CHARACTERISATION OF REACTIVE HYDRIDE COMPOSITES

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Borohydrides are among the most promising materials for mobile fuel cell applications, due to their high percentage weight hydrogen (>10 % wt. H_2), that exceed the DOE targets (4.5 % wt. H_2)(1). $Zn(BH_4)_2$ derivatives are of great interest due to their low decomposition temperature and diverse crystal structures(2). The main concern regarding the use of borohydrides for mobile applications is that B_2H_6 gas release upon decomposition, which poisons the nafion membranes of PEMFC.

MgH_2 reduces the amount of B_2H_6 released in borohydrides during decomposition, and it is commonly used to form reactive hydride composites(3, 4). The production of B_2H_6 is reduced due to the MgB_2 formation upon dehydrogenation, as presented by equation 1. Likewise, CaH_2 has also displayed similar properties to MgH_2 regarding reversible boride formation shown in equation 2(5).

$$2MBH_4 + MgH_2 \leftrightarrow 2MH + MgB_2 + 4H_2 \quad (1)$$

$$6MBH_4 + CaH_2 \leftrightarrow 6MH + CaB_6 + 10H_2 \quad (2)$$

The reversible formation of borides enhances the viability of reactive hydride composite storage materials(6). Here we present the differences between boride formation of CaH_2 and MgH_2 upon dehydrogenation when coupled with $NaZn_2(BH_4)_5$ and the consequential B_2H_6 release.

$NaZn_2(BH_4)_5$ was synthesised then mechanically ball milled with MgH_2 and CaH_2 in separate batches; the stoichiometric ratios of which are 1:0, 1:1 and 1:2. Raman and PXRD were used to characterise the structures compared to the literature. DSC and TGA were then used to characterise how the stoichiometric changes alters thermolysis. The results presented characterise alternate decomposition pathways caused by MgH_2 and CaH_2 and the subsequent B_2H_6 release.

References:

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