Looking for ambient pressure superhydrides: application to the Y-Fe-H system

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Abstract

Computational studies have successfully predicted the dramatic uptake of hydrogen by metals under pressure, leading to the experimental synthesis of superhydrides. These materials demonstrate exceptional properties, such as high-temperature superconductivity, hydrogen storage and superionicity, like in LaH_{10} [1,2,3]. Up to now, most of the studies have been performed on binary hydrides in the 100 GPa range and none of the discovered superhydrides could be recovered at ambient pressure. Ternary hydrides offer possibilities to stabilize such superhydrides at ambient pressure, and potentially recover their properties [4]. While many ternary superhydrides have now been predicted by calculations, a frustratingly low number of them have actually been synthesized, and none of them were recovered at ambient pressure.

We have undertaken the search of ternary superhydrides in the system Y-Fe-H. Our experimental strategy relies on the use of pre-hydrogenated precursors $YFe_2H_{4.2}$ [5]. Our first experiments showed a spontaneous hydrogen uptake under pressure up to 50 GPa, which plateaued at YFe_2H_7 [6]. Subsequent laser heating at 80 GPa on these samples lead to the discovery of the superhydride $Y_3Fe_4H_{20}$ [7], whose full structure was obtained by coupling calculations and experiments. Remarkably, this compound remains metastable upon decompression down to ambient pressure for more than a day.

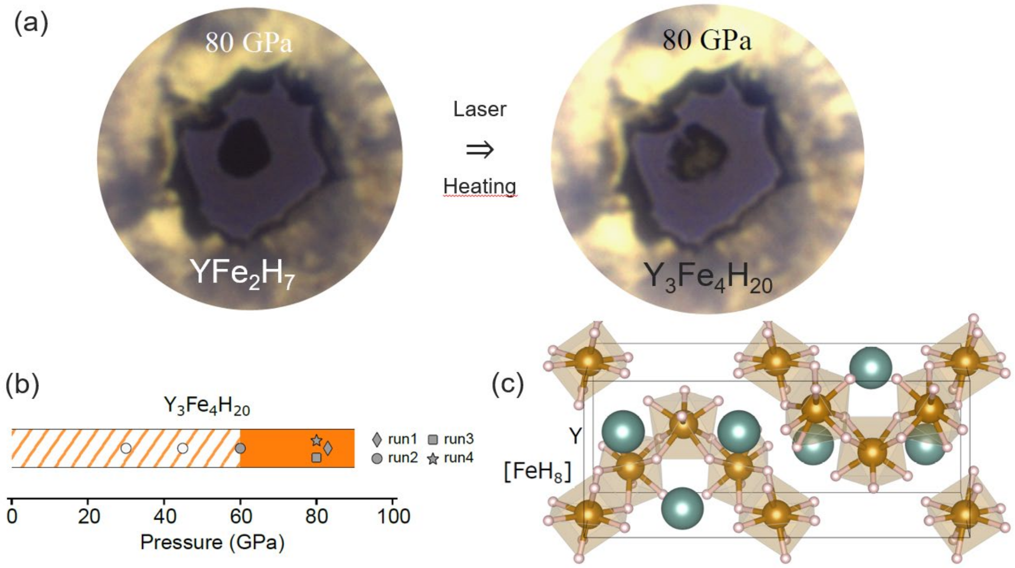

Figure 1: (a) Optical images taken before and after laser heating on a Y-Fe-H compound. (b) Stability (orange area) and metastability (dashed lines) phase diagram of $Y_3Fe_4H_{20}$, obtained after multiple heatings performed at different pressures. (c) Full structure of $Y_3Fe_4H_{20}$, which includes Y atoms and FeH_8 units.

References

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