Lightweight Intermetallics for Hydrogen Storage

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– A Member of the DOE Metal Hydride Center of Excellence –

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Project ID # STP27

GE Program Overview

Timeline

- Project start date: FY05
- Project end date: FY09
- Percent complete: *New Project*

Budget

- Expected Total Project Funding:

Phase I - 3 years:	*$2.00M*
– DOE Share:	$1.60M
– GE Share:	$0.40M
Phase II - 2 years:	*$1.47M*
– DOE Share:	$1.18M
– GE Share:	$0.29M

- Funding for FY05:

  $450K (DOE), $112K (GE)

Barriers

Right heat of formation

Absorption / desorption kinetics

Hydrogen capacity and reversibility

Targets

Gravimetric capacity: > 6%

Volumetric capacity: > 0.045 kg H_2/L

Min/max desorption temp: -30 / 85°C

Partners

- Member of DOE MHCoE
- Collaborations with MHCoE partners on modeling and characterization
- Member of the Coordinating Council of DOE MHCoE

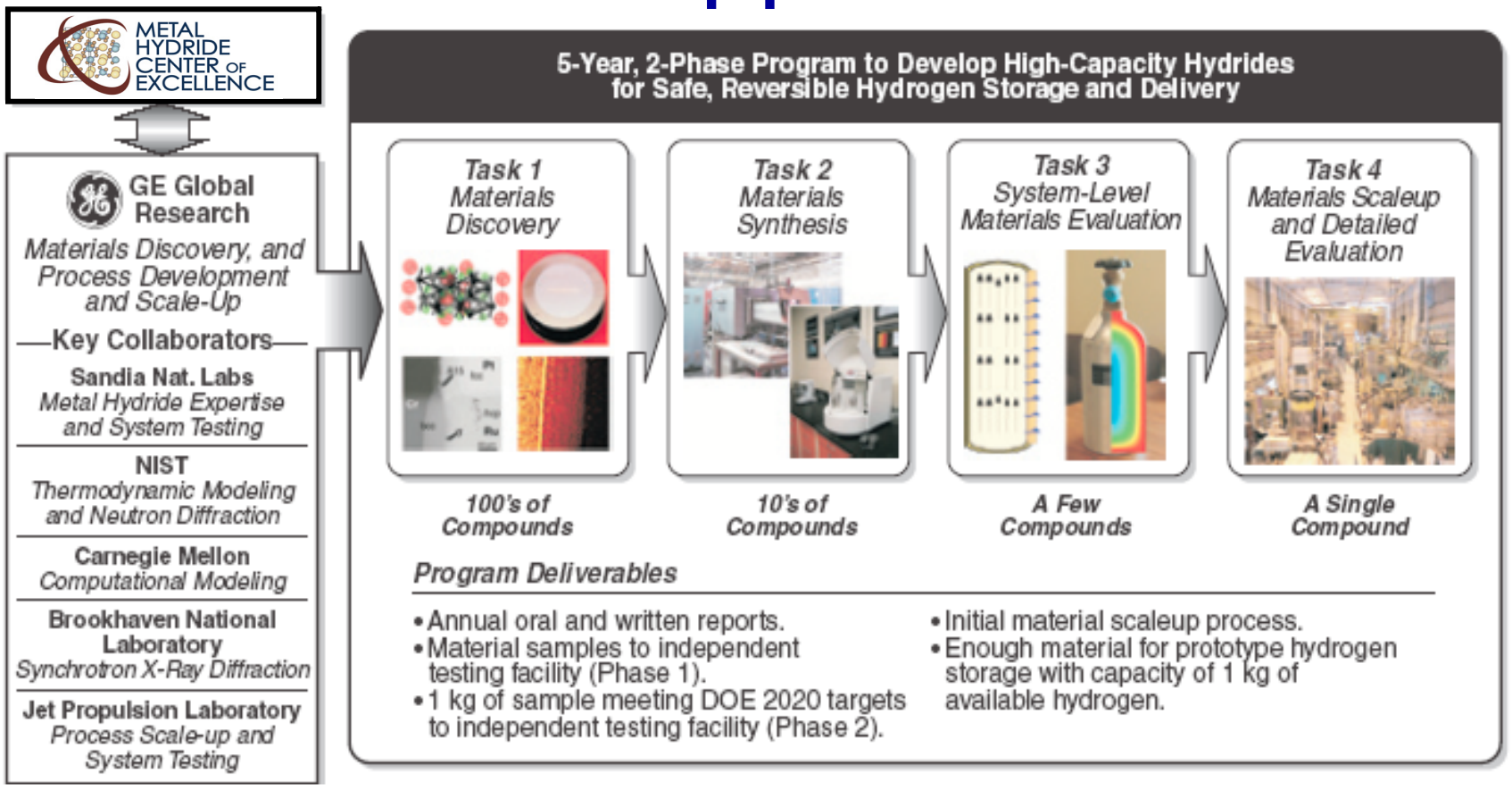
GE Program Objective

Discover and develop a high capacity (> 6 wt.%) lightweight hydride that is practical and inexpensive for reversible vehicular hydrogen storage and delivery systems, capable of meeting or exceeding the 2010 DOE/FreedomCAR targets.

FY05 Goals

- Develop a high-efficiency combinatorial synthesis and high-throughput screening methodology for metal hydride discovery
- Identify hydrides from combinatorial samples and validate them through gram-quantity sample tests

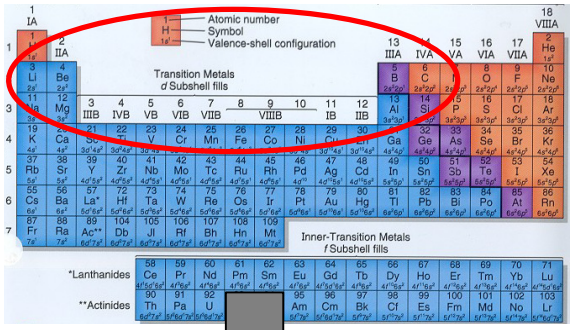
GE Approach

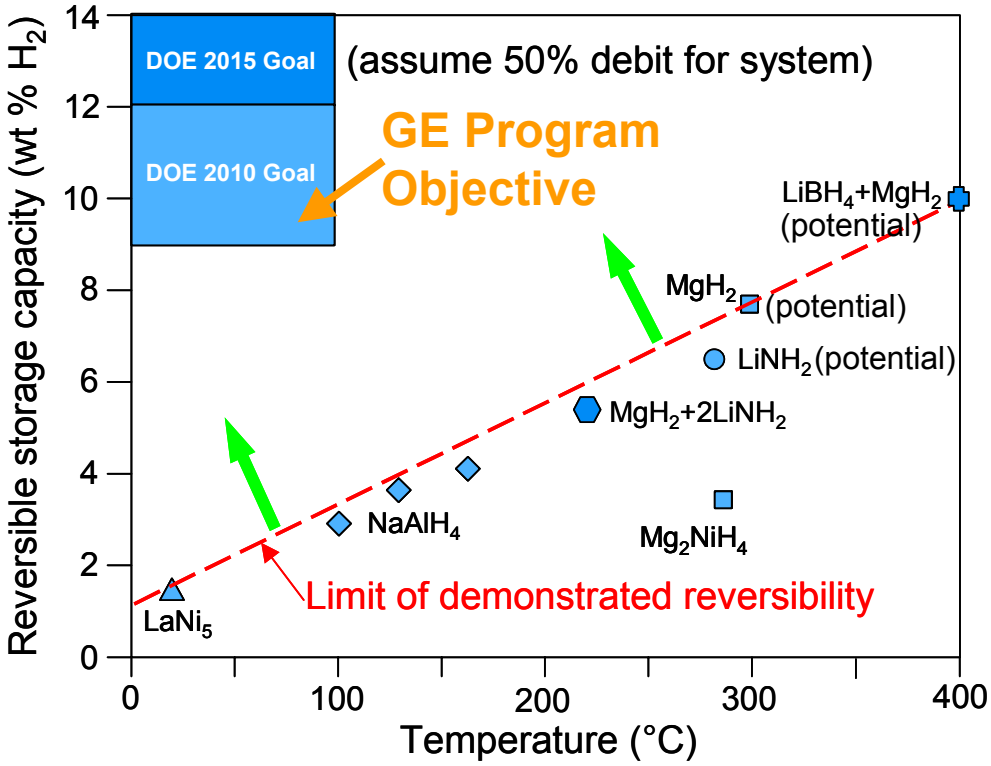


Materials Discovery Acceleration: *Design for Six Sigma coupled with…*

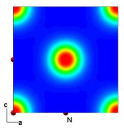
- Materials Expertise: Development & Processing
- High Throughput Screening (HTS): Composition Design Space
- Characterization: Composition, Microstructure & Performance
- System Performance: Characterization & Predictive Modeling
- Focused multi-disciplinary team

GE Metal Hydride Discovery Process

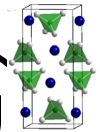




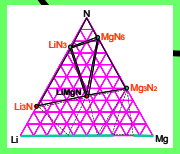
System Requirements
Thermodynamics
Reaction Path
Diffusion
Safety



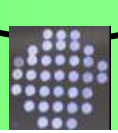
Modeling

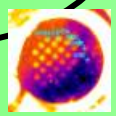


Concepts

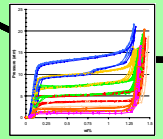


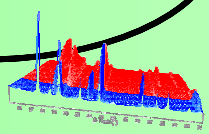
Combi & HTS





Synthesis & Characterization





New Hydrides

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GE Lightweight Intermetallics Approach

- **Focus:**

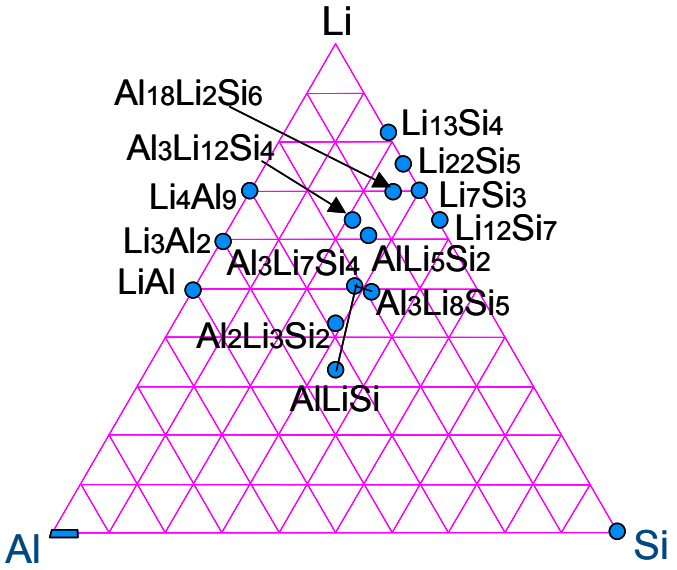
  Lightweight aluminides & silicides of Li, Mg, and Na (potential to 6 wt.%)

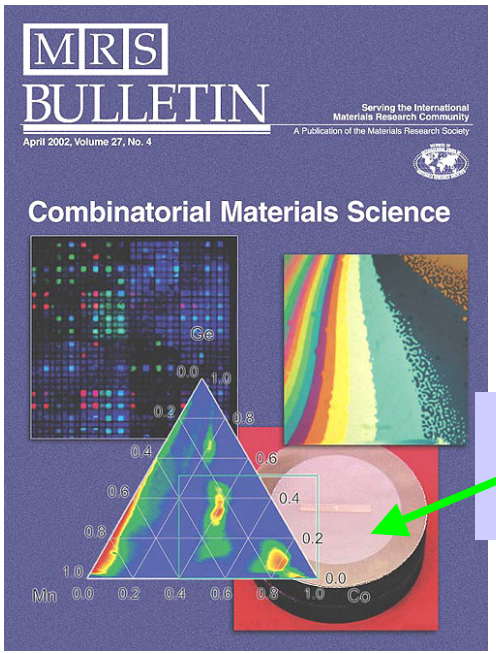
- **Opportunity:**

  Many intermetallic compounds exist in aluminide and silicide systems

- **Develop & Validate:**

  Combinatorial synthesis and high-throughput screening methodologies for hydride discovery in the target temperature – pressure – kinetics design space

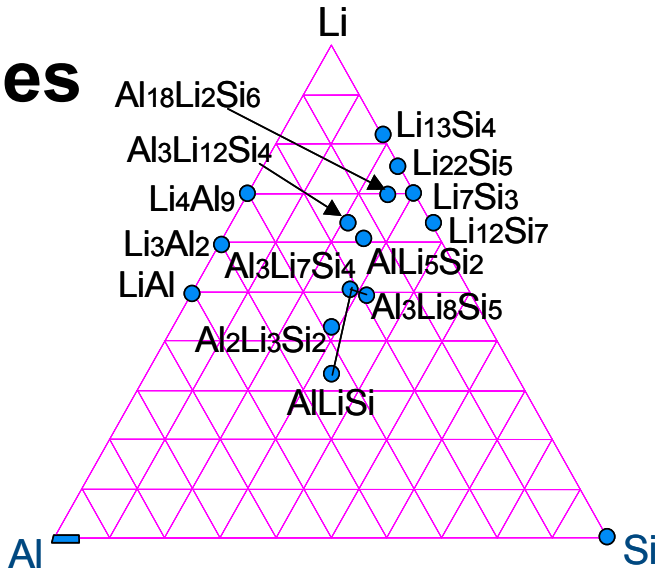




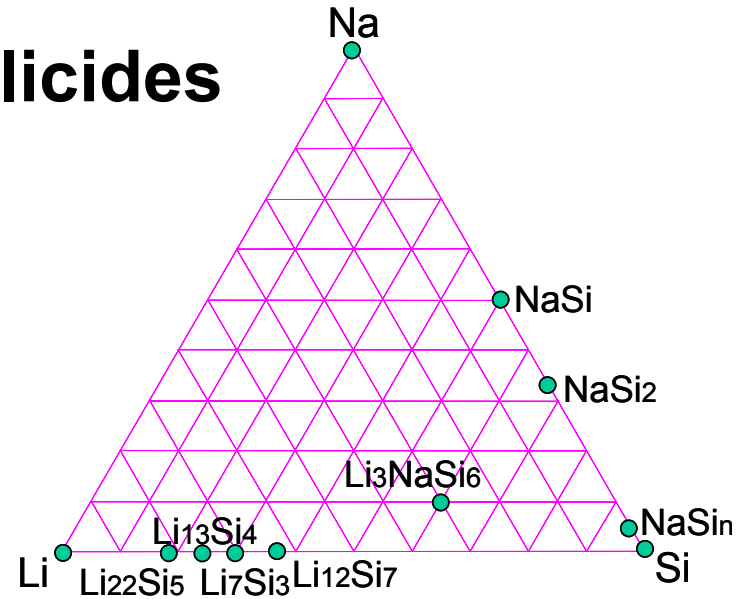
Diffusion multiple

Aluminides and Silicides

Aluminides



Silicides

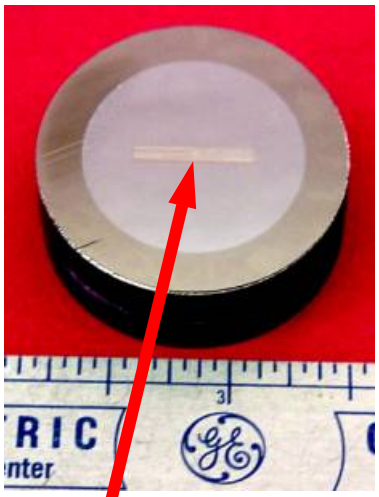


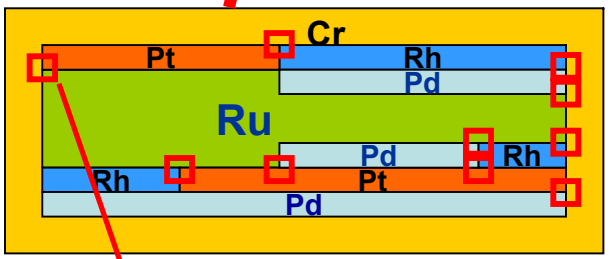
- **Space to be screened:** Al-Li, Al-Li-Si, Al-Li-Mg, Al-Ga, Al-Li-Cu, Al-Li-Mn, Al-Mg-Zn, Al-Mg-Cu, Al-Li-Ge, Al-Li-Si, …

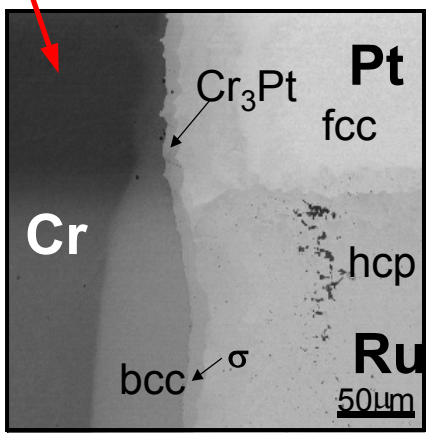
- **Space to be screened:** Li-Si, Li-Mg-Si, Mg-Si, Na-Si, Li-Na-Si, Na-Al-Si, Li-Na-Al-Si Li-Na-Si, …

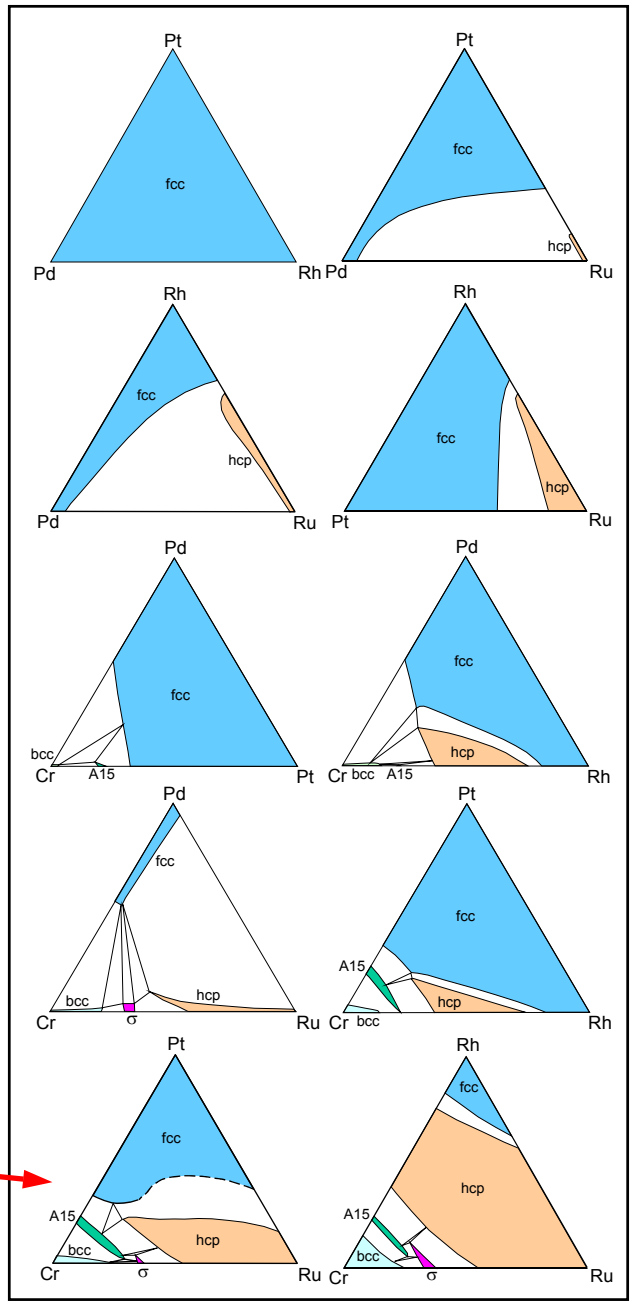
- **Al and Si are lightweight, high availability & low cost**
- **Many compounds known to exist but not evaluated for H_2 storage**
- **Minimal risk of forming volatile hydrides (*e.g.*, BH_3, NH_3)**

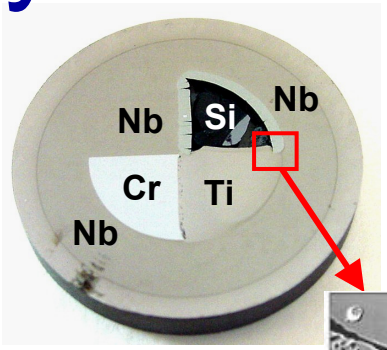
Diffusion Multiples & Alloy Development

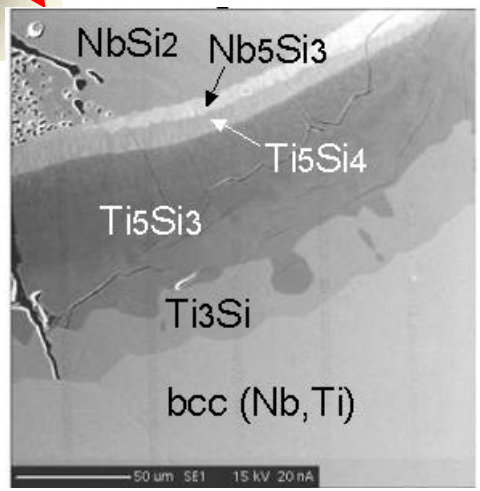


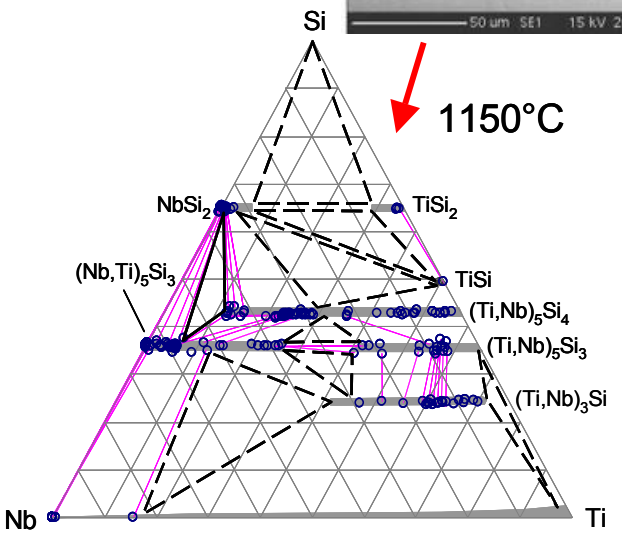












Synthesize many compounds simultaneously

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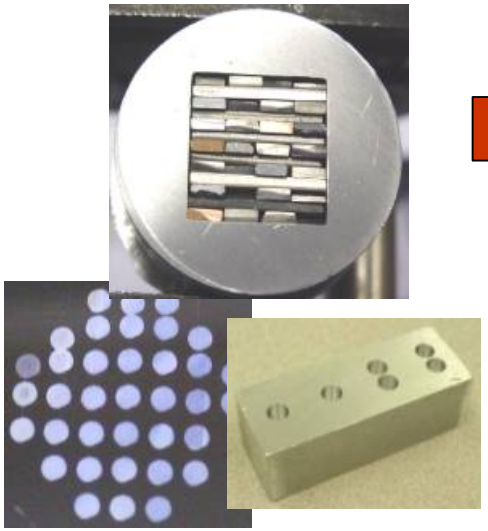
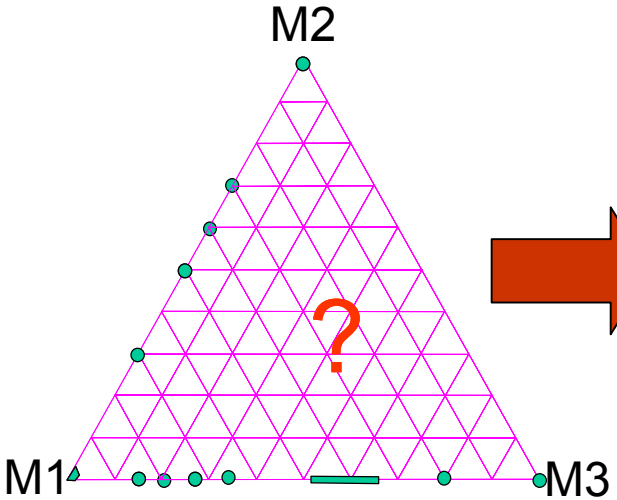
Combinatorial Synthesis & HTS

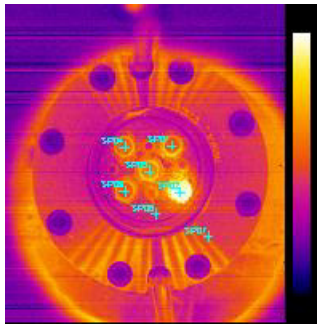


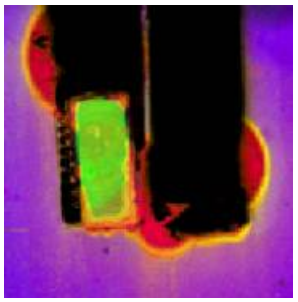


React @ desired T and atmosphere

- Slice & polish
- 1st-level characterization

Charge with D_2





Screening with thermography

Screening with time-of-flight secondary ion mass spectroscopy

Identify, synthesize & test leads

Effective combi synthesis methods developed

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Combinatorial Synthesis & HTS: Results

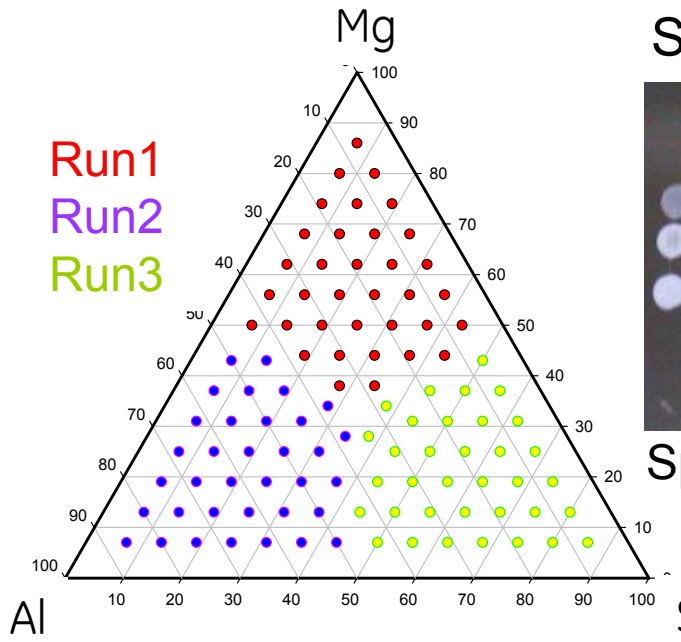
Thin-film methods

Synthesis

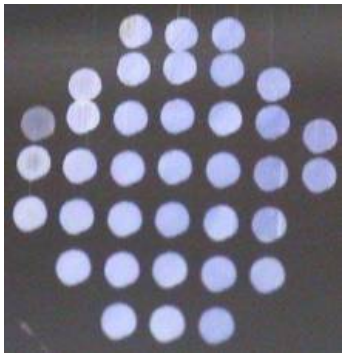
- Complementary to diffusion multiple
- Great for exploring Mg, Al, Si alloys
- Map phase diagram at 6% intervals, 3 runs, 5hrs.
- 7 target co-sputtering, DC and RF power

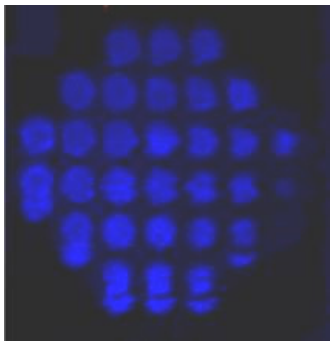
Screening

- Optical reactor capability, 350 °C, 55 atm.

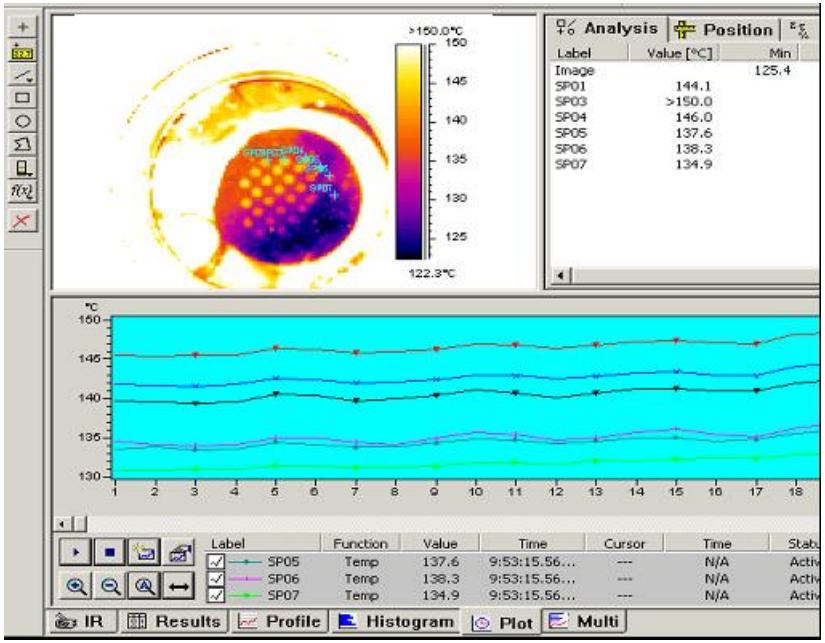


Start Mg_3-$Al_{0.03}$ End $Mg_{0.03}Al_3$





Sputtered Array Imaging A/B ratio



Screen for H_2 storage with thermography

Thermography is an effective screening tool

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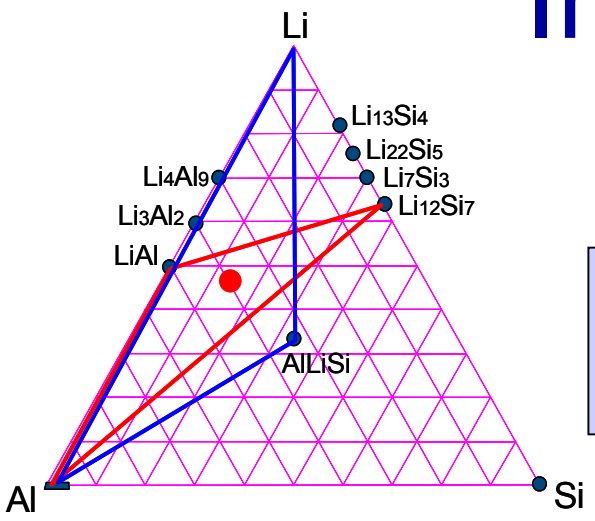
In-Situ XRD: Results



Literature:

$LiAlSi + 0.45\ H_2 \leftrightarrow LiAlSiH_{0.9}$ 535°C, 80-82 bar

New result: 300-380°C, < 135 bar

$AlLi + Li_{12}Si_7 + Al + H_2 \leftrightarrow LiAlSiH_{0.9} + LiH + (Al)$

$LiAlSiH_{0.9}$

Charging kinetics are *very* fast

LiAl

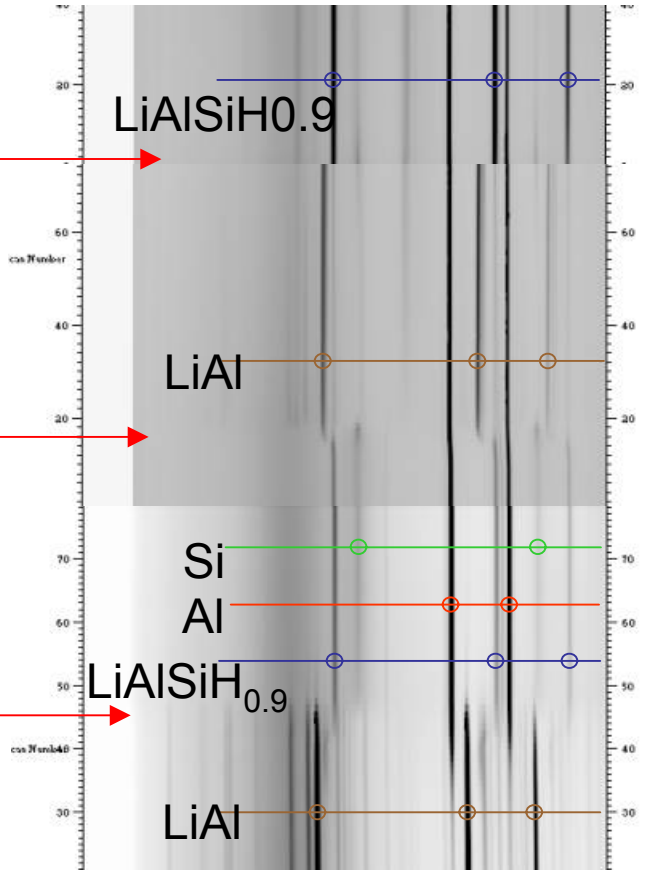
LiAl (Al)

Decomposition without intermediates at 380 °C

$LiAlSiH_{0.9} + Si + Al$

Hydrogenation via intermediates at 300 °C

$LiAl + Li_{12}Si_7 + Al$



380°C
135 bar

310-380°C
2 bar

75-300°C
135 bar

First intermetallic hydride in non-transition metal alloys

GE Lightweight Intermetallics Progress

1. Designed new diffusion multiple configuration and tested for alkali metals
2. Demonstrated the screening capability of thermography and ToF-SIMS
3. Studied/screened several compounds in the Li-Al-Si ternary system

   – *This system has the first reversible intermetallic hydride in non-transition metal alloys*

Future Work

Remainder of FY ’05:

- Team with modeling partners to identify promising concepts/systems
- Continue to make combi samples & screen the aluminides and silicides composition space
- Synthesize lab quantities of compounds identified from combi screening to validate the methodology

FY ’06:

- Continue with the hydride discovery task (Task 1)
- Begin Task 2: materials synthesis
- Prepare Task 3: system-level materials evaluation models and setup

GE Lightweight Intermetallics for Hydrogen Storage: Plan