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Synthesis and dehydriding properties of perovskite-type hydrides

High-Temperature Materials Science（Environmental Materials Science）
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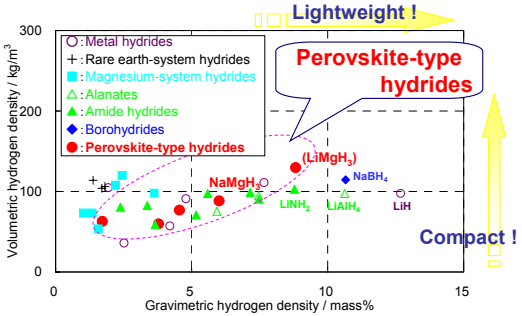
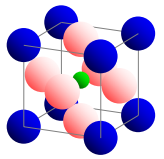
Introduction



Volumetric versus gravimetric hydrogen density

What is
"perovskite structure" ?

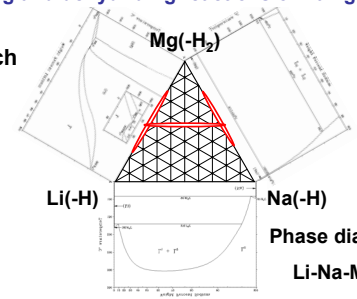


ABX_3
- *A*, *B* : cation, X : anion
- ionic radius ･･･ *A* ～ X > *B*
- coordination numbers ･･･ *A* : 12、*B* : 6
- cubic, tetragonal, orthorhombic, rhombohedral
- oxides, nitrides, carbides, halides
- synthesis of hydrides ･･･
  high temperature (> 500 K) under hydrogen atmosphere

Purpose

(I) Synthesis of $Li_xNa_{1-x}MgH_3$ (x = 0 ～ 1.0) by milling process
(II) Hydriding and dehydriding reactions of $NaMgH_3$

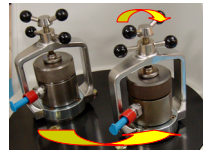
Approach



Phase diagram of
Li-Na-Mg-H system

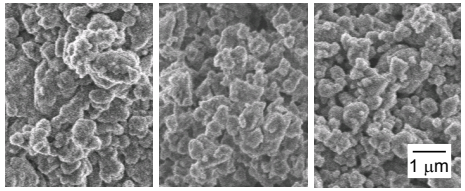
Experimental Procedures

Synthesis
Milling process（under hydrogen, 20 hours）
Apparatus : planetary ball mill (Fritsch P-7)
Starting :mixtures of powder
LiH (99.9%), NaH (95 %), MgH_2 (90 % + Mg)



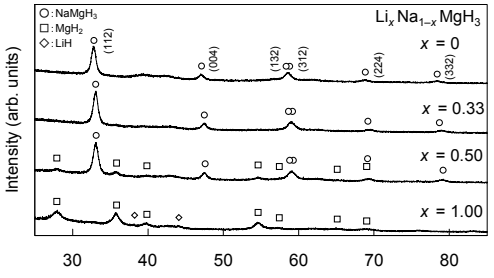
Measurements
SEM observation, powder XRD, thermal analysis

Results and Discussion



x = 0　x = 0.50　x = 1.00

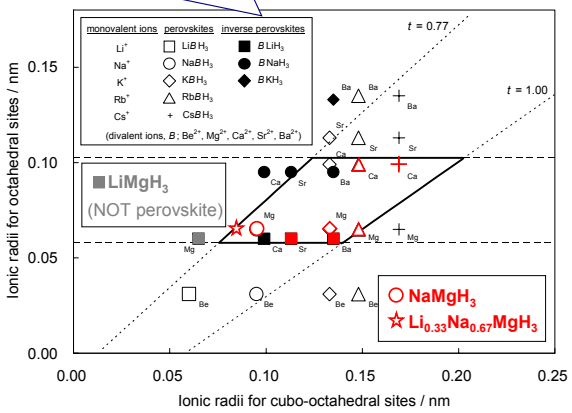
SEM images of $Li_xNa_{1-x}MgH_3$ (x = 0, 0.50 and 1.00)



XRD profiles of $Li_xNa_{1-x}MgH_3$ (x = 0, 0.33, 0.50 and 1.00)

Formation ability of perovskite hydrides

(1) Goldschmidt tolerance factor
(2) Pauling's first rule
(3) Charge neutrality
(4) Stability of inverse perovskite



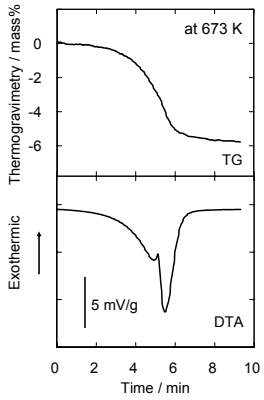
Geometric restrictions of perovskite hydrides ABH_3

Hydriding properties of $NaMgH_3$

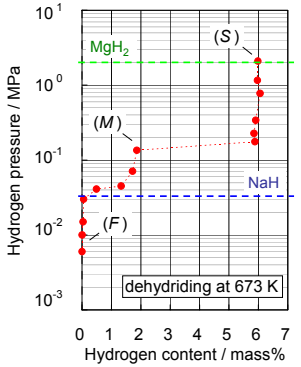
Hydriding reactions of $NaMgH_3$

$NaMgH_3 \rightarrow NaH + Mg + H_2$
$\rightarrow Na + Mg + 3/2H_2$

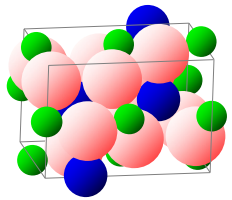
Reversible !



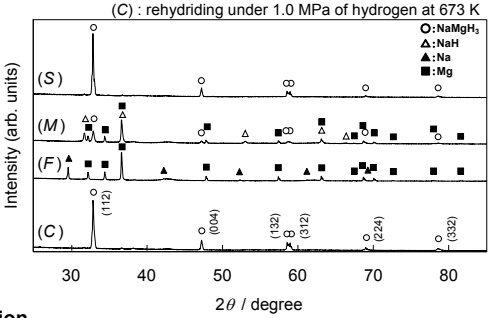
Thermal analysis of $NaMgH_3$



Hydrogen pressure-composition (*p-c*) isotherm of $NaMgH_3$



Crystal structure of $NaMgH_3$
Rönnebro et al., *J. Alloys Comp.*, 299 (2000) 101.



XRD profiles of $NaMgH_3$

K. Ikeda, Y. Nakamori, S. Orimo, *Acta Mater.*, 53 (2005) 3453.

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Summary

(I) $Li_xNa_{1-x}MgH_3$ (x = 0 ～ 0.33) with the perovskite structure was synthesized by mechanical milling alone. Formation ability of perovskite hydrides can be reasonably explained using the Goldschmidt tolerance factors.

(II) Reversible hydriding and dehydriding reactions of perovskite-type hydrides were confirmed in $NaMgH_3$. Nearly 6.0 mass% of hydrogen was released from $NaMgH_3$ within 8 min at 673 K.