

# Lightweight Intermetallics for Hydrogen Storage

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Niskayuna, NY

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

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# 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<sub>2</sub>/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

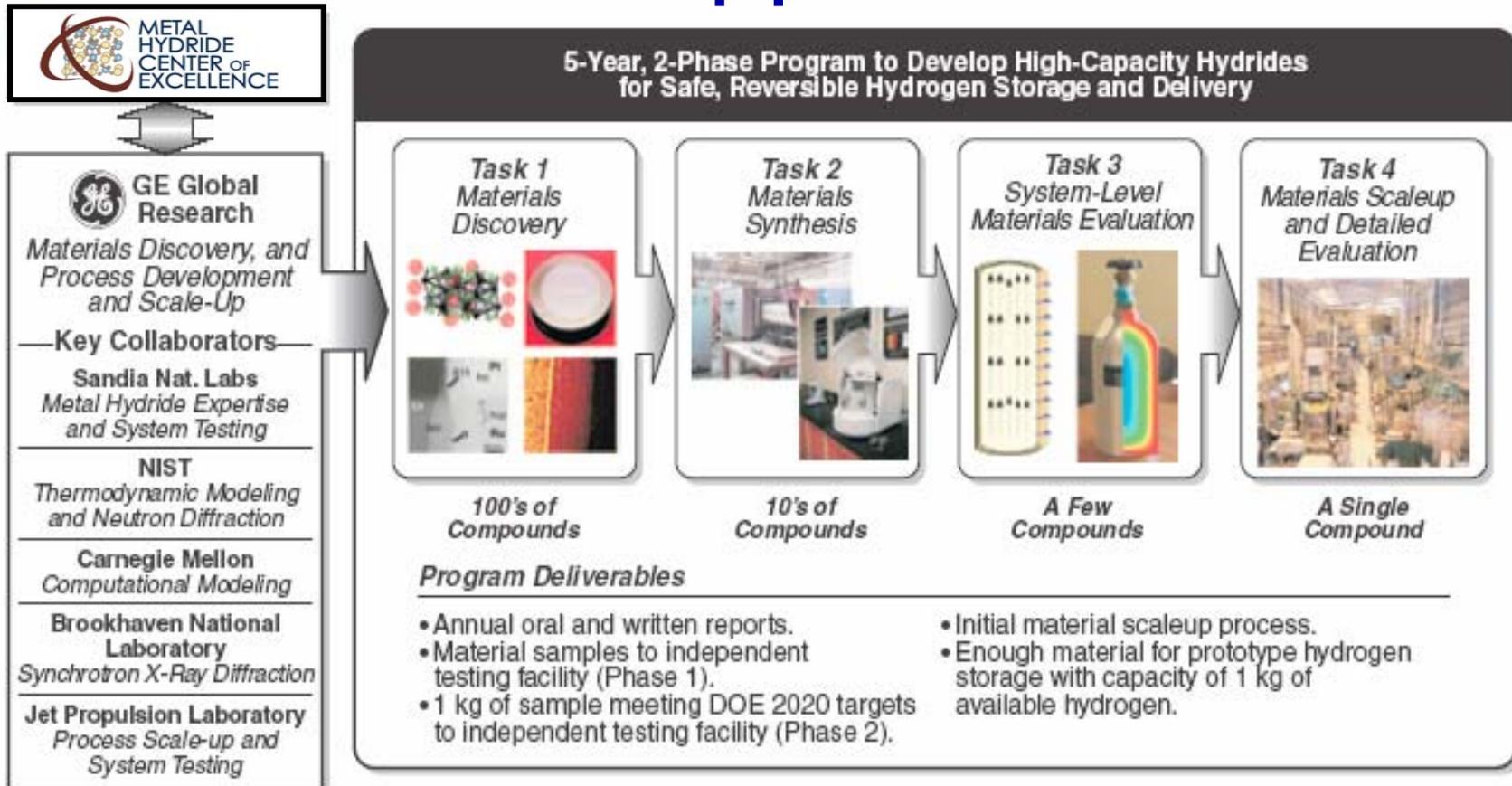
# GE Program Objective

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

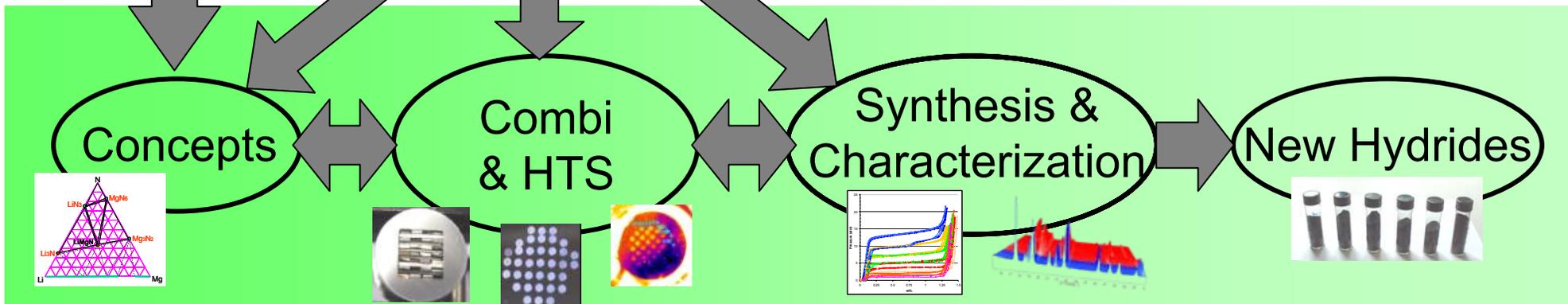
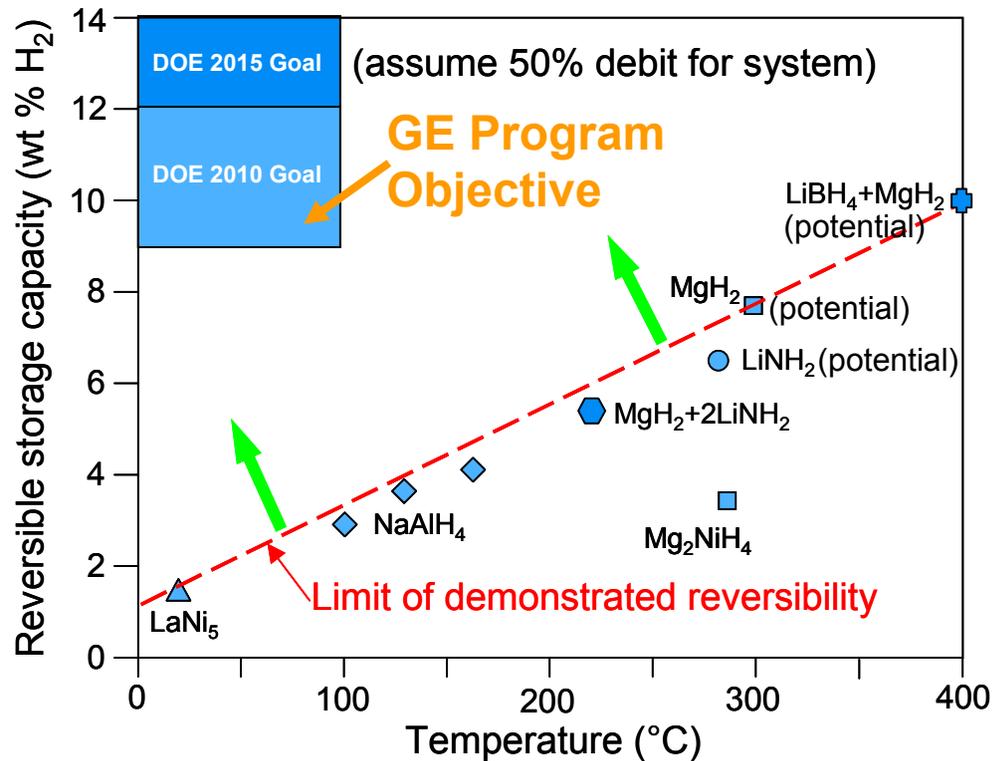
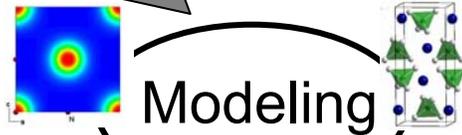
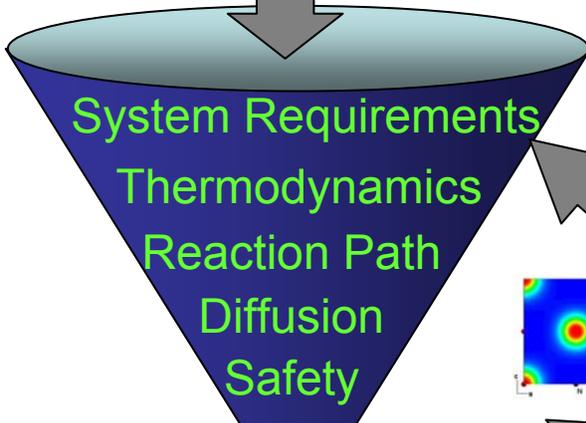


## Materials Discovery Acceleration: *Design for Six Sigma coupled with...*

- 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

Periodic table showing elements categorized by groups (IA to VIIIA) and periods (1 to 7). A red circle highlights the transition metals (groups IIIA to VIIIA) and inner-transition metals (lanthanides and actinides).



# GE Lightweight Intermetallics Approach

- **Focus:**

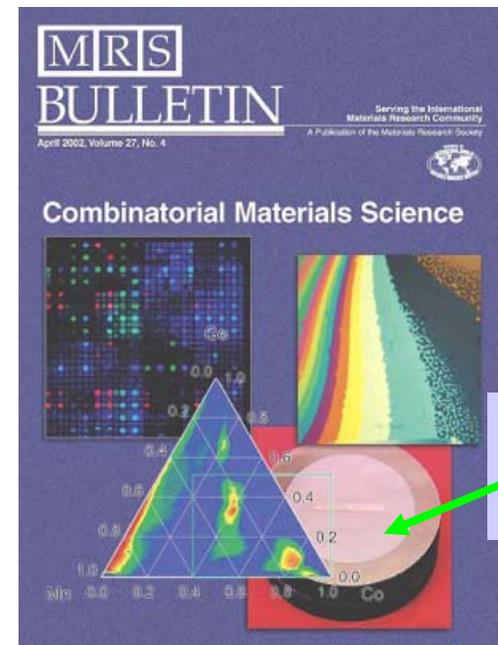
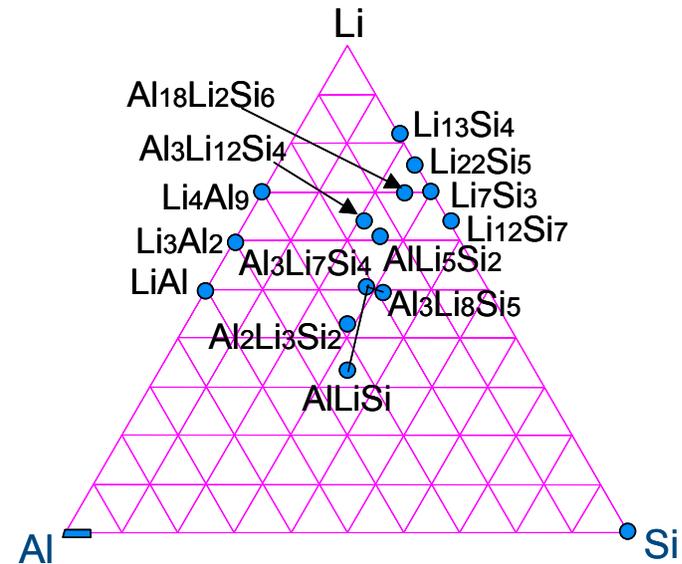
Lightweight aluminides & silicides of Li, Mg, and Na (potential to 6 wt.%)

- **Opportunity:**

Many intermetallic compounds exist in aluminide and silicide systems

- **Develop & Validate:**

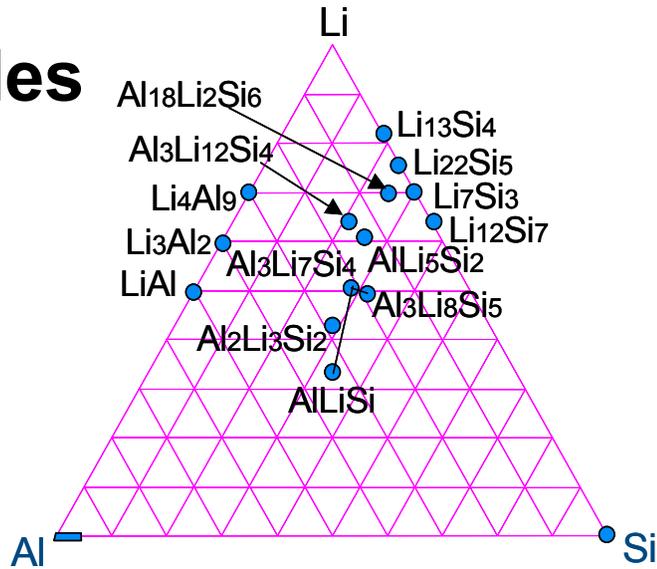
Combinatorial synthesis and high-throughput screening methodologies for hydride discovery in the target temperature – pressure – kinetics design space



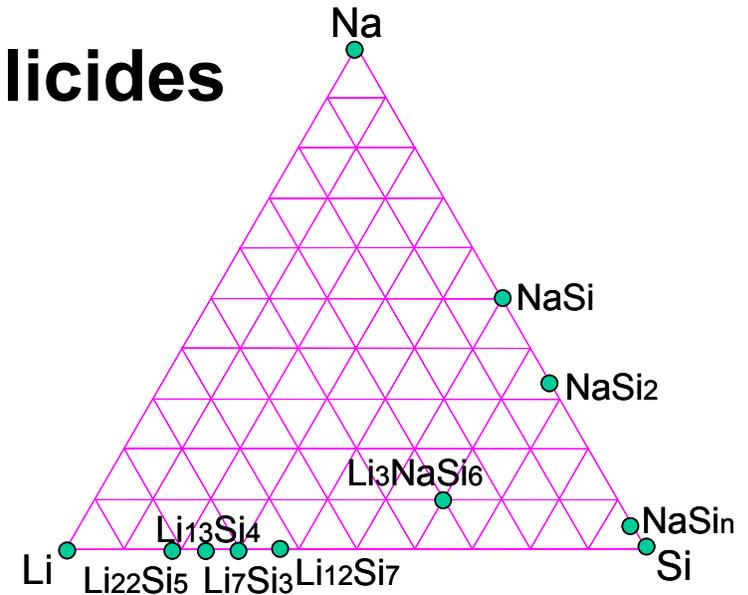
Diffusion multiple

# Aluminides and Silicides

## Aluminides



## Silicides

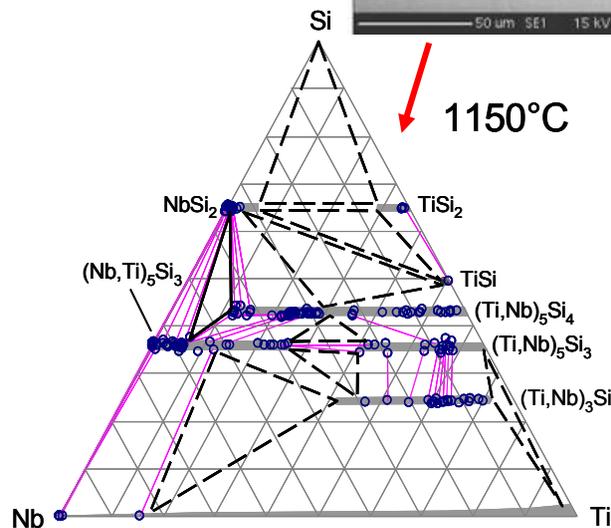
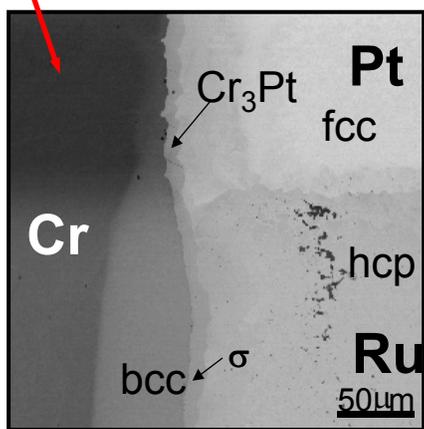
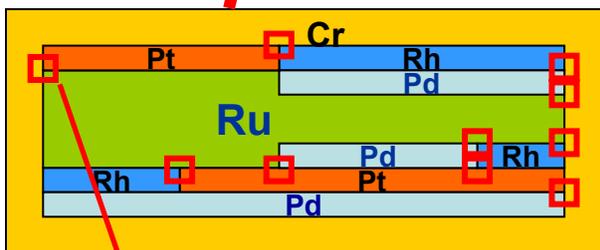
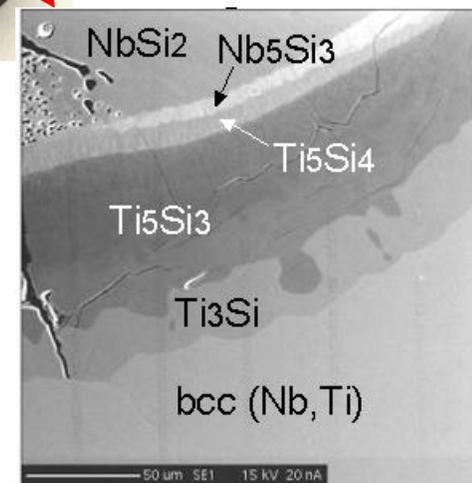
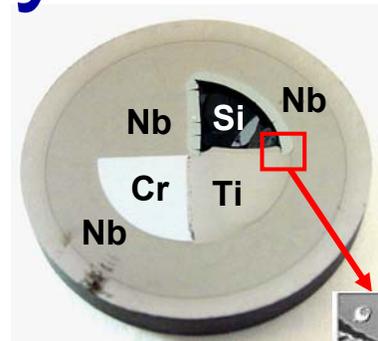
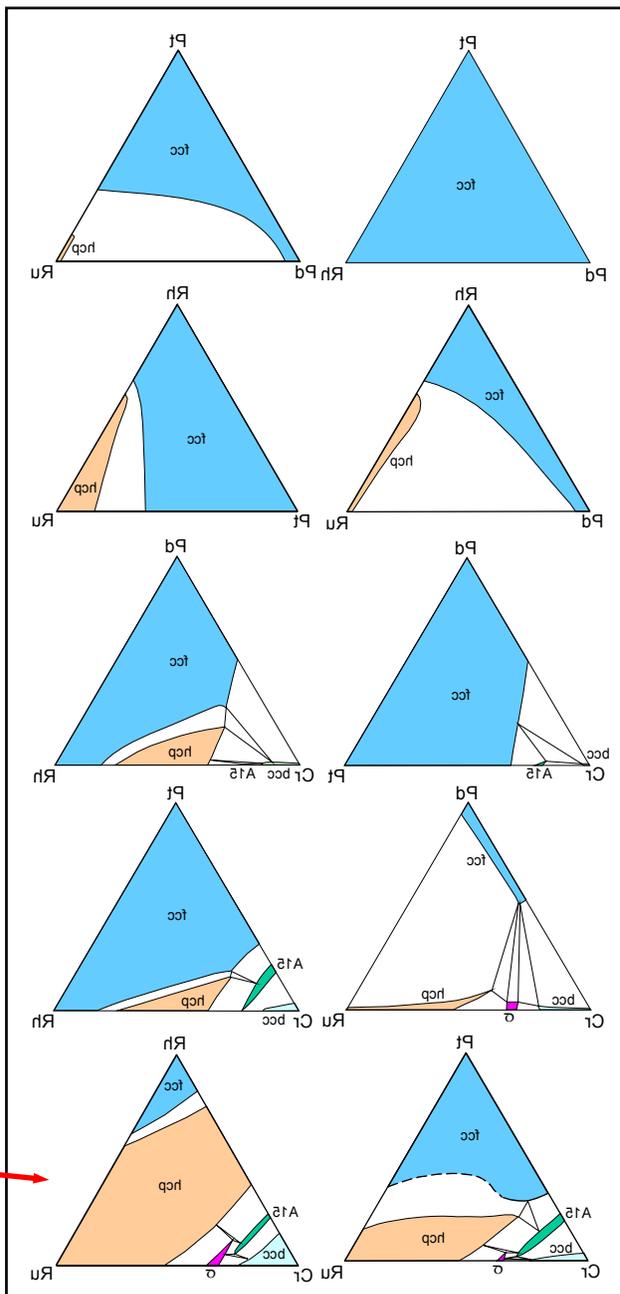
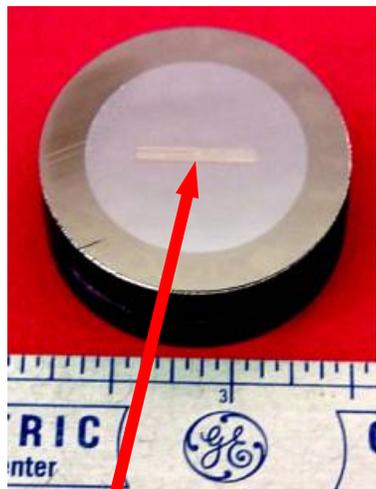


- **Space to be screened:** Al-Li, Al-Li-Si, Al-Li-Mg, Al-Ga, Al-Li-Cu, Al-Li-Mn, Al-Mg-Zn, Al-Mg-Cu, Al-Li-Ge, Al-Li-Si, ...

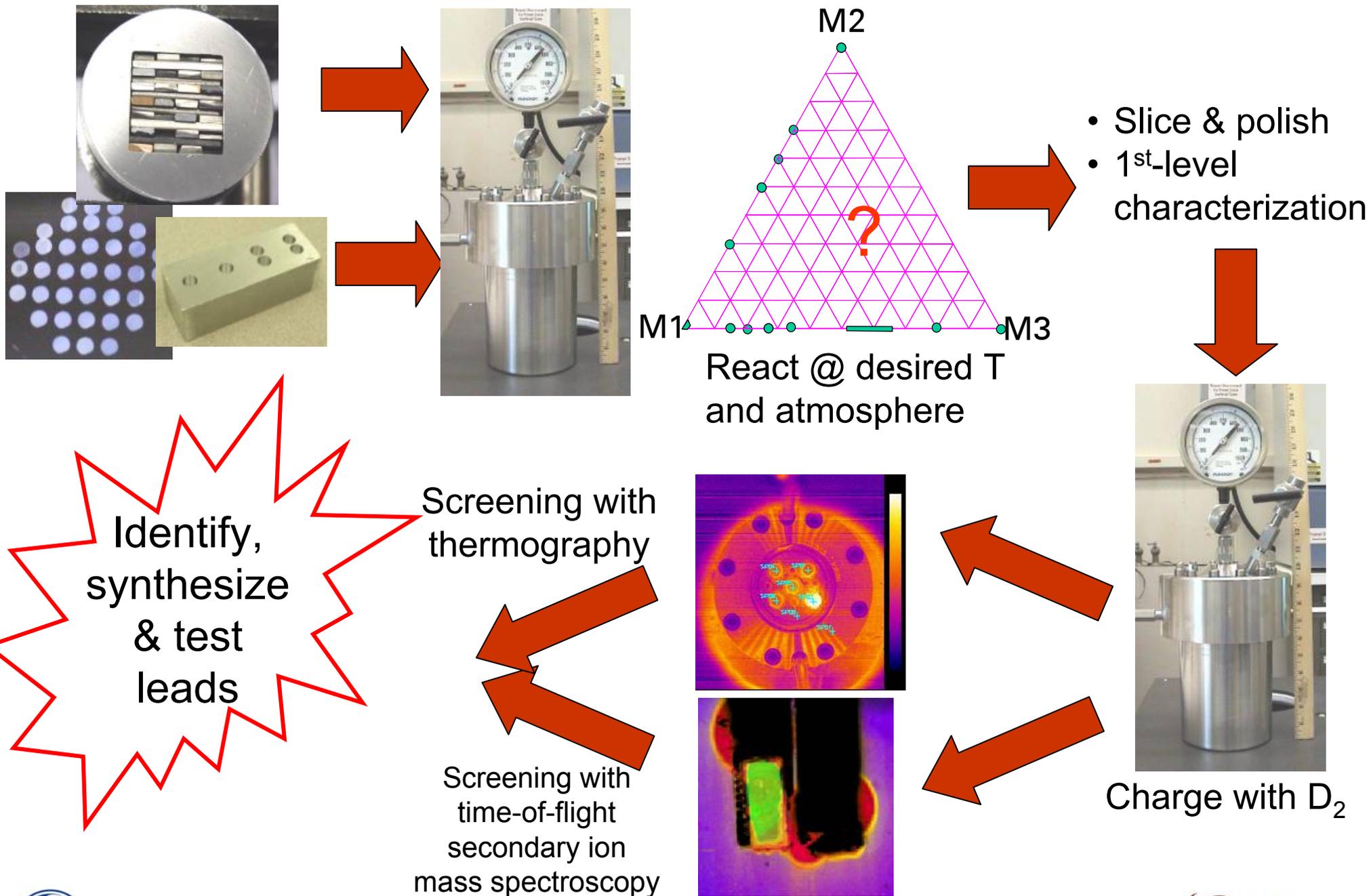
- **Space to be screened:** Li-Si, Li-Mg-Si, Mg-Si, Na-Si, Li-Na-Si, Na-Al-Si, Li-Na-Al-Si, Li-Na-Si, ...

- **Al and Si are lightweight, high availability & low cost**
- **Many compounds known to exist but not evaluated for H<sub>2</sub> storage**
- **Minimal risk of forming volatile hydrides (e.g., BH<sub>3</sub>, NH<sub>3</sub>)**

# Diffusion Multiples & Alloy Development



# Combinatorial Synthesis & HTS



# Combinatorial Synthesis & HTS: Results

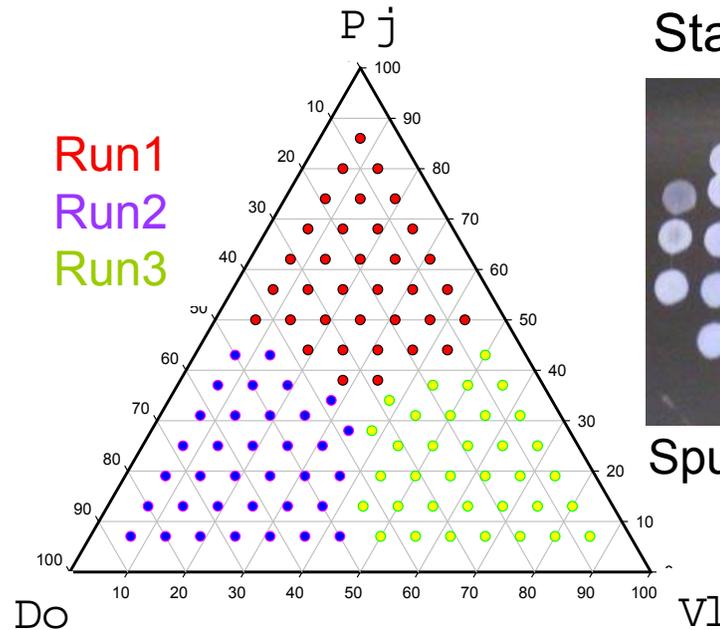
## Thin-film methods

### 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

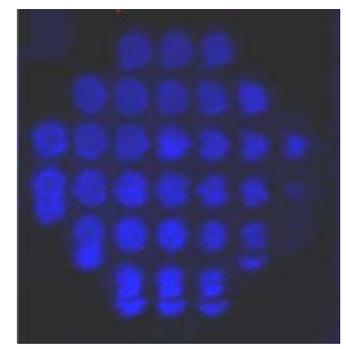
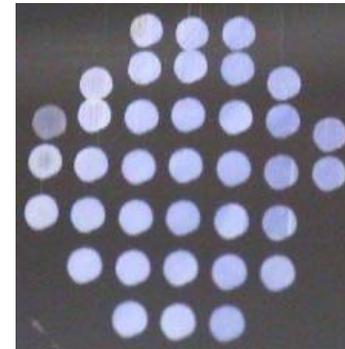
### Screening

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

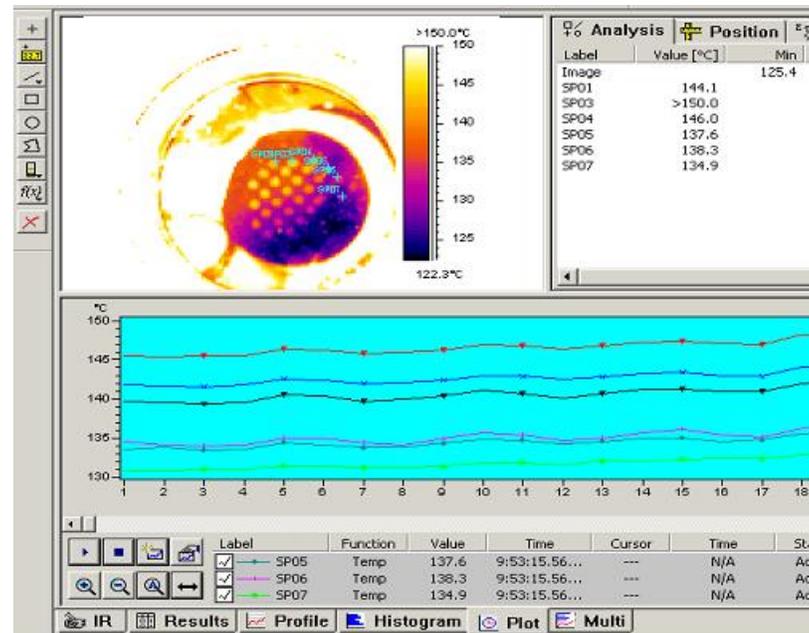


Start  $Mg_3-Al_{0.03}$

End  $Mg_{0.03}Al_3$

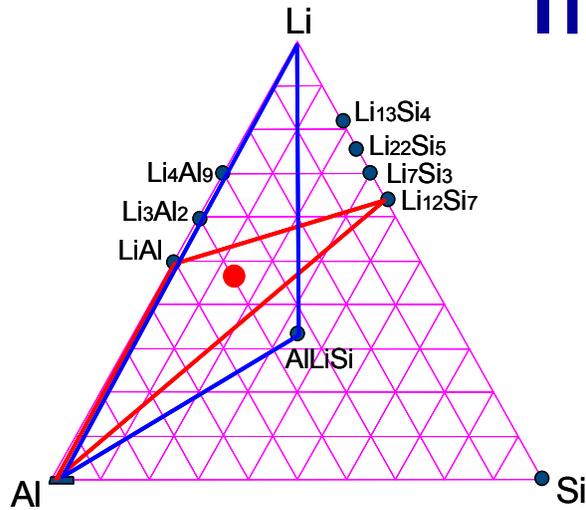


Sputtered Array Imaging A/B ratio



Screen for  $H_2$  storage with thermography

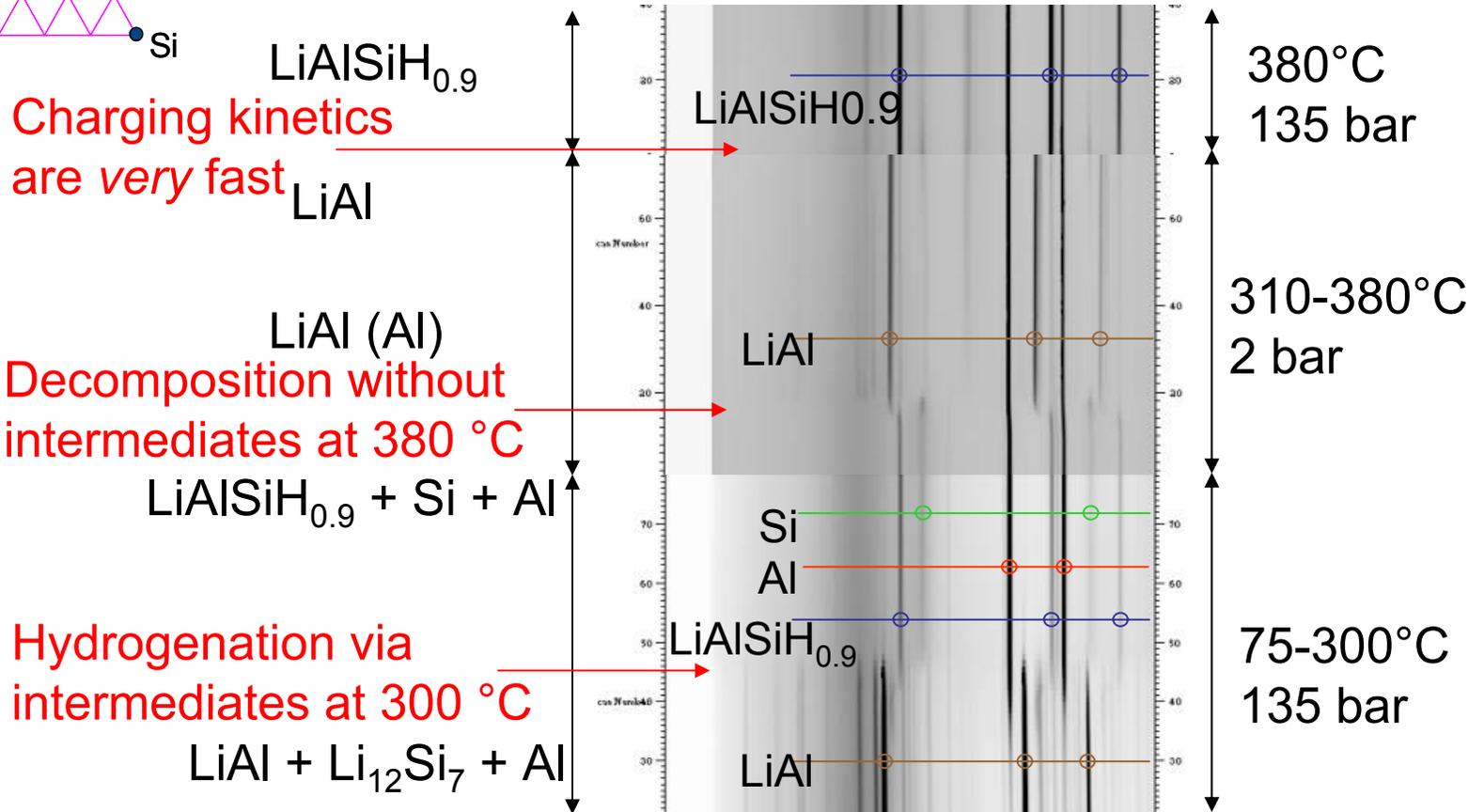
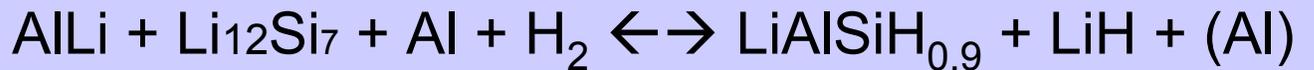
# In-Situ XRD: Results



Literature:



**New result: 300-380°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

