Study of the Influence of NaCl and LiCl on the Decomposition of $Sr(AlH_4)_2$

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The suitability of complex hydrides such as alanates for solid-state hydrogen storage applications, especially regarding the transition to a renewable energy-based economy, is being widely discussed. Advances in the field of mechanochemistry allowed the preparation of alanates also by ball milling. In order to characterise the alanates themselves, often simply the obtained mixtures consisting of the alanate and the by-product were investigated [1]. For that purpose, the by-product is assumed to be inert. We reviewed the validity of this assumption by investigating the decomposition behaviour of $Sr(AlH_4)_2$ + 2 NaCl and $Sr(AlH_4)_2$ + 2 LiCl mixtures, synthesised by ball milling.

TG-DSC measurements (Sensys DSC, SETARAM) were used for a general characterisation of the thermal dehydrogenation of the different mixtures. We found the by-product to not affect the decomposition of $Sr(AlH_4)_2$ itself, but that of $SrAlH_5$. To investigate the influence of LiCl and NaCl on the dehydrogenation pathway of $SrAlH_5$ in more detail, the decomposition products were analysed by means of XRD and the feasibility of possible decomposition reactions was assessed from a thermodynamic point of view.

While NaCl does not affect the decomposition pathway, LiCl alters the dehydrogenation reactions by acting as a reactant. Instead of decomposing directly to SrH_2 and $SrAl_4$ (R1), $SrAlH_5$ dehydrogenates in two separate steps when LiCl is present in the sample. First SrHCl and Al (R2) and then $SrAl_4$ (R3) is formed.

$$SrAlH_5 + Al \rightarrow 0.5\ SrAl_4 + 0.5\ SrH_2 + 2\ H_2 \quad \text{(R 1)}$$

$$SrAlH_5 + LiCl \rightarrow SrHCl + Al + LiH + 1.5\ H_2 \quad \text{(R 2)}$$

$$0.5\ SrHCl + 2\ Al + 0.5\ LiH \rightarrow 0.5\ SrAl_4 + 0.5\ LiCl + 0.5\ H_2 \quad \text{(R 3)}$$

The different effects of LiCl and NaCl correspond to the differing stability of LiH ($\Delta_f H°(298)$ = -90.5 kJ/mol [2]) and NaH ($\Delta_f H°(298)$ = -56.4 kJ/mol [2]). Due to the high stability of LiH its formation is thermodynamically favoured and thus the addition of LiCl changes the decomposition reactions of $Sr(AlH_4)_2$.

References

[1] K. Suárez-Alcántara, J. R. Tena-Garcia, R. Guerrero-Ortiz, *Materials* **2019**, *12*, 2724-2787.
[2] A. Roine, *HSC Chemistry*, Metso Outec, Pori, **2021**.