Clean-limit superconductivity in $\text{Im}3m$ $\text{H}_3\text{S}$ synthesized from sulfur and hydrogen donor ammonia borane

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We present detailed studies of the superconductivity in high-pressure $\text{H}_3\text{S}$. X-ray diffraction measurements show that cubic $\text{Im}3m$ $\text{H}_3\text{S}$ was synthesized from elemental sulfur and hydrogen donor ammonia borane ($\text{NH}_3\text{BH}_3$). Our electrical transport measurements confirm superconductivity with a transition temperature $T_c \approx 197 \text{ K}$ at 153 GPa. From the analysis of both the normal state resistance and the slope of the critical field, we conclude that the superconductivity is described by clean-limit behaviour. A significant broadening of the resistive transition in finite magnetic field is found, as expected for superconductors. We identify a linear temperature-over-field scaling of the resistance at the superconducting transition which is not described by existing theories.

The discovery of superconductivity in $\text{H}_3\text{S}$ at a critical temperature of $T_c \sim 200 \text{ K}$ revolutionized the search for high-temperature superconductivity [1]. Since then, high-temperature superconductivity has been observed in a number of binary hydrides at high pressures including LaH$_{10}$, CeH$_9$, and YH$_3$ and in carbonaceous sulfur hydride [1–6]. Extreme pressures of typically more than 100 GPa are required for the synthesis and study of these hydride compounds. The high hydrogen stoichiometries yield the high density of electronic states, high-frequency phonon modes, and strong electron-phonon coupling necessary for a high-$T_c$ in phonon mediated superconductivity [5–9]. Both synthesis and experimental studies of high-temperature hydride superconductors remain very challenging due to the high pressures needed.

Synthesis of hydride superconductors is typically done by laser heating precursors in situ at high pressures. Only in the initial work by Drozdov et al. was superconducting $\text{H}_3\text{S}$ synthesized from the dissociation of molecular $\text{H}_2\text{S}$ at high pressures [1, 10–12]. All recent studies synthesized $\text{H}_3\text{S}$ from elemental sulfur and either molecular hydrogen or a hydrogen donor material as precursors using laser heating [3, 13–19]. Whilst molecular hydrogen affords the cleanest synthesis route, loading hydrogen into a diamond anvil cell (DAC) is technically much more demanding. Thus, it is not easily adapted for wide-spread and detailed studies of superconductivity in hydrides by the global physics community. Hence, it is important to establish synthesis routes using hydrogen donor materials like ammonia borane. For some hydrides this can be further simplified with evaporated samples of starting elements such as yttrium or lanthanum [17, 20].

Detailed understanding of the superconductivity in hydride compounds requires structural information, e.g. from x-ray diffraction (XRD) to complement information about the superconducting properties – ideally on the same sample. Transition temperatures up to 203 K have been linked to the cubic $\text{Im}3m$ phase of $\text{H}_3\text{S}$ at a pressure of 155 GPa [1, 21]. At pressures below $\approx$ 140 GPa a rhombohedral distortion leads to a lower symmetry $R3m$ phase with a reduced $T_c$ [22]. Other phases have been reported but have not been probed for superconductivity [10, 11, 14, 15, 19].

Superconductivity in $\text{H}_3\text{S}$ has been confirmed with multiple probes despite the limitations and challenges of measurements in DACs. The most common evidence stems from the observation of zero resistance for various samples by the group of Eremets and the suppression of the resistive transition in magnetic field [1, 13, 21]. In addition, a suppression of $T_c$ has been observed for samples with deuterium substitution [1, 21] roughly in agreement with the expected isotope effect predicted by computational studies [7, 23]. A diamagnetic signal has been observed in DC magnetisation measurements [1, 18], nuclear resonant scattering [24], and in AC susceptibility by [12]. Recently, Minkov et al. have presented detailed magnetisation studies of $\text{H}_3\text{S}$ synthesized from sulfur and ammonia borane from which they extract the lower critical field and London penetration depth [18]. Here, we present electrical resistance measurements demonstrating superconductivity in $\text{H}_3\text{S}$ synthesized with this novel route using ammonia borane and sulfur.

Our successful synthesis of $\text{Im}3m$ $\text{H}_3\text{S}$ is evident from the XRD data collected on our sample at 153 GPa as presented in Figure 1. After loading sulfur and ammonia borane, we applied 153 GPa and subsequently laser heated the sample in a small area (cf. section I of the supplementary information for synthesis details [25, 26]). In the laser-heated area, we clearly observe an XRD pattern in excellent agreement with $\text{Im}3m$ $\text{H}_3\text{S}$ as demonstrated in Figure 1 (a). (see section II of the supplementary information [25] and references therein [27, 28] for details of the XRD measurements) In particular, we observe no splitting of the (110) Bragg peak at $2\theta = 7.6^\circ$ and hence conclude that a rhombohedral distortion is absent in our sample. This is in agreement with the stability range of...
FIG. 1. Powder x-ray diffraction showing $Im\bar{3}m \text{H}_3\text{S}$. Powder patterns taken with a 30 s acquisition time and corrected for diffuse scattering. Panels (a) and (b) show the integrated patterns at locations where $Im\bar{3}m \text{H}_3\text{S}$ and elemental sulfur (S-V) are respectively present. Vertical ticks indicate expected peak positions for the different phases (gray corresponds to cubic boron nitride). (c) Spatial mapping of Bragg reflections associated with S-V and $Im\bar{3}m \text{H}_3\text{S}$ phases. Contacts visible in gray, with the S-V and H$_3$S regions shown in blue and red respectively. (d) and (e) Unfurled area detector images of powder patterns presented in (a) and (b). Diffuse background correction details are discussed in section SII of the supplementary materials[25]. (f). Photo of the sample. Labels mark the electrical contacts, while the blue and red lines demarcate the sulfur and H$_3$S respectively.

the $Im\bar{3}m$ phase above 140 GPa established from previous XRD measurements [10]. The $Im\bar{3}m$ phase in our sample consists of larger crystallites compared to the elemental sulfur as evident from the spots in the detector images Figure 1 (d) and (e). Yet, a preferred orientation appears to be absent as indicated by the good agreement with the Rietveld refinement of the XRD pattern in Figure 1 (a). For the $Im\bar{3}m \text{H}_3\text{S}$ phase, we find a unit cell volume of 29.5(1) $\text{Å}^3$ in good agreement with previous calculations (29.2 $\text{Å}^3$)[29] and with earlier XRD studies at similar pressures (29.8 $\text{Å}^3$) where H$_3$S is synthesized using elemental precursors [10, 22]. Outside the laser-heated area, we find XRD patterns in excellent agreement with elemental sulfur (S-V) in its rhombohedral $\beta$-Po structure (cf. Figure 1 (b)).

Both the XRD mapping and optical image (Figure 1 (c) and (f)) of our sample demonstrate that $Im\bar{3}m \text{H}_3\text{S}$ has formed in an area of $\approx 15 \text{µm} \times 15 \text{µm}$. In the optical image, this region is darker than the grainy, metallic elemental sulfur surrounding it and contains a reflective region in its centre. This black region likely marks boron nitride residue from the dissociation of ammonia borane, with weak Bragg reflections associated with boron nitride also visible in Figure 1 (a), whilst the central reflective area constitutes an exposed surface of $Im\bar{3}m \text{H}_3\text{S}$ with metallic reflectivity. Below, we demonstrate that $Im\bar{3}m \text{H}_3\text{S}$ in our sample displays metallic electrical resistance. The XRD mapping of the characteristic peaks (Figure 1) confirms that the entire dark region (including the reflective centre) has been transformed to $Im\bar{3}m \text{H}_3\text{S}$ whilst the remainder of the sample is pure elemental sulfur. In addition, we observe the XRD peaks of tungsten and gold from our electrodes at the outer edges of the area scanned with XRD (gray areas in Figure 1 (c)).

Formation of superconducting $Im\bar{3}m \text{H}_3\text{S}$ in our sample is evident from resistivity measurements presented in Figure 2, which show a large drop in resistance ($\approx 80 \%$) at $T_c = 197 \text{K}$ (see SI III for further details). Before laser heating, we observe the expected behaviour of elemental sulfur at high pressure: the resistance is metallic and features the superconducting transition of elemental sulfur at 17 K [30, 31]. After laser heating, the resistance shows a major drop at $T_c = 197 \text{K}$ which we associate with the formation of superconducting H$_3$S. Below $T_c$, a residual resistance of $\approx 20 \%$ remains which stems from residual elemental sulfur in the measurement path using the contacts $V_{\pm}$. With six electrodes, the voltage
drop associated with the superconducting transition can be measured in four-point configuration on both sides of the sample. Using the electrodes (labelled $V\pm$ in Figure 1 f) close to the $Im3m$ $H_3S$ part of the sample we find an 80\% drop of the resistance. By contrast, the electrodes further away (labelled $V_2\pm$) yield a drop of less than 25\%. This shows that superconducting $H_3S$ is present closer to the electrodes $V\pm$ whilst unreacted sulfur dominates the transport behaviour sensed between electrodes $V_2\pm$. Hence, we associate the resistive transition with superconductivity of the $Im3m$ phase detected close to the $V\pm$ electrodes.

The resistance contribution originating from $H_3S$ is extracted in Figure 2 (b). Here, the residual resistance from elemental sulfur is subtracted over the full temperature range. For this, we identify the parameters describing the normal state resistance of elemental sulfur from a Bloch-Grüneisen (BG) fit

\[
R(T) = R_0 + B \left( \frac{T}{\Theta_D} \right)^n \int_0^{\Theta_D/T} \frac{z^n dz}{(e^z - 1)(1 - e^{-z})} \tag{1}
\]

between $20K \leq T \leq 150K$ as shown by the dotted line in Figure 2 (a). Here, $R_0$ is the residual resistance of the normal state, $B$ quantifies the magnitude of the resistance contribution from electron-phonon scattering, and $\Theta_D$ is the Debye temperature. The exponent $n$ assumes different values depending on whether scattering is intra-band ($n = 5$) or inter-band ($n = 3$) [32]. We use parameters specific to elemental sulfur established from fits to $R(T)$ before laser heating as shown by the dotted line in Figure 2 (a). Here, $R_0$ and $B$ are fitted to the sulfur contribution in the resistance after laser heating (dashed line in Figure 2 (a)). [34] We obtain the resistance contribution ($\Delta R$) of $H_3S$ by subtracting the fit representing the residual sulfur. This corresponds to the assumption of a series-resistor network which is guaranteed below $T_c$ by the superconducting state of $H_3S$ and likely satisfied above $T_c$ given the proximity of the sensing electrodes to the $H_3S$ phase in our sample. The resulting curve for the resistance of $H_3S$ is shown in Figure 2 (b).

The normal state behaviour of $Im3m$ $H_3S$ can be well fitted by the BG form (Equation 1) as shown by the dashed line in Figure 2 (b). The limited temperature range f the normal state ($200K \leq T \leq 300K$) does not allow to determine the exponent $n$ for $H_3S$, $n = 3$ and $n = 5$ yield very similar fits to the data. We fix the exponent to the most common value $n = 5$, i.e. assuming that intra-band scattering is dominant in $Im3m$ $H_3S$ but highlighting the resulting uncertainty to other quantities. We find a Debye temperature $\Theta_D = 1260K$ ($\Theta_D = 1570K$ for $n = 3$) that is considerably larger than for elemental sulfur, reflecting the increased phonon energies stemming from lattice vibrations involving hydrogen. $\Theta_D$ is in good agreement with the characteristic phonon frequency calculated by Errea et al. [7]. We note that the Fermi-liquid (FL) quadratic temperature dependence of the resistance ($R = R_0 + AT^2$) discussed in previous work [13] is consistent with the crossover range of the BG form as shown in the inset Figure 2 (c). However, the magnitude of the temperature-dependent resistance is much more consistent with the electron-phonon scattering associated with the BG form than the electron-electron scattering associated with the FL form. Specifically, using the lateral dimensions $15\mu m \times 15\mu m$ and a plausible thickness of $2\mu m$ of the $H_3S$ phase of the sample we estimate the resistivity and the specific magnitude $B' = 7 \times 10^{-9}\Omega \mu m$ of the

\[
\frac{\Delta R(T)}{T} = B\left(\frac{T}{\Theta_D}\right)^n \int_0^{\Theta_D/T} \frac{z^n dz}{(e^z - 1)(1 - e^{-z})}
\]

Figure 2. High $T_c$ superconducting $H_3S$. (a) Electrical resistance before and after laser heating (LH) measured on two different pairs of contacts (cf. labels in Figure 1 f)). The normal resistance of elemental sulfur before laser heating (blue) has been fitted with Equation 1 (dotted line) for $20K \leq T \leq 290K$. The contribution from sulfur after laser heating has been fitted for $35K \leq T \leq 150K$ with Equation 1 (dashed line) using $\Theta_D$ and $n$ found for elemental sulfur before laser heating. (b) The contribution from $H_3S$ has been extracted by subtracting the Bloch-Grüneisen (BG) form of the residual sulfur (dashed line in (a)). Vertical arrow marks $T_c = 197K$ taken as the intersection between linear fits to the superconducting transition and to the normal state resistance. BG and Fermi-liquid (FL) fits to the normal-state resistance of $H_3S$ ($T \leq 205K$) are shown as dashed and dotted lines respectively. Inset (c) shows the resistance of $H_3S$ versus $T^2$ together with both fits.
 electron-phonon contribution as well as the specific magnitude of the FL contribution $A' = 2.4 \times 10^{-12} \text{mK}^{-2}$. Whilst the uncertainty of $A'$ and $B'$ is dominated by the uncertainty of the sample thickness $\approx 50\%$, we can compare to values for other metals. $B'$ is comparable in magnitude to values for simple monovalent metals [32] but $A'$ is at least one order of magnitude larger than for transition metals [35]. Hence, this comparison suggests that the normal-state resistance of $1 \text{m3m} \text{H}_3\text{S}$ is dominated by electron-phonon scattering.

We estimate the mean free path in our $\text{H}_3\text{S}$ sample to be $l \approx 8 \text{nm}$. For this, we use the sample dimensions of the $\text{H}_3\text{S}$ part to estimate the residual resistivity $\rho_0 \approx 8 \times 10^{-8} \text{m} \Omega$ and the Drude transport equation applied to a single-band free-electron approximation $\rho = \frac{\hbar (3\pi^2)^{1/3}}{(n^{2/3} e^2 \rho_0)}$ with the charge carrier concentration $n \approx 8.5 \times 10^{22} \text{cm}^{-3}$ determined from Hall effect measurements [13].

Further evidence for the superconducting nature of the transition at $T_c = 197 \text{K}$ stems from our measurements in magnetic fields up to 14 T. In Figure 3(a), we show that the transition is shifted to lower temperature in magnetic field. The temperature-dependence of the upper critical field, $H_{c2}(T)$, associated with superconductivity of $\text{H}_3\text{S}$ is in agreement with the behaviour reported earlier by Mozaeffari et al. (cf. Figure 3(c)) [13]. Our samples and those of Mozaeffari et al. have been synthesized with different methods, from sulfur and ammonia borane or hydrogen respectively. This is very likely to lead to different concentrations of impurities as indicated by the difference of resistance ratios at room temperature and low temperature estimated for the normal-state $\text{RRR} = \frac{R(300 \text{K})}{R_{\text{normal}}(T \to 0)} = 3$ and $r = 1.9$ for our sample and that of Mozaeffari et al., respectively. The fact that we observe good agreement of $B_{c2}(T)$ between our samples and those of Mozaeffari et al. suggests that the superconducting properties are independent of impurity concentrations, i.e. in the clean limit. By contrast, the samples obtained via dissociation of $\text{H}_2\text{S}$ by Drozdov et al. [1] showed a much smaller resistance ratio $r \sim 1$ and a larger slope at the critical field suggesting an enhancement due to a limited mean free path, i.e. in the dirty limit.

The upper critical field of a superconductor is determined by the orbital and Pauli pair-breaking effects. Near $T_c$, the Pauli pair-breaking is negligible for conventional superconductors and hence, we use the slope of the critical field $\frac{dB_{c2}}{dT} = -0.58(3) \text{K}^{-1}$ to estimate the coherence length, $\xi_0$, and Fermi velocity, $v_F$. In the clean limit, the slope of the critical field is given by

$$\left. -\frac{dB_{c2}}{dT} \right|_{T_c} = \frac{\Phi_0}{2\pi(0.74)^2 c^2 T_c}$$

where $\Phi_0 = \hbar/2e$ is the flux quantum. From this, we obtain the coherence length $\xi_0 = 2.2 \text{nm}$. Comparison of the coherence length with the mean free path ($\xi_0 < l$) justifies applicability of the clean limit relations. We estimate the Fermi velocity using

$$\xi_0 = \frac{\hbar v_F}{\pi \Delta_0} \approx \frac{\hbar v_F}{\pi \gamma k_B T_c}$$

where the numerical factor $\gamma \approx 2.0(4)$ reflects the expected strong coupling behaviour associated with the high-temperature superconductivity in $\text{H}_3\text{S}$. Based on these assumptions, we obtain $v_F^{\text{exp}} = 3.8(7) \times 10^6 \text{m s}^{-1}$.

The obtained Fermi velocity is significantly lower than expected from DFT calculations. We employ Wien2k to calculate the band structure of $\text{H}_3\text{S}$ based on the experimental lattice parameters from our XRD results. (Details of the DFT calculation can be found in section IV of the supplementary information [25] and references therein[36, 37].) Our band structure looks very similar to earlier reports [38]. The Fermi velocity at the Fermi

![Figure 3: Suppression of superconducting transition in magnetic field.](image-url)
form with offset has been reported for YH
linearly as demonstrated in Figure 3(d). A similar linear
Upon application of a magnetic field, $\Delta c = \frac{T - T_c}{T_c}$ is the normalized temperature and
In zero field, our sample features a sharp transition with
conducting transition can be influenced by many factors
transition in magnetic field. The width of the super-
strong renormalisation of the Fermi velocity due to the
experimental result $v_F^{\text{exp}} \approx 3.8 \times 10^5 \text{ m s}^{-1}$. The reduced
Fermi velocity in experiment compared to DFT confirms
of the Fermi velocity $\langle v_F \rangle$ is shown as a colormap plot over the Fermi surface of H$_3$S. A considerable variation of $v_F$ is found over several of the Fermi-surface sheets. Within a simple single-band model we can compare the global average of the Fermi velocity $\langle v_F \rangle = 1.6 \times 10^6 \text{ m s}^{-1}$ with our experimental result $v_F^{\text{exp}} \approx 3.8 \times 10^5 \text{ m s}^{-1}$. The reduced Fermi velocity in experiment compared to DFT confirms strong renormalisation of the Fermi velocity due to the strong electron-phonon coupling in H$_3$S.

We observe a clear broadening of the superconducting transition in magnetic field. The width of the superconducting transition can be influenced by many factors including inhomogeneities in composition and pressure. In zero field, our sample features a sharp transition with $\Delta T_c = T_{c \text{onset}} - T_{c50\%} = 0.5 \text{ K}$ suggesting a good homogeneity of our sample and small pressure gradients. Upon application of a magnetic field, $\Delta T_c(H)$ increases linearly as demonstrated in Figure 3(d). A similar linear form with offset has been reported for YH$_3$ [17]. The broadening of the transition is most visible in the inset Figure 2(b). An increase in transition width is in general

energy is shown as a colormap over the Fermi surface in Figure 4. A considerable variation of $v_F$ is found over several of the Fermi-surface sheets. Within a simple single-band model we can compare the global average of the Fermi velocity $\langle v_F \rangle$ is shown as a colormap plot over the Fermi surface of H$_3$S as obtained with DFT calculations. Fermi surface sheets 1, 3, and 5 are shown in top panel, sheets 2 and 4 in bottom panel.

Infinite magnetic field, flow of the flux lattice can increase the width of the superconducting transition. Near $T_c$, the flow of the flux lattice is determined by the activation energy required to overcome pinning leading to the expectation that the resistance scales as $t^{3/2}/h$ [40]. Here $t = (T - T_c)/T_c$ is the normalized temperature and $h = B/B_c(T = 0)$ the normalized field. Alternatively, the suppression of filamentary superconductivity in finite magnetic fields can cause changes to the superconducting transition – usually leading to a sharper transition with a lower $T_c$. By analysing the scaling behaviour of a large portion of the resistive transition, we focus on the contributions arising from the bulk of our H$_3$S phase – the suppression of filamentary superconductivity does not usually lead to a scaling form of the resistance. In our sample of H$_3$S, we find reasonable scaling of a large proportion of the superconducting transition as demonstrated in Figure 5. Good scaling is found for a functional form

$$
\frac{R}{R_{\text{normal}}} = f \left( \frac{t^\beta}{h + \alpha} \right)
$$

linear in temperature, i.e. with $\beta = 1$. To determine $h$, we use $B_c2(T = 0) = 88 \text{ T}$ estimated by Mozaffari et al. [13]. The constant $\alpha = 0.019$ reflects the finite width of the superconducting transition in zero magnetic field associated with sample inhomogeneities, strain, or other non-thermal causes suggesting that Equation 4 implies a temperature-over-field scaling of the intrinsic superconducting transition in H$_3$S. Notably, the scaling of Equation 4 leads to much better collapse of the data than a form involving $\beta = 3/2$ predicted by Tinkham et al. [40] (cf. Figure 5(b)). Whilst a precise determination of $\beta$, i.e. discriminating exponents close to unity will require further measurements over a wider field range the quality of the data collapse in Figure 5 suggests that linear temperature-over-field scaling dominates the fluctuations of the superconducting transition in H$_3$S. A linear form Equation 4 is consistent with data on MgB$_2$ and other hydride superconductors [41]. Yet, we note that the linear transition width and linear temperature-over-field scaling in H$_3$S cannot be associated with granular anisotropic superconductivity like in MgB$_2$ [42] as H$_3$S is cubic. Hence, the linear temperature-over-field scaling of the resistance in H$_3$S suggest that a new model might be required to describe the broadening of the superconducting transition in hydride superconductors.

I. CONCLUSION

Im$3m$ H$_3$S can be synthesized from elemental sulfur and ammonia borane. Superconductivity is evident from a sudden drop in resistance which is found to shift to lower temperatures and broaden upon application of magnetic field. Two experimental observations suggest

FIG. 4. The magnitude of the Fermi velocity is shown as color map over the Fermi surface of H$_3$S as obtained with DFT calculations. Fermi surface sheets 1, 3, and 5 are shown in top panel, sheets 2 and 4 in bottom panel.
that the superconductivity follows clean-limit behaviour. (i) The critical field curve is found to be identical for different samples at the same pressure synthesized in different ways, i.e. independent of different levels of impurities. (ii) Our estimated mean free path is longer than the coherence length extracted from the slope of the critical field. A significant broadening of the superconducting transition in finite field is found and follows a linear $t/(h + \alpha)$ scaling which suggests that a new model is required to describe the fluctuations in proximity to the superconducting transition in hydrides.

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**ADDITIONAL INFORMATION**

Data are available at the University of Bristol data repository data.brins [43].

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