In Situ Energy-Dispersive XAS and XRD Study of the Superior Hydrogen Storage System MgH$_2$/Nb$_2$O$_5$

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Figure 1. Schematic illustration of the experimental setup for hydrogen cycling. The valves are indicated by “On/Off” (two-position valve) and “R” (remote-controlled two-position valve).
Figure 2. Selected EDXAS spectra (initial, after heating in hydrogen, and the first desorption) of (a) physically mixed (PM) sample and ball milled (BM) sample compared to (b) measured reference samples.
Figure 3. Energy of Nb absorption K-edge at 0.8 normalized absorbance ($E_{0.8}$) versus time with energy of measured niobium references (oxidation state in parentheses) enclosed for comparison.
Figure 4. Selected EDXAS spectra of the (a) PM sample and (b) BM sample (see also Figure 3) in the Nb edge region.
Figure 5. Sample phase composition estimated by linear combination of reference samples Nb, NbO, NbO$_2$, and Nb$_2$O$_5$. 
Figure 6. XRD diffraction pattern evolution of the regions of characteristic peaks for (a) Nb$_2$O$_5$, (b) MgO, and (c) Mg/MgH$_2$ peaks for the PM sample. The initial spectrum in (c) has been amplified by a factor of 15 to show the Mg contribution in the initial sample.
Figure 7. XRD pattern evolution of the regions of characteristic peaks for (a) Nb$_2$O$_5$, (b) MgO, and (c) Mg/MgH$_2$ peaks for the BM sample.
Figure 8. Sample phase composition estimated by linear combination of reference samples Nb, NbO, NbO$_2$, and Nb$_2$O$_5$. 

\[ \text{NbO}_a + (a - b)\text{Mg} \rightarrow (a - b)\text{MgO} + \text{NbO}_b \] (1)

\[ \text{NbO}_a + (a - b)\text{MgH}_2 \rightarrow (a - b)\text{MgO} + \text{NbO}_b + (a - b)\text{H}_2 \uparrow \] (2)
Thank You!