Cyclic stability of the in-situ formed Mg-based nanocomposite catalyzed by YH_2

Qian Li [a, b, *], Yang Li [a], Bin Liu [a], Xionggang Lu [a], Tengfei Zhang [c], Qinfen Gu [d]

[a] *State Key Laboratory of Advanced Special Steels & Shanghai Key Laboratory of Advanced Ferrometallurgy & School of Materials Science and Engineering, Shanghai University, Shanghai 200444, China*

[b] *Materials Genome Institute, Shanghai University, Shanghai 200444, China*

[c] *Division of Material Science and Engineering, Hokkaido University, Sapporo 0600808 Japan*

[d] *Australian Synchrotron, 800 Blackburn Rd, Clayton 3168, Australia*

* Corresponding author: shuliqian@shu.edu.cn

1. Apparent activation energy for dehydrogenation of 40th-cycled $Mg+Mg_2Ni+YH_2$ nanocomposite

The dehydrogenation tests for $Mg+Mg_2Ni+YH_2$ nanocomposite were performed at 250, 300 and 350 °C with an initial state of vacuum, using a Sievert-type apparatus (Suzuki Shokan Co., Ltd.). The apparent activation energy for dehydrogenation of 40th-cycled $Mg+Mg_2Ni+YH_2$ nanocomposite was evaluated from the Arrhenius plot of the characterization time (t_c) as follows:

$$\ln(1/t_c) = \ln(1/B_t) - \frac{E_a}{RT}, \quad (1)$$

where E_a is the apparent activation energy, and B_t is a constant. t_c was obtained by fitting the dehydrogenation curves with the diffusion-controlled formula of Chou-model [1, 2], as follows:

$$\xi = 1 - (1 - \sqrt{\frac{t}{t_c}})^3, \quad (2)$$

Fig. S1 shows the dehydrogenation curves with fitting results. Fig. S2 shows the fitting result of the Arrhenius plot. It is learned that the apparent activation energy for the dehydrogenation of 40th-cycled $Mg+Mg_2Ni+YH_2$ nanocomposite is 40.7 kJ/mole. This value is slightly higher than that of MgH_2 with nano-coating of multi-valence Ti-based catalysts (30.8 kJ/mole) [3], but much lower than those of commercial MgH_2(135 kJ/mole) [4], high energy ball-milled MgH_2 (96 kJ/ kJ/mole) [4], doped $TiCl_3$ (67.8

kJ/mole) [5], Nb_2O_5 (62.8 kJ/mole) [6] and TiH_2 (58.4 kJ/mole H_2) [7]. This outstanding dehydrogenation kinetics is due to that the sample has been fully activated after 40 de/hydrogenation cycles, not only resulting in extensive networks of cracks running throughout the Mg particles (see Fig. 4(c) in the manuscript), but also generating vast number of YH_2 nano particles evenly and densely distributed on the surface and within the matrix of Mg particles (see Fig. 4(d), Fig. 5(c) and (d) in the manuscript).

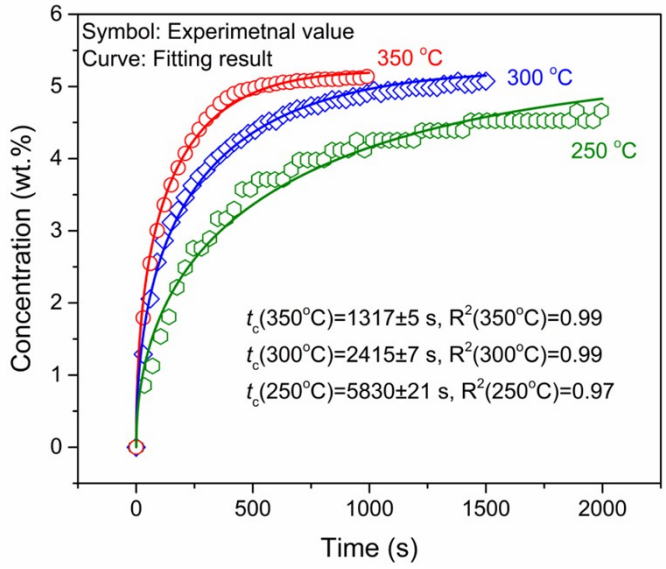

Figure S1. Dehydrogenation curves of 40th-cycled Mg+Mg_2Ni+YH_2 nanocomposite with fitting results

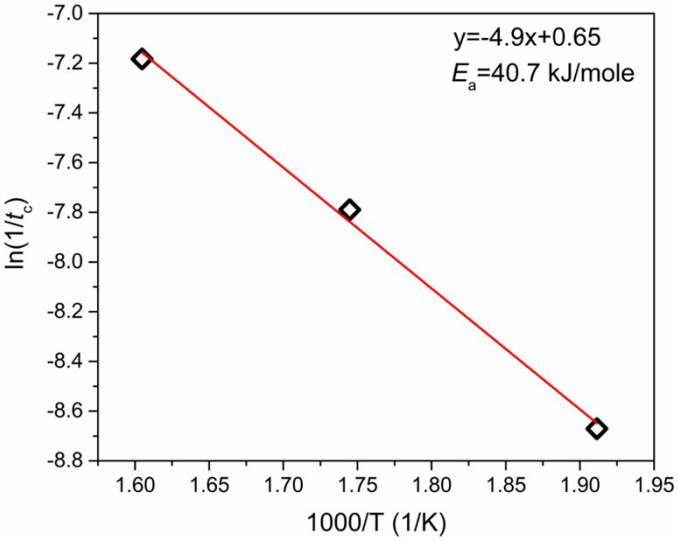

Figure S2. The fitting result of the Arrhenius plot.

References

[1] K. Chou, Q. Li, Q. Lin, L. Jiang and K. Xu, Int. J. Hydrogen Energy, 2005, 30(3), 301-309.

[2] Y.P. Pang, Q. Li, Int. J. Hydrogen Energy, 2016, 41(40), 18072-18087.

[3] J. Cui, H. Wang, J.W. Liu, L.Z. Ouyang, Q.A. Zhang, D.L. Sun, X.D. Yao and M. Zhu, J. Mater. Chem. A, 2013, 1(18), 5603-5611.

[4] N. Bazzanella, R. Checchetto and A. Miotello, Appl. Phys. Lett., 2004, 85(22), 5212-5214.

[5] Y.J. Choi, J. Lu, H.Y. Sohn and Z.Z. Fang, J. Power Sources, 2008, 180(1), 491-497.

[6] O. Friedrichs, F. Agueyzinsou, J. Fernandez, J. Sanchezlopez, A. Justo, T. Klassen, R. Bormann and A. Fernandez, Acta Mater., 2006, 54(1), 105-110.

[7] J. Lu, Y. J. Choi, Z. G. Fang and H. Y. Sohn, J. Am. Chem. Soc. 2010, 132, 6616-6617.