High-temperature superconductivity on the verge of a structural instability in lanthanum superhydride

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The possibility of high, room-temperature superconductivity was predicted for metallic hydrogen in the 1960s. However, metallization and superconductivity of hydrogen are yet to be unambiguously demonstrated and may require pressures as high as 5 million atmospheres. Rare earth based “superhydrides”, such as LaH10, can be considered as a close approximation of metallic hydrogen even though they form at moderately lower pressures. In superhydrides the predominance of H-H metallic bonds and high superconducting transition temperatures bear the hallmarks of metallic hydrogen. Still, experimental studies revealing the key factors controlling their superconductivity are scarce. Here, we report the pressure and magnetic field dependence of the superconducting order observed in LaH10. We determine that the high-symmetry high-temperature superconducting Fm-3m phase of LaH10 can be stabilized at substantially lower pressures than previously thought. We find a remarkable correlation between superconductivity and a structural instability indicating that lattice vibrations, responsible for the monoclinic structural distortions in LaH10, strongly affect the superconducting coupling.
For phonon-mediated superconductors, a high transition temperature necessitates light atomic masses. The lightest atom available to compose a crystal lattice is hydrogen, which forms covalently bonded molecular dimmers under ambient conditions. Transforming pure molecular hydrogen, with the aid of pressure, into a metal with an atomic lattice and into a superconductor has been a long-standing challenge and the subject of contention for the high-pressure community. Yet, chemical pre-compression with certain elements reduces the pressure required for metallization; thus, stable hydrogen-rich phases can be synthesized by the current high-pressure technology. With the discovery of a superconducting transition at the critical temperature $T_c = 203$ K in H$_3$S at 150 GPa\(^1\), the search for hydrogen-rich high-temperature superconductors (HTSs) has intensified, with the recent report of room-temperature superconductivity in C-S-H system with a maximum $T_c$ of 288 K\(^2\). A new family of rare-earth hydrides, such as LaH$_{10}$\(^3,4\) and YH$_6$\(^5\), opened a path to a significant increase in $T_c$, which is predicted to reach 305–326 K in YH$_6$\(^6\).

While in H$_3$S the crystal lattice is formed by H-S covalent bonds, LaH$_{10}$ forms a clathrate-like structure, where each La atom is locked at the center of a H$_3$S hydrogen cage. The interatomic distances between hydrogen atoms in LaH$_{10}$ are close to the H–H distance predicted for atomic metallic hydrogen near $p = 500$ GPa\(^6\). Due to the short H–H distances and the high hydrogen content, LaH$_{10}$ can be considered as “doped” metallic hydrogen. A pronounced isotope effect on $T_c$ when hydrogen is substituted by its heavier isotope deuterium, confirmed that the superconductivity in HTS hydrides is induced by electron–phonon interactions\(^7\). However, there is a dearth of experimental studies on HTS hydrides due to the very limited number of measurement techniques available at such extreme pressures. Here we explore the superconductivity and the structure of the lanthanum hydride family over a wide range of pressures, temperatures, and magnetic fields. We find that superconductivity in LaH$_{10}$ is strongly affected by a crystal lattice instability toward symmetry-lowering distortions. A similar dramatic change in the $T_c(p)$ dependence for another HTS hydride H$_3$S was also linked to a structural phase transition\(^8-11\). The present study firmly establishes the connection between HTS and soft phonon modes that are responsible for the structural instability in hydrides.

**Results and discussion**

The relation between crystal structure and superconductivity. Metallic lanthanum readily reacts with hydrogen at high pressures and temperatures yielding the clathrate-like superhydride LaH$_{10}$. We found that the superconducting $Fm-3m$ phase of LaH$_{10}$ can be synthesized at pressures much lower than ~150–170 GPa\(^3,4,12,13\) as reported earlier. Specifically, the powder X-ray diffraction data show that the sample prepared in the present study under 138 GPa is comprised of the dominant $Fm-3m$ phase of LaH$_{10}$. The minor impurity phases are attributed to two hexagonal close-packed (hcp) phases with the P6$_3$/mmc space group but with a different c/a ratio (~1.63 for hcp-I and ~1.48 for hcp-II) and a composition close to LaH$_{10}$ (Fig. 1). Both impurity phases were also found in various samples prepared via the direct chemical reaction between hydrogen and lanthanum or lanthanum trihydride in the previous work\(^6\) and did not distinctly affect the $T_c$ of the superconducting $Fm-3m$ phase, which has the highest $T_c$ in the lanthanum–hydrogen system\(^9\).

The persistence of the high-pressure, high-symmetry phase of LaH$_{10}$ at pressures as low as 138 GPa corroborates recent theoretical calculations that take quantum effects into account\(^14,15\). In contrast to the classical ab initio calculations\(^8,14,15\), which predict structural distortions in the $Fm-3m$ LaH$_{10}$ below ~230 GPa, the inclusion of the zero-point energy stemming from quantum atomic fluctuations lowers the enthalpy of the high-symmetry phase and stabilizes it at pressures as low as 129 GPa\(^14\).

The LaH$_{10}$ sample under 138 GPa still exhibits a narrow superconducting transition toward zero resistance with a high $T_c$ of 243 K, slightly lower than the maximum $T_c$ of ~250 K reported for LaH$_{10}$ at ~150–170 GPa\(^3,14,13\), in accordance with a “dome-shape” pressure dependence of $T_c$ for the $Fm-3m$ phase of LaH$_{10}$\(^3\). No intrinsic hysteresis between cooling and warming $R(T)$ curves was observed (Supplementary Fig. 1). The resistivity $p$ of LaH$_{10}$ is estimated to be $(0.3 \pm 0.1) \text{ m}\Omega\cdot\text{cm}$ at $T = 300$ K and is higher than the value reported for H$_3$S\(^16\). The large error bar is mainly due to the uncertainty on the thickness of the sample.

After the abrupt decompression from 138 to 120 GPa, some reflections from the ancestral cubic phase became split (Fig. 1) and the $T_c$ dropped to 191 K (Fig. 2). The powder X-ray diffraction patterns of the new distorted phase can be reasonably indexed within the $C2/m$ space group (Fig. 1b). The refined cell parameters and the coordinates of the heavier La atoms in a good agreement with theoretical models for the $C2/m$ LaH$_{10}$ phase\(^14,17,18\). According to the theoretical calculations\(^14\), the monoclinic scenario of the structural distortions is energetically more favorable than two alternative orthorhombic and rhombohedral distortions of the $Fm-3m$ phase of LaH$_{10}$ on decompression.

We found that these monoclinic structural distortions are reversible, and the high-symmetry phase can be restored if the pressure is increased. The observed $T_c$ increases rapidly within a short pressure range with increasing pressure and reaches 241 K at 136 GPa (Fig. 2a). The broadening of the superconducting transition in Fig. 2a is likely caused by the deterioration of the phase crystallinity during variations of the pressure. The continuous change of the lattice volume during the $Fm-3m$–$C2/m$ phase transition is in close agreement with both the experimental\(^3\) and theoretical\(^19\) equations of state for LaH$_{10}$ indicating the retention of the LaH$_{10}$ composition (Supplementary Fig. 2). In addition, predictions suggest that the composition should not change during any structural distortion scenario for the $Fm-3m$ phase of LaH$_{10}$ upon decreasing pressure\(^14,17,18\).

The pressure dependence of $T_c$ in Fig. 2 displays two distinct regions—a low-pressure region characterized by a sharp rise in $T_c$, and a high-pressure region with a much more moderate dome-like $T_c(p)$ dependence, with a clear boundary between the two regions at 135 GPa. This distinct shape in $T_c(p)$ in LaH$_{10}$ closely resembles the $T_c$ variation first discovered in the hydride H$_3$S, where a sharp but continuous drop in $T_c$ was attributed to the change of the crystalline structure\(^8,10,11\). Multiple distorted hydrogen arrangements from a high-symmetry $Fm-3m$ phase are predicted for LaH$_{10}$ as well\(^14\). One of the predictions reports a stable LaH$_{10}$ $Fm-3m$ phase at high pressures, with symmetric H positions and a $T_c$ of 259 K at 170 GPa. The drop in pressure is predicted to stabilize a distorted $R-3m$ phase of LaH$_{10}$ with $T_c = 206$ K at 150 GPa\(^18\). A $T_c$ ~ 229–245 K was calculated for the $C2/m$ phase, although the calculations were performed for $p = 200$ GPa, which is substantially higher than the values presented here\(^17\).

The softening of lattice vibrations. A likely explanation for the drastic change in the dependence of $T_c$ with pressure <135 GPa is a structural phase transition in LaH$_{10}$. The lack of a discontinuous jump in $T_c$ in LaH$_{10}$ and in H$_3$S\(^8,10\) points to a continuous symmetry-lowering lattice distortion or a phase transition of the second order or weakly first order. We calculated phonon dispersion relations for the high-symmetry $Fm-3m$ and distorted $C2/m$ phases of LaH$_{10}$ and identified the lattice vibrations that soften upon decompression and can be linked to the
Fig. 1 Structural data for LaH$_{10}$ synthesized from La and excess H$_2$. a, b Rietveld refinement for Fm-3m phase of LaH$_{10}$ at 138 GPa and C2/m phase of LaH$_{10}$ at 120 GPa, respectively. The peaks originating from the hcp-I (a = 3.668(4) Å; c = 5.914(11) Å; V = 68.9(1) Å$^3$ at 138 GPa) and hcp-II (a = 3.750(3) Å; c = 5.561(7) Å; V = 67.7(1) Å$^3$ at 138 GPa) impurity phases are indicated through blue and red dashes, respectively. The refined ratio between the main and the impurity phases is provided in the left bottom corner of each figure. The main structural building block, two connected LaH$_{32}$ polyhedra, are shown in the middle inserts for each phase. Large blue and small black spheres correspond to La and H atoms, respectively. c, d The original powder X-ray diffraction patterns at 138 and 120 GPa, respectively. New reflections appear at 120 GPa due to the monoclinic distortions.

Fig. 2 The superconducting transitions in LaH$_{10}$. a The electrical resistance in LaH$_{10}$ after the synthesis under 138 GPa (red curve), after the abrupt decompression down to 120 GPa (brown curve), and upon a gradual increase in pressure from 120 to 136 GPa (blue, green, purple, and black curves). The data measured at 138 GPa on the upper panel are divided by 9 for better presentation. b Pressure dependence of $T_c$ in LaH$_{10}$ measured in the present study (black symbols) and from a prior study$^3$ (open red symbols). Insets: photos of the DAC loaded with a La flake and after the synthesis of LaH$_{10}$ through laser-assisted heating.
dashed lines extrapolate the slope of the high-temperature superconducting transition (left line) toward the asymptotic trace representing the high-field normal state magnetoresistance (right line) at 170 K, respectively. The intersection between two lines provides an estimation of the upper critical field ($H_{c2}$). The intersection of the first line with the horizontal axis indicates the irreversibility field ($H^*$) for the high-temperature superconducting phase.

**Table 1** Summary of sample properties and the associated WHH fit parameters: the critical temperature, the upper critical field at $T=0$ K, coherence length at $T=0$ K, BCS Fermi velocity, calculated bare-band Fermi velocity, and the slope of $H_{c2}$ at the critical temperature.

| Sample structure | $p$ (GPa) | $T_c$ (K) | $H_{c2}(0)$ (T) | $\xi(0)$ (nm) | $BCS \, \nu_F \times 10^5$ m/s | Band $\nu_F \times 10^5$ m/s | $dH_{c2}/dT|_{Tc}$ (T/K) |
|------------------|-----------|-----------|----------------|--------------|-----------------------------|-----------------------------|--------------------------|
| C2/m LaH$_{10}$ | 120       | 189       | 133.5          | 1.57         | 2.17                        | 3.73                        | −1.12                    |
| Fm-3m LaH$_{10}$| 136       | 246       | 143.5          | 1.514        | 2.77                        | 4.99                        | −0.83                    |

observed lattice distortion (Supplementary Fig. 4). The calculated phonon dispersions show that the Fm-3m phase is dynamically stable at 200 GPa. However, the softening of the low-lying H-H “wagging” vibration modes along the Γ–X direction is found in the phonon spectrum (Supplementary Figs. 4 and 5), which leads to a structural instability toward the monoclinic C2/m distortion. The classical harmonic treatment of atomic vibrations for the Fm-3m phase of LaH$_{10}$ shows negative phonon frequencies at pressures <180 GPa.

The transformation of the crystallographic structure from a higher- to a lower-symmetry phase is governed by the phonon softening in the vicinity of a structural transition has been reported in a number of superconducting families, ranging from Sn nanostructures, A15 compounds, intercalated graphite, ternary silicides, and even some elements under pressure. The symmetry-lowering distortion in the H sub-lattice in LaH$_{10}$ is driven by the softening of the low-lying H-H vibration modes below 500 cm$^{-1}$ (Supplementary Figs. 4 and 5), leading to a stronger electron–phonon interaction in the Fm-3m phase, which is characterized by a coupling constant $\lambda = 2 \int_0^\infty \alpha^2 F(\omega) \omega^{-1} \, d\omega$, where $\omega$ is the phonon frequency, $F(\omega)$ is the phonon density of states, and $\alpha^2$ is an average square electron–phonon matrix element. While the light atomic mass of hydrogen is a necessary requirement for phonon-coupled HTS, $T_c$ is also strongly affected by $\lambda$, with a peak in $T_c$ predicted for large $\lambda \sim 2–2.5$, which should occur in the vicinity of the lattice instability in HTS hydrides.

**Lattice distortion effect on superconducting parameters.** The impact of the structural instability on the key parameters of the superconducting phase, including the upper critical field, $H_{c2}$, and the superconducting coherence length, $\xi$, for the Fm-3m and C2/m phases of LaH$_{10}$ was confirmed through magnetotransport measurements. The samples were electrically connected in a van der Pauw configuration (Fig. 2c, inset), making the measurements of both resistivity and Hall effect possible. The LaH$_{10}$ sample under 120 GPa was measured up to 45 T in direct current (DC) magnetic fields, and the LaH$_{10}$ sample under 136 GPa was measured in a 65 T pulsed magnet.

The magnetoresistance (MR) of LaH$_{10}$ collected at fixed temperatures is shown in Fig. 3. Under external magnetic fields, the superconducting transitions span tens of teslas, which correlates with the broadening of the superconducting transition at zero field (Fig. 2a). The normal state MR above $H_{c2}$ is nearly field and temperature independent, with a clear kink at the onset of superconductivity at $H_{c2}$. For the consistency with prior studies, the $H_{c2}$ values are determined as the intersection between the straight line extrapolations of the normal state MR and the slope of the superconducting transition by a method similar to the one followed in ref. 16. The irreversibility field of the high-temperature superconducting phase ($H^*$) is taken by extrapolating the leading edge of the transition to the horizontal axis (Supplementary Fig. 6). The Hall resistance signal measured above $T_c$ is consistent with the electron-like Fermi surface (Supplementary Fig. 7).

Upper critical field measurements in H$_2$S HTS hydride have independently verified a large $\lambda \sim 2$16. We find a substantially larger $H_{c2}$ for LaH$_{10}$ and determined that magnetic fields of the order of 100 T are required to distinguish between a strongly coupled scenario with a large $\lambda$ and the more commonly employed Werthamer–Helfand–Hohenberg (WHH) model derived in the weakly coupling limit, $\lambda \ll 1$131. To extract the key superconducting properties of LaH$_{10}$ and explore the effects of the structural transition on its superconductivity, we fit the temperature dependence of $H_{c2}$ to the WHH (Fig. 3c and Table 1) formalism. The WHH model fits our data well for fields up to 60 T, which is our upper measurement limit. The WHH model considers the combined effects of the magnetic field on the orbital motion and on the spin of the electrons: $H_{c2}^2 = H_{orb}^{-2} + H_{p}^{-2}$. The transformation of the crystallographic structure from a higher- to a lower-symmetry phase is governed by the phonon softening in the vicinity of a structural transition has been reported in a number of superconducting families, ranging from Sn nanostructures, A15 compounds, intercalated graphite, ternary silicides, and even some elements under pressure. The symmetry-lowering distortion in the H sub-lattice in LaH$_{10}$ is driven by the softening of the low-lying H-H vibration modes below 500 cm$^{-1}$ (Supplementary Figs. 4 and 5), leading to a stronger electron–phonon interaction in the Fm-3m phase, which is characterized by a coupling constant $\lambda = 2 \int_0^\infty \alpha^2 F(\omega) \omega^{-1} \, d\omega$, where $\omega$ is the phonon frequency, $F(\omega)$ is the phonon density of states, and $\alpha^2$ is an average square electron–phonon matrix element. While the light atomic mass of hydrogen is a necessary requirement for phonon-coupled HTS, $T_c$ is also strongly affected by $\lambda$, with a peak in $T_c$ predicted for large $\lambda \sim 2–2.5$, which should occur in the vicinity of the lattice instability in HTS hydrides. The classical harmonic treatment of atomic vibrations for the Fm-3m phase of LaH$_{10}$ shows negative phonon frequencies at pressures <180 GPa.

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where \( H_{orb} \) and \( H_p \) are the orbital-limited and spin-limited (Pauli) critical fields, respectively. We obtain \( H_p(0) \) values of 352 T at 120 GPa and 457 T at 136 GPa. \( H_p(0) \) values are larger by a factor of ~3 when compared to the \( H_c(0) \) values listed in Table 1, indicating predominantly orbital-limited upper critical fields in HTS LaH\(_{10}\), which is similar to H\(_3\)S\(_{16}\). The WHH fit provides a reasonable estimate of the superconducting coherence length \( \xi = \sqrt{\phi_0/2\pi H_c} \), where \( \phi_0 \) is the magnetic flux quantum. There is a significant drop in \( T_c \) in the distorted phase of LaH\(_{10}\) at 120 GPa when compared to the LaH\(_{10}\) sample at 136 GPa. Surprisingly, \( H_c(0) \) only drops by a small amount and thus \( \xi(0) \) remains nearly unchanged. \( \xi \) is linked to both \( T_c \) and the Fermi velocity \( v_F : \xi \sim \sqrt{\phi_0/k_B T_c} \) within the BCS theory\(^6\), but the \( \xi \sim v_F/T_c \) rule should remain valid for other models, thus signaling a lower value for \( v_F \) in the \( C2/m \) phase at 120 GPa when compared to that in the \( Fm-3m \) phase at 136 GPa. The onset of the lattice distortion is expected to be strongly affected by the electron dispersion, e.g. via the flattening of the bands at the boundaries of the new Brillouin zone, which may lead to a drop in \( v_F \) so that \( \xi \) and \( H_c \) remain high despite the drop in \( T_c \) in the \( C2/m \) phase. We calculated the \( v_F \) values along the Fermi surfaces in the first Brillouin zone for both \( C2/m \) and \( Fm-3m \) phases (Fig. 4a). The average calculated \( v_F \) values are listed in Table 1 alongside with the BCS values obtained from \( H_c(0) \). The calculated \( v_F \) values are larger than BCS values mainly because the calculations do not account for the renormalization of the bare-band \( v_F \) due to electron–phonon coupling. Nevertheless, the model provides a more reliable estimate of the relative change in \( v_F \). The calculations confirm a ~30% drop in \( v_F \) in the \( C2/m \) phase as observed in the high-field experiments. A comparative review of the \( v_F \) values for other hydrogen-rich HTS families, which can be extracted from the published \( H_c \) data, as well as the present study, reveal a surprisingly narrow distribution close to ~2.5 × 10\(^5\) m/s (Fig. 4b). A similar universal Fermi velocity was first noticed in the HTS cuprates, with a surprisingly similar average value of ~2.7 × 10\(^5\) m/s\(^3\)\(^2\). This similarity points to a renormalization of the charge carrier band dispersion both in the cuprates and in the hydrides via a strong coupling to low-lying excitations near the Fermi level, the same coupling that is commonly considered to be responsible for the high-temperature superconductivity.

In conclusion, we have measured the properties of the superconducting LaH\(_{10}\) compound as a function of pressure, temperature, and high magnetic fields. We find evidence for a pressure-induced \( Fm-3m \rightarrow C2/m \) structural transition in LaH\(_{10}\) at \( p_c = 135 \) GPa, resulting in a steep but continuous decrease in \( T_c(p) \) below \( p_c \). A likely mechanism for the structural instability is phonon softening associated with a gradual distortion of the lattice, as proposed for another HTS hydride H\(_3\)S. We established key superconducting quantities of superhydrides under high magnetic fields, including upper critical fields and coherence lengths. We found that the drop in the Fermi velocity in LaH\(_{10}\) is consistent with the distortion-induced changes in the Brillouin zone. The proximity of a peak in \( T_c \) to a symmetry-lowering structural transition, which is now experimentally established for at least two HTS hydride families, indicates that the tuning of the soft phonon modes should be viewed as one of the main pathways toward maximizing \( T_c \) in the hydrogen-rich superconductors.

**Methods**

**Diamond anvil cell.** The superconducting sample of LaH\(_{10}\) were synthesized in situ in a miniature diamond anvil cell (DAC) with a maximum diameter of 8.8 mm and a body length of ~30 mm. The DAC was designed by reworking and modifying the
Zero field electrical transport measurements. Zero field electrical resistance was measured through a four-probe technique in van der Pauw geometry with currents ranging from $10^{-4}$ A to $10^{-3}$ A at $p = 138$ GPa to $136$ GPa. No apparent effect of the current value on the measured $T_c$ was observed. The electrical measurements are presented in a warming part of a thermal cycle as it yields a more accurate temperature reading: the sample was warmed up slowly (0.2 K/min) under nearly isothermal environmental conditions (no coolant flow). The temperature measured by a Si diode thermometer attached to the DAC with an accuracy of ±1 K. $T_c$ was determined at the onset of superconductivity—at the point of apparent deviation in the temperature dependence of the resistance from the normal metallic behavior.

Magnetotransport measurements. MR and Hall effect measurements under high magnetic fields were conducted in the 45 T hybrid magnet and in the 65 T pulsed magnet at the National High Magnetic Field Laboratory. A copper thermal shield was placed around the DAC during DAC field measurements. The thermal shield was heated uniformly to reduce the thermal gradients, and a secondary Cernox thermometer was attached to the DAC stage for accurate measurements of the sample temperature. There is no observable heating from the ramping of the magnetic field rates up to 3 T/min. The Hall effect was measured for the sample at 120 GPa above $T_c$ in the hybrid DC magnet from 11.5 to 45 T. Reverse-field reciprocity method was employed to determine Hall resistance $R_{xy}$ because the field direction of the hybrid magnet cannot be reversed during the day shift. A high-frequency (290 kHz) lock-in amplifier technique was employed to measure sample MR in 65 T pulsed magnet. AC field measurements were performed using DFT using the Perdew–Burke–Ernzerhof generalized gradient approximation. Phonon dispersion calculations were performed with the density functional perturbation theory. Ultrasonic pseudopotentials for La and H were used with a kinetic energy cutoff of 80 Ry. To reliably calculate the phonon dispersion, we have employed dense $k$-meshes and $q$-meshes for all the phonon frequencies: 8 x 8 x 4 k-meshes and 4 x 4 x 2 q-meshes for the C2/m-LaH$_{10}$ structure and 12 x 12 x 12 $k$-meshes and 6 x 6 x 6 $q$-meshes for the Fm-3m-LaH$_{10}$ structure. The visualization of the atomic vibrations was done by using a visualization tool (http://henriqemiranda.github.io/phono2e.html). For visualizations in three-dimensions of the Fermi surfaces associated with the electronic states on the Fermi surfaces in the first Brillouin zone, we have used FermiSurfer open software drawing code (http://fermisurfer.osdn.jp/).

Data availability
The data that support the findings of this study are available in Open Science Framework with the identifier: https://doi.org/10.17605/OSF.IO/RUIWJA. Source data are provided with this paper.

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Author contributions

D.S., V.S.M. and F.F.B. designed the research and wrote the paper; V.S.M. prepared the samples, collected synchrotron X-ray diffraction data, performed electrical transport measurements without external magnetic field, and processed the structural data; D.S., F.F.B., S.M., L.B. and M.J.E. performed electrical transport measurements under external magnetic fields and processed the data; D.S., F.F.B., S.M. and V.B.P. assisted with the synchrotron X-ray diffraction experiments; Y.S. and Y.M. performed structural relaxation, electronic structures, and phonon calculations. M.J.E. designed the diamond anvil cell. All authors contributed to writing the paper.

Competing interests

The authors declare no competing interests.

Additional information

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