

# Universal Fermi velocity in highly compressed hydride superconductors

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## AFFILIATIONS

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## ABSTRACT

The Fermi velocity  $v_F$  is one of the primary characteristics of any conductor, including any superconductor. For conductors at ambient pressure, several experimental techniques have been developed to measure  $v_F$ , and, for instance, Zhou *et al.* [Nature **423**, 398 (2003)] reported that high- $T_c$  cuprates exhibited a universal nodal Fermi velocity  $v_{F,\text{univ}} = (2.7 \pm 0.5) \times 10^5$  m/s. However, there have been no measurements of  $v_F$  in highly compressed near-room-temperature superconductors (NRTS), owing to experimental challenges. Here, to answer the question of the existence of a universal Fermi velocity in NRTS materials, we analyze the full inventory of data on the ground-state upper critical field  $B_{c2}(0)$  for these materials and find that this class of superconductors exhibits a universal Fermi velocity  $v_{F,\text{univ}} = (1/1.3) \times [2\Delta(0)/k_B T_c] \times 10^5$  m/s, where  $\Delta(0)$  is the ground-state amplitude of the energy gap. The ratio  $2\Delta(0)/k_B T_c$  varies within a narrow range  $3.2 \leq 2\Delta(0)/k_B T_c \leq 5$ , and so  $v_{F,\text{univ}}$  in NRTS materials lies in the range  $2.5 \times 10^5$  m/s  $\leq v_{F,\text{univ}} \leq 3.8 \times 10^5$  m/s, which is similar to the range of values found for the high- $T_c$  cuprate counterparts of these materials.

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## I. INTRODUCTION

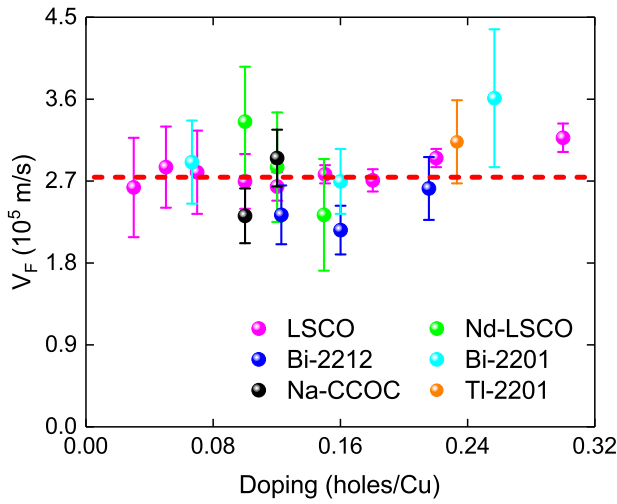
Since pivotal experimental discovery of the first near-room-temperature superconductor (NRTS) H<sub>3</sub>S by Drozdov *et al.*,<sup>1</sup> nearly two dozen highly compressed hydrogen-rich superconducting phases have been synthesized in binary and ternary systems.<sup>2–17</sup> Experimental studies of NRTS are well supported by first-principles calculations,<sup>18–30</sup> but experimental characterizations of NRTS phases are limited by the narrow range of techniques that are available for materials inside diamond anvil cells (DACs).<sup>25–27</sup> These comprise x-ray diffraction (XRD) phase analysis, Raman spectroscopy, and magnetoresistance measurements,<sup>31–35</sup> although, with the use of some advanced techniques, Hall effect measurements can also be performed.<sup>31</sup> Because of this, only two characteristic values of the superconducting state of the NRTS phases are commonly extracted from experimental data, namely, the transition temperature  $T_c$  and the extrapolated value for the ground-state upper critical field  $B_{c2}(0)$  or the ground-state superconducting coherence length  $\xi(0)$ , which can be derived from the Ginzburg–Landau<sup>36</sup> expression

$$\xi(0) = \sqrt{\frac{\phi_0}{2\pi B_{c2}(0)}}, \quad (1)$$

where  $\phi_0 = h/2e$  is the superconducting flux quantum, with  $h$  being Planck's constant and  $e$  the electric charge of the electron.

Other important parameters of NRTS materials, among which we can mention the Fermi velocity  $v_F$ , have not been measured to date, owing to the challenges of performing such measurements on samples inside DACs. However, considering that all NRTS superconductors are hydrides, there is an expectation that these materials will exhibit a universal Fermi velocity  $v_{F,\text{univ}}$ , as has been discovered in cuprates, for which  $v_{F,\text{univ}} = (2.7 \pm 0.5) \times 10^5$  m/s, as reported by Zhou *et al.*<sup>37</sup> (see Fig. 1).

The theoretical motivation for the quest for a universal Fermi velocity in NRTS comes, on the one hand, from the recent understanding<sup>38</sup> that sulfur in H<sub>3</sub>S is analogous to the oxygen in cuprates, and, on the other hand, from the fact that highly compressed hydrides fit nicely with the main global scaling laws for superconductors.<sup>39–43</sup> However, it should be noted that an analysis



**FIG. 1.** Universal nodal Fermi velocity  $v_{F,\text{univ}} = (2.7 \pm 0.5) \times 10^5$  m/s for cuprate superconductors. These are the raw data reported by Zhou *et al.*<sup>37</sup> for  $(\text{La}_{2-x}\text{Sr}_x)\text{CuO}_4$  (LSCO),  $(\text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x)\text{CuO}_4$  (Nd-LSCO),  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  (Bi-2212),  $\text{Bi}_2\text{Sr}_2\text{CuO}_6$  (Bi-2201),  $(\text{Ca}_{2-x}\text{Na}_x)\text{CuO}_2\text{Cl}_2$  (Na-CCOC), and  $\text{Ti}_2\text{Ba}_2\text{CuO}_6$  (TI-2201).

of whether these materials also comply with other scaling laws for superconductors<sup>44,45</sup> requires more experimental data on normal-state resistivity  $\rho(T)$ <sup>31,46–48</sup> and ground-state London penetration depth  $\lambda(0)$ .<sup>1,49,50</sup>

Here, we report the results of our search for a universal Fermi velocity in NRTS materials, based on an analysis of the full inventory of values for the ground-state upper critical field  $B_{c2}(0)$  in these materials. We find that a universal Fermi velocity,  $v_{F,\text{univ}}$ , does indeed exist in NRTS materials and obeys the empirical law

$$v_{F,\text{univ}} = \frac{1}{1.3} \times \frac{2\Delta(0)}{k_B T_c} \times 10^5 \text{ m/s}, \quad (2)$$

where  $k_B$  is Boltzmann's constant and  $\Delta(0)$  is the ground-state superconducting energy gap.

## II. DESCRIPTION OF APPROACH

In the Bardeen–Cooper–Schieffer (BCS) theory of superconductivity,<sup>51</sup> the ground-state coherence length  $\xi(0)$  and the amplitude of the ground-state energy gap  $\Delta(0)$  are linked through the expression

$$\xi(0) = \frac{\hbar v_F}{\pi \Delta(0)}, \quad (3)$$

where  $\hbar$  is the reduced Planck's constant. BCS theory also involves a dimensionless ratio

$$\alpha = \frac{2\Delta(0)}{k_B T_c}. \quad (4)$$

Substitution of Eqs. (3) and (4) into Eq. (1) gives the dependence of the ground-state upper critical field on the transition temperature:

$$B_{c2}(0) = \left[ \frac{\pi \phi_0 k_B^2}{8 \hbar^2} \right] \frac{\alpha^2}{v_F^2} T_c^2, \quad (5)$$

where the multiplicative prefactor in square brackets is a constant:

$$A = \left[ \frac{\pi \phi_0 k_B^2}{8 \hbar^2} \right] = 1.38 \times 10^7 \text{ T m}^2 / (\text{s}^2 \text{ K}^2). \quad (6)$$

Thus, if hydrogen-rich superconductors exhibit a universal Fermi velocity  $v_{F,\text{univ}}$ , then a fit of the full inventory of the  $B_{c2}(0)$  vs  $T_c$  dataset to the equation

$$B_{c2}(0) = A f T_c^\beta, \quad (7)$$

where  $\beta$  and  $f = \alpha^2 / v_F^2$  are free fitting parameters, should reveal that

$$\beta \cong 2, \quad (8)$$

and, if this is the case, then the universal Fermi velocity  $v_{F,\text{univ}}$  can be calculated from the deduced free-fitting parameter  $f$  as

$$v_{F,\text{univ}} = \frac{\alpha}{\sqrt{f}} = \frac{1}{\sqrt{f}} \frac{2\Delta(0)}{k_B T_c}. \quad (9)$$

It should be noted that  $\alpha = 2\Delta(0)/k_B T_c$  in highly compressed hydrogen-rich superconductors varies within the range<sup>4,8,12,27,42,49,52–55</sup>

$$3.2 \leq \frac{2\Delta(0)}{k_B T_c} \leq 5, \quad (10)$$

where the lower limit is the value deduced from experiment<sup>42,50,52</sup> and the upper limit is based on the many results obtained from first-principles calculations, which always predict  $4.3 \leq 2\Delta(0)/k_B T_c$  in NRTS materials,<sup>4,8,12,27,53–55</sup> including very high values of  $2\Delta(0)/k_B T_c \cong 5.0$  for some NRTS phases.<sup>4,8,12,27</sup>

## III. EXTRAPOLATION MODEL FOR THE GROUND-STATE UPPER CRITICAL FIELD

Equation (7) has the ground-state upper critical field  $B_{c2}(0)$  as dependent variable. However, it is important to note that this value can be determined by the use of several extrapolative models<sup>56–59</sup> that utilize experimental  $B_{c2}(T)$  data measured at high reduced temperatures  $T/T_c$ . The primary reason why there is a necessity for extrapolative models is that all highly compressed hydrogen-rich superconductors have  $B_{c2}(T \rightarrow 0 \text{ K}) > 20$  T, which cannot be measured by the conventional and widely used Physical Property Measurement System (manufactured by Quantum Design), for which the highest measurable magnetic field  $B_{\text{appl}} = 9\text{--}16$  T (depending on the specific model). It should be also stressed that  $B_{c2}(T \rightarrow 0 \text{ K})$  for the NRTS compounds  $\text{H}_3\text{S}$ ,  $\text{LaH}_{10}$ ,  $\text{YH}_6/\text{YH}_9$  and  $(\text{La},\text{Y})\text{H}_{10}$  are so high that even measurements at the best available quasi-DC

magnetic field facilities worldwide<sup>31,48,60</sup> cover only the range of reduced temperatures  $\frac{1}{2} \lesssim T/T_c$ .

In this paper, from the several extrapolative  $B_{c2}(T)$  models that are available,<sup>56–59</sup> we use the following analytical approximate expression from Werthamer–Helfand–Hohenberg (WHH) theory,<sup>61,62</sup> which was proposed by Baumgartner *et al.*<sup>59</sup>

$$B_{c2}(T) = \frac{1}{0.693} \frac{\phi_0}{2\pi\xi^2(0)} \left[ \left(1 - \frac{T}{T_c}\right) - 0.153 \left(1 - \frac{T}{T_c}\right)^2 - 0.152 \left(1 - \frac{T}{T_c}\right)^4 \right], \quad (11)$$

where  $\xi(0)$  and  $T_c \equiv T_c(B = 0)$  are two free fitting parameters (this equation is referred to as the B-WHH model hereinafter). Equation (11) was originally proposed for the extrapolation of  $B_{c2}(T)$  data for neutron-irradiated Nb<sub>3</sub>Sn alloys,<sup>59</sup> and recently several research groups have found that provides good approximations for a variety of superconducting materials.<sup>4,63–68</sup> On this basis, in the present study, we used Eq. (11) as a good, robust and simple analytical tool to extrapolate the  $B_{c2}(T)$  curve to the low-temperature high-field region.

It is a necessary to describe the criterion for extracting  $B_{c2}(T)$  datasets from experimentally measured  $R(T, B_{\text{appl}})$  curves. Several criteria are available for the definitions of  $T_c$ ,  $B_{c2}(T)$ , and  $T_c(B_{\text{appl}})$ , which have been discussed recently for the case of NRTS in Ref. 69. We have found<sup>69,70</sup> that the best match between the electron–phonon coupling constant  $\lambda_{e\text{-ph}}$  extracted from  $R(T, B_{\text{appl}} = 0)$  curves and the  $\lambda_{e\text{-ph}}$  computed by first-principles calculation is obtained when  $T_c$  is defined at a value of the ratio  $R(T)/R_{\text{norm}}$  that is as low as practically possible (where  $R_{\text{norm}}$  is the normal-state resistance just above the transition). By analyzing the full inventory of  $R(T, B_{\text{appl}})$  data for NRTS materials herein, we have come to the conclusion that owing to noise and slope issues with real-world  $R(T, B_{\text{appl}})$  curves and the fact that highly compressed superhydrides contain several superconducting phases, the appropriate criterion is

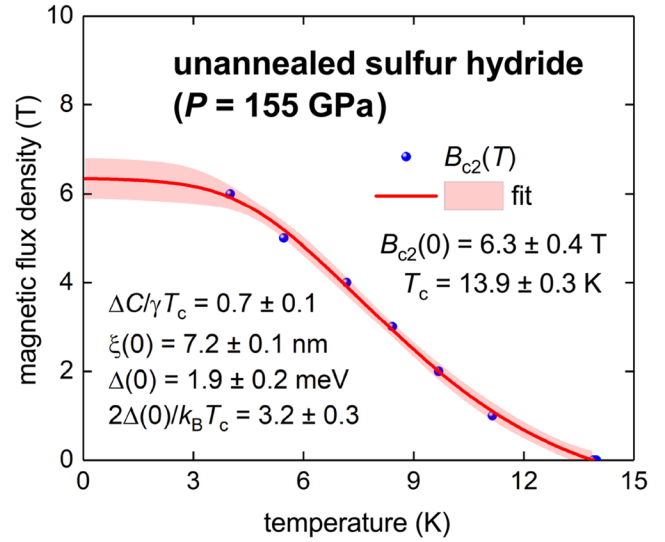
$$\frac{R(T, B_{\text{appl}})}{R(T_c^{\text{onset}}, B_{\text{appl}})} = 0.05, \quad (12)$$

and we use this henceforth in this study.

## IV. RESULTS

### A. Unannealed highly compressed sulfur hydride

In the first paper on NRTS superconductors, Drozdov *et al.*<sup>1</sup> reported  $R(T, B_{\text{appl}})$  data for unannealed highly compressed sulfur hydride ( $P = 155$  GPa) in their Fig. 3(a). By using the criterion of Eq. (12) [which is  $R(T, B_{\text{appl}})_{\text{criterion}} = 23$  m $\Omega$  for the  $R(T, B_{\text{appl}})$  curves shown in bottom insert in Fig. 3(a) in Ref. 1], we extracted the  $B_{c2}(T)$  dataset for this sample, which is shown in Fig. 2. Because this  $B_{c2}(T)$  dataset covers a significant part of the full temperature range  $0 \text{ K} < T \leq T_c$ , there was no need to use an extrapolative fit, and instead we fitted this dataset to the model in Ref. 52, which allowed to



**FIG. 2.** Upper critical field data  $B_{c2}(T)$  and data fit to Eqs. (13) and (14) for unannealed highly compressed sulfur hydride ( $P = 190$  GPa). The raw  $R(T, B_{\text{appl}})$  dataset was that reported by Drozdov *et al.*<sup>1</sup> The deduced values of  $\xi(0)$ ,  $\Delta(0)$ ,  $T_c$ , and  $\Delta C/\gamma T_c$  are shown on the figure. The 95% confidence bands are shown by the pink shaded area. The fit quality is  $R = 0.9985$ .

deduce  $\Delta(0)$ ,  $2\Delta(0)/k_B T_c$ , and  $\Delta C/\gamma T_c$  (the last of which is the relative jump in electronic specific heat at  $T_c$ , with  $\gamma$  being the so-called Sommerfeld constant):

$$B_{c2}(T) = \frac{\phi_0}{2\pi\xi^2(0)} \left[ \frac{1.77 - 0.43 \left(\frac{T}{T_c}\right)^2 + 0.07 \left(\frac{T}{T_c}\right)^4}{1.77} \right]^2 \times \left\{ 1 - \frac{1}{2k_B T} \int_0^\infty \frac{d\varepsilon}{\cosh^2 \left[ \frac{\sqrt{\varepsilon^2 + \Delta^2(T)}}{2k_B T} \right]} \right\}, \quad (13)$$

where the temperature-dependent superconducting gap  $\Delta(T)$  is given by<sup>71,72</sup>

$$\Delta(T) = \Delta(0) \tanh \left[ \frac{\pi k_B T_c}{\Delta(0)} \sqrt{\eta \frac{\Delta C}{\gamma T_c} \left( \frac{T_c}{T} - 1 \right)} \right], \quad (14)$$

with  $\eta = 2/3$  for  $s$ -wave superconductors.

We used Eqs. (13) and (14) to extract  $\xi(0)$ ,  $\Delta(0)$ ,  $T_c$ , and  $\Delta C/\gamma T_c$  from  $B_{c2}(T)$  datasets for a variety of superconductors, including two highly compressed hydride phases of H<sub>3</sub>S,<sup>52</sup> SnH<sub>12</sub>,<sup>42</sup> V<sub>3</sub>Si,<sup>73</sup> and several iron-based superconductors.<sup>73</sup> However, it should be stressed that the approach using Eqs. (13) and (14) is only applicable for  $B_{c2}(T)$  datasets defined by Eq. (12) or by a stricter criterion.

One of the most important deduced parameters,  $\alpha = 2\Delta(0)/k_B T_c = 3.2 \pm 0.3$ , is in remarkable agreement with the corresponding values deduced for highly compressed annealed H<sub>3</sub>S ( $P = 155$ – $160$  GPa),  $\alpha = 3.20 \pm 0.02$ <sup>49</sup> and  $3.55 \pm 0.31$ ,<sup>52</sup> and for highly compressed annealed SnH<sub>12</sub> ( $P = 190$  GPa),  $\alpha = 3.28 \pm 0.18$ .<sup>42</sup> The deduced  $\Delta C/\gamma T_c = 0.7 \pm 0.1$  is also below the weak-coupling

limit of BCS theory  $\Delta C/\gamma T_c = 1.43$ , as is the corresponding value for the annealed H<sub>3</sub>S material,  $\Delta C/\gamma T_c = 1.2 \pm 0.3$ .<sup>52</sup> It should be mentioned that to deduce  $\Delta C/\gamma T_c$  with higher accuracy requires more  $B_{c2}(T)$  data points, especially at  $T \sim T_c$ . The deduced  $B_{c2}(0)$  and  $T_c$  are given in Table I.

## B. Annealed highly compressed hydrides

We processed reported  $R(T, B_{\text{appl}})$  datasets for several annealed highly compressed hydrides by using Eq. (12) to extract  $B_{c2}(T)$  datasets. The obtained datasets were fitted to Eq. (11), and the deduced values are given in Table I. These materials are as follows:

1. Sulfur superhydride H<sub>3</sub>S ( $P = 155$  and  $160$  GPa), for which the raw data were reported by Mozaffari *et al.*<sup>31</sup>
2. Cerium superhydride CeH<sub>*n*</sub> ( $P = 88, 137,$  and  $139$  GPa), for which the raw data were reported by Chen *et al.*<sup>12</sup>
3. Lanthanum superhydride LaH<sub>10</sub> ( $P = 120, 136$  GPa), for which the raw data were reported by Sun *et al.*<sup>60</sup>
4. Yttrium superhydride/superdeuteride YH<sub>6</sub>/YD<sub>6</sub> ( $P = 172$  and  $200$  GPa), for which the raw data were reported by Troyan *et al.*<sup>4</sup>
5. Lanthanum–yttrium superhydride (La,Y)H<sub>10</sub> ( $P = 182, 183,$  and  $186$  GPa), for which the raw data were reported by Semenok *et al.*<sup>8</sup>
6. Tin superhydride SnH<sub>12</sub> ( $P = 190$  GPa), for which the raw data were reported by Hong *et al.*<sup>11</sup>
7. Thorium superhydrides ThH<sub>9</sub> and ThH<sub>10</sub> ( $P = 170$  GPa), for which the raw data were reported by Semenok *et al.*<sup>16</sup>

The respective fits are shown in Figs. S1–S7 in the [supplementary material](#).

## C. Analysis of $B_{c2}(0)$ vs $T_c$ for superhydride phases

All deduced  $B_{c2}(0)$  and  $T_c$  values for superhydride phases are collected in Table I, where we have also added data for the Th<sub>4</sub>H<sub>15</sub> phase reported by Satterthwaite and Toepke.<sup>74</sup>

The full dataset from Table I is shown in Fig. 3, together with the fit to Eq. (7). Although this dataset has a large scatter, it can be seen in Fig. 3(a) that the free-fitting power-law exponent  $\beta = 2.07 \pm 0.14$  is practically undistinguishable from the expected value  $\beta \equiv 2$  [Eq. (5)]. When  $\beta$  is the free-fitting parameter [Fig. 3(a)], the deduced  $f = (1.19 \pm 0.90) \times 10^{-10} \text{ s}^2/\text{m}^2$  has a large uncertainty. However, when  $\beta$  is fixed to 2 [Fig. 3(b)], the free-fitting parameter  $f$  can be deduced with high accuracy as

$$f = \frac{\alpha^2}{v_{F,\text{univ}}^2} = (1.68 \pm 0.08) \times 10^{-10} \text{ s}^2/\text{m}^2, \quad (15)$$

from which we can obtain

$$v_{F,\text{univ}} = \frac{\alpha}{1.30 \pm 0.03} \times 10^5 \text{ m/s} \cong \frac{1}{1.3} \times \frac{2\Delta(0)}{k_B T_c} \times 10^5 \text{ m/s}. \quad (16)$$

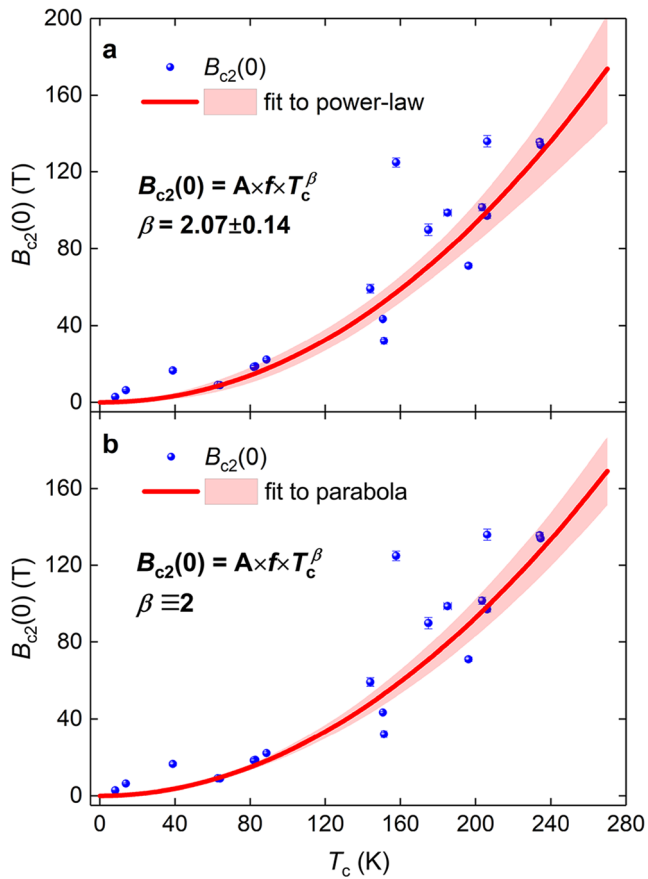
By substituting the lower [ $2\Delta(0)/k_B T_c = 3.2$ ] and upper [ $2\Delta(0)/k_B T_c = 5.0$ ] limits of the ratio  $2\Delta(0)/k_B T_c$  [Eq. (10)] into Eq. (16), we can establish the lower and upper limits of  $v_{F,\text{univ}}$  in superhydrides:

$$2.5 \times 10^5 \text{ m/s} \lesssim v_{F,\text{univ}} \lesssim 3.8 \times 10^5 \text{ m/s}. \quad (17)$$

The deduced  $v_{F,\text{univ}}$  for hydrogen-rich superconductors [Eq. (16)] is similar to the corresponding value for high- $T_c$  cuprates,  $v_{F,\text{univ}} = (2.7 \pm 0.5) \times 10^5 \text{ m/s}$ ,<sup>37</sup> if Eq. (10) is taken into account.

**TABLE I.** Deduced  $B_{c2}(0)$  and  $T_c$  values for hydrogen-rich superconductors for which raw  $R(T, B_{\text{appl}})$  data are available to date.

Phase and data source	Figures	Pressure (GPa)	$T_c$ (K)	$\Delta T_c$ (K)	$B_{c2}(0)$ (T)	$\Delta B_{c2}(0)$ (T)
Unannealed sulfur hydride [Fig. 3(a) in Ref. 1]	2	155	13.9	0.3	6.3	0.4
Annealed H <sub>3</sub> S (Fig. 3 in Ref. 31)	S1(a)	155	185	2	98.8	1.2
Annealed H <sub>3</sub> S (Figs. S1 and S2 in Ref. 31)	S1(b)	155	196.1	0.6	71.1	1.1
Annealed H <sub>3</sub> S (Fig. 3 in Ref. 31)	S1(c)	160	143.9	1.4	59.2	2.3
Annealed CeH <sub>9</sub> [Fig. S7(a) in Ref. 12], cooling	S2(a)	88	38.8	0.4	16.5	1
Annealed CeH <sub>9</sub> [Fig. 1(c) in Ref. 12], warming	S2(b)	139	88.6	0.3	22.2	0.7
Annealed CeH <sub>9</sub> [Fig. 1(d) in Ref. 12], cooling	S2(c)	137	81.9	0.7	18.4	0.7
Annealed CeH <sub>9</sub> [Fig. 1(d) in Ref. 12], warming	S2(d)	137	82.7	0.7	18.7	0.6
Annealed LaH <sub>10</sub> [Fig. 3(a) in Ref. 60]	S3(a)	120	174.8	0.8	90	3
Annealed LaH <sub>10</sub> [Fig. 3(b) in Ref. 60]	S3(b)	136	206.2	0.8	136	3
Annealed YD <sub>6</sub> [Fig. S13(a) in Ref. 4]	S4(a)	172	157.7	0.2	124.9	2.4
Annealed YH <sub>6</sub> [Fig. S16(c) in Ref. 4]	S4(b)	200	206.2	0.2	97.2	1.4
Annealed (La,Y)H <sub>10</sub> [Fig. S27(b) in Ref. 8]	S5(a)	183	203.5	0.2	101.6	1.8
Annealed (La,Y)H <sub>10</sub> [Fig. S28(a) in Ref. 8]	S5(b)	182	234	0.1	135.8	1.5
Annealed (La,Y)H <sub>10</sub> [Fig. S28(a) in Ref. 8]	S5(c)	186	234.5	0.1	134	1
Annealed SnH <sub>12</sub> [Fig. 4(a) in Ref. 11], cooling	S6(a)	190	62.8	0.4	9	0.2
Annealed SnH <sub>12</sub> [Fig. 4(a) in Ref. 11], warming	S6(b)	190	64.1	0.5	8.9	0.2
Annealed ThH <sub>9</sub> [Fig. 4(a) in Ref. 16]	S7(a)	170	151.2	1.5	32	0.9
Annealed ThH <sub>10</sub> [Fig. 4(a) in Ref. 16]	S7(b)	170	150.6	0.4	43.4	0.6
Th <sub>4</sub> H <sub>15</sub> (Ref. 74)		Ambient	8.2	0.15	2.75	0.25



**FIG. 3.** Total  $B_{c2}(0)$  vs  $T_c$  dataset for hydrogen-rich superconductors deduced in this work (Table 1) and data fits to (a) Eq. (7) and (b) Eq. (5). (a) Free-fitting  $\beta = 2.07 \pm 0.14$  and  $f = (1.19 \pm 0.90) \times 10^{-10} \text{ s}^2/\text{m}^2$ ; the fit quality is  $R = 0.9361$ . (b)  $\beta = 2.0$  (fixed) and free-fitting  $f = (1.68 \pm 0.08) \times 10^{-10} \text{ s}^2/\text{m}^2$ ; the fit quality is  $R = 0.9354$ .

## V. DISCUSSION

The primary assumption of the Migdal–Eliashberg (ME) theory of electron–phonon-mediated superconductivity<sup>75–77</sup> is that the ratio of characteristic phonon energy  $\hbar\omega_D$  (where  $\omega_D$  is the Debye frequency) to the Fermi energy  $E_F$  is very small,  $\hbar\omega_D/E_F \ll 1$ . In normal metals  $\hbar\omega_D/E_F \lesssim 10^{-2}$ ,<sup>78–82</sup> and this is why ME theory is quantitatively accurate. However, for many high-temperature superconductors, the application of ME theory cannot be justified. In fact, in our previous studies,<sup>69,70</sup> we deduced the Debye temperature  $T_\theta \cong 1500$  K, in highly compressed  $\text{H}_3\text{S}$  from a fit of experimentally measured temperature-dependent resistance  $R(T)$  to the Bloch–Grüneisen equation.<sup>83,84</sup> This temperature can be converted into the Debye energy  $k_B T_\theta = \hbar\omega_D \cong 0.13$  eV, and, considering that the Fermi energy was deduced in our previous study<sup>52</sup> as  $E_F = 0.5\text{--}1.0$  eV, we can conclude that  $0.13 \leq \hbar\omega_D/E_F \leq 0.26$ , and thus ME theory<sup>75,76</sup> does not provide an exact description of highly compressed  $\text{H}_3\text{S}$ .

The first concern that nonadiabatic effects (i.e., effects beyond ME theory<sup>75,76</sup>) are important in highly compressed  $\text{H}_3\text{S}$  was expressed by Pietronero *et al.*,<sup>82</sup> who also pointed out that: “. . . The fingerprints of non-adiabatic effects are: – position of the material in the Uemura diagram; . . .” Although the traditional way to position a material in the Uemura plot requires knowledge of the ground-state London penetration depth  $\lambda(0)$  (which has only recently been reported for  $\text{H}_3\text{S}$ <sup>46</sup>), the present author utilized the ground-state coherence length  $\xi(0)$  [deduced from the  $B_{c2}(T)$  data] and found<sup>52</sup> that  $\text{H}_3\text{S}$  falls into the unconventional superconductors band in the Uemura plot.<sup>41</sup> In later work,<sup>42,85–88</sup> it was established that  $\text{LaH}_{10}$ ,  $\text{Th}_4\text{H}_{15}$ ,  $\text{ThH}_9$ ,  $\text{ThH}_{10}$ ,  $\text{YH}_6$ ,  $\text{SH}_{12}$ , and  $\text{H}_3(\text{S},\text{C})$  also fall into the unconventional superconductors band in the Uemura plot. This is direct evidence that the ratio  $\hbar\omega_D/E_F$  in superhydrides has values well above those typical of conventional superconductors,  $\hbar\omega_D/E_F \lesssim 10^{-2}$ .

On the basis of the derived universal Fermi velocity in superhydrides,  $v_{F,\text{univ}}$  [Eq. (16)], we can conclude that the strength of the nonadiabatic effects in a superhydride (as quantified by the ratio  $\hbar\omega_D/E_F$ ) can be revealed if the Debye temperature  $T_\theta$  of the compound can be deduced from the normal part of the temperature-dependent resistance  $R(T)$ .<sup>69,70,86</sup> It should be noted that the Debye temperature in superhydrides varies from  $T_\theta \cong 870$  K ( $\text{D}_3\text{S}$ ,  $P = 173$  GPa<sup>69</sup>) up to  $T_\theta \cong 1700$  K ( $R3m$ -phase of  $\text{H}_3\text{S}$ ,  $P = 133$  GPa<sup>69</sup>).

An analysis of the first experimental  $R(T)$  data<sup>89</sup> measured for metallic hydrogen phase III (compressed at  $P = 402$  GPa) revealed that  $T_\theta \cong 730$  K.<sup>70</sup> If we assume that metallic hydrogen phase III complies with the established  $v_{F,\text{univ}}$  [Eq. (16)] and that it has  $2\Delta(0)/k_B T_c = 3.53$  and exhibits no effective mass enhancement, then the ratio  $\hbar\omega_D/E_F$  can be estimated as  $\hbar\omega_D/E_F = 0.3$ . This implies that metallic hydrogen should exhibit pronounced nonadiabatic effects,<sup>78–82</sup> which could prevent the emergence of a superconducting state in this metal at high temperature.

It should be also mentioned that first principles calculations (FPC) are an essential part of current NRTS phase searches.<sup>27</sup> The accuracy and powerful capabilities of FPC became obvious after the pivotal prediction of the  $\text{Im}3m - \text{H}_3\text{S}$  phase,<sup>90,91</sup> which was later discovered experimentally.<sup>1</sup> Another achievement of the FPC approach was demonstrated recently when Li *et al.*<sup>92</sup> and Ma *et al.*<sup>93</sup> reported the discovery of a calcium superhydride phase with transition temperature  $T_c = 200\text{--}215$  K (at a pressure  $P = 160\text{--}190$  GPa), which was predicted by Wang *et al.*<sup>94</sup> in 2012. However, it should also be mentioned that the superconductivity predicted by FPC in some binary systems (e.g.,  $\text{AlH}_3$ <sup>95,96</sup>), has never been observed experimentally. This implies that further development of FPC techniques to take account of non-adiabatic effects is highly desirable.

Overall, remarkable progress has been achieved in this field from the first theoretical predictions of high-temperature superconductivity in metallic hydrogen<sup>97,98</sup> and hydrogen-dominated alloys<sup>74,99</sup> five decades ago to the remarkable experimental and FPC results<sup>1,27</sup> reported recently. It should be stressed that all the primary discoveries in the field (e.g., the direct searches for and syntheses of the  $\text{H}_3\text{S}$ ,  $\text{LaH}_{10}$ , and  $\text{YH}_6$  phases) have come from a perfect conjunction of theory and experiment. An excellent example of this is the story of the discovery of near-room-temperature superconductivity in highly compressed sulfur

hydride.<sup>1</sup> In February 2014, Li *et al.*<sup>100</sup> reported results of FPC calculations for highly compressed sulfur hydride. These calculations showed that at  $P = 160$  GPa, the sulfur hydride retains the composition of  $\text{H}_2\text{S}$  and that this compound exhibits a superconducting transition temperature of  $T_c \sim 80$  K. In November 2014, an alternative theoretical result was reported by Duan *et al.*,<sup>91</sup> who performed thorough FPC using USPEX software<sup>101–103</sup> and predicted that sulfur hydride would decompose into a mixture of elemental sulfur and an  $(\text{H}_2\text{S})_2\text{H}_2$  phase at high pressure. This result was in a good accord with an earlier report by Strobel *et al.*,<sup>104</sup> who showed experimentally that at  $P > 3.2$  GPa, the  $\text{H}_2\text{S}$ – $\text{H}_2$  mixture exhibited structural ordering with the formation of the  $(\text{H}_2\text{S})_2\text{H}_2$  phase (with four formula units per unit cell). The predicted transition temperature for the  $(\text{H}_2\text{S})_2\text{H}_2$  phase was  $T_c = 191$ – $204$  K at  $P = 200$  GPa.<sup>91</sup> On December 1, 2014, Drozdov *et al.*<sup>105</sup> reported a milestone experimental result on the observation of  $T_c \approx 190$  K in sulfur hydride compressed at  $P > 150$  GPa.

Another remarkable story should also be mentioned here, namely, the discovery of the  $Fm\bar{3}m$ – $\text{LaH}_{10}$  phase, for which  $T_c \cong 274$ – $286$  K at  $P = 210$  GPa was theoretically predicted by Liu *et al.*<sup>106</sup> in June 2017. This NRTS phase was experimentally discovered by Drozdov *et al.*<sup>107</sup> on August 21, 2018, and, two days later, Somayazulu *et al.*<sup>108</sup> confirmed this discovery.

## VI. CONCLUSIONS

In this study, we have proposed that hydrogen-rich superconductors exhibit a universal Fermi velocity  $v_F$ , which is given by empirical expression  $v_{F,\text{univ}} = (1/1.3) \times [2\Delta(0)/k_B T_c] \times 10^5$  m/s. Considering that the gap-to-transition temperature ratio  $2\Delta(0)/k_B T_c$  in hydrogen-rich superconductors varies within the range  $3.2 \leq 2\Delta(0)/k_B T_c \leq 5.0$ , we conclude that  $v_{F,\text{univ}}$  varies within the range  $2.5 \times 10^5$  m/s  $\leq v_{F,\text{univ}} \leq 3.8 \times 10^5$  m/s.

The Debye temperature  $T_\theta$  can be deduced from the temperature-dependent resistance  $R(T)$  of the conductor,<sup>69,83,84</sup> and so this universal Fermi velocity  $v_F$  in superhydrides [Eq. (16)] can be used to calculate the ratio  $\hbar\omega_D/E_F$ , which determines the strength of nonadiabatic effects in the superconductor. Calculations for metallic hydrogen phase III (compressed at  $P = 402$  GPa) have shown that  $\hbar\omega_D/E_F = 0.3$ , which implies strong nonadiabatic effects in this metal.

## SUPPLEMENTARY MATERIAL

See the [supplementary material](#) for the  $B_{c2}(T)$  fits to Eq. (11) for highly compressed superhydrides.

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## AUTHOR DECLARATIONS

### Conflict of Interest

The author has no conflicts to disclose.

### Author Contributions

**Evgeny F. Talantsev:** Conceptualization (lead); Data curation (lead); Formal analysis (lead); Investigation (lead); Methodology (lead); Validation (lead); Visualization (lead); Writing – original draft (lead); Writing – review & editing (lead).

### DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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