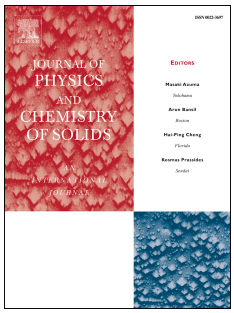
Accepted Manuscript



Synergistic effects of transition metal halides and activated carbon nanofibers on kinetics and reversibility of MgH_2

Praphatorn Plerdsranoy, Sophida Thiangviriya, Palmarin Dansirima, Puttimate Thongtan, Dechmongkhon Kaewsuwan, Narong Chanlek, Rapee Utke

PII: S0022-3697(18)30779-0

DOI: 10.1016/j.jpcs.2018.09.001

Reference: PCS 8714

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 28 March 2018

Revised Date: 30 June 2018

Accepted Date: 3 September 2018

Please cite this article as: P. Plerdsranoy, S. Thiangviriya, P. Dansirima, P. Thongtan, D. Kaewsuwan, N. Chanlek, R. Utke, Synergistic effects of transition metal halides and activated carbon nanofibers on kinetics and reversibility of MgH_2, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.09.001.

Synergistic effects of transition metal halides and activated carbon nanofibers on kinetics and reversibility of MgH_2

Praphatorn Plerdsranoy[1], Sophida Thiangviriya[1], Palmarin Dansirima[1], Puttimate Thongtan[1], Dechmongkhon Kaewsuwan[3], Narong Chanlek[3], Rapee Utke[*, 1, 2]

[1]School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand.

[2]Center of Excellent on Advanced Functional Materials (CoE-AFM), Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand.

[3]Synchrotron Light Research Institute, Nakhon Ratchasima 30000, Thailand.

MgH_2 doped with transition metal halides (TiF_4, NbF_5, and $ZrCl_4$) and activated carbon nanofibers (ACNF) for reversible hydrogen storage is prepared by ball milling technique. Transition metal halides provide catalytic effects for de/rehydrogenation kinetics, while ACNF benefits thermal conductivity and hydrogen permeability as well as prevents particle agglomeration during cycling. Significant reduction of onset and main dehydrogenation temperatures of MgH_2 (ΔT=243 and 158 °C, respectively) are achieved by doping with 5-10 wt. % of NbF_5, ACNF-TiF_4 and ACNF-NbF_5. During the 1st cycle, the latter samples liberate 4.7-5.0 wt. % H_2 within 1 h 30 min, whereas MgH_2 doped with ACNF reaches only 1.5 wt. % H_2. The reaction between MgF_2 and NbH_x (x<1) (MgH_2-NbF_5 and MgH_2-ACNF-NbF_5) during dehydrogenation results in the formation of new catalytic active species of Nb-F-Mg favoring kinetics. Upon four hydrogen release and uptake cycles, kinetics and reversibility within 1 h 30 min of MgH_2-ACNF-NbF_5 are preserved at 5.0 wt. % H_2, while those of MgH_2-NbF_5 and MgH_2-ACNF-TiF_4 decay to 4.4 wt. % H_2. Activation energy (E_A) for dehydrogenation of MgH_2 considerably decreases from 140.0±10.2 to 37.8±1.5 kJ/mol after doing with ACNF-NbF_5. Superior performance of MgH_2-ACNF-NbF_5 to MgH_2-NbF_5 is due to synergistic effects of NbF_5 and ACNF. In the case of MH_2-ACNF-TiF_4, the disappearance of active species benefiting kinetic properties and the formation of thermally stable TiH_2 account for inferior hydrogen content reversible.

* Corresponding author (Email: rapee.g@sut.ac.th)