\[\mu\text{SR and magnetometry study of superconducting 5\% Pt doped IrTe}_2\]

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We present magnetometry and muon spin rotation (\(\mu\)SR) measurements of the superconducting dichalcogenide \(\text{Ir}_0.95\text{Pt}_{0.05}\text{Te}_2\). From both sets of measurements we calculate the penetration depth and thence superfluid density as a function of temperature. The temperature dependence of the superfluid densities from both sets of data indicate fully gapped superconductivity that can be fit to a conventional s-wave model and yield fitting parameters consistent with a BCS weak coupling superconductor. We therefore see no evidence for exotic superconductivity in \(\text{Ir}_0.95\text{Pt}_{0.05}\text{Te}_2\).

INTRODUCTION

Transition metal dichalcogenides have been studied for many years in an effort to understand their diverse properties \cite{1,2}. These materials are layered quasi-two dimensional systems that frequently exhibit charge density wave (CDW) ordering that is not yet fully understood \cite{2}. Furthermore, the crystal structure of these materials is amenable to substitution and intercalation of a wide variety of dopant atoms to allow tuning through a broad range of electronic properties \cite{3}. In particular, these systems provide a valuable avenue to study the interplay of structural transitions and superconductivity as in many cases superconductivity emerges after the CDW transition is suppressed by doping or applied pressure \cite{4,8}.

IrTe\(_2\) is a member of this group of compounds. It undergoes a structural transition at about 270 K \cite{9} from the trigonal \(\text{P3}_{\text{\textit{m}}1}\) space group to triclinic \(\text{PT}\) \cite{10,12}. Recent work has shown that this structural transition is associated with a charge density wave that has a periodicity 6 times larger than the underlying lattice \cite{13,15}. Substituting Ir with Pd, Pt, or Rh \cite{7,16,18} or intercalation with Cu \cite{19} suppresses the structural transition and leads to superconductivity with a maximum \(T_C\) of 3 K and \(H_{C2}\) \(\approx\) 0.1 T. Intercalation with other transition metals also suppresses the structural transition but does not lead to superconductivity, possibly as a result of competing magnetism \cite{20}. Measurements of \(T_C\) as a function of hydrostatic pressure in Pt-substituted IrTe\(_2\) have shown that increasing the temperature of the structural transition decreases \(T_C\), which shows that the appearance of superconductivity is directly related to the disappearance of the structural transition \cite{21}.

IrTe\(_2\) is of particular interest as both Ir and Te have high atomic numbers. Spin orbit coupling is therefore expected to be high which may lead to exotic states such as topological superconductivity \cite{22,23}. Determining the superconducting symmetry is important as unconventional (non s-wave) symmetry is required for superconductors to be topologically non-trivial \cite{23}.

Previous measurements of the superconducting symmetry by thermal conductivity \cite{24} and STM \cite{25} suggest conventional s-wave superconductivity. However, the thermal conductivity measurements cannot conclusively rule out odd-parity p-wave superconductivity, and STM measurements are inherently a surface technique and so the state they probe may not be representative of the bulk superconductivity. Furthermore, no penetration depth measurements have been conducted on this material. These measurements are important, as the temperature dependence of the penetration depth gives information about the symmetry of the superconducting gap \cite{26}.

Muon spin rotation (\(\mu\)SR) is a powerful technique that can be used to study the magnetic penetration depth of type II superconductors in the vortex state \cite{26}. In this technique spin-polarized muons are implanted up to a few hundred \(\mu\)m into the sample where they precess in the local magnetic field and decay, emitting positrons that are detected to gain information about the local magnetic field. Importantly, the muons are implanted far enough into the sample that this can be considered a truly bulk technique. Therefore, surface effects that may change the states measured by techniques such as STM will not be a factor in these measurements.

In this paper we present complementary \(\mu\)SR and SQUID magnetometry measurements of the penetration depth of \(\text{Ir}_0.95\text{Pt}_{0.05}\text{Te}_2\). These measurements indicate an s-wave superconducting state, with gap and \(T_C\) values that are consistent with a conventional BCS weak-coupling superconductor.

EXPERIMENTAL METHODS

Single crystals of \(\text{Ir}_0.95\text{Pt}_{0.05}\text{Te}_2\) with sizes of a couple mm\(^3\) were grown using the self flux growth method \cite{27}.

Muon spin rotation (\(\mu\)SR) experiments were performed at the TRIUMF laboratory in Vancouver, Canada. We used the Pandora dilution refrigerator spectrometer on the M15
surface-muon beam line. This instrument gives access to temperatures between 0.03 K and 10 K with the sample mounted on a silver cold finger, magnetic fields up to 5 T with a superconducting magnet, and a time resolution of 0.4 ns. The field is applied parallel to the incoming muon beam direction, and we performed measurements with the muon spin rotated perpendicular to the field direction (SR). These experiments were performed on an unaligned collection of small (<1-2 mm) irregularly shaped single crystals mounted on a 1 x 2 cm silver plate using Apiezon N-grease. We used the μSRfit software package to analyze the μSR data.

Magnetometry measurements were performed at McMaster University using a Quantum Design XL-5 MPMS with an iHelium He³ cryostat insert for measurements down to 0.5 K. Magnetization vs. temperature curves were measured both on a subset of unaligned crystals from the μSR sample weighing 238 mg (polycrystalline sample), and on an aligned single crystal plate weighing 4.72 mg with dimensions 2.4 mm x 1.5 mm x 0.35 mm (C-axis). Magnetization vs. field curves were measured with fields up to 0.15 T and temperatures ranging from 0.5 to 3 K using the single crystal plate. Alignment of the single crystal was verified with Laue X-Ray diffraction prior to the magnetometry measurements.

RESULTS AND DISCUSSION

Figure 1 shows a temperature scan of the magnetization taken with an applied field of 300 Oe after cooling in zero field on the polycrystalline sample for comparison with the μSR data. This data shows strong diamagnetism, indicating that our sample is superconducting with a $T_c$ of about 2.3 K at $H_{ext} = 300$ Oe.

Muons that land in a superconducting sample with an applied field between $H_{C1}$ and $H_{C2}$ see an asymmetric field distribution arising from the vortex state that will have the form shown in Fig. 2 (d) inset. The experimental data from such a measurement, even on an ideal vortex lattice, will always show some broadening of this distribution due to the finite lifespan of the muon and time-window of the experiment. In practice, inhomogeneities in a sample will cause additional broadening of the field distribution that is difficult to rigorously account for. This is particularly important for the case of a polycrystalline sample where varied orientation and possible slight differences between the properties of different grains will broaden the signal. For our sample, we fit the field distribution to a three component model shown in Eq. 1 similar to that used by Khasanov et al. in measurements on high $T_c$ cuprates. This fit has two Gaussian-relaxing components representing the asymmetric superconducting line shape, and one non-relaxing component representing the silver background. These fits are made in the time domain to avoid Fourier transform broadening and to properly

Figures 2 (a-c) show μSR time spectra measured in an applied external field of 300 Oe $< H_{C2}$ transverse to the muon spins at 0.03 K, 1 K, and 2 K after field cooling the sample to ensure a uniform vortex lattice. This data shows a relaxing oscillating signal, with a beat evident in the lower temperatures along with a non-relaxing signal that persists to large times. This indicates the presence of more than one component to the signal, and can be more easily visualized by looking at the Fourier transform (FT) of the 0.03 K data found in Fig. 2 (d). We interpret the two peaks in the FT as arising from muons missing the sample and landing in the silver sample holder (peak at ≈ 300 G) and those hitting the sample and probing the superconducting state (lower field peak).

![Fig. 1. Magnetization measurements on a polycrystalline sample of Ir₀.₉₅Pt₀.₀₅Te₂ measured in a field of 300 Oe after cooling in zero field.](image1)

![Fig. 2. SR μSR time spectra of Ir₀.₉₅Pt₀.₀₅Te₂ measured in an applied field of 300 Oe at (a) T=0.03 K, (b) T=1 K, and (c) T=2 K. (d) Fourier transform of the μSR data collected in an applied field of 300 Oe at T=0.03 K. The inset in (d) shows the theoretical field distribution of a superconductor using the London model.](image2)
use the experimental error bars for weighting.

\[ A = A_T \left[ C \left( F \cos(\gamma_B B_1 t) + (1 - F) \cos(\gamma_B B_2 t) e^{-0.5(\sigma_1 t)^2} \right) \\
+ (1 - C) \left( \cos(\gamma_B B_2 t) e^{-0.5(\sigma_2 t)^2} \right) \right] \]

Here, \( C \) and \( F \) are temperature independent values giving the ratio of the three components, \( B_1 \) is the temperature independent mean field for the silver site, \( B_2 \) is the temperature dependent mean sample field, and \( \sigma_i \) are the temperature dependent Gaussian relaxation rates.

In this case the penetration depth can be determined from the equation [29]:

\[ \lambda = \sqrt{\frac{0.043\sqrt{2} \gamma B \phi_0}{\sqrt{\langle (\Delta F)^2 \rangle}}} \]

Here, \( \gamma = 135.538 \) MHz/T is the muon gyromagnetic ratio, \( \phi_0 = 2.06783 \) Wb is the flux quantum, and \( \langle (\Delta F)^2 \rangle \) is the central second moment (variance) of the fit frequency distribution. \( \langle (\Delta F)^2 \rangle \) is given by Eq. 3 which can be derived by considering that the second moment of a sum of two Gaussian distributions is the sum of the individual second moments, and that the central second moment is the second moment minus the square of the mean [31].

\[ \langle (\Delta F)^2 \rangle = R_1 \sigma_1^2 + R_2 \sigma_2^2 + R_1 R_2 (\gamma_B B_1 - \gamma_B B_2)^2 \]

Here, \( \sigma_i \) are the relaxation rates, \( B_i \) are the mean fields, and \( R_i \) are the relative weights of the two components.

These fits gave values of \( C = 0.7046, F = 0.37 \), and the temperature dependent values shown in Fig. 3. The temperature dependence of the fit parameters indicate that \( T_C \approx 2.25 \) K, consistent with that from our magnetization measurements at the same field. From the \( \sigma_T \) we calculated the temperature-dependent penetration depth using Eq. 2 this is shown in Fig. 4 (blue squares). This penetration depth diverges towards infinity approaching \( T_C \) and at low temperature \((T < 0.5 \) K) has an average value of \( 119 \pm 2 \) nm with very weak temperature dependence (linear fit slope of \( 4 \pm 3 \) nm \( \approx \) 0). This behavior is consistent with what is expected for a conventional fully gapped superconductor that should asymptote to a constant low temperature value.

To compare with the penetration depth measured by \( \mu \)SR, we also performed magnetization vs. field measurements at a range of temperatures below \( T_C \) on a single crystal plate. As our field in these measurements was applied using a superconducting coil, there will always be some trapped flux in the magnet, resulting in an offset from the expected field set by applying current. We corrected for this by doing a linear fit of the low-field MvH data of the ZFC field scans and subtracting the resulting field offset. This indicated a trapped flux of \( \approx 2.5 \) Oe for the \( H \parallel C \)-axis measurements, and \( \approx 7.5 \) Oe for \( H \perp C \)-axis. Blue squares are from \( \mu \)SR using a Gaussian fit.
field applied parallel to the C-axis, and $D_\perp = 0.1124$ for the field applied perpendicular to the C-axis, using the formula found in Ref. [32]. The internal field is then calculated as $H_{int} = H_{ext} - DM$. This gives low temperature effective ZFC internal fields of 176 G for $H \parallel$ C-axis, and 55 G for $H \perp$ C-axis which indicate that either 98% or 84% of the volume is superconducting. The discrepancy between these two numbers may indicate some inaccuracy in our estimation of the demagnetization factors, but this uncertainty does not substantially affect the conclusions we have reached.

\[ -4\pi M = \frac{\alpha \phi_0}{8\pi \lambda^2} \ln \left( \frac{\beta H_{c2}}{H} \right). \]  
(4)

Here, $M$ is the magnetization in G, $\phi_0$ is the flux quantum, $\lambda$ is the effective zero field penetration depth, $\alpha$ and $\beta$ are constants which depend on the field range being fit. We therefore plotted $M$ vs. $\ln(H)$, and fit the resulting linear regime to determine $\lambda$ from the slope ($s$) as,

\[ \lambda = \sqrt{\frac{\alpha \phi_0}{8\pi s}}. \]  
(5)

We used an $\alpha$ value of 0.7 in the following analysis, appropriate to higher field ranges [33]. However, it is important to note that changing this value will only result in a rescaling of the penetration depth; it will not affect the temperature dependence. Examples of these linear fits are shown in Fig. 6 (c) and (d). The resulting penetration depths are plotted alongside that measured by $\mu$SR in Fig. 4 (green circles and red triangles).

This analysis gives low-temperature penetration depths of $\lambda_{\parallel}(0) = 91$ nm and $\lambda_{\perp}(0) = 125$ nm, which shows that the anisotropy in this material is not large. The low temperature penetration depth measured by $\mu$SR (120 nm) falls between these two values, which is expected as the polycrystalline $\mu$SR sample should result in an averaging of the two penetration depths. The $\mu$SR value is closer to the $\lambda_{\perp}$ value, which may indicate some preferential orientation of the polycrystalline sample. However, as the $\mu$SR data is measured at

![Magnetization measurements on a single crystal sample of Ir$_{0.95}$Pt$_{0.05}$Te$_2$ in a field of 50 Oe applied (a) perpendicular to the C-axis and (b) parallel to the C-axis. Closed circles show measurements after cooling in zero applied field and open circles show measurements after cooling with the field applied.](image)

![Magnetization vs. internal field curves measured at 0.5 K (black squares) and 2 K (red circles) for (a) $H \parallel$ C-axis and (b) $H \perp$ C-axis. (c-d) Magnetization vs. $\ln(H)$ curves along with linear fits to the high-field region (solid lines) measured at 0.5 K (black squares) and 2 K (red circles) for (c) $H \parallel$ C-axis and (b) $H \perp$ C-axis.](image)

The magnetization of a type II superconductor in the reversible regime near $H_{c2}$ can be approximated using the London model as [33].
dependence of our data is consistent with Ir
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7. These data all show good agreement with the fits, therefore
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the critical temperature.

From the penetration depth, we determined the normalized
superfluid density, \( n_s \), in each case as,

\[
\frac{n_s(T)}{n_s(0)} = \frac{\lambda^2(0)}{\lambda^2(T)}. \tag{6}
\]

The resultant superfluid densities are plotted in Fig. 7. This
figure allows us to look at the temperature dependencies of
the superfluid density in each case without the confounding
possible normalization issues discussed above. The inset in
Fig. 7 shows these superfluid densities plotted vs. normalized
temperature (\( T/T_c \)) and shows that the temperature dependence
of the superfluid density measured by the two methods is essen-
tially the same aside from the shift in \( T_c \). Estimating \( H_{c2} \)
from our MvH scans gives approximate values of 300 G for
\( H \perp \) C-axis and 225 G for \( H \parallel \) C-axis at \( T = 2.3 \) K, the \( T_c \)
measured from \( \mu \)SR at 300 G. From these values we would expect
a somewhat lower \( T_c \) at 300 G (closer to 2.1 K), but the discrepancy is not large. The likely explanation is that
there is some variation between individual crystal grains, and
that the one we used for the single-crystal measurements has a
slightly lower \( T_c \) compared to the polycrystalline aggregate
used for the \( \mu \)SR measurements.

To determine whether our data matches what would be ex-
pected of a fully gapped superconductor, we fit these super-
fluid densities to the formula [35],

\[
n_s(T) = C \left[ 1 - 2 \int_{\Delta}^{\infty} dE \frac{\partial F}{\partial E} \frac{E}{\sqrt{E^2 - \Delta^2}} \right]. \tag{7}
\]

Here, \( C \) is a scaling constant, \( E \) is the energy difference
above the Fermi energy, \( F = \frac{1}{2\pi^2 n_B} \frac{1}{\sqrt{1 + \frac{E}{T_c}}} \) is the Fermi function,
\( k_B \) is the Boltzmann constant, and \( \Delta \) is the gap, which we
approximate using the interpolation formula [35],

\[
\Delta(T) = \Delta_0 \tanh \left( 1.742 \sqrt{T_c \frac{T}{T_c} - 1} \right). \tag{8}
\]

Here, \( \Delta_0 \) is the zero temperature value of the gap, and \( T_c \) is
the critical temperature.

The results of these fits are shown as the solid lines in Fig.
7. These data all show good agreement with the fits, therefore
our data is consistent with Ir\(_{0.95}\)Pt\(_{0.05}\)Te\(_2\) being a fully gapped
superconductor. In particular, the data show a flat temperature
dependence of \( n_s \) at low temperatures, which suggests that
there are no nodes in the gap and hence the majority of the
carriers are fully gapped. We find no evidence in these fits
for unconventional superconductivity, however there are some
exotic states such as p-wave \( k_x \pm ik_y \), that are fully gapped and
would be indistinguishable from s-wave in our measurements
[36].

Furthermore, we can compare the fit values for \( T_c \) and \( \Delta_0 \)
showed in Table I to the expected constant \( \frac{2\Delta_0}{k_B T_c} = 3.5 \) for a
BCS weak coupling superconductor. The data show a range
between 3.57 and 3.9 for this ratio, which is close to the ex-
pected ratio. Our data are consistent with STM measurements
on Ir\(_{0.95}\)Pd\(_{0.05}\)Te\(_2\) that found a value of \( \frac{2\Delta_0}{k_B T_c} = 3.6\) [25]. This
indicates that differently doped (Pd vs. Pt) IrTe\(_2\) display sim-
ilar superconducting properties.

| \(\mu\)SR     | \(\Delta_0\) (meV) | \(T_c\) (K) | \(\frac{2\Delta_0}{k_B T_c}\) |
|-------------|------------------|------------|-----------------------------|
| SQUID Perpendicular | 0.351           | 2.28       | 3.57                        |
| SQUID Parallel     | 0.463           | 2.84       | 3.90                        |
|                 | 0.463           | 2.92       | 3.68                        |

TABLE I. Parameters used for the superfluid density fits to Eq. [7]
shown in Fig. 7.

FIG. 7. Normalized superfluid density determined from magnetiza-
tion measurements and \( \mu \)SR measurements. Red triangles are from
magnetometry with \( H \perp \) C-axis. Green circles are from magne-
tometry with \( H \parallel \) C-axis. Blue squares are from the \( \mu \)SR data. Solid
lines show BCS fits to the data using Eq. [7].

CONCLUSION

We have presented penetration depth and superfluid density
data of Ir\(_{0.95}\)Pt\(_{0.05}\)Te\(_2\) determined from SQUID magnetome-
try and \( \mu \)SR. These data are consistent with conventional BCS
weak coupling s-wave superconductivity in Ir\(_{0.95}\)Pt\(_{0.05}\)Te\(_2\), with a zero temperature gap of \( \Delta_0 = 0.46 \) meV in zero field.
The gap decreases to 0.35 meV at $H_{ext} = 300$ G as expected from the corresponding drop in $T_C$ over the same field range. We see no evidence for nodes in the gap which suggests that d-wave pairing symmetry does not appear in this material. However, we are unable to distinguish p-wave and s-wave pairing as some p-wave states may be fully gapped.

Finally, our work shows that the temperature dependence of the penetration depths measured by two very different techniques ($\mu$SR and magnetometry) are consistent with one another. This strengthens the conclusions we can draw from one technique alone, and is to our knowledge the first quantitative comparison of the results of the two techniques on the same material.

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