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ESRF HIGHLIGHTS 2021

Towards a better understanding of high-temperature superconductivity in superhydrides at ultrahigh pressures

The search for room-temperature superconductors is one of the most important problems in physics. Recently, high-temperature superconductivity was demonstrated in superhydrides at ultrahigh pressures. XAS, XRD and Raman measurements at 180 GPa were combined to elucidate the nature of pressure-induced rearrangements in the electronic and atomic structure in YH_3.

Searching for new high-temperature superconductors is one of the most important problems in physics and chemistry. For decades after the discovery of cuprates in 1986, only unconventional superconductors (SC) that do not follow the theory developed by J. Bardeen, L. Cooper, and R. Schrieffer (BCS) had shown high-temperature superconductivity. In 2015, the record critical temperature (Tc) for SC of 203 K in hydrogen sulfide at 160 GPa was observed **[1]**, suggesting that room-temperature superconductivity described by the BCS-Eliashberg theory is realistic. Soon afterwards, nearly room-temperature SC at 250 K in LaH_{10} **[2]** and at 243 K in YH_9 **[3]** was discovered at a pressure above 200 GPa. Even higher Tc above room temperature is predicted for YH_{10} **[4]** and Li_2MgH_{16} **[5]**.

These new findings urged for a better understanding of hydrogen interaction mechanisms with the heavy atom sublattice in metal hydrides under high pressure at the atomic scale. Therefore, the pressure-induced rearrangements of the electronic and atomic structure at the local and bulk scale, which may inhibit or favour superconductivity, were studied in the archetypal metal hydride YH_3 (**Figure 19**).

X-ray absorption spectroscopy (XAS) and X-ray diffraction (XRD) measurements carried out at beamline **BM23** were combined with Raman spectroscopies to study YH_3 under ultrahigh pressures up to 180 GPa, and also at low temperatures (10-300 K, 39 GPa). High-pressure Y K-edge extended X-ray absorption fine structure (EXAFS) data on YH_3 were collected up to 180 GPa in a diamond anvil cell equipped with nano-polycrystalline diamonds, ensuring glitch-free signals with a high signal-to-noise ratio up to $16.5 Å^{-1}$ in momentum space. Complementary XRD data were acquired sequentially to probe the phase transitions and lattice parameter evolutions (**Figure 20**).

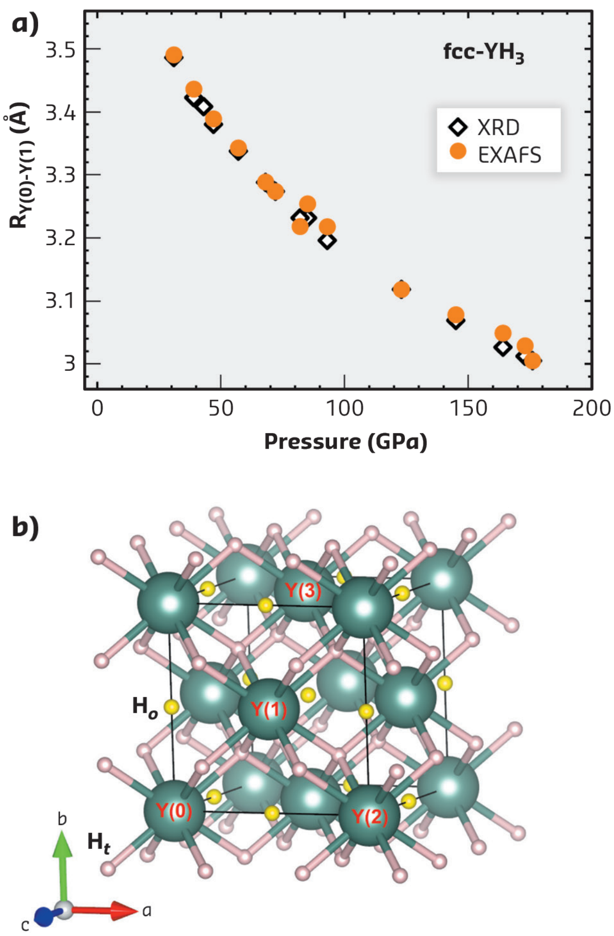
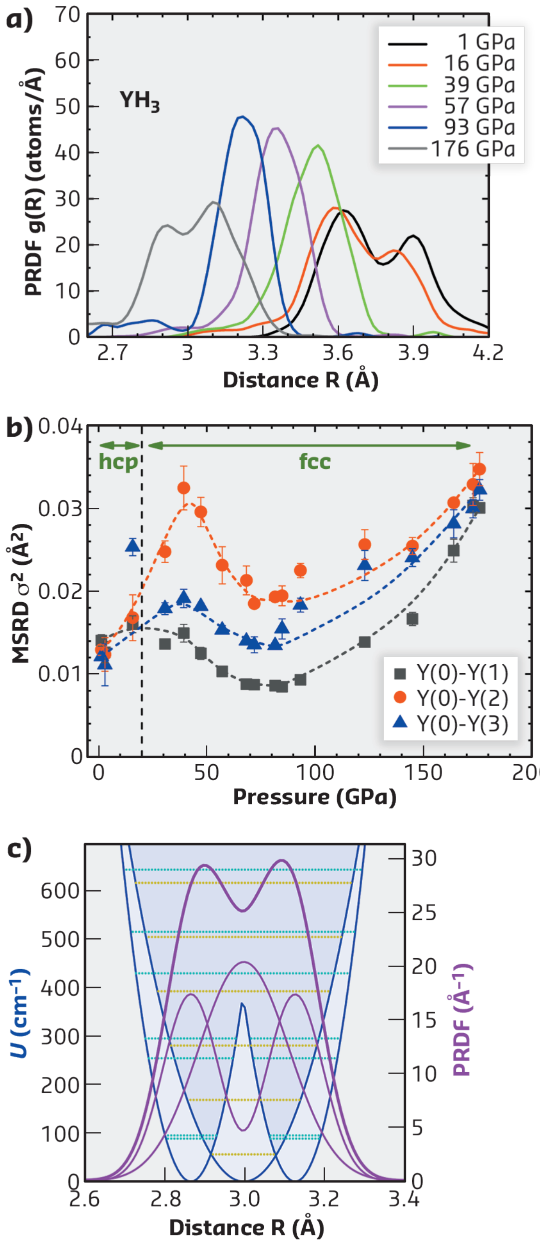


Fig. 19: a) Pressure dependence of the interatomic distance R(Y0)-(Y(1)) for fcc YH_3 obtained from XRD versus EXAFS data. **b)** Structure of the metal hydride YH_3.

Fig. 20: a) Pressure dependences of pair radial distribution function (PRDF) of the first Y(0)-Y(1) shell at different pressures up to 176 GPa. **b)** Pressure evolution of the mean square relative displacement (MSRD) for the three nearest Y-Y shells around Y(0) atoms. **c)** Double-well vibrational potential of Y atoms at 176 GPa.



The combination of the experimental methods made it possible to implement a multiscale length study of YH_3, covering short-, medium- and long-range. X-ray absorption near-edge structure (XANES) data demonstrate a strong effect of hydrogen on the density of 4d yttrium states that increases with pressure, and EXAFS data evidence a strong anharmonicity, manifested as yttrium atom vibrations in a double-well potential. The crystal lattice instability arising due to the Jahn-Teller effect was found to manifest itself as local (short-range) lattice distortions, which inhibit superconductivity in YH_3 at low pressures. That, in turn, reconciles many controversies observed previously in this compound and provides valuable information concerning the nearly room-temperature superconductivity recently found at high pressures. These results will contribute to a better understanding of the hydrogen interaction mechanism with the heavy atom sublattice and high-temperature superconductivity in metal hydrides.

More recently, yttrium hydrides with the compositions of YH_6 and YH_9 were synthesised in a diamond anvil cell, and superconductivity in the YH_6 and YH_9 phases was demonstrated with a maximal Tc of ~220 K at 183 GPa and ~243 K at 201 GPa, respectively. Further work at beamline **BM23** has focused on carrying out XRD and XAS measurements on these samples under ultrahigh pressure.

PRINCIPAL PUBLICATION AND AUTHORS

Local electronic structure rearrangements and strong anharmonicity in YH_3 under pressures up to 180 GPa, J. Purans (a,b), A.P. Menushenkov (b), S.P. Besedin (c), A.A. Ivanov (b), V.S. Minkov (c), I. Pudza (a), A. Kuzmin (a), K.V. Klementiev (d), S. Pascarelli (e,f), O. Mathon (e), A.D. Rosa (e), T. Irifune (g), M.I. Eremets (c), *Nat. Commun.* **12**, 1765 (2021); https://doi.org/10.1038/s41467-021-21991-x
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