REPORT

MA-4601 “Structural Investigation of Novel Ternary Hydrides - Near Room-temperature Superconductors”

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Research goals

Within this proposal, we planned to study the crystal structure of ternary superconducting hydrides: La-Y-H, Mg-Y-H, Ca-Y-H. We expected that the crystal structure of these ternary polyhydrides will be determined for the first time. We planned to confirm formation of cubic $CaYH_{12}$, $LaYH_{12}$ and $Y_xMg_{1-x}H_6$, as well as non-stoichiometric ternary hydrides, in accordance with the results of computer modelling.

Results

Diamond anvil cells (DACs) loaded by (Mg,Y)-H and (Ca,Y)-H samples were broken during laser heating or a few days later, before its sending to ESRF. Four DACs loaded by $La_xY_{(1-x)}$-H turned to be more stable and crashed only after the one day of XRD measurements at the ID15B beamline. Four measured DACs (named M1, M2, SL1 and SL3) had the following parameters:

DAC	Pressure, GPa	Sample size, µm	Sample
M1	180	30	LaY/BH_3NH_3
M2	180	32	La_2Y/BH_3NH_3
SL1	180	29	La_4Y/BH_3NH_3
SL3	170	29	Y_4La/BH_3NH_3

The La-Y alloys for the loading of DACs were prepared by an arc melting (2000-2500 ^{o}C, 10 seconds) of La/Y pellets in Ar atmosphere at pressure of 6 bar. According to the results of scanning electron microscopy (SEM), X-ray diffraction and energy-dispersive analysis (EDX), the obtained alloys consisted of *hcp*-La_4Y (SL1), *hcp*-La_2Y (M2) and mixtures of La_2Y+Y_2La (M1) and La_2Y+Y_2La + Y (SL3).

Pulsed laser heating of La/Y micro samples, taken from obtained La/Y alloys and mixed with NH_3BH_3, was carried out at 1500-2000 K with duration of several microseconds. After the heating the La/Y particles expanded, became black, and the pressure in DACs, measured via both Raman signals of diamond and hydrogen, dropped to 180±2 GPa (M1, M2, SL1) and 170±2 GPa (SL3).

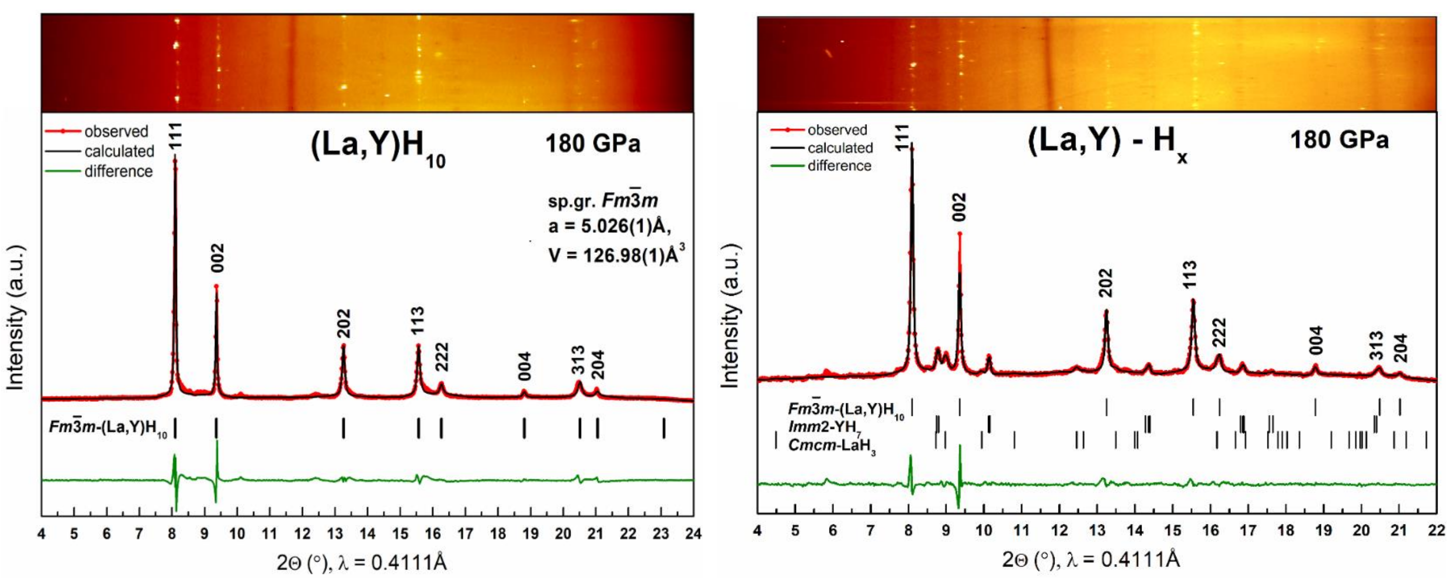

Figure 1. (Left) Le Bail refinement of the unit cell parameters of *Fm*-3*m*-$(La,Y)H_{10}$ sample in M2 DAC. (Right) LeBail refinement of the cell parameters of *Fm*-3*m*-$(La,Y)H_{10}$, *Imm2*-YH_7 and *Cmcm*-LaH_3 (M1 DAC).

Results of the synthesis were examined through powder X-ray diffraction of synchrotron radiation, wavelength of 0.4111 Å, at the ID15B ESRF beamline (Figure 1). In all 4 cells the main phase was *Fm*-3*m*-(La,Y)H_{10} with a cell volume by 0.5-0.83 Å^3 lower than the cell volume of *Fm*-3*m*-LaH_{10} at 170-180 GPa, respectively. This corresponds to the sample composition of La_3YH_{40} or $La_{0.75}Y_{0.25}H_{10}$, which is close to the loaded one (M2, SL1). The cleanest samples were in the DACs SL1 and M2, while in M1 and SL3 we have detected previously described impurities: pseudocubic *Imm2*-YH_7 (Figure 1, right chart) and, probably, *Cmcm*-LaH_3 (Figure 2).

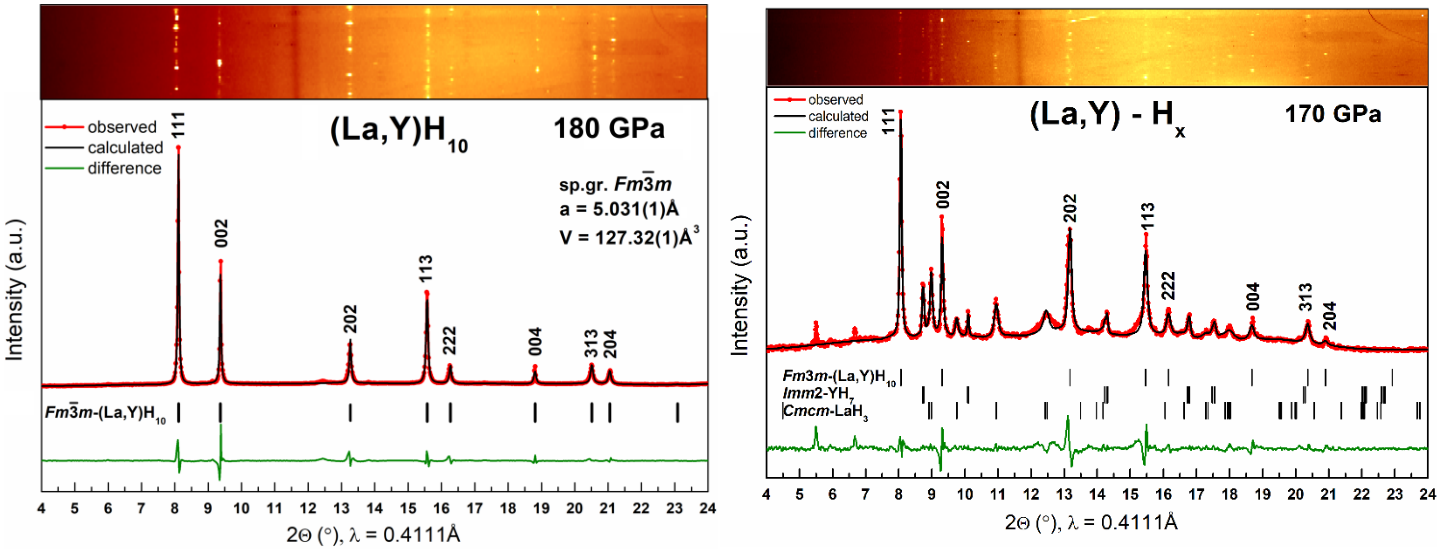

Figure 2. (left) Le Bail refinement of the unit cell parameters of *Fm*-3*m*-(La,Y)H_{10} sample in SL1. (Right) Le Bail refinement of the cell parameters of *Fm*-3*m*-(La,Y)H_{10}, *Imm2*-YH_7 and *Cmcm*-LaH_3 phases in SL3 DAC.

Experimental lattice parameters and unit cell volumes of $Fm\bar{3}m$-(La,Y)H_{10} (Z = 4), *Imm2*-YH_7 (Z = 2), and *Cmcm*-LaH_3 (Z = 4) are given below:

$Fm\bar{3}m$-(La,Y)H_{10}			
DAC	Pressure, GPa	*a*, Å	*V*, Å^3
M1	180	5.038(1)	127.86(2)
M2	180	5.026(1)	126.98(2)
SL1	180	5.031(1)	127.32(1)
SL3	170	5.071(1)	130.40(1)

$Imm2$-YH_7					
DAC	Pressure, GPa	*a*, Å	*b*, Å	*c*, Å	*V*, Å^3
M1*	166	3.29(4)	3.33(6)	4.68(7)	51.50
SL3	170	3.303(1)	3.322(2)	4.672(2)	51.25(2)
M1	180	3.279(2)	3.305(2)	4.641(2)	50.30(1)

$Cmcm$-LaH_3					
DAC	Pressure, GPa	*a*, Å	*b*, Å	*c*, Å	*V*, Å^3
M1	180	2.791(4)	10.492(5)	2.657(3)	77.83(2)
SL3	170	2.737(2)	10.507(3)	2.727(2)	78.44(3)

*Taken from previous investigation of Y-H system.

Conclusion: within this project, we were able to synthesize a ternary *fcc* lanthanum-yttrium superhydride (decahydride) La_3YH_{40}, in which about 25% of La atoms were replaced by Y atoms without changing the cubic structure of the hydrogen sublattice. The latter explains the high-temperature superconductivity observed for the synthesized samples.