

ARTICLE

Sustainable NaAlH₄ production from recycled automotive Al alloy

Received 00th January 20xx,
Accepted 00th January 20xx

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DOI: 10.1039/x0xx00000x

Supporting Information

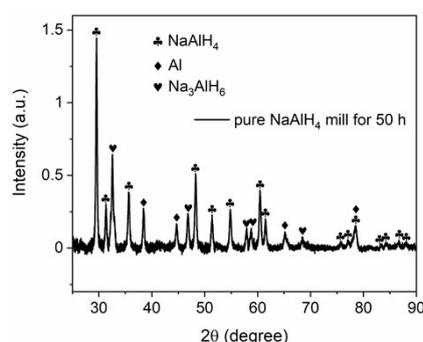


Fig. S1 XRD pattern ($\lambda = 1.54184 \text{ \AA}$) of the NaH + pure Al mixture collected after 50 h's ball milling under about 83 bar of hydrogen.

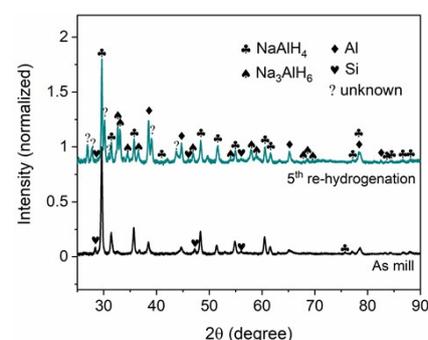


Fig. S2. XRD patterns of the as-milled, and 5th re-hydrogenation of the less pure NaAlH₄.

Table S1 Fitting models and their corresponding kinetic reaction equations used for the hydrogenation curves of the less pure NaAlH₄¹.

Model types	Kinetic rate models	Fitting equations
Diffusion models	D1 one-dimensional diffusion	$\alpha^{2/0.25}$
	D2 two-dimensional diffusion	$(\alpha + (1 - \alpha) * \ln[\frac{1}{1 - \alpha}]) / 0$
	D3 Jander equation for three-dimensional diffusion	$[(1 - [(1 - \alpha)]^{(1/3)})]^{2/0.0}$
	D4 Ginstling-Braunshtein equation for three dimensional diffusion	$(1 - 2/3 [\alpha - (1 - \alpha)]^{(2/3)}) /$
Geometrical contraction models	R2 two-dimensional interface controlled	$(1 - [(1 - \alpha)]^{(1/2)}) / 0.29285$
	R3 three-dimensional interface controlled	$(1 - [(1 - \alpha)]^{(1/3)}) / 0.20625$
Nucleation and growth models	F1 JMA- n = 1	$(- \ln[\frac{1}{1 - \alpha}]) / 0.6931$
	F2 JMA- n = 1/2	$(- \ln[\frac{1}{[(1 - \alpha)]^{(1/2)}}]) / 0.5$
	F3 JMA- n = 1/3	$(- \ln[\frac{1}{[(1 - \alpha)]^{(1/3)}}]) / 0.5$
	F4 JMA- n = 1/4	$(- \ln[\frac{1}{[(1 - \alpha)]^{(1/4)}}]) / 0.5$

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

References

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