Superconducting properties of pseudobinary telluride Chevrel phase \( \text{Mo}_4\text{Re}_2\text{Te}_8 \)

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Received 6 June 2022, revised 29 August 2022
Accepted for publication 1 September 2022
Published 7 October 2022

Abstract

Unconventional superconductivity in the Chevrel phase (CP) offers a wide structural aspect to understand the superconducting ground state. A detailed investigation of the superconducting properties of Re-based pseudobinary telluride CP \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) is reported. It crystallizes in a trigonal structure, with the space group \( R\bar{3}H \) having a superconducting transition temperature at \( T_C = 3.26(3) \text{ K} \) with a fully gapped superconducting state in the moderate electron–phonon coupling limit.

Keywords: Chevrel phase, superconductivity, pseudobinary telluride

(Some figures may appear in colour only in the online journal)

1. Introduction

Unconventional superconductors are an integral part of the new phase of quantum matter, exhibiting additional broken symmetries (e.g. time-reversal or rotational symmetry) with the global gauge symmetry, \( U(1) \). The Chevrel phase (CP) superconductor is a crucial member of the unconventional superconductor family, providing a broader aspect of interactions and structural impact on the superconducting ground state [1]. The CP has a perplexing array of unconventional superconducting properties, including an extremely high upper critical magnetic field, multicomponent and multiband superconductivity, magnetic field-driven or magnetically ordered superconductivity, reentrant superconductivity and many more [2–8]. Additionally, classical CPs exhibit various crystal structures based on the coupling manner of its building blocks (or Mo clusters) [9–12], which produces quasi-1D superconductors [13] and interesting topological properties [14].

CPs are extensively known for their relatively high value of upper critical field, and it is believed that the high spin–orbit splitting by a large Sommerfeld coefficient, \( \gamma_n \), ascribed to low-lying phonons, is responsible for it [15, 16]. The observed large superconducting gap value in CPs is also similar to the superconductivity mediated by soft phonons (low-lying phonons) with a strong electron–phonon coupling, as recently observed in IrGe [17], BaPd\(_2\)As\(_2\) [18] and SrPt\(_3\)P [19]. Furthermore, the superconducting properties of CPs depend on the intercluster Mo–Mo distance [12, 20]. The partial substitution at the Mo site can change the metallic compound \( \text{Mo}_6X_8 \) (here \( X \) is the chalcogenide) into semiconducting sulphides and selenides [21, 22] while in contrast, tellurides of this family become superconductors [20, 23, 24]. Most studies on the unconventional superconducting properties of CPs have primarily focused on rare-earth intercalated sulphides and selenides [21, 22] while in contrast, tellurides of this family become superconductors [20, 23, 24]. Most studies on the unconventional superconducting properties of CPs have primarily focused on rare-earth intercalated sulphides and selenides. However, to date, the high upper critical field and pairing mechanism in CPs are not properly understood. Along with this, the superconducting properties of CP tellurides are largely unexplored. This can provide details about the electron–electron interaction, electron–phonon coupling and spin–orbit coupling effect on the nature of superconductivity and the pairing mechanism, which can be helpful in understanding the unconventional in the superconducting state of CPs. Detailed studies of new CPs are essential for a deeper insight into the superconducting ground state and gap symmetry.
In this work, we investigate the superconducting properties of a less-explored Re-based pseudobinary telluride CP, Mo$_4$Re$_2$Te$_8$, where Re is partially substituted at the Mo site. This study comprises two different prospects; firstly, the presence of Re in the Mo cluster will increase the spin–orbit coupling strength (SOC) and affect the phononic distribution by changing the related interactions of the CP system. Secondly, this compound can address the ambiguity in Re-based superconductors regarding the possible reason for time-reversal symmetry (TRS) breaking. Compounds such as Re$_2$X ($X = Zr, Hf, Ti$), a non-centrosymmetric family, show spontaneous field presence and breaking TRS, regardless of the element X [25–27], while other non-centrosymmetric compounds, such as Re$_2$Y ($Y = Ta, W$) and the Re–B system [28–30], preserve the TRS. Furthermore, the uncertainty in TRS breaking in centrosymmetric Re is also intriguing [31, 32] and raises more questions about the role of the associated structure and Re concentration in TRS breaking. In this regard, investigating more Re-based superconductors is necessary, and the Re-based pseudobinary telluride CP Mo$_4$Re$_2$Te$_8$ provides that platform with a new structural aspect and different Re concentration. We have performed temperature-dependent measurements of AC transport, magnetization and specific heat under different magnetic fields, which allows deducing the superconducting characteristic parameters with other electronic parameters of Mo$_4$Re$_2$Te$_8$. A moderate electron–phonon coupling with s-wave gap symmetry is indicated by specific heat measurement. Moreover, the initial band structure calculations suggest the importance of SOC on the electronic states of Mo$_4$Re$_2$Te$_8$ along with the dominance of the d state of Re and Mo atoms in the density of states (DOS) at the Fermi level.

2. Experimental details

A polycrystalline sample of the nominal composition Mo$_4$Re$_2$Te$_8$ was prepared by the solid-state reaction method, where the constituent elemental powder of Mo (99.99%), Re (99.99%) and Te (99.9999%) was mixed together in a stoichiometric ratio. The palletized form of the mixture was sealed in an evacuated quartz ampoule and heated to between 1150 °C and 1200 °C for a few days. The powder x-ray diffraction (XRD) pattern was obtained using a PANalytical diffractometer equipped with Cu K$_\alpha$ radiation ($\lambda = 1.5406$ Å). Magnetic measurements were performed on a superconducting quantum interference device of magnetic property measurement system (MPMS-3, Quantum Design). Transport and specific heat measurements were carried out using a physical property measurement system (PPMS, Quantum Design). The four-probe technique was used to measure the AC transport, and the two-$\tau$ relaxation method was used for specific heat measurement.

3. Results and discussion

3.1. Sample characterization

The recorded XRD pattern for Mo$_4$Re$_2$Te$_8$ was refined using Fullprof software [33]. Rietveld refinement confirms Mo$_4$Re$_2$Te$_8$ crystallization in the trigonal structure having a space group $R\bar{3}H$, and figure 1 shows the refined pattern with the goodness of fit value equal to 4.2. The additional peaks in the XRD pattern with smaller intensities belong to elemental Mo and Re, marked respectively with a hash and an asterisk (figure 1), and have only a small fraction in the majority phase $R\bar{3}H$. However, no impact of the unreacted Mo and Re is observed in the superconducting properties of Mo$_4$Re$_2$Te$_8$. The refined lattice parameters of Mo$_4$Re$_2$Te$_8$ are tabulated together with the parent compound Mo$_6$Te$_8$ in table 1. The Mo$_6$–$_x$Re$_x$Te$_8$ ($x = 2$) cluster, the building block of the crystal structure, is displayed in the inset of figure 1.

3.2. Superconducting and normal state properties

3.2.1. Electrical resistivity. The temperature dependence of resistivity, $\rho(T)$, for Mo$_4$Re$_2$Te$_8$ under a zero magnetic field is shown in figure 2(a). The onset of the sharp drop in resistivity is recorded at a temperature, $T_{C, \text{onset}} = 3.54(2)$ K, with a transition width of $\Delta T = 0.3$ K (figure 2(b)). The observed $T_C$ $\propto$ $\rho(T)$ dominates with the reported value [23, 24]. The increasing behavior of low temperature (normal -state) $\rho(T)$ demonstrates the metallic nature of Mo$_4$Re$_2$Te$_8$. Hence, the $\rho(T)$ temperature dependence is analyzed using the equation:

\[
\rho(T) = \rho(0) + C(1 - T/T_C)^{\beta}.
\]
The magnetization moment under temperature variation of Mo$_4$Re$_2$Te$_8$ was measured at 1 mT in both zero-field-cooled warming (ZFCW) and field-cooled cooling (FCC) mode, as shown in figure 3(a). The onset of the diamagnetic signal of the compound is noted at $T_{C,\text{onset}} = 3.26(3)$ K, where the deviation of the FCC curve from the ZFCW depicts the flux pinning in the sample. The inset of figure 3(a) shows the magnetization loop under a magnetic field variation of $\pm 4$ T at 1.8 K for Mo$_4$Re$_2$Te$_8$. The full magnetization loop confirms the type-II superconductivity with bulk pinning in the sample, and represents an irreversible nature of magnetization, $H_{irr} = 1.54$ T, where further increase in the applied magnetic field de-pins the vortices.

The lower critical field value, $H_{C1}(0)$, is extracted from the magnetization dependence on the magnetic field measured at different temperatures up to $T_C$, as shown in the inset of figure 3(b). The linear deviation from the Meissner effect (entering the vortex region) is considered as the $H_{C1}$ for the respective isotherm. The temperature dependence of $H_{C1}$ for Mo$_4$Re$_2$Te$_8$ is shown in figure 3(b) and fitted using the Ginzburg–Landau (GL) equation, given as

$$H_{C1}(T) = H_{C1}(0) \left[ 1 - \left( \frac{T}{T_C} \right)^2 \right].$$ \hspace{1cm} (2)

The estimated value of $H_{C1}(0)$ from the fitting is 0.49(1) mT. Furthermore, the value of the upper critical field, $H_{C2}(0)$, is computed via variation of the transition temperature under applied magnetic fields. The applied increasing magnetic field shifts the superconducting transition temperature to a lower value as observed in the resistivity, magnetization and specific heat measurements. The inset of figure 3(c) represents the same via the resistivity measurement, where $T_C$ is recorded at the 90% drop in normal-state resistivity value. The variation of the upper critical field value, $H_{C2}$, with the reduced temperature, $t = T/T_C$, is fitted with the Ginzburg–Landau equation,

$$H_{C2}(t) = H_{C2}(0) \left[ \frac{(1 - t^2)}{(1 + t^2)} \right].$$ \hspace{1cm} (3)

The well-fitted data are shown in figure 3(c), providing an upper critical field of $H_{C2}(0) = 5.08(7)$ T, $5.62(6)$ T and $5.78(4)$ T from the magnetization, specific heat and resistivity data, respectively.

The effect of an applied external magnetic field in superconductors is described by two mechanisms: (a) orbital decoupling and (b) the Pauli limiting effect. The orbital limiting field is where the increased kinetic energy of one electron breaks the Cooper pair, given by the Wartherm–Helfand–Hohenberg expression [44, 45],

$$H_{C2}^{\text{orbital}}(0) = -\alpha T_C \left. \frac{dH_{C2}(T)}{dT} \right|_{T=T_C}$$ \hspace{1cm} (4)

Here, $\alpha$ is considered to be 0.69 for the dirty limit superconductor. The initial slope $-\frac{dH_{C2}(T)}{dT}$ in the vicinity of $T_C$ is 1.58(1) T for Mo$_4$Re$_2$Te$_8$, which evaluates the orbital limiting field, $H_{C2}^{\text{orbital}}(0) = 3.55(4)$ T. From the Bardeen–Cooper–Schrieffer (BCS) theory of superconductors, another effect Pauli limiting field is represented as $H_{C2}^{\text{Pauli}}(0) = 1.86 T_C$ [46, 47], with $T_C = 3.26(3)$ K, and $H_{C2}^{\text{Pauli}}(0)$ becomes 6.00(5) T. Moreover, the relative strength of the two magnetic effects, the orbital and Pauli limiting field, is measured by the Maki parameter [48], $\alpha_M = \sqrt{2}H_{C2}^{\text{Pauli}}(0)/H_{C2}^{\text{orbital}}(0) = 0.84(2)$.
The close value of \( \alpha_M \) to one demonstrates the non-negligible effect of the Pauli limiting field in the Cooper pair breaking. Along with this, the proximity of the upper critical field value \( (H_{C2,p}(0) = 5.78(4) \text{ T}) \) to the Pauli limiting field is also compelling and similar to other Re-based superconductors, which shows unconventional superconductivity [25, 49, 50].

The superconducting characteristic length parameters were calculated from the upper and lower critical field values. The relation between \( H_{C2}(0) \) and the Ginzburg–Landau coherence length, \( \xi_{GL}(0) \) [51], \( H_{C2}(0) = \frac{\Phi_0}{\pi \xi_{GL}(0)^2} \), where \( \Phi_0 = 2.07 \times 10^{-15} \text{ Tm}^2 \) is the quantum flux, gives \( \xi_{GL}(0) = 80(1) \text{ Å} \). The lower critical field, \( H_{C1}(0) \), and coherence length, \( \xi_{GL}(0) \), are related to the penetration depth, \( \lambda_{GL}(0) \), as follows [52]:

\[
H_{C1}(0) = \frac{\Phi_0}{4\pi \lambda_{GL}(0)} \left( \ln \frac{\lambda_{GL}(0)}{\xi_{GL}(0)} + 0.12 \right) \tag{5}
\]

providing \( \lambda_{GL}(0) = 1325(40) \text{ nm} \). Moreover, the value of the Ginzburg–Landau parameter, \( \kappa_{GL} = \frac{\lambda_{GL}(0)}{\xi_{GL}(0)} \), is calculated to be 165(7), indicating a strong type-II superconductivity in Mo\(_4\)Re\(_2\)Te\(_8\), consistent with the previously studied CPs. The thermodynamic critical field is also evaluated using the relation \( H_c = \sqrt{\frac{H_{C2}(0)H_{C1}(0)}{\ln(\frac{H_{C2}(0)}{H_{C1}(0)})}} [52] \) and obtains the value \( H_c = 22(1) \text{ mT} \) for Mo\(_4\)Re\(_2\)Te\(_8\).

### 3.2.3. Specific heat.

The bulk superconductivity is further probed by specific heat versus temperature measurement at zero applied magnetic field for Mo\(_4\)Re\(_2\)Te\(_8\). Figure 4(a) shows the jump in specific heat data at \( T_{C,mid} = 3.23(6) \text{ K} \) estimated from the midpoint. Above \( T_c \), the normal-state region of specific heat is fitted using the Debye relation, \( C/T = \gamma_n + \beta_3 T^3 \), where \( \gamma_n \) is the Sommerfeld coefficient and \( \beta_3 \) is the lattice constant. Fitting of the data provides the parameters as \( \gamma_n = 24.7(8) \text{ mJ mol}^{-1} \text{ K}^{-2} \) and \( \beta_3 = 5.95(4) \text{ mJ mol}^{-1} \text{ K}^{-4} \). Furthermore, the change in superconducting transition temperature with the applied magnetic field is shown in figure 4(b).

The specific heat measurement also allows us to calculate several other parameters. The lattice constant parameter, \( \beta_3 \), is used to extract information about the phonons and provides the Debye temperature, \( \theta_D \). Using the relation \( \theta_D = \left( \frac{12\pi^4 R N}{5\beta_3} \right)^{1/3} \), where \( R \) is the universal gas constant and \( N = 14 \) the number of atoms per formula unit, the estimated value of \( \theta_D \) is 166(1) K. The obtained value of \( \theta_D \) from the specific heat measurement matches the value from the resistivity measurement. The Sommerfeld coefficient, \( \gamma_n \), is related to the single-particle DOS at the Fermi level by the expression \( \gamma_n = \left( \frac{2\pi^2}{3} \right) D(E_F) \), and the operation yields \( D(E_F) = 10.5(3) \text{ states eV}^{-1} \text{ f.u.}^{-1} \). The information on the electron–phonon coupling strength can also be extracted from McMillian theory, where the dimensionless quantity \( \lambda_{e-ph} \) is stated by the relation [53].
\[
\lambda_{\text{e-ph}} = \frac{1.04 + \mu^* \ln(\theta_0/1.45TC)}{(1 - 0.62\mu^*)\ln(\theta_0/1.45TC)} - 1.04
\] (6)

Here, \(\mu^*\) is typically assumed to be 0.13 for intermetallic superconductors. The values \(\theta_0 = 166(1)\) K and \(T_C = 3.23(6)\) K, provide the value \(\lambda_{\text{e-ph}} = 0.67(2)\), suggesting that the telluride CP Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8} is a moderately coupled superconductor. Even though the high DOS at the Fermi level, large contribution to the lattice-specific heat, \(\beta_3\), and parameter \(\gamma_n/T_C = 7.6\) mJ mol\(^{-1}\) K\(^{-3}\) of Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8} are comparable to SnMo\textsubscript{4}S\textsubscript{8}, PbMo\textsubscript{4}S\textsubscript{8}, and Ag\textsubscript{1-}\textsubscript{j}Mo\textsubscript{j}S\textsubscript{8}, possessing a strong electron–phonon coupling, Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8} has moderate coupling. The ratio \(\gamma_n/T_C\) indicates the scale of the transition temperature with the DOS at \(E_F\) [3, 4].

The symmetry associated with the superconducting gap can be understood by analyzing the electronic specific heat temperature dependence in the superconducting region. The electronic contribution to the specific heat is calculated by subtracting the phononic contribution from the total specific heat at zero field. Theoretically, it can be computed from \(C_s = \gamma_n \omega_0^2 T / \pi^2\), with \(S\) being the entropy in the superconducting region and within the BCS approximation has the form

\[
S = -\frac{6\gamma_n}{\pi^2} \left( \frac{\Delta(0)}{\omega_0} \right) \int_0^\infty \left[ f(\xi) + (1 - f) \ln(1 - f) \right] dy \] (7)

where \(f(\xi) = \exp(E(\xi))/k_BT + 1\)\(^{-1}\) is the Fermi function. \(E(\xi) = \sqrt{\xi^2 + \Delta(\xi)^2}\) is the excitation energy of the quasi-particle measured relative to the Fermi level, with \(\gamma = \xi/\Delta(0)\) and \(\Delta(\xi)\) being the temperature-dependent gap function. In the isotropic s-wave BCS approximation, the gap function can be written as \(\Delta(\xi) = \text{tanh}(\sqrt{1.82(1.018)/(1/\xi) - 1})^{0.51}\) with \(t = T/T_C\). Figure 4(c) displays the variation of electronic specific heat, \(C_s\), with temperature, fitted with the BCS s-wave model. The well-fitted data in the superconducting region yield \(\Delta(0)/k_BT_C = 1.81(4)\), while the specific heat jump value \(\Delta C/\gamma_n T_C = 1.44(8)\). Both of these values, \(\Delta(0)/k_BT_C\) and \(\Delta C/\gamma_n T_C\), are close to the BCS predicted values (1.76 and 1.43) in the weak coupling limit. Hence, this indicates that Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8} is a weakly coupled superconductor. However, to understand the exact structure of the superconducting gap and the nature of the pairing state, low-temperature specific heat below 1.9 K is required.

3.2.4. Electronic properties and the Uemura plot. To gain an insight into the electronic properties, we have performed band structure calculations using the full potential linear augmented plane wave method as implemented in Wien2k [54, 55]. We used a \(k\)-point mesh of \(10\times10\times10\) within the first Brillouin zone, and the generalized gradient approximation exchange-correlation functional of Perdew, Burke, and Ernzerhof [56]. SOC was included for all the elements in the calculations. The energy and charge convergence criteria were set to 0.01 meV and \(10^{-5}\) electronic charge per f.u., respectively. The Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8} structure was simulated by substituting Re in the place of two Mo atoms in Mo\textsubscript{5}Te\textsubscript{8}. The electronic band structure between the high-symmetry points [57] in the Brillouin zone and the DOS of Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8} is shown in figure 5. The inclusion of SOC for Re significantly modifies the band dispersion, while SOC in Mo and Te does not have much influence, indicating that the high SOC of Re plays an important role in Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8}. Two doubly degenerate bands, \(B_1\) and \(B_2\), shown in red and blue color respectively, are dispersing in a large energy window in the vicinity of the Fermi level (\(E_F\)) and cross \(E_F\) at different \(k\) points of the Brillouin zone. The Fermi level lies almost in the middle of band \(B_1\), while band \(B_2\) remains almost empty. The system is close to cubic (rhombohedral angle \(= 92.12\)\(^\circ\)), and the high-symmetry points \(P, Z, Q, P_l\) and \(Q_l\) are almost equivalent where a small electron pocket (band \(B_2\)) is seen in the band structure. At the same time, a large hole pocket is centered around the \(\Gamma\) point (band \(B_1\)), as also observed from the Hall measurement, suggesting dominant hole carriers.

Strong hybridization between the Mo/Re \(d\) states and Te \(p\) states is observed in the DOS plot (figure 5). The calculated value of total DOS at \(E_F\) is 9.87 states eV\(^{-1}\) f.u.\(^{-1}\), in qualitative agreement with the values obtained from the specific heat experiment.

Furthermore, in order to quantify the London penetration depth, \(\lambda_L\), electronic mean free path, \(l_e\), and to verify the dirty-limit superconductivity for Mo\textsubscript{4}Re\textsubscript{2}Te\textsubscript{8}, a set of equations are implemented. The Fermi vector, \(k_F\), is estimated from the quasiparticle number density by the relation, \(k_F = (3\pi^2n)^{1/3}\); here, \(n = 1.21(3) \times 10^{28} m^{-3}\) from the normal Hall measurement, hence \(k_F = 0.71(2) \) \(\AA^{-1}\). The Sommerfeld coefficient, \(\gamma_n\), and \(k_F\) are used for effective mass value estimation by the relation \(m^* = (h k_F)^2/\pi^2 n k_F^2\), with \(k_F\) being the Boltzmann constant, and \(m^*\) becomes 3.2(3) \(m_e.\) Moreover, in consideration of Drude’s model, the mean free path is defined as \(l_e = \nu_F \tau\), where \(\tau\) is the scattering time given by \(\tau^{-1} = n e^2 \rho_0/m^* \nu_F\). \(\nu_F\) is the Fermi velocity, stated as \(\nu_F = h k_F/m^*\). Including the respective values of \(m^*\), \(k_F\), \(n\), and residual resistivity, \(\rho_0 = 2.95(1) m\Omega cm\), the scattering time \(\tau\) and the Fermi velocity \(\nu_F\) are evaluated, which provides the mean free path, \(l_e = 0.81(9) \) \(\AA\). From BCS theory [51], the coherence length \(\xi_0\) is approximated as \(0.18 h\nu_F/k_BT_C\), hence becoming 1074(202) \(\AA\).
for \( T_C = 3.26 \text{ K} \). The huge difference between the coherence length and mean free path \( \xi_0 > l_c \) puts \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) in the dirty-limit superconductor. Furthermore, the London penetration depth \( \lambda_L \) is expressed as \( \lambda_L = \left( \frac{m^*}{\mu_0 ne^2} \right)^{1/2} \) and calculated to be 86(1) nm. The characteristic nature of poor metal with the short mean free path of the known CPs is also observed in our telluride CP compound \( \text{Mo}_4\text{Re}_2\text{Te}_8 \).

The CP has been classified as an unconventional superconductor based on their \( \frac{T_C}{T_F} \) ratio provided by Uemura et al [1]. The ratio for the CP lies in the range 0.01 \( \leq \frac{T_C}{T_F} \leq 0.1 \) with high-\( T_F \), organic, heavy-fermion, and other unconventional superconductors. For a 3D system, assuming a spherical Fermi surface, the Fermi temperature, \( T_F \), is given by the relation [58]

\[
k_B T_F = \frac{\hbar^2}{2 (3\pi^2)^2/3 n^{2/3} m^*},
\]

where \( n \) is the quasiparticle number density per unit volume and \( m^* \) is the effective mass of the quasiparticles. Considering the values of \( n \) and \( m^* \) as listed in table 2, from equation (8), we get \( T_F = 6980(845) \text{ K} \) for \( \text{Mo}_4\text{Re}_2\text{Te}_8 \). The ratio \( \frac{T_C}{T_F} = 0.0005 \) places \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) in the region of Re-based compounds, having \( \text{Re}_2\text{Te}_5 \) [59] on its left side and other compounds having same composition on its right side [25, 26, 31, 49], with the elemental Re [31], as shown in figure 6.

Irrespective of the short mean free path, large contribution of lattice-specific heat, high DOS at the Fermi level, and moderate electron–phonon coupling in the pseudobinary compound \( \text{Mo}_4\text{Re}_2\text{Te}_8 \), the exotic character of the extremely high upper critical field value of CPs is absent. As -above-mentioned parameters but with the strong electron–phonon coupling are accounted to be the possible reason for high upper critical field value in well-known CPs [15, 16]. Hence, strong electron–phonon coupling might be a possible requirement to enhance the upper critical field beyond a limit in CPs. However, the comparable value of the upper critical field to the Pauli paramagnetic limit suggests a possible unconventional nature of its superconducting ground state as observed in many Re-based superconductors [25, 49]. Notably, such a large value of the upper critical field has not been observed in any other Te superconductors, with the exception of the iron-based chalcogenide superconductors [62]. Moreover, the Uemura classification of \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) places it in an interesting position between the two different Re concentration systems. In addition, a recent first-principles study of CP \( \text{PbMo}_5\text{S}_6 \) questions its position in the Uemura plot and suggests the phonon-driven superconductivity with a significant contribution of strong Coulombic repulsion in the compound [63]. Hence, to assure the unconventional nature and superconducting gap symmetry of \( \text{Mo}_4\text{Re}_2\text{Te}_8 \), further microscopic investigations are required.

### Table 2. Parameters in the superconducting and normal state of \( \text{Mo}_4\text{Re}_2\text{Te}_8 \)

| Parameters | Unit | \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) |
|------------|------|-------------------------------|
| \( T_C \) | K    | 3.26(3)                       |
| \( H_C^* \) | mT   | 0.49(1)                       |
| \( H_C^0 \) | T    | 5.78(4)                       |
| \( H_C^* \) | T    | 6.00(5)                       |
| \( H_C^0 \) | T    | 3.55(4)                       |
| \( \xi_0 \) | Å    | 80(1)                         |
| \( \lambda_L \) | nm   | 1325(40)                      |
| \( k_T \) | 165(7)                      |
| \( \gamma_n \) | mJ mol\(^{-1}\) K\(^{-2}\) | 24.7(8)                       |
| \( \theta_D \) | K    | 166(1)                        |
| \( \Delta_C/\gamma_n T_C \) | 1.44(8) |
| \( \Delta(0)/k_B T_C \) | 1.81(4) |
| \( v_F \) | \( 10^4 \text{ m s}^{-1} \) | 2.6(2)                        |
| \( n \) | \( 10^{23} \text{ m}^{-3} \) | 1.21(3)                       |
| \( T_F \) | K    | 6980(845)                      |
| \( T_C/T_F \) | 0.0005(1) |
| \( m^*/m_e \) | 3.2(3) |

**Figure 6.** A plot between \( T_C \) and \( T_F \) representing the unconventional superconductor family. \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) is shown, which is close to the conventional superconductor band region regardless of the other CP, which lies in the unconventional band [60, 61].

### 4. Conclusion

To summarize, Re-based pseudobinary telluride CP \( \text{Mo}_4\text{Re}_2\text{Te}_8 \) is investigated, and a superconducting transition at \( T_C = 3.26(3) \text{ K} \) is recorded. XRD analysis confirms the phase purity and trigonal structure crystallization. The AC resistivity shows the poor metallic character of the sample with a short mean free path. The magnetization measurements suggest type-II superconductivity with an upper critical field of \( H_C^* = 5.78(4) \text{ T} \), close to the Pauli limiting field. The specific heat data measured in zero applied magnetic field present a jump value of \( \Delta C/\gamma_n T_C = 1.44(8) \) with fully gapped superconductivity in \( \text{Mo}_4\text{Re}_2\text{Te}_8 \). Initial band structure calculations also depict a significant contribution of Re in the DOS at the Fermi level, with a notable spin–orbit coupling impact of Re on the band dispersion. A detailed microscopic study (e.g. muon spectroscopy) combined with detailed theoretical calculations of the electronic structure is required to...
understand the superconducting ground state, possible pairing mechanism and the role of Re on the superconducting properties of this compound.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgments

A K acknowledges the funding agency Council of Scientific and Industrial Research (CSIR), Government of India, for providing an SRF fellowship (Award No. 09/1020 (0172)/2019-EMR-I). R P S acknowledges the Science and Engineering Research Board, Government of India, for the Core Research Grant CRG/2019/001028.

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