Materials for Hydrogen Storage

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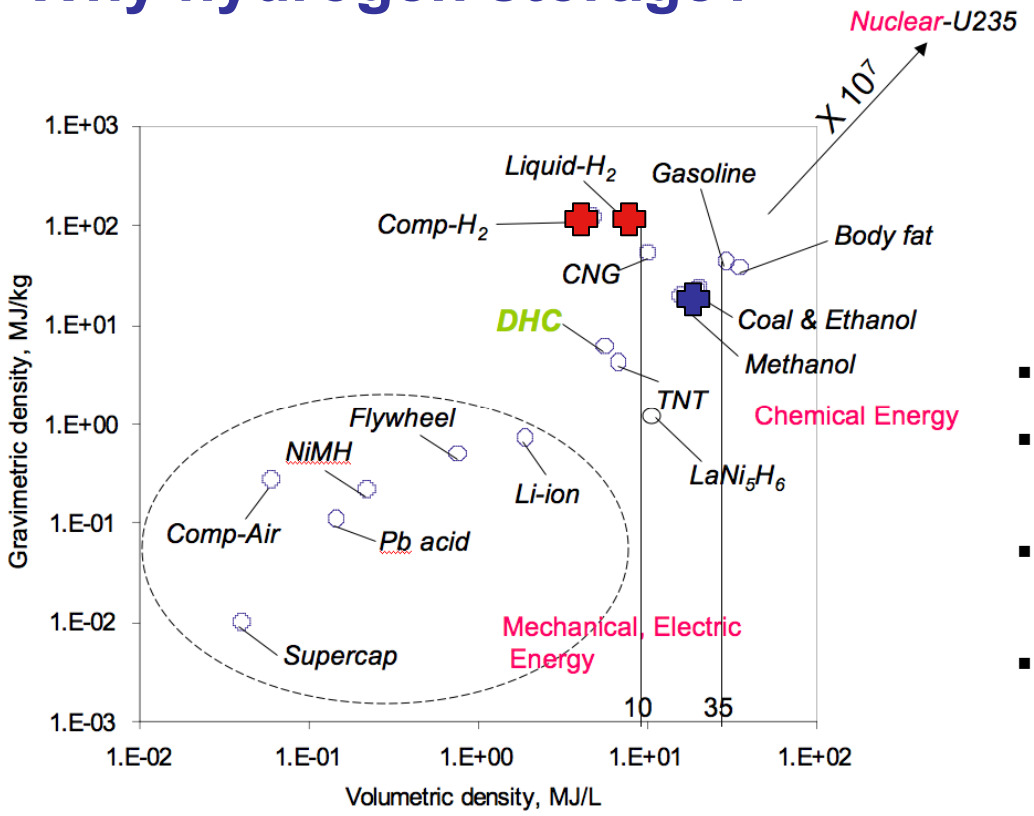
Why hydrogen storage?

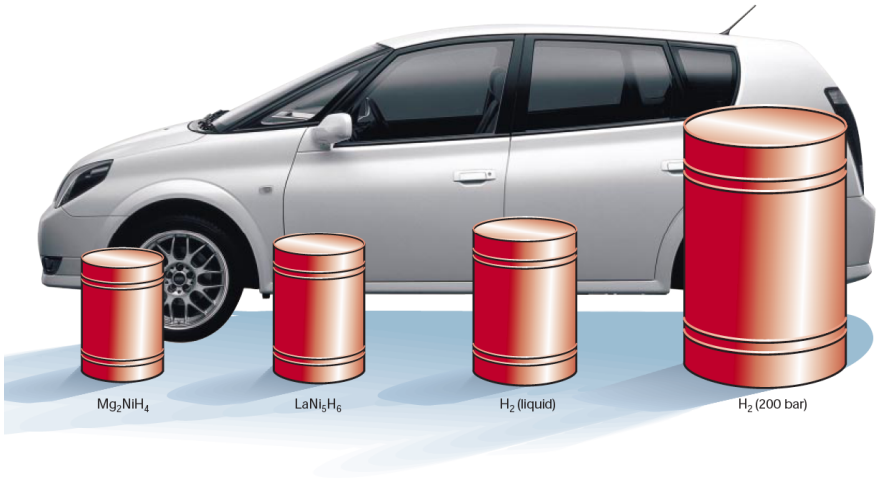


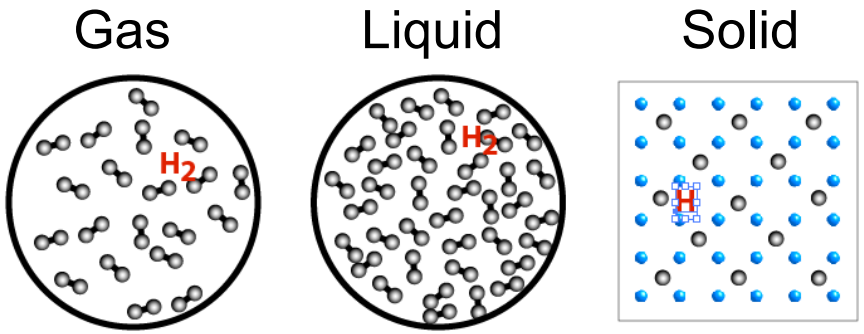
$$2H_2+O_2->2H_2O$$

How to compact H for automotive applications ?

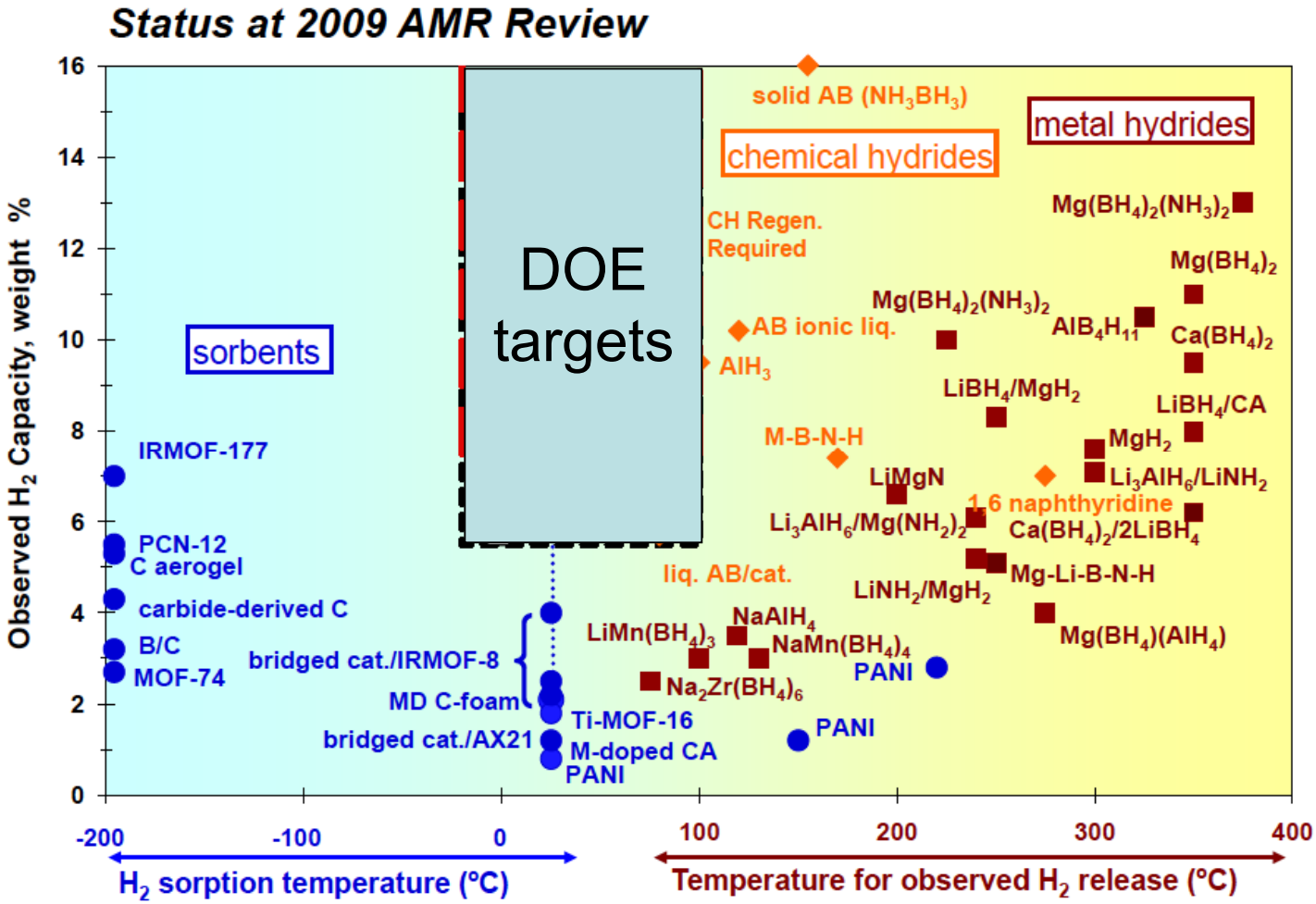
(6 kg of H per 300 miles)

- Weight and volume of container
- Time of compaction/fueling (5 min/6 kg)
- Temperature and pressure (<150 C˚ and 0.3/1.2 MPa)
- Other issues: cost, cycling, heat of reaction





Solid-state hydrogen storage



Our studies of hydrogen storage materials

Interstitial hydrides

(Ti,Zr)TM_2 Laves alloys for Ni-MH batteries; bcc-based alloys

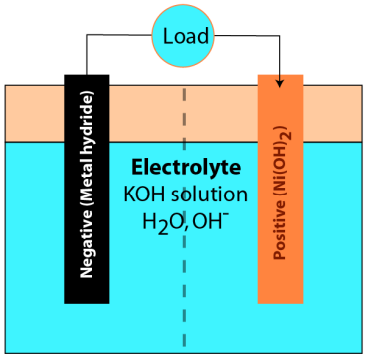
Complex hydrides ($Mg(BH_4)_2$, $LiAlH_4$ etc)

Raman/PCI, IR emissivity/PCI

Films

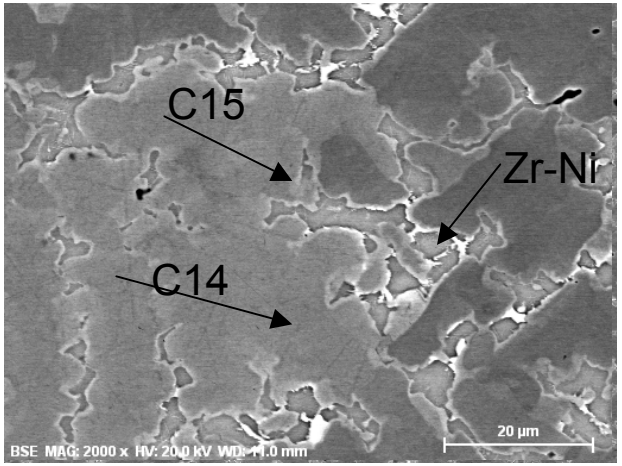
Combinatorial high-throughput, kinetics

Ni-MH electrochemical cell



$M + H_2O + e^- \xrightarrow{charge} MH + OH^-$

$Ni(OH)_2 + OH^- \xrightarrow{charge} NiOOH(\beta) + H_2O + e^-$



•$Ti_{12.5}$ Zr_{21} V_{10} $Ni_{40.9}$ $Co_{1.5}$ $Cr_{8.5}$ $Mn_{5.6}$

Prediction of a microstructure in multicomponent systems (CALPHAD, solidification path by THERMO-CALC)

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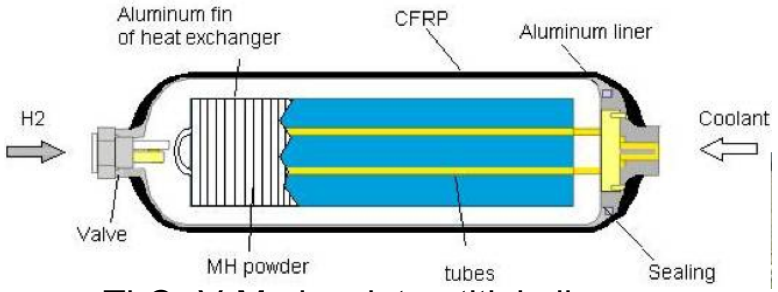
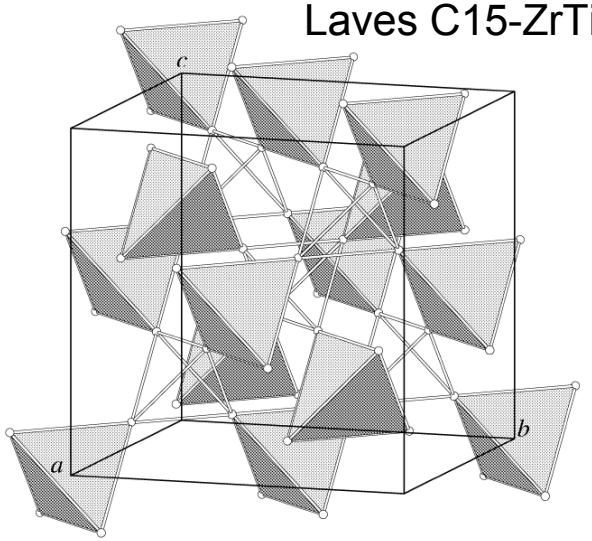
High-Pressure Metal Hydride Tank for Fuel Cell Vehicles (Toyota)



Ti-Cr-V-Mn bcc interstitial alloys

Laves C15-$ZrTi_2H_4$



Maximizing H capacity in compounds: Distribution of hydrogen in interstitial sites (tetrahedral, octahedral, other)

$AB_2H_{(3\text{-}6)}$ compare to AB_2T_{12}

Chemistry (energy) of T: AB_3, A_2B_2, A_4etc

Max occupancy for multicomponent compound

Path of filling the sites (blocking effect)

Effect on PCI curves

Stress

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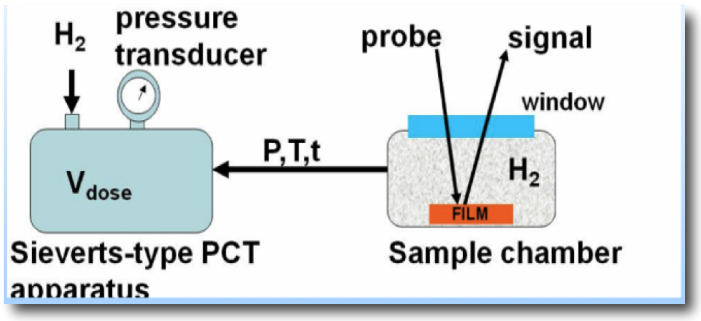
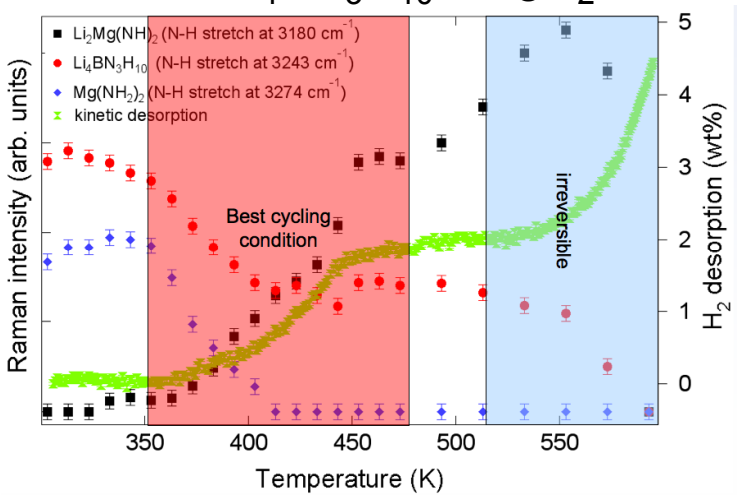
Combinatorial high-throughput, kinetics



Nano $Li_4BN_3H_{10}$ - MgH_2



Identifying phases, modeling Raman or IR vibration modes

Calculating Raman intensities as a function of phase fraction or concentration in solid solution

Understanding optics, scattering from irregular surfaces (powders), depth

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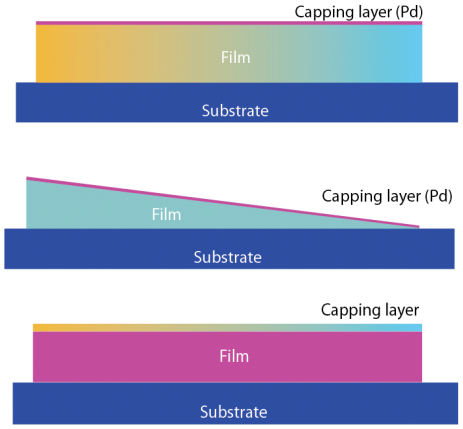

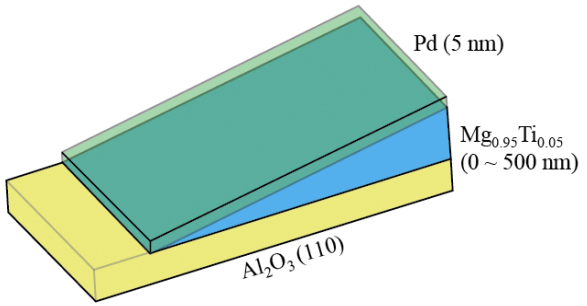

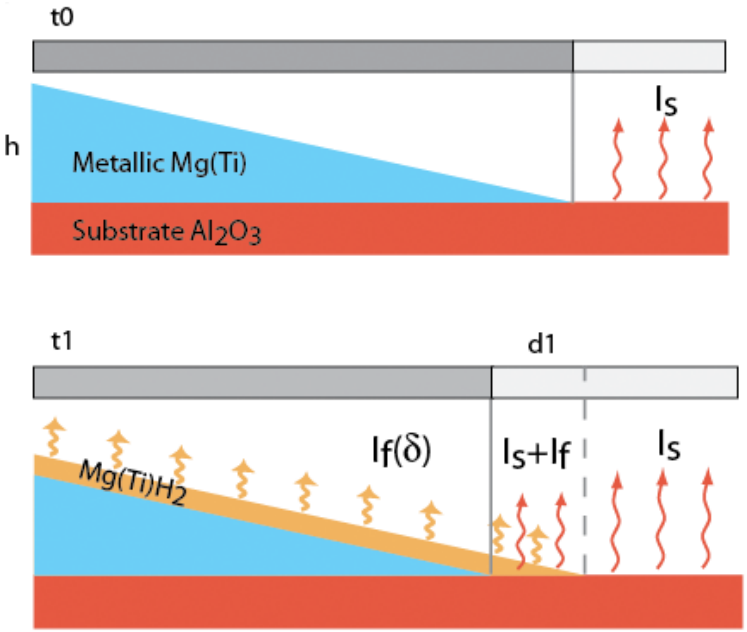

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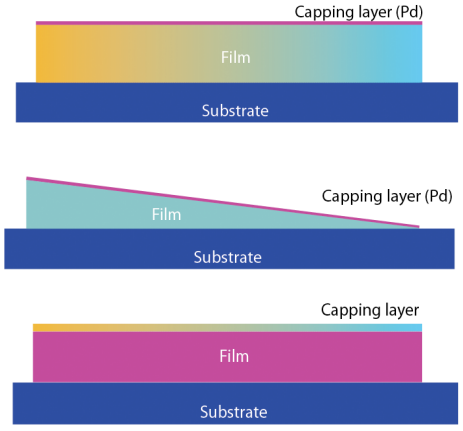
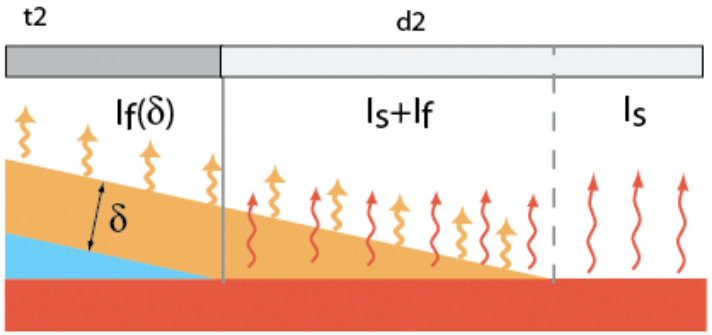
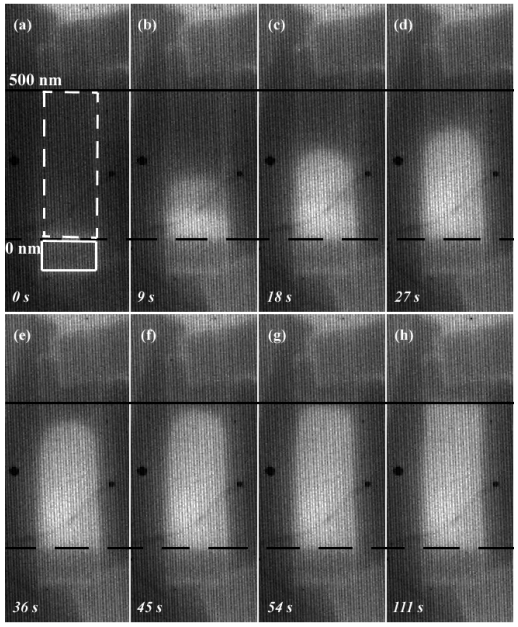
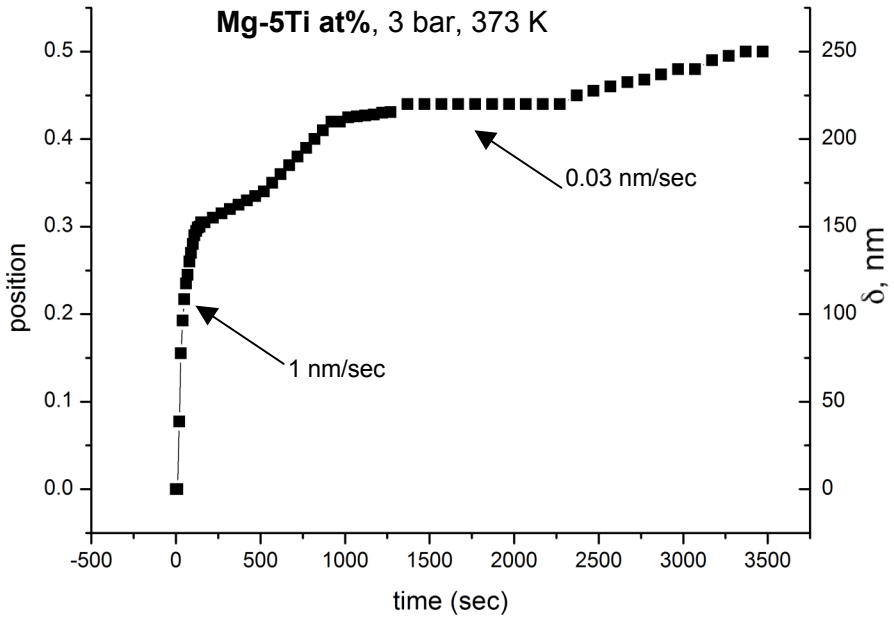




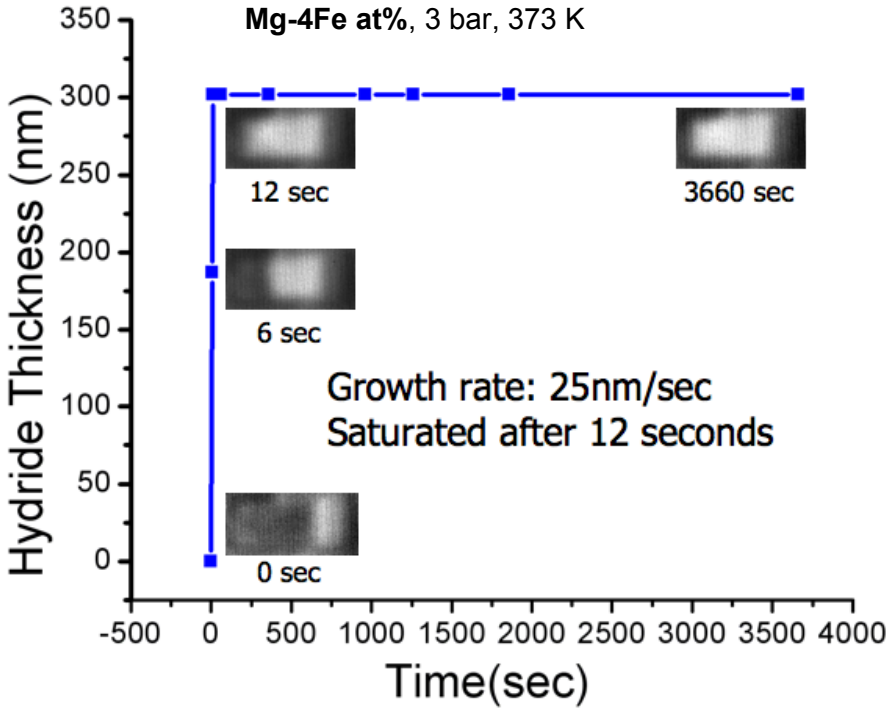


IR imaging: kinetics of growth in Mg-TM wedge films

Mg, Mg-Ti

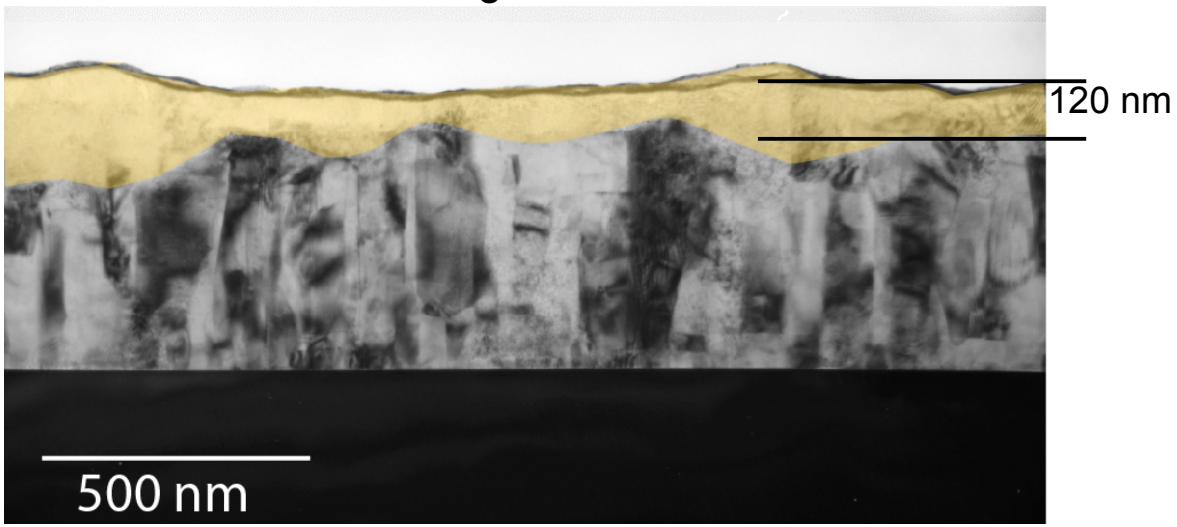


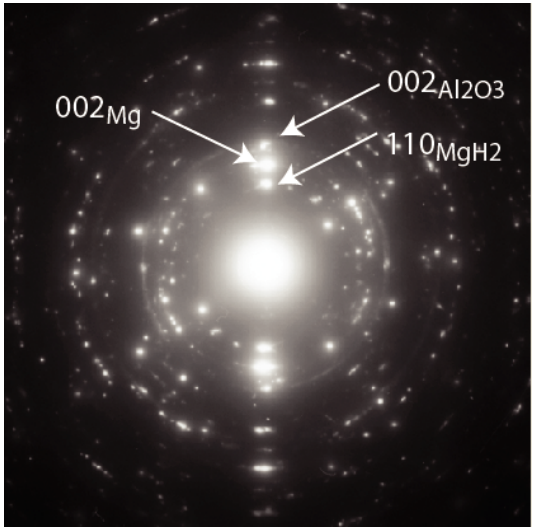
Mg-Fe



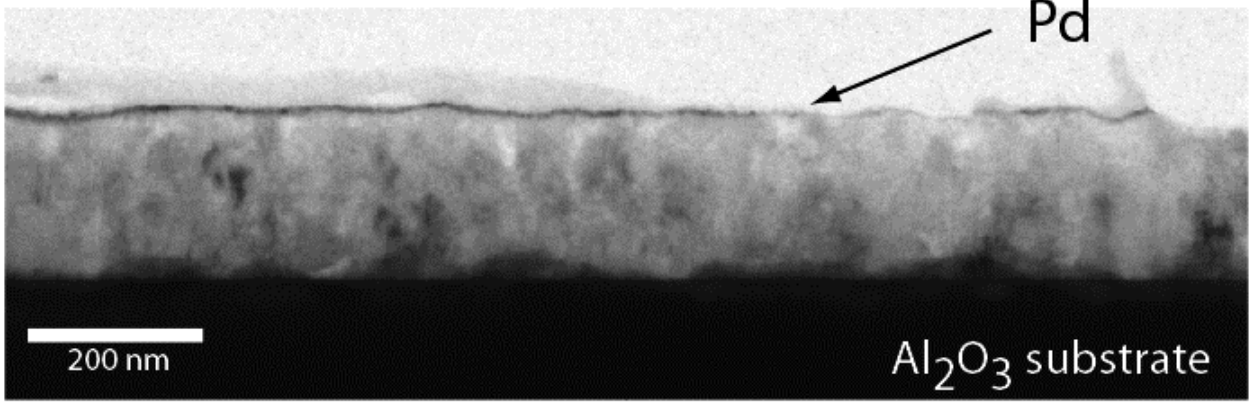
Hydrogenated Mg-Ti and Mg-Fe wedge films: TEM

Cross-sectional TEM, Mg-5Ti at% film

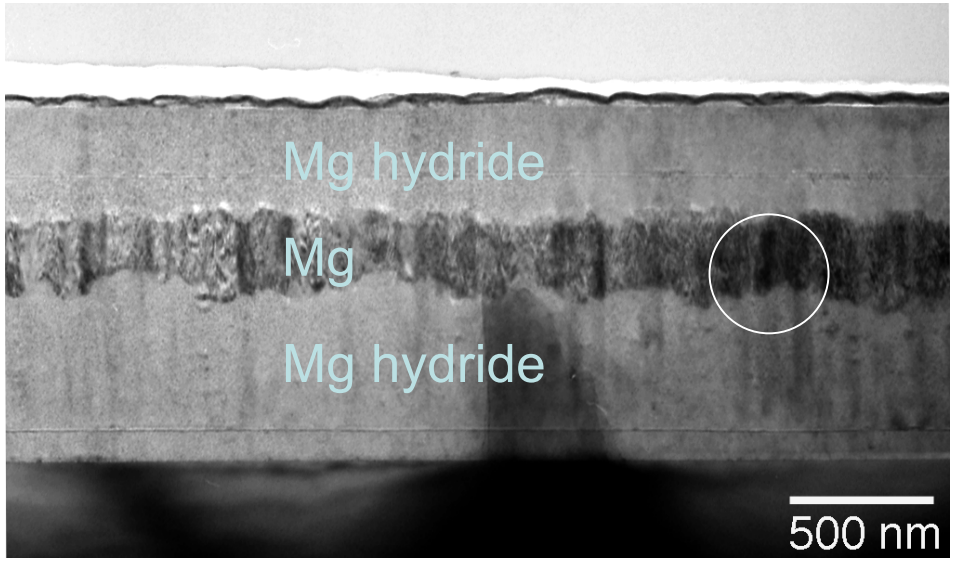


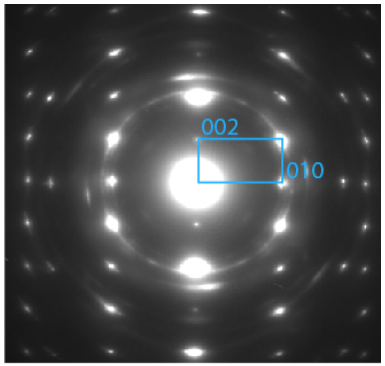


Cross-sectional TEM, Mg-4Fe at% film

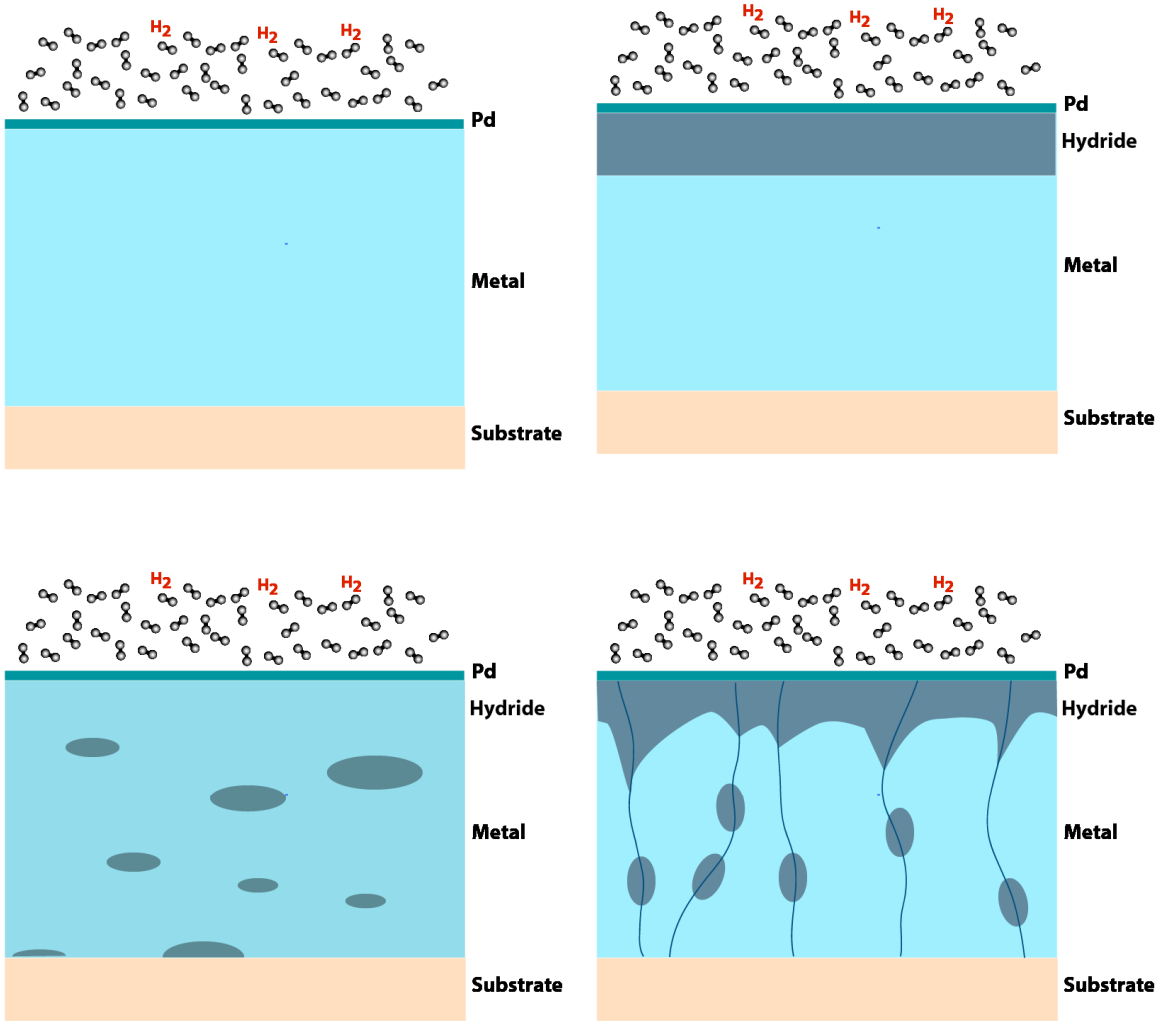


Thick hydrogenated Mg-4Fe film





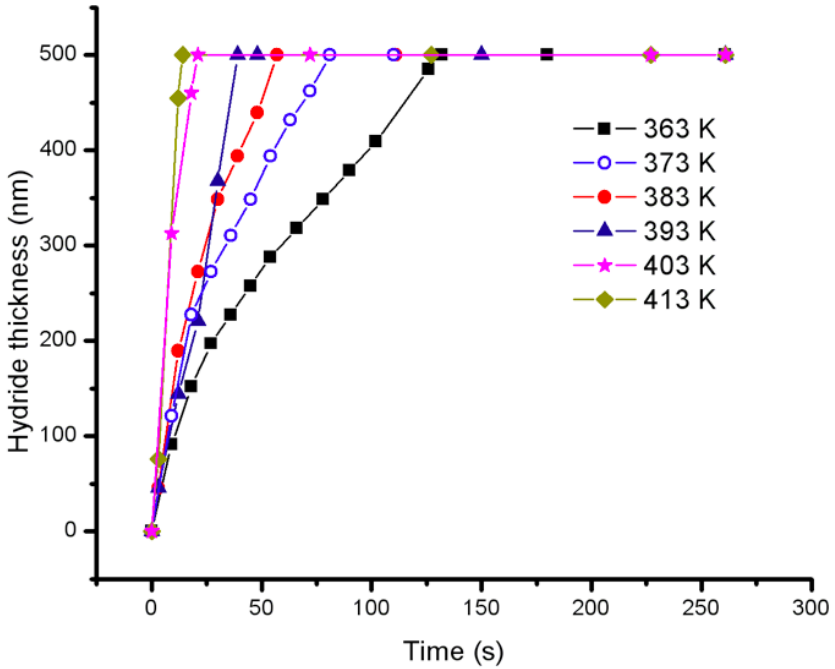
Different scenarios for formation of hydride phase in films



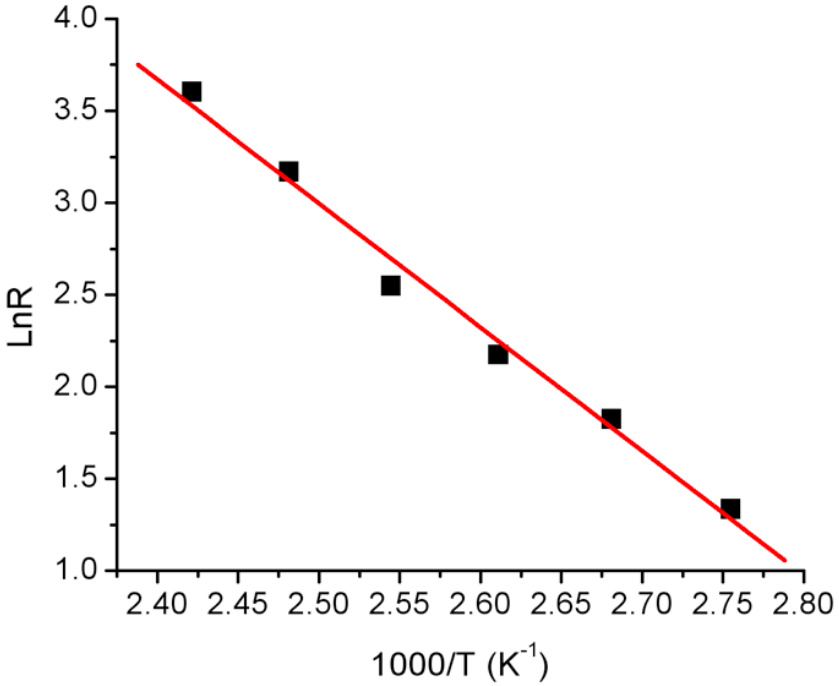
To be taken into account

1. Dissociation of H_2
2. Interaction with Pd
3. Diffusion in M
4. Diffusion in MH
5. Nucleation
6. Growth
7. Effect of defects

Kinetics of hydride growth in Mg-4Fe wedge films



Plot of approximate MgH_2 layer thickness as a function of hydrogenation time. Films hydrogenated under 0.1 MPa hydrogen pressure at 363 K, 373 K, 383 K, 393 K, 403 K and 413 K.



Arrhenius plot of the hydride growth rate as a function of 1/T. An activation energy obtained from this plot is ~56 +/- 3 kJ/mole

What 56 kJ/mole means?