Supplementary Materials: Hydrogen Sorption in Erbium Borohydride Composite Mixtures with $LiBH_4$ and/or LiH

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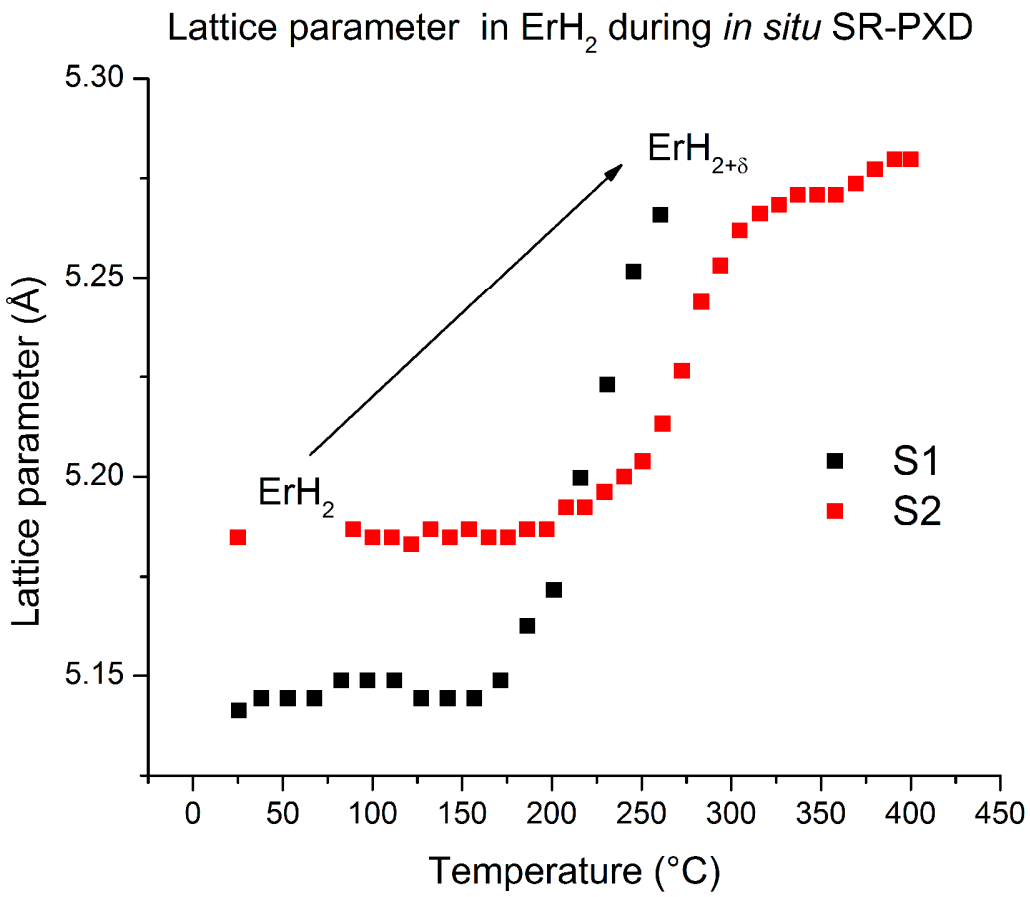

Figure S1. SR-PXD data of thermal desorption of S1 and S2. Shown is the increasing lattice parameter of ErH_2 for S1 (black curve) and S2 (red curve). Reason of the increase in lattice parameter is probably a hydrogenation reaction of ErH_2 to $ErH_{2+\delta}$ with ($0 \leq \delta \leq 1$), possibly ErH_3, rather than pure thermal expansion. λ = 0.77787 Å.

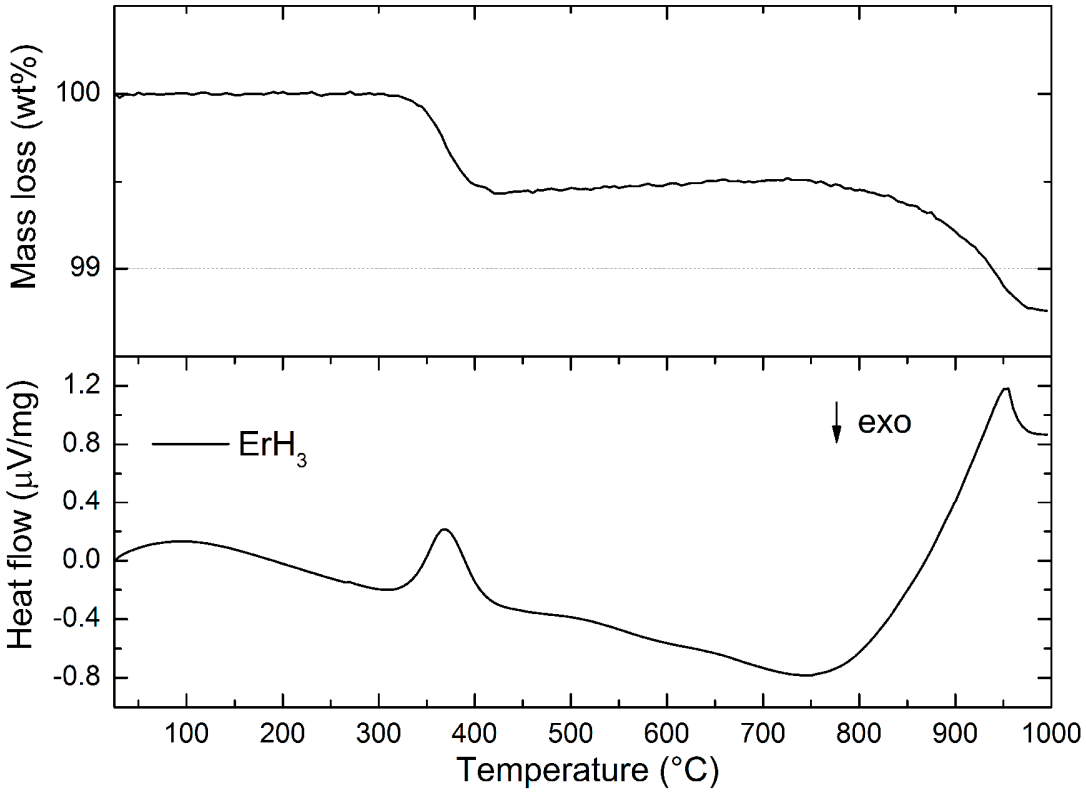

Figure S2. TG-DSC data of pure ErH_3 between 25 and 1000 °C. The first endothermic peak corresponds to the reduction of ErH_3 to ErH_2 and is consistent with the weight loss. The second endothermic peak corresponds to the reduction of ErH_2 to Er and is also consistent with the weight loss.

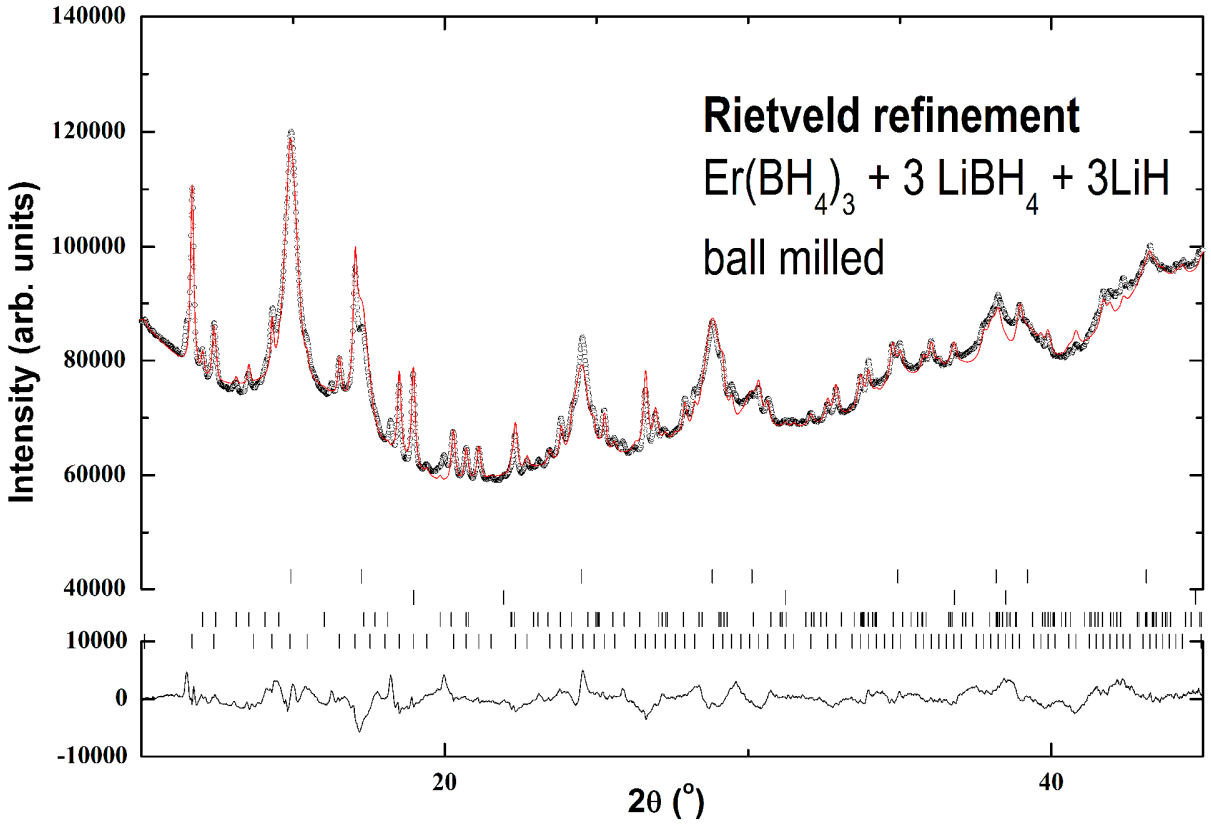

Figure S3. SR-PXD Rietveld refinement and difference plot of S2 after ball milling and storage in Argon atmosphere for 9 month. Observed (circles) and calculated (red line) patterns and difference plot (below). Vertical tick marks for the Bragg peak positions for (from top): 1. *c*-ErH_3 with 32.1(1) wt% 2. LiH with 0.0(9) wt% 3. $LiBH_4$ with 38.2(16) wt%, 4. $Er(BH_4)_3$ with 29.7(1) wt%; R_{wp} = 1.33%. λ = 0.7778 Å.

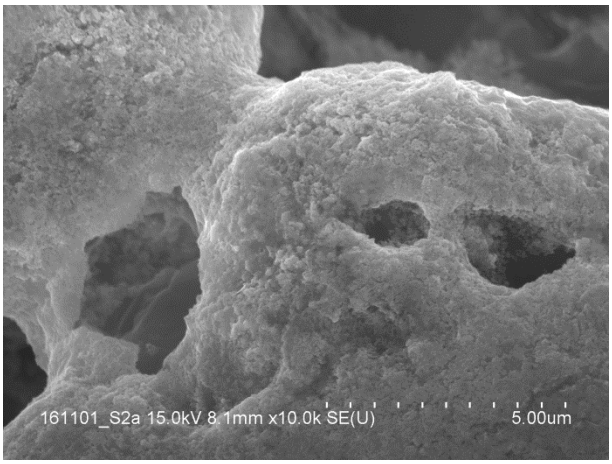

Figure S4. SEM image of the absorbed S1 after conductivity measurements. Showing surface morphologies of the absorbed sample. Magnification 10.000.

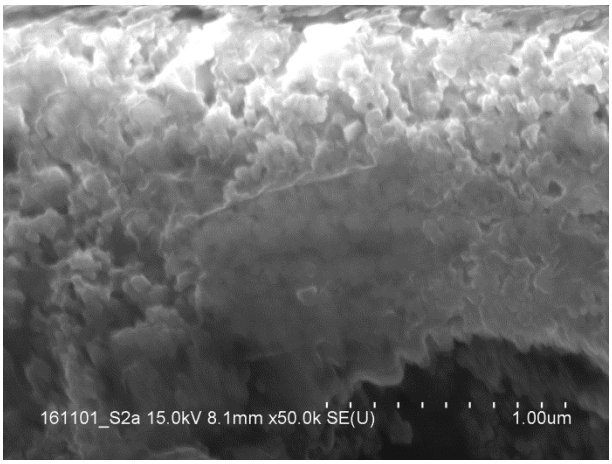

Figure S5. SEM image of the absorbed S1 after conductivity measurements. Magnification 50.000.

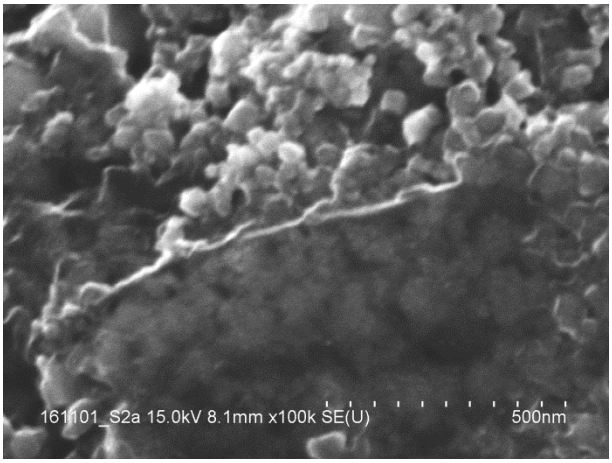

Figure S6. SEM image of the absorbed S1 after conductivity measurements. Magnification 100.000.

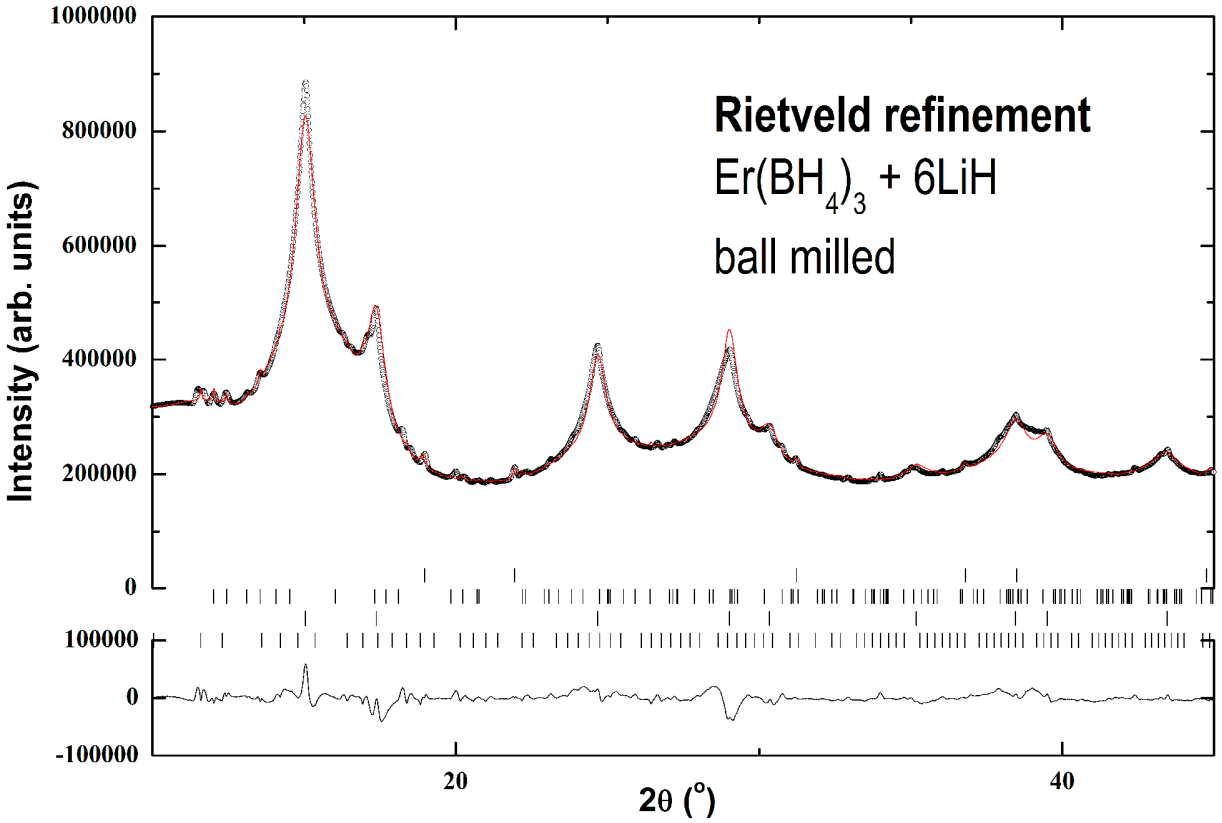

Figure S7. SR-PXD Rietveld refinement and difference plot of S1 after ball milling. Observed (circles) and calculated (red line) patterns and difference plot (below). Vertical tick marks for the Bragg peak positions for (from top): 1. LiH with 24.8(2) wt% 2. $LiBH_4$ with 29.9(3) wt%, 3. *c*-ErH_3 with 44.1(4) wt%; 4. $Er(BH_4)_3$ with 1.1(2) wt%. R_{wp} = 2.65%. λ = 0.7778 Å.

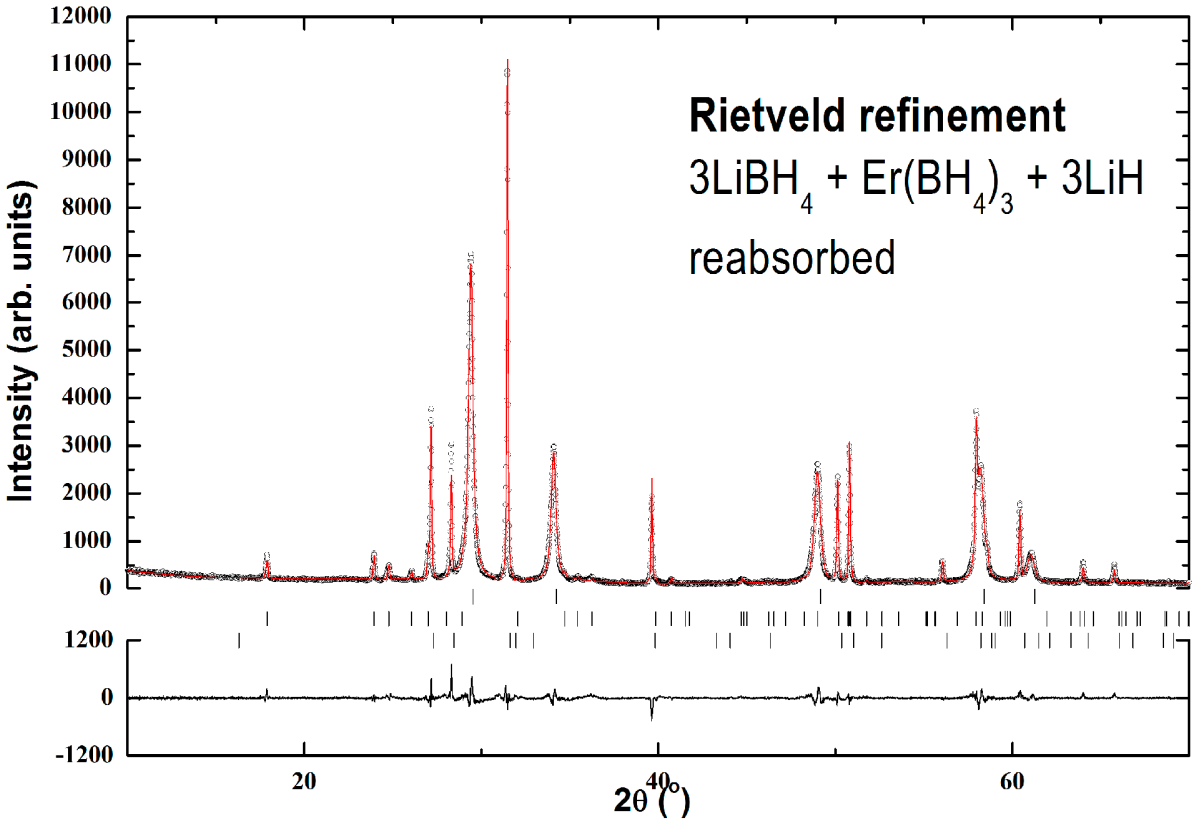

Figure S8. PXD Rietveld refinement and difference plot of S2 after first reabsorption. Observed (circles) and calculated (red line) patterns and difference plot (below). Vertical tick marks for the Bragg peak positions for (from top): 1. *c*-ErH_3 in *Fm*-3*m* with 27.4(2) wt%; 2. $LiBH_4$ with 58.1(2) wt%, 3. *t*-ErH_3 in *P*-3*c*1 with 14.45(4) wt%. R_{wp} = 8.32%. λ = 1.54059Å.

Table S1. Atomic positions (x, y, z) and displacement factor (U_{iso}) refined for Er and B in $Er(BH_4)_3$ with data from Fig. S3. Estimated standard deviations in brackets.

Atom	Position	X	y	z	U_{iso}
Er1	8*c*	0.2168(1)	0.2168(1)	0.2168(1)	0.0235(4)
B1	24*d*	0.197(4)	0.255(8)	0.965(4)	0.018(17)
H1	24*d*	0.2892	0.2539	0.0231	0.00032
H2	24*d*	0.1039	0.2248	0.0335	0.00032
H3	24*d*	0.1736	0.3472	0.9186	0.00032
H4	24*d*	0.2012	0.1633	0.8931	0.00032