Formation ability and hydriding properties of perovskite hydrides

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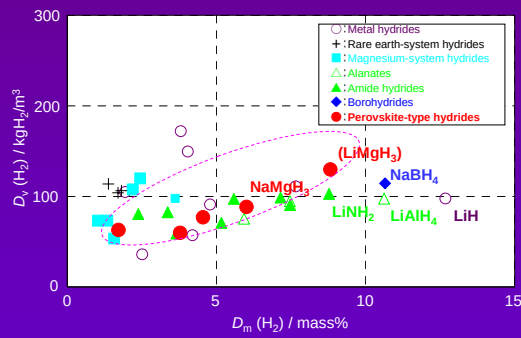
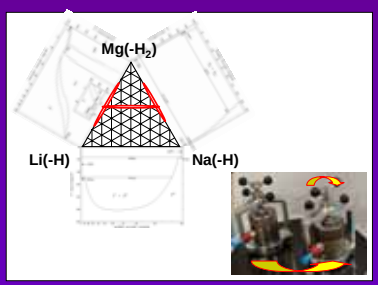
Introduction

Perovskite compounds show attractive physical and chemical properties such as high temperature superconductivity, ionic/electron conductivity, catalysis, and so on. Although some ternary hydrides also exhibit the perovskite structures, the material functions and even fundamental properties of the **perovskite "hydrides"** have not been clarified yet. So, we focus on the "***formation ability***" and "***hydriding properties***" of the perovskite hydrides.



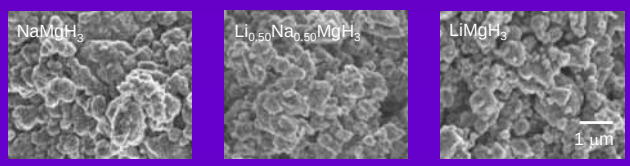
Perovskite structure ABX_3 ...

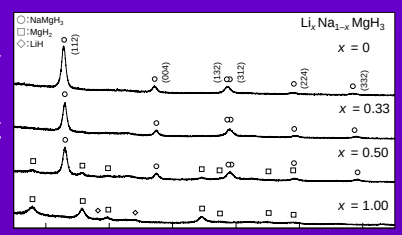
- ***A***, ***B*** : cation, ***X*** : anion
- ionic radius ... ***A*** ～ ***X*** > ***B***
- coordination numbers ... ***A*** : 12, ***B*** : 6
- cubic, tetragonal, orthorhombic, rhombohedral
- oxides, nitrides, carbides, halides
- hydrides
  synthesis ... high temp. (> 500 K) under H_2 atmosphere
  structure, reactivity, function ... unknown



Results and Discussion

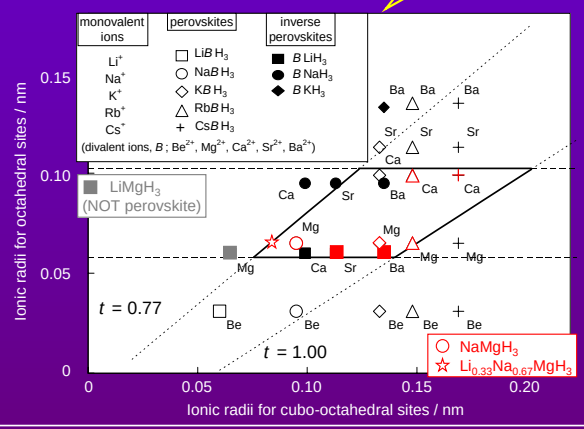
Formation ability of perovskite hydrides





Geometric restrictions of perovskite hydrides ABH_3

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



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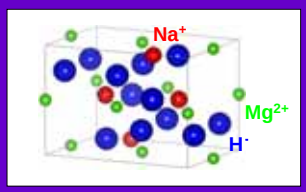
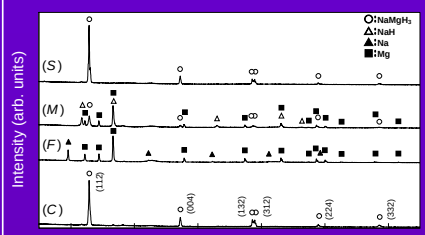
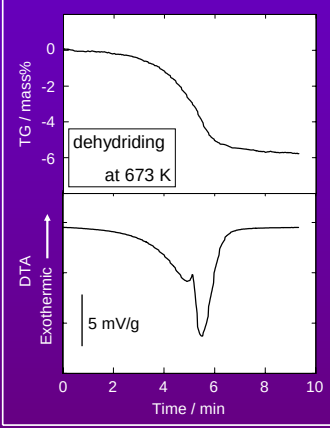
Hydriding properties of $NaMgH_3$

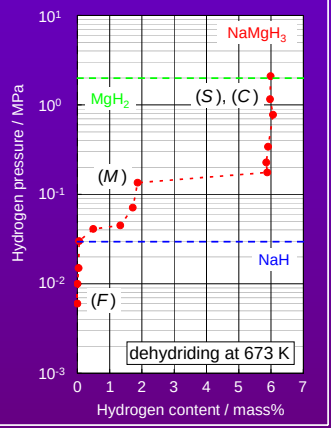




$NaMgH_3$ → $NaH + Mg + H_2$ → $Na + Mg + 3/2H_2$

Reversible !





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Conclusions

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