Electronic Supplementary Material (ESI) for Nanoscale

Excellent Catalytic Effects of Highly Crumpled Graphene Nanosheets on Hydrogenation/dehydrogenation of Magnesium Hydride

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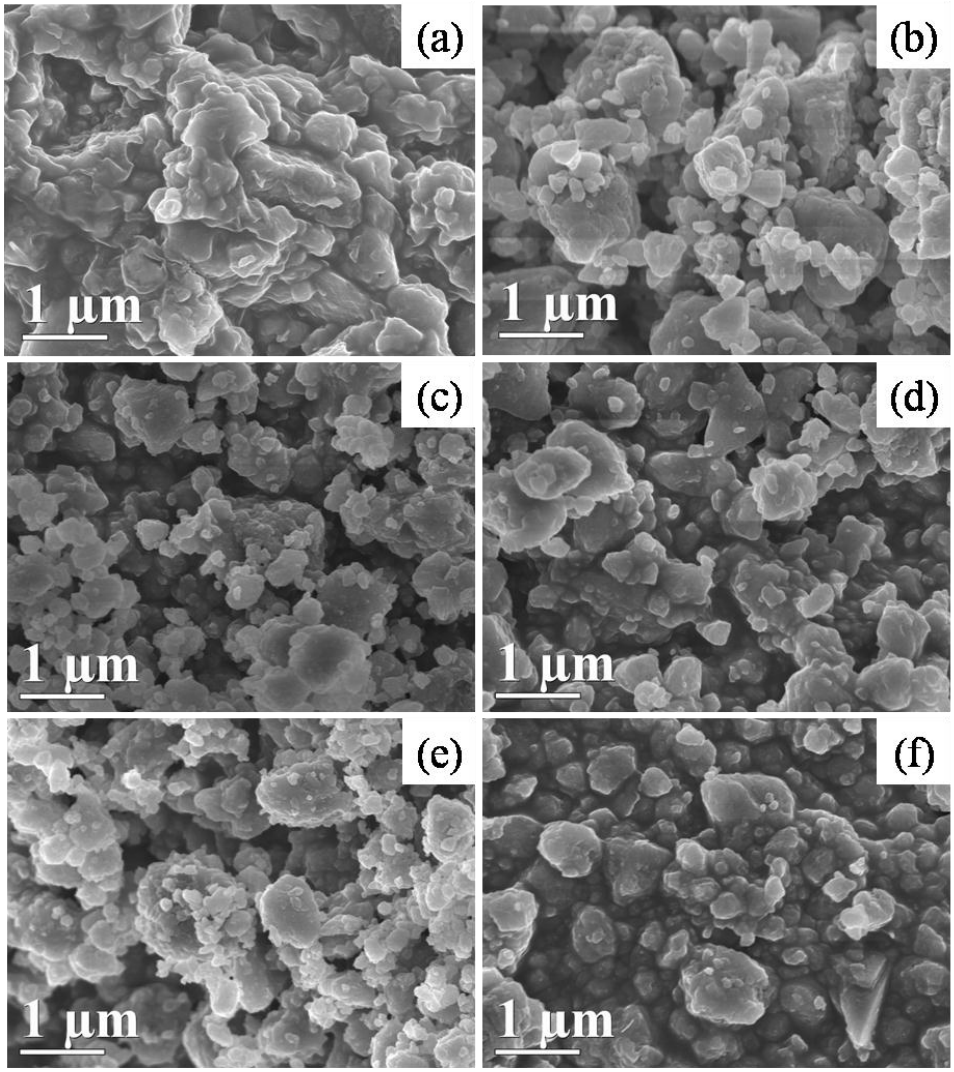

Fig. S1 SEM images of (a) MgH_2-5GNS-1h, (b) MgH_2-5GNS-5h, (c) MgH_2-5GND-10h, (d) MgH_2-5GNS-15h, (e) MgH_2-5GNS-20h, and (f) MgH_2-20h, respectively.

Table S1 Kinetic data obtained from the absorption experiments of different samples at different temperature.

sample	Temperature (℃)	slope (n)	-lnk	Ea (kJ mol^{-1})
MgH_2-5wt% -5GNS-1h	300	0.66	4.35	123.3
	200	0.96	9.52	
	150	1.01	13.6	
MgH_2-5wt% -5GNS-5h	300	0.52	4.09	102.2
	200	0.81	8.60	
	150	0.84	11.7	
MgH_2-5wt% -5GNS-10h	300	1.04	3.36	94.8
	200	0.97	7.70	
	150	0.93	10.4	
MgH_2-5wt% -5GNS-15h	300	1.10	3.0	86.8
	200	0.97	6.82	
	150	0.91	9.46	
MgH_2-5wt% -5GNS-20h	300	1.16	2.94	76.2
	200	1.10	6.42	
	150	1.01	8.59	
MgH_2-20h	300	0.95	3.54	99.0
	200	0.96	7.76	
	150	1.02	10.93	

Notes on calculation of reaction rate k and activation energy Ea:

The obtained absorption data can be well fitted by Johnson-Mehl-Avrami equation as follows[1, 2]:

$$kt = [-\ln(1-\alpha)]^{1/n}$$

Where α is the fraction of metal already becomes hydride at time t, n is the dimensionality of MgH_2 growth. Plotting the data as:

$$\ln(-\ln(1-\alpha)) \text{ Versus } \ln(t)$$

Yields a straight line where n=slope and $k = e^{(y-\text{intercept})/\text{slope}}$.

The rate constant k is a function of temperature T and pressure P. Hence, it can be written in the following form[3]:

$$k = k(P) \cdot k(T) = k(P) \cdot K_0 \exp(-\frac{Ea}{RT})$$

For determining the activation energy through the Arrhenius equation, the values of k were corrected for the difference in driving forces during the measurements. Separate hydrogen absorption kinetics experiments of the MgH_2-5wt%GNS show that the rate constant $k(P,T_0)$ follows the parabolic relationship.

$$k(P) = 1 - \sqrt{P/P_{eq}}$$

P is the H_2 pressure during the reaction and P_{eq} is the equilibrium H_2 pressure.

References:

1. J. F. Fernández and C. R. Sánchez, *J. Alloys. Compd.*, 2002, **340**, 189-198.
2. P. Rudman, *J. Appl. Phys.*, 1979, **50**, 7195-7199.
3. B. Zahiri, M. Danaie, X. Tan, B. S. Amirkhiz, G. A. Botton and D. Mitlin, *J. Phys. Chem. C*, 2011, **116**, 3188-3199.