superconductivity in these new compounds. Note that the presence of two bands crossing the Fermi level was indeed confirmed by ab-initio band structure calculations presented in $^7$, $^10$. On the other hand the specific heat data of SrPt$_3$P were found to be well described within a single band, single $s$–wave gap approach with the zero-temperature gap value $\Delta = 1.85$ meV $^6$.

In this paper we report on the results of muon-spin rotation ($\mu$SR) studies of the magnetic penetration depth ($\lambda$) as a function of temperature and magnetic field of the novel superconductor SrPt$_3$P. Below $T \simeq T_c/2$ the superfluid density ($\rho_s \propto \lambda^{-2}$) becomes temperature independent which is consistent with a fully gapped superconducting state. The full temperature dependence of $\rho_s(T)$ is well described within a single $s$-wave gap scenario with the zero-temperature gap value $\Delta = 1.58(2)$ meV. On the other hand, $\lambda$ was found to increase with increasing magnetic field as is observed in multi-band superconductors or superconductors with nodes in the energy gap. The upper critical field demonstrates a pronounced upward curvature thus pointing to a multi-band nature of the superconducting state of SrPt$_3$P. Our results indicate that SrPt$_3$P is a two-band superconductor with equal gaps but different coherence length parameters $\xi_i$ within two Fermi surface sheets.

The sample preparation and the magnetization experiments were performed at the ETH-Zürich. Polycrystalline samples of SrPt$_3$P were prepared using cubic anvil high-pressure and high-temperature technique. Coarse powders of Sr, Pt, and P elements of high purity (99.99%) were weighed according to the stoichiometric ratio 1:3:1, thoroughly grounded, and enclosed in a boron nitride container, which was placed inside a pyrophyllite cube with a graphite heater. All procedures related to the sample preparation were performed in an argon-filled glove box. In a typical run, a pressure of 2 GPa was applied at room temperature. While keeping the pressure constant, the temperature was ramped up in 2 h to the maximum value of 1050 °C, maintained for 20–40 h, and then decreased to room temperature in 1 h. Afterwards, the pressure was released, and the sample was removed. All high-pressure prepared samples demonstrate large diamagnetic response with the superconducting transition temperature of $\approx 8.4$ K (see the inset in Fig. $^1$). The powder x-ray diffraction patterns are consistent with those reported in Ref. $^6$.

Measurements of the upper critical field $B_{c2}$ were performed using a Quantum Design 14 T PPMS. The temperature dependence of $B_{c2}$ was obtained from zero field-cooled magnetization curves $[M_{ZFC}(T)]$ measured in constant magnetic fields ranging from 0.3 mT to 4 T (see Fig. $^1$). For each particular field the corresponding superconducting transition temperature $T_c(B)$ was taken as an intersect of the linearly extrapolated $M_{ZFC}(T)$ curve in the vicinity of $T_c$ with $M_{ZFC} = 0$ line (see the in-
The first term of Eq. (1) represents the response of the superconducting part of the sample. Here $A_{sc}$ denotes the initial asymmetry; $\sigma_{sc}$ is the Gaussian relaxation rate due to the FLL; $\sigma_0$ is the contribution to the field distribution arising from the nuclear moment and which is found to be temperature independent, in agreement with the ZF results (not shown); $B_{int}$ is the internal magnetic field sensed by the muons and $\phi$ is the initial phase of the muon-spin ensemble. The second term with the initial asymmetry $A_b$, small $\sigma_0 < 0.3 \, \mu s^{-1}$ and $B_0$ close to the applied field corresponds to the background muons stopping in the cryostat and in nonsuperconducting parts of the sample.

Figure 2 shows the temperature dependence of $\sigma_{sc}$ in four different fields 0.05, 0.15, 0.3, and 0.45 T. As expected, $\sigma_{sc}$ is zero in the paramagnetic state and starts to increase below the corresponding $T_c(B)$. Upon lowering $T$, $\sigma_{sc}$ increases gradually reflecting the decrease of the penetration depth $\lambda$ or, correspondingly, the increase of the superfluid density $\rho_s \propto \lambda^{-2}$. The overall decrease of $\sigma_{sc}$ with increasing applied field is partially caused by the decreased width of the internal field distribution upon approaching $B_{c2}$. In order to quantify such an effect, one can make use of the numerical Ginzburg-Landau model, developed by Brandt [33]. This model predicts the magnetic field dependence of the second moment of the magnetic field distribution, i.e. the $\mu$SR depolarization rate:

$$
\sigma_{sc}[\mu s^{-1}] = 4.83 \times 10^4 (1 - B/B_{c2}) \times
$$

set it Fig. 1, $B_{c2}(T)$ curve exhibits a pronounced upward curvature around $\sim 6 - 6.5$ K. Linear fits of $B_{c2}(T)$ in the vicinity of $T_c$ and for $T < 0.6 K$ yield $d B_{c2}/dT = -0.45$ and $-0.77 \, T/K$, respectively. Open circles correspond to $B_{c2}(T)$ data points from Ref. [6]. They are in perfect agreement with our data thus implying that the upturn on $B_{c2}(T)$ reported here is indeed a generic property of SrPt$_3$P compound. Note that an upward curvature of $B_{c2}(T)$ was also observed previously for a number of materials such as Nb [11, 12], V [11], NbSe$_2$ [13, 15], MgB$_2$ [16, 18], borocarbides and nitrides [19, 21], heavy fermion systems [22], various iron-based [23, 25] and cuprate superconductors [26, 27] and was often associated with two-band superconductivity.

The temperature and the magnetic field dependence of the magnetic penetration depth $\lambda$ were determined from transverse-field (TF) $\mu$SR data [28]. The experiments were carried out at the $\pi$E1 beam line at the Paul Scherrer Institute (Villigen, Switzerland). The data were analyzed using the free software package MUSRFIT [29]. In a polycrystalline sample the magnetic penetration depth $\lambda$ can be extracted from the Gaussian muon-spin depolarization rate $\sigma_{sc}(T) \sim \lambda^{-2}$, which reflects the second moment of $\langle \gamma \mu_B^2 \rangle$ that is the muon g-imagnetic ratio of the magnetic field distribution due to the flux-line lattice (FLL) in the mixed state [30, 32]. The TF- $\mu$SR data were analyzed using the asymmetry function:

$$
A(t) = A_{sc} \exp[-(\sigma_{sc}^2 + \sigma_{2}^2) t^2/2] \cos(\gamma \mu B_{sc} t + \phi) + A_b \exp(-\sigma_b^2 t^2/2) \cos(\gamma \mu B_0 t + \phi)
$$

FIG. 1: (Color online) The temperature dependence of the upper critical field $B_{c2}$ of SrPt$_3$P. The crosses and the circles correspond to two different samples. The solid lines are linear fits of $B_{c2}(T)$ in the vicinity of $T_c$ and for $T \leq 6$ K. Open circles are $B_{c2}(T)$ data points from Ref. [6]. The inset shows the temperature dependence of the zero field-cooled magnetization $M_{ZFC}$ measured at $\mu_0 H = 0.3$ mT.

FIG. 2: (Color online) The temperature dependence of the depolarization rate $\sigma_{sc}$ caused by formation of FLL in SrPt$_3$P in fields of 0.05, 0.15, 0.3, and 0.45 T. The red solid line is the fit of Eq. (1) to $\sigma_{sc}(B)$ data with $\lambda^{-2} = 46(1) \mu m^{-2}$, $B_{c2} = 1.6(1)$ T. The dashed black line represents $\sigma_{sc}(B)$ as expected for $\lambda^{-2} = 38(1) \mu m^{-2}$ and $B_{c2} = 4.5$ T obtained in magnetization experiments.


\[ \times [1 + 1.21(1 - \sqrt{B/B_c})^3] \lambda^{-2}[\text{nm}^{-2}]/(T - T_c)^2 \] (2)

The insert of Fig. 2 shows the evolution of \( \sigma_{sc} \) at \( T = 1.7 \) K as a function of the applied magnetic field \( B \). Each data point was obtained after cooling the sample in the corresponding field from above \( T_c \) to \( 1.7 \) K. Under the assumption of field independent \( \lambda \) the dependence of \( \sigma_{sc} \) on \( B \) was analyzed by means of Eq. (2) using the values of the upper critical field \( B_{c2} \) as obtained in magnetization experiments \( B_{c2}(1.7) \) K \( \approx 4.5 \) T, see Fig. 1. It is clear from the inset of Fig. 3 that the theoretical \( \sigma(B) \) is not in agreement with the data. If \( B_{c2} \) is kept as a free parameter in the analysis, the fit yields \( B_{c2} = 1.6(1) \) T which is clearly inconsistent with the magnetization data. Therefore one has to conclude that the field independence of \( \lambda \), which was implicitly assumed in Eq. (2), is not valid (the discussion on field dependence of \( \lambda \) comes later in the paper). The low-temperature value of \( \lambda \) at \( B = 0 \) \( [\lambda(0, B = 0)] \) could be estimated by extrapolating two theory lines shown in the inset of Fig. 2 to \( B = 0 \). This results in \( \lambda(0, B = 0) = 155 \pm 10 \) nm.

\[ \frac{\lambda^{-2}(T)}{\lambda^{-2}(0)} = \frac{\rho_s(T)}{\rho_s(0)} = 1 + 2 \int_{\Delta(T)}^{\infty} \left( \frac{\partial f}{\partial E} \right) \frac{E \, dE}{\sqrt{E^2 - \Delta(T)^2}}. \] (3)

Here \( \lambda^{-2}(0) \) and \( \rho_s(0) \) are the zero-temperature values of the magnetic penetration depth and the superfluid density, respectively, and \( f = [1 + \exp(E/k_B T)]^{-1} \) is the Fermi function. The temperature dependence of the gap is approximated by \( \Delta(T)/\Delta(0) = \tanh[\{1.82[1.018(T_c/T - 1)]^{0.51}\}] \] \( \Delta(0) \) is the maximum gap value at \( T = 0 \). The fit results in \( \Delta(0, B)/k_B T_c(B) = 4.35(4) \), \( \lambda^{-2}(T)/\lambda^{-2}(1.7 - 3.5 K) = 1.021(6), \) and \( T/T_c(B) = 0.972(3) \). For \( T_c(B) = 0 \) \( \approx 8.4 \) K (see Fig. 1) we get \( \Delta(T = 0, B = 0) = 1.58(2) \) meV. Note that this value of the superconducting gap is close to \( \Delta = 1.85 \) meV obtained from zero-field specific heat data by Takayama et al. [6].

It is noteworthy that there is no need to introduce more that one gap parameter or to consider more complicated gap symmetry in order to satisfactorily describe \( \lambda^{-2}(T) \) data. A fit using two superfluid density components with \( s \)-wave gaps \( \Delta_1 \) and \( \Delta_2 \): \( \lambda^{-2}(T) = \lambda_{1s}^{-2}(T, \Delta_1) + \lambda_{2s}^{-2}(T, \Delta_2) \), as well a fit using an isotropic \( s \)-wave gap function result in higher \( \chi_0^1 \) than obtained for the single \( s \)-wave model described above. From the analysis of \( \lambda^{-2}(T) \) data alone one could therefore conclude that SrPt_3P is a a single band \( s \)-wave superconductor. Note that the similar conclusion was reached by Takayama et al. [6] based on specific heat data. In the following we will suggest that this was a premature conclusion obtained without considering the field dependence of \( \lambda \).

As follows from the inset in Fig. 3 the field increase from 0.05 up to 0.45 T leads to decrease of \( \lambda^{-2} \) by almost a factor of 2. In a single band \( s \)-wave superconductors \( \lambda \) is independent on the magnetic field [31, 35, 37]. A dependence of \( \lambda \) on \( B \) is expected for superconductors containing nodes in the energy gap or/multigap superconductors [32, 36, 38, 40]. In the later case the superfluid density within one series of bands is expected to be suppressed faster by magnetic field than within the others [39, 40].

The single \( s \)-wave gap behavior of \( \lambda^{-2}(T) \) (see Fig. 3 and the discussion above) and the multi-band features following after the upper critical field \( B_{c2} \) and \( \lambda^{-2}(B) \) measurements (Fig. 1 and the inset on Fig. 3) allow us to assume that SrPt_3P is a two-band superconductor with energy gaps being equal within both bands.

Within a two-gap model the deviation from the simple field independence of \( \lambda \) as well as the appearance of upward curvature of the upper critical field could reflect the occurrence of two distinct coherence lengths \( \xi_1 \) and \( \xi_2 \) for two bands (associated to the corresponding upper critical field values \( B_{c2,i} = \phi_0/(2\pi\xi_i^2) \) [39, 44]. For BCS
superconductors the zero-temperature coherence length obeys the relation \( \xi \propto \langle v_F \rangle / \Delta_1 \) (\( \langle v_F \rangle \) is the averaged value of the Fermi velocity). One could assume, therefore that in SrPt\( _3 \)P the difference between \( \xi_1 \) and \( \xi_2 \) could be caused by the different Fermi velocities (\( \langle v_{F,1} \rangle \neq \langle v_{F,2} \rangle \)), while gaps remain the same (\( \Delta_1 = \Delta_2 \)).

The statement about different \( \langle v_F \rangle \)'s in two Fermi surface sheets of SrPt\( _3 \)P is fully confirmed by the calculated band structure [7–10]. According to Refs. [7–10] there are two bands crossing the Fermi level having significantly different \( v_F \)'s. The ratio of \( v_F \)'s is, e.g., \( \zeta \approx 2 \) along \( \Gamma - X \) and \( \zeta \approx 3 - 4 \) along \( \Gamma - Z \) directions of the Brillouin zone. It is worth to note that different Fermi velocities on the different superconducting bands suppose to be a common feature of multi-band superconductors as e.g. MgB\( _2 \) [15–17], borocarbides [20, 17], Fe-based superconductors [18, 19] etc.

![Diagram](image)

**FIG. 4:** (Color online) Schematic diagram representing relations between the various types of a single-band, two-band and multi-band superconductors.

Note SrPt\( _3 \)P studied here is different from the most famous two-band superconductor MgB\( _2 \). In SrPt\( _3 \)P the charge carriers in both bands suppose to be almost equally coupled to the phonons. Indeed, according to the band structure calculations of Nekrasov et al. [9] the carriers in two bands correspond to the relatively similar \( p_d \sigma \) antibonding states of Pt(II)-P and Pt(II)-P ions, and are coupled to the same low-lying phonon modes confined on the ab plane. In MgB\( _2 \) only the \( \sigma \) band carriers are coupled strongly to the so called \( E_{2g} \) phonons, while the coupling of both, the \( \sigma \) and the \( \pi \), bands to the harmonic \( B_{1g}, A_{2u}, \) and \( E_{1u} \) phonons is negligible [50]. We may conclude, therefore, that MgB\( _2 \) and SrPt\( _3 \)P correspond to two limiting cases of two-band superconductivity with the energy gaps being nonequal (\( \Delta_1 \neq \Delta_2 \), as in MgB\( _2 \)) and equal (\( \Delta_1 = \Delta_2 \), as in SrPt\( _3 \)P). At the same time SrPt\( _3 \)P remains the "true" two-band superconductor since, due to nonequal Fermi velocities (\( \langle v_{F,1} \rangle \neq \langle v_{F,2} \rangle \)), the carriers in various bands "respond" differently to the magnetic field (as shown here based on \( B_{c2}(T) \) and \( \lambda(B) \) studies and by Takayama et al. [6] based on the observation of nonlinear temperature behavior of the Hall resistivity).

By following the above presented arguments we propose a schematic diagram describing relations between the single-, two-, and the multi-band superconductivity (see Fig. 4). The single-band superconductor has one gap and one averaged over the Fermi surface Fermi velocity (\( \langle v_F \rangle \)). There are two type of two-band superconductors with energy gaps being equal (\( \Delta_1 = \Delta_2 \)) and nonequal (\( \Delta_1 \neq \Delta_2 \)). Both of these types are characterized, however, by nonequal \( \langle v_F \rangle \)'s. The "transition" from the two- to the multi-band superconductivity may occur by three different routes. (i) All gaps in all bands crossing the Fermi level are equal (\( \Delta_1 = \Delta_2 \ldots = \Delta_n \)). This is probably the case for the optimally doped LaFeAsO\( _{0.9} \)F\( _{0.1} \) having five Fermi surfaces (as most other Fe-based superconductors, see e.g. Ref. [1] and references therein). As shown by Luetkens et al. [51] the temperature evolution of the superfluid density of LaFeAsO\( _{0.9} \)F\( _{0.1} \) is well described within the single \( s^- \)-wave gap approach, while \( \lambda^{-2} \) depends strongly on the magnetic field. It should be noted, however that the presence of two distinct gaps in LaFeAsO\( _{0.9} \)F\( _{0.1} \) were reported by Gonnelli et al. [52] based on the result of point contact Andreev reflection experiment. (ii) Gaps in some Fermi sheets are equal but in others are not (\( \Delta_1 = \Delta_2 \ldots = \Delta_k \neq \Delta_{k+1} \ldots = \Delta_n \)). A good example is the optimally doped Ba\( _{1-x} \)K\( _x \)Fe\( _2 \)As\( _2 \) where three gaps are equal (\( \zeta \approx 9 \) meV) while the last gap was found to be of approximately eight times smaller (\( \zeta \approx 1.1 \) meV) [48, 53]. (iii) Gaps in all the Fermi sheets are different (\( \Delta_1 \neq \Delta_2 \ldots \neq \Delta_n \)).

To summaries, the temperature and the magnetic field dependence of the magnetic penetration depth \( \lambda \) in SrPt\( _3 \)P superconductor (\( T_c \approx 8.4 \) K) were studied by means of muon-spin rotation. Below \( T \approx T_c / 2 \) the superfluid density \( \rho_s \propto \lambda^{-2} \) is temperature independent which is consistent with a fully gapped superconducting state. The full \( \rho_s(T) \) is well described within the single \( s^- \)-wave gap scenario with the zero-temperature gap value \( \Delta = 1.58(2) \) meV. At the same time \( \lambda \) was found to be strongly field dependent which is the characteristic feature of the nodal gap and/or multi-band systems. The multi-band nature of the superconducting state in SrPt\( _3 \)P was further confirmed by observation of an upward curvature of the upper critical field. To conclude, all above presented results show SrPt\( _3 \)P to be a two-band superconductor with the equal gaps but different coherence lengths \( \xi_i \) associated with the two Fermi surface sheets.

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