

Enhancement Effect of Bimetallic Amide $\text{K}_2\text{Mn}(\text{NH}_2)_4$ and in-situ Formed KH and Mn_4N on the Dehydrogenation/Hydrogenation Properties of Li-Mg-N-H System

Gökhan Gizer ¹, Hujun Cao ^{1,2}, Julián Puszkiel ^{1,3,*}, Claudio Pistidda ¹, Antonio Santoru ¹, Weijin Zhang ², Teng He ², Ping Chen ², Thomas Klassen ^{1,4}, Martin Dornheim ^{1,*}

¹ Nanotechnology Department, Helmholtz-Zentrum Geesthacht, Max-Planck Straße 1, 21502, Geesthacht, Germany

² Dalian National Laboratory for Clean Energy Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, P. R. China

³ Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Centro Atómico Bariloche, Av. Bustillo km 9500, S.C. de Bariloche, Argentina

⁴ Institut für Werkstofftechnik, Helmut-Schmidt-Universität, Holstenhofweg 85, 22043 Hamburg, Germany

*Correspondence: julian.puszkiel@hzg.de; martin.dornheim@hzg.de

Supplementary Data

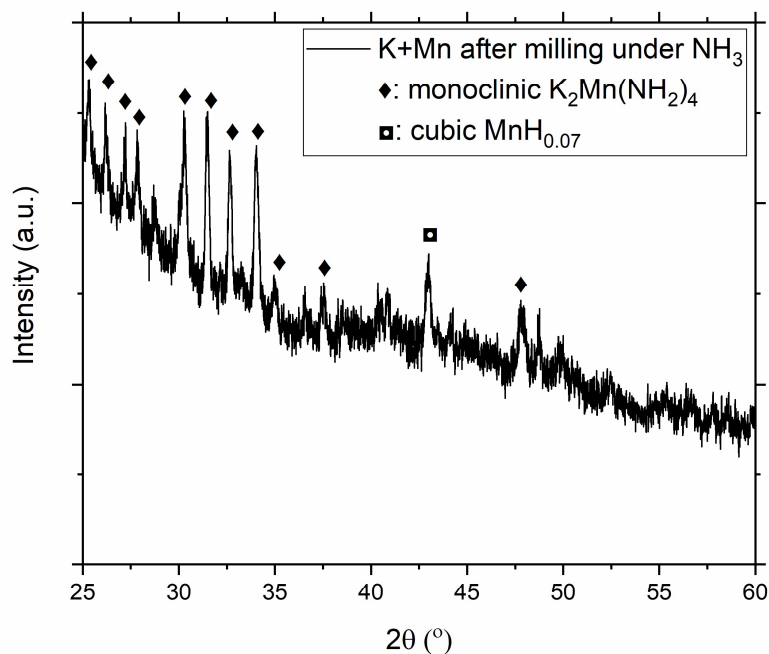


Figure S1 PXD pattern of K and Mn after ball milling under NH_3 . $\lambda=\text{Cu}$, $\text{K}\alpha$. Based on Rietveld refinement, weight fraction of $\text{K}_2\text{Mn}(\text{NH}_2)_4$: 95 wt.%, $\text{MnH}_{0.07}$: 5wt. %

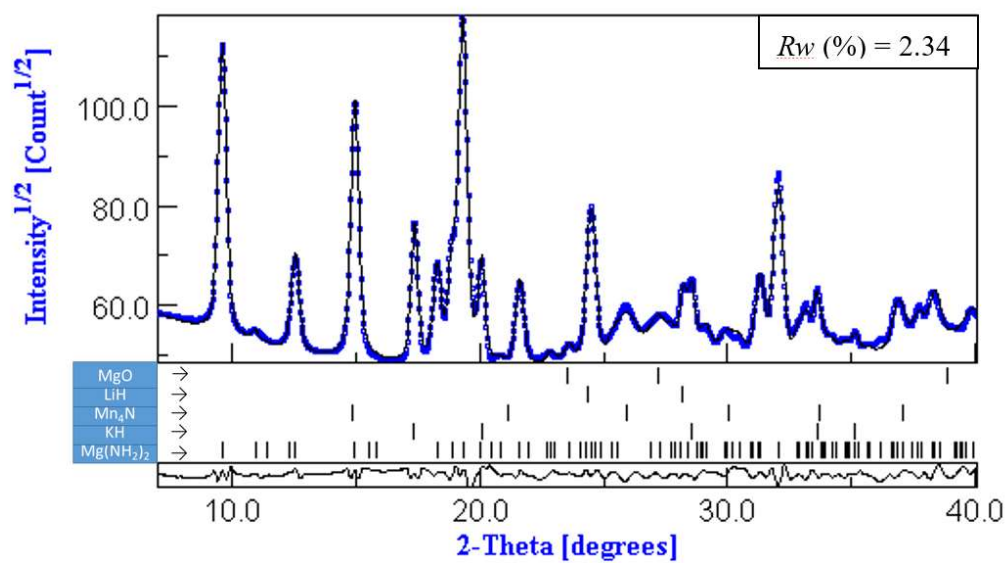


Figure S2 SR-PXD pattern of the Mg-Li-5KMn after rehydrogenation, $\lambda = 0.9941$ Å. Blue dots: Measurement data, Black line: Calculated fit

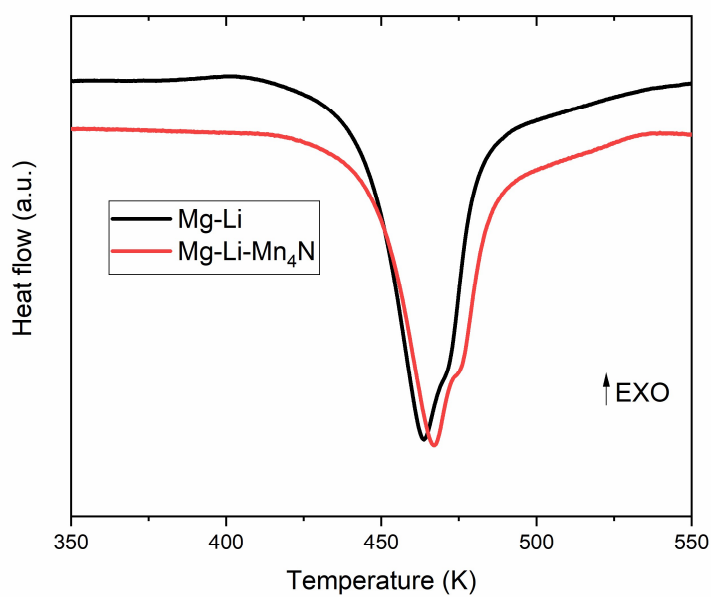


Figure S3 DSC curves of Mg-Li and 5 mol % Mn₄N containing Mg-Li samples. Heating rate: 3K/min

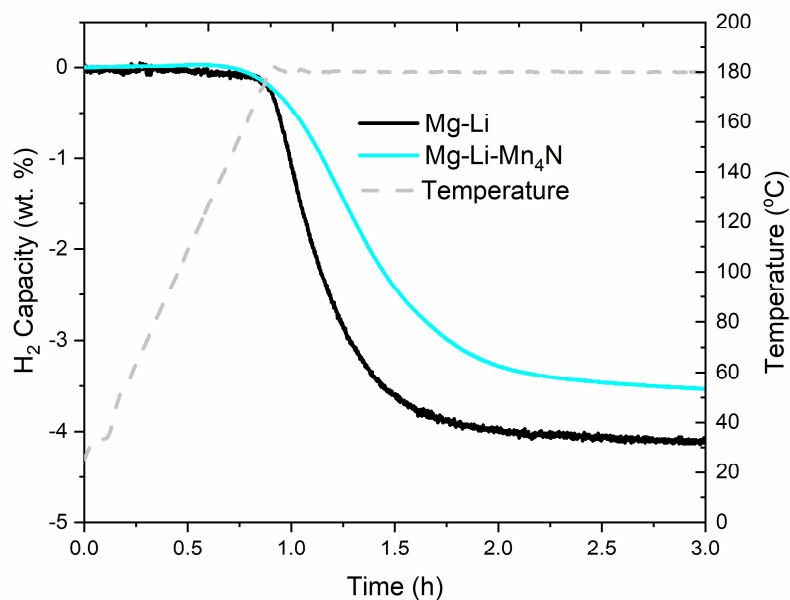


Figure S4 H₂ release curves of Mg-Li and 5 mol % Mn₄N containing Mg-Li samples under 1 bar of H₂. Heating: RT → 180 °C, 3°C/min

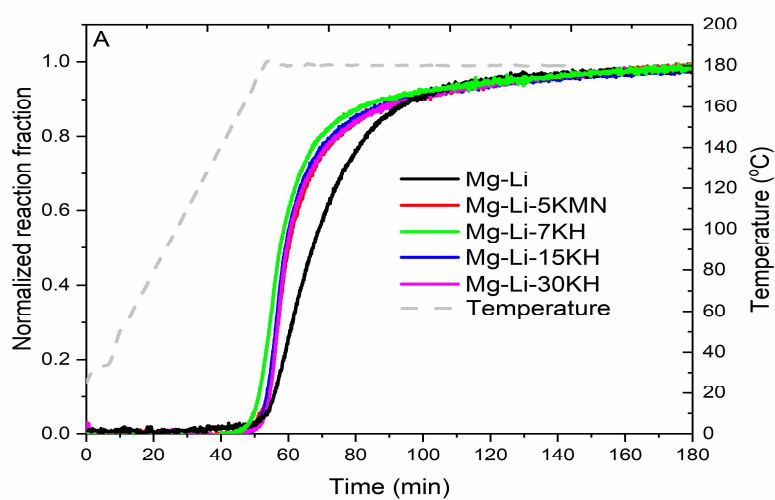


Figure S5 Non-isothermal normalized dehydrogenation kinetics of prepared samples. Heating was applied from room temperature until 180 °C, with a heating rate of 3 °C/min. Dehydrogenation was carried out under 1 bar of H₂.

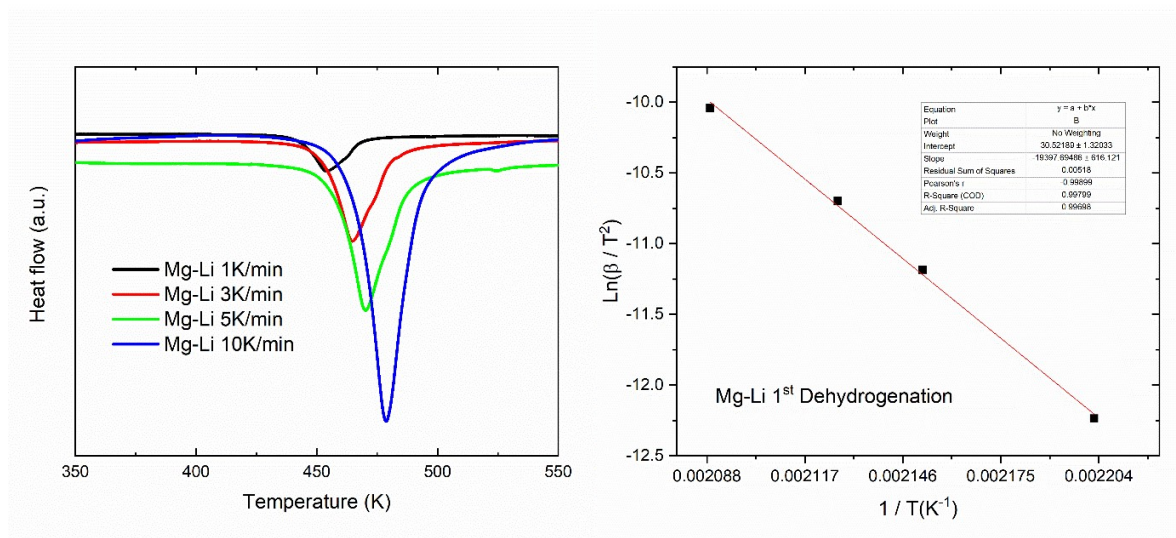


Figure S6 DSC and corresponding Arrhenius plots of Mg-Li at the 1st dehydrogenation

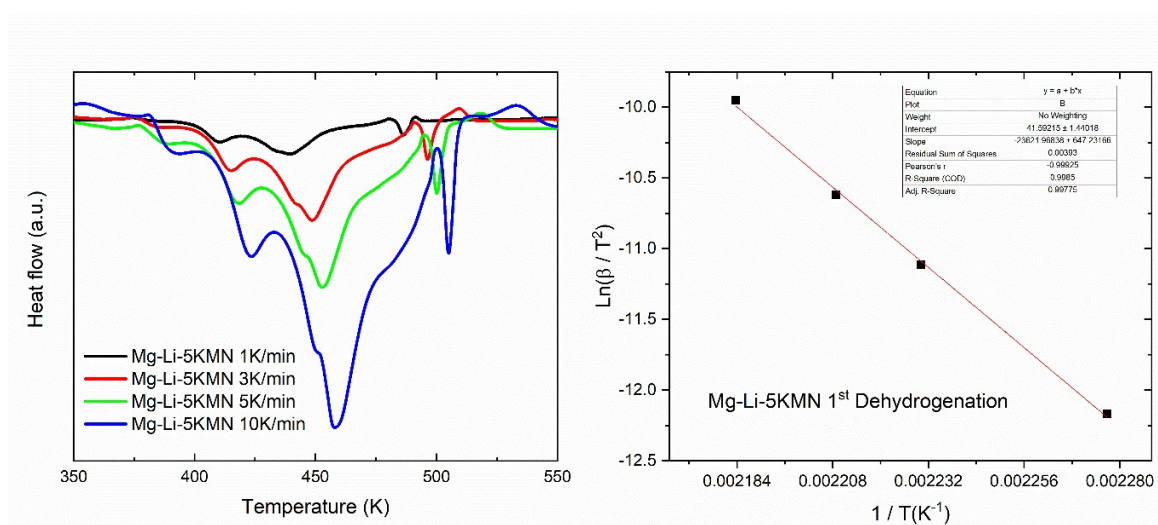


Figure S7 DSC and corresponding Arrhenius plots of Mg-Li-5KMn at the 1st dehydrogenation

Table S1 Calculation of the kinetic constant applying the Arrhenius equation.

Composition	A (1/s)	E _a (kJ/mol)	1 st Dehydrogenation $k = A \cdot \exp [-E_a/RT]$	H ₂ capacity x k (wt.%/s)
Mg-Li	3.49E+17	161±5	0.1	0.4
Mg-Li-5KMn	2.70E+22	196±5	0.7	2.5