Integrated Computational Materials Engineering (ICME) for Mg: International Pilot Project (Part 1))

John E. Allison
Ford Motor Company / USAMP

April 9, 2010

Project ID
LM012

Overview

Timeline

- Project start date: Feb 2007
- Project end date: Feb 2012
- Percent complete: 60%

Budget

- Total project funding
  - DOE share: $1M
  - Contractor share: $1M
- Funding received in FY09
  - $215,052
- Funding for FY10
  - $223,000

Barriers

- Barriers addressed:
  - Design data & modeling tools
  - Manufacturabiity
  - Performance
  - Cost

Partners

- 3 US Universities
- 3 US Companies
- TMS
- Lead: USAMP

USAMP

Relevance to Materials Technologies
Lightweight Materials Goals

- Application of Mg alloys in body applications may result in up to 45% mass savings.
- The development and utilization of ICME tools will enable an early assessment and optimization of the primary performance characteristics to ensure that key performance metrics are met.
- Development and utilization of ICME tools will enable optimization of manufacturing processes and design to reduce costs of Mg component.
- Current Mg alloys have limitations for use in some body applications. ICME tools will enable cost effective development of new alloys to meet cost/performance requirements

USAMP

Goals – What we are trying to do

- Establish, demonstrate and utilize an ICME knowledge infrastructure for magnesium in body applications for:
  - Microstructural engineering
  - Process and product optimization
  - Future alloy development

- Attract materials researchers into Mg field & leverage their efforts by providing a collaboration space for coupling high quality data and models.

- Identify and fill technical gaps in fundamental knowledge base

USAMP

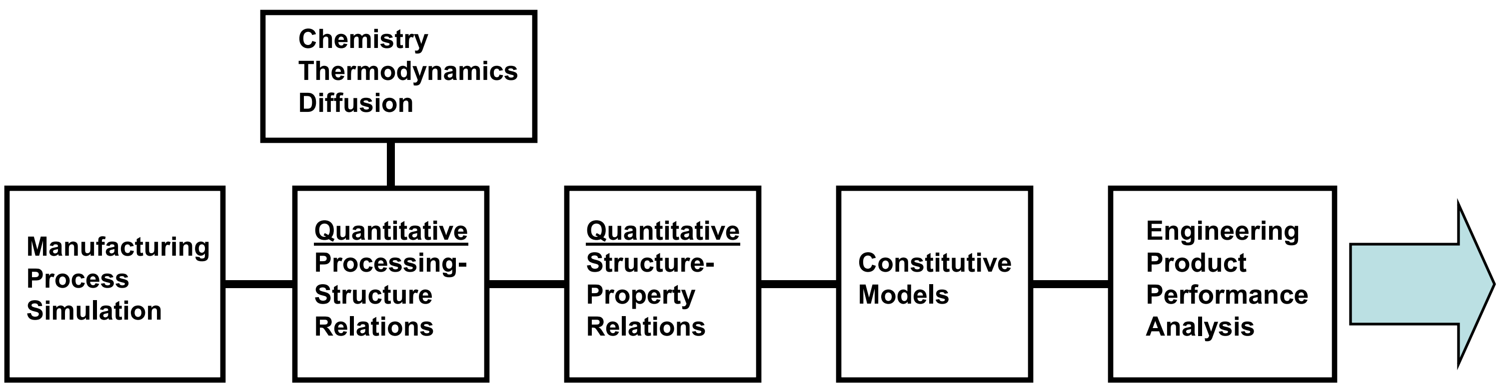
Milestones

- Milestone 1: Infrastructure Demonstration (March 2009)
  - *Demonstrate a cyber-infrastructure data to enable integration and collaboration*
- Milestone 2: ICME Progess Demonstration (March 2010):
  - Demonstrate substantial progress in all task areas
  - Demonstrate integration with manufacturing simulation
- Milestone 3: Application to MFERD Phase II (September/October 2011)
  - Demonstrate ability of ICME tools to link manufacturing and predict performance of MFERD demonstration structure & validate the results *(Dec 2012)*
- Milestone 4: Enhanced ICME (January/December 2012)
  - Demonstrate enhanced ICME for Mg capability linked with manufacturing and design CAE tools and optimization

USAMP

The Approach – Develop ICME Tools for Mg in Body Applications

Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.*

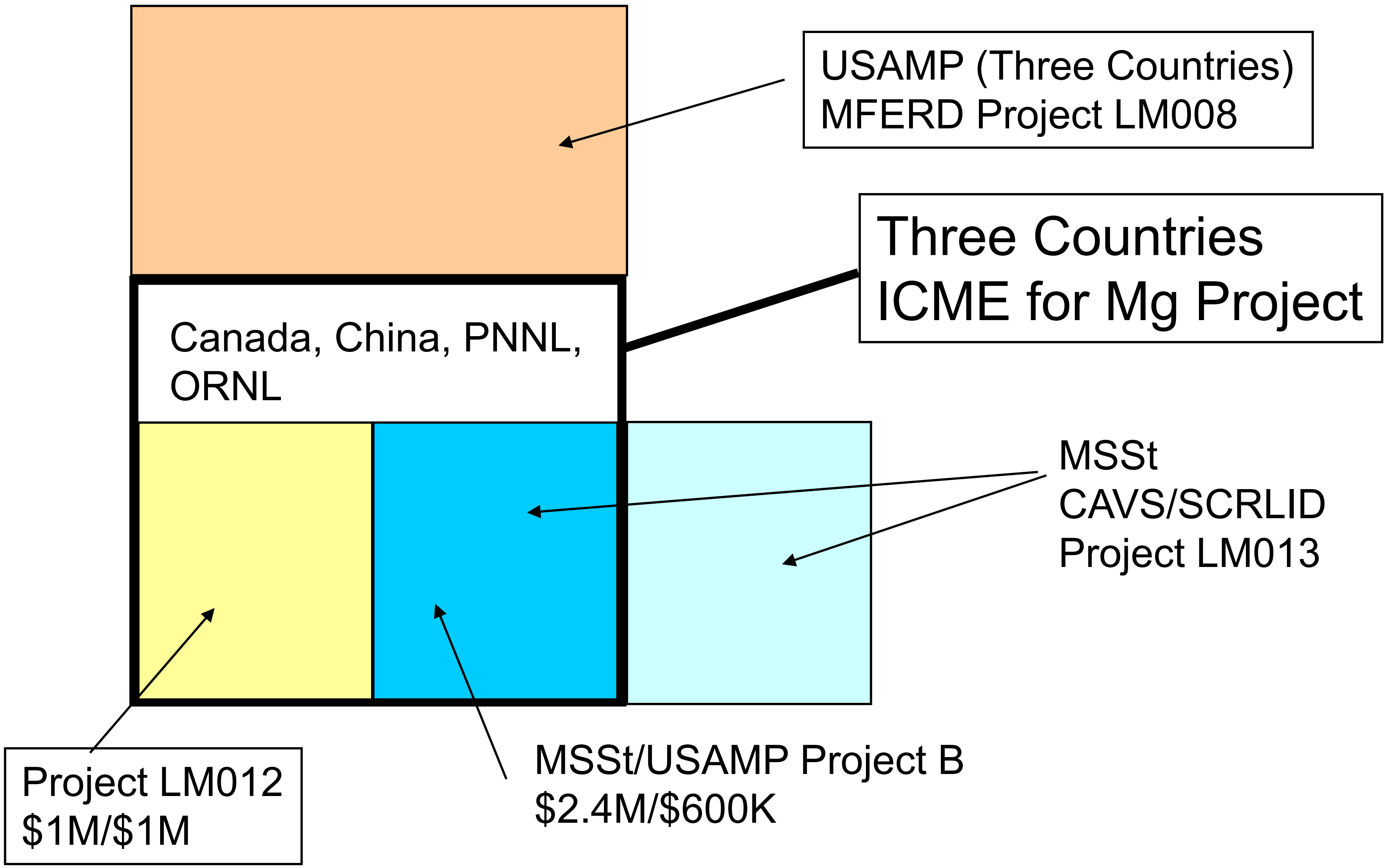


- Process & product optimization
- Innovation

* NAE ICME Report, 2008

USAMP

Program Integration



US Mg ICME Team

- **Ford**
- **GM**
- **McCune & Associates**
- **Northwestern University**
- **University of Michigan**
- **University of Virginia**
- **Materials Informatics Inc**
- **The Minerals, Metals and Materials Society (TMS)**
- **ThermoCalc Inc**
- **MagmaSoft**
- ***Mississippi State University****
- ***Lehigh University****
- ***Oak Ridge National Lab****
- ***Pacific Northwest Labs****

•Not funded in this project LM012

USAMP

International Partners – China*

- **Tsinghua University**
- **Northeastern University**
- **Central South University**
- **Shanghai JiaoTong University**

International Partners – Canada*

- **CANMET-MTL**

•Not funded in this project LM012

USAMP

ICME for Mg Program Task Goals

- ***Task 1: Cyberinfrastructure:*** *Establish a Mg ICME Cyberinfrastructure (CI) (MSSt, PNNL & USAMP)*

- **Task 2: Calculated Phase Diagrams:** Establish a Phase Diagram_and Diffusion Infrastructure (within CI)

- ***Task 3: Extruded Mg:*** *Establish quantitative processing-structure-property relationships for extruded Mg and integrate with Mfg simulation and constitutive models (MSSt & USAMP)*

- **Task 4: Sheet Mg:** Establish quantitative processing-structure-property relationships for sheet Mg and integrate with Mfg simulation and constitutive models

- **Task 5: Cast Mg:** Establish quantitative processing-structure-property relationships for Super Vacuum high pressure Die Cast (SVDC) Mg and integrate with Mfg simulation and constitutive models

USAMP

Task 2. Calculated phase equilibria & diffusion

Goal: Establish a Phase Diagram and Diffusion Infrastructure (within CI)

Accomplishments:

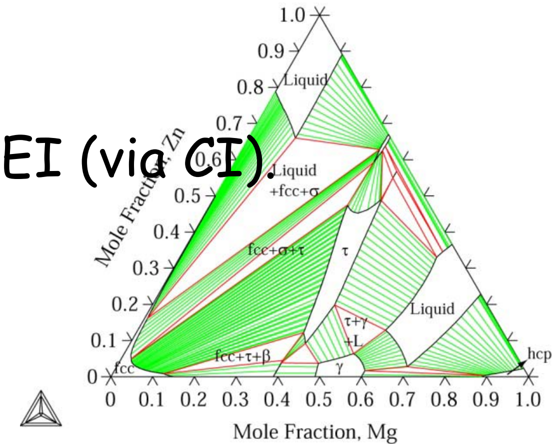
- Completed development of & demonstrated Extensible, Self-Optimizing Phase Equilibria Infrastructure (ESPEI) framework

- ESPEI being established on CI

- Completed significant DFT calculations for 6 Mg-Al-X system (X=Si, Ti, Mn, Fe, Zn, and Zr)

- DFT results in process of downloading to ESPEI (via CI).

- *Characterized diffusion for Al in Mg*



ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure

For Magnesium Alloys

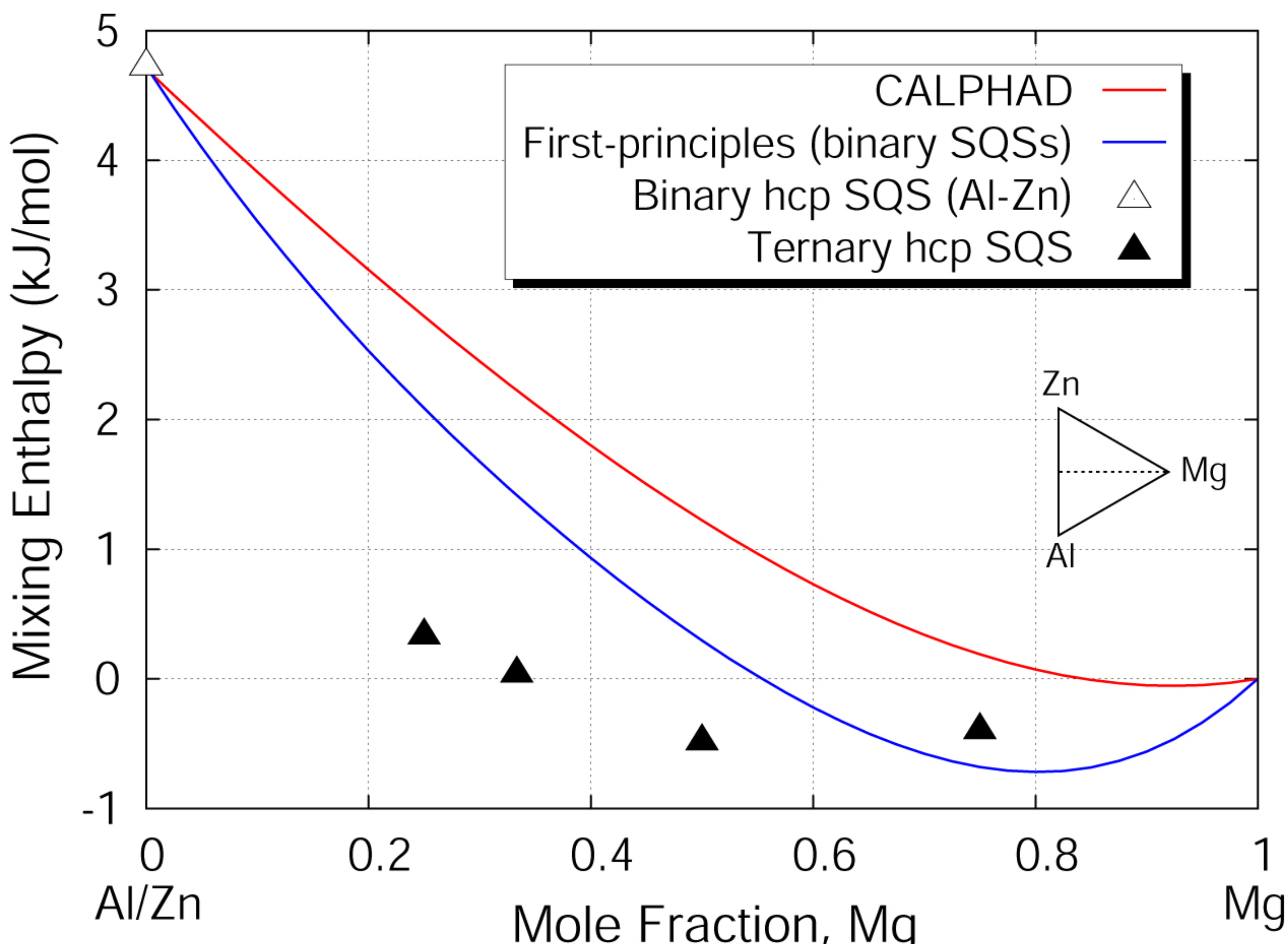
- Enthalpy of formation
- Enthalpy of mixing
- Heat capacity
- Entropy of formation
- Entropy of mixing
- Driving force
- Activity (standard)
- Gibbs energy of formation
- Gibbs energy of mixing
- Mole Gibbs energy
- Activity (nonstandard form)
- Crystal structure
- Magnetism
- Curie/Néel temperature
- …

Conditions:

- Reference states
- Compositions
- Pressure
- Temperature

- Measurement
- First-principles
- Empirical Estimation

Completed DFT Calculations of mixing enthalpies for Mg-Al-Zn system



Northwestern Univ

USAMP

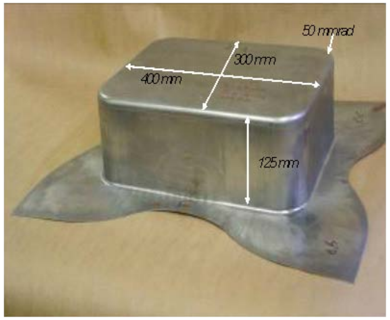
Task 3: ICME for Sheet

<u>Goal:</u> Establish quantitative processing-structure-property relationships for sheet Mg and integrate with Mfg simulation and constitutive models

Accomplishments:

- Selected alloy and focal component
- Simulated forming and formed components
- Developed modeling approach that explains anisotropy effects and differences between single crystal and polycrystals
- Calibrated constitutive models for the Mg sheet alloy AZ31 applied to warm forming simulation & compared with experimental results

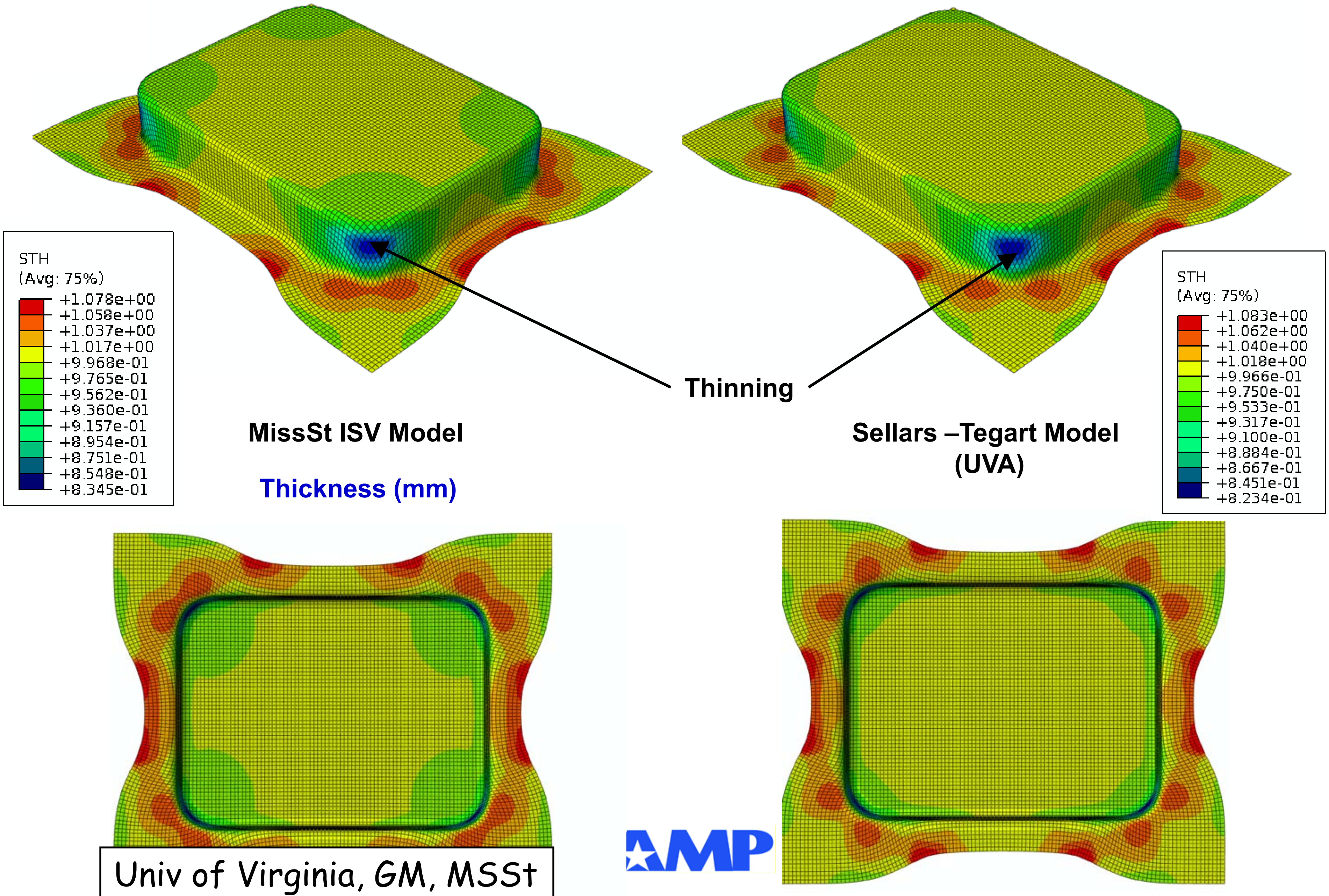
Pan Die Geometry

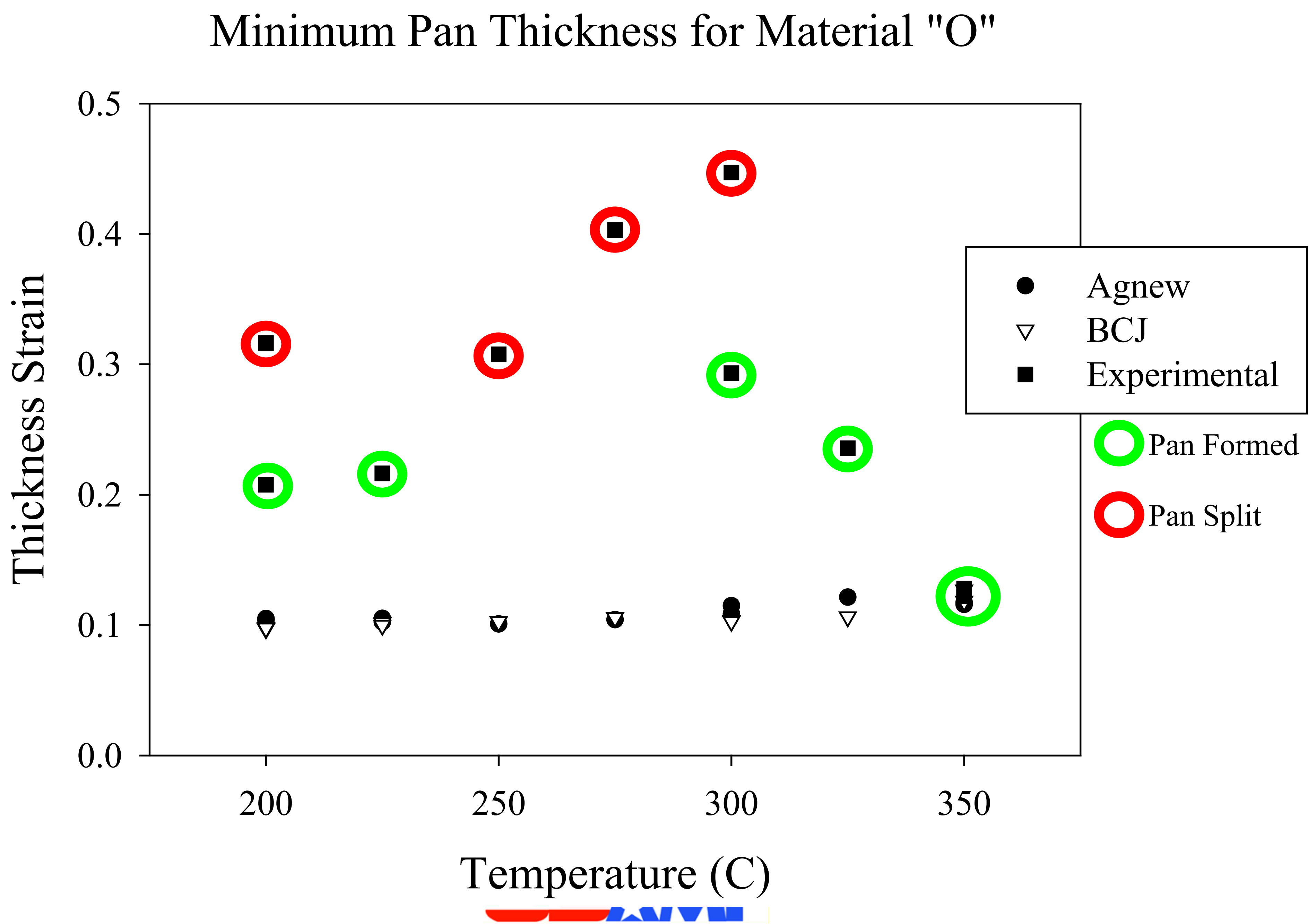


Mg Alloy: AZ31

USAMP

Sheet Metal Forming Simulation @ 473K





Minimum Pan Thickness for Material "O"
Thickness Strain
0.0
0.1
0.2
0.3
0.4
0.5
200
250
300
350
Temperature (C)
Agnew
BCJ
Experimental
Pan Formed
Pan Split

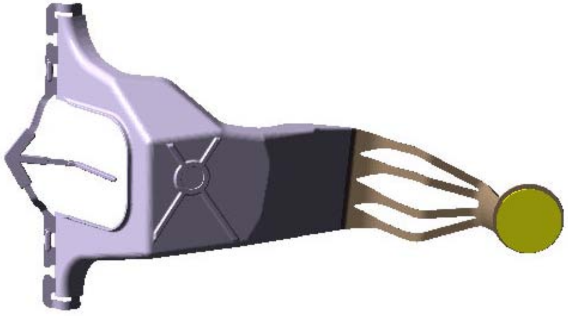
Task 5. ICME for Super Vacuum HPDC (SVDC)

Goal: Establish quantitative processing-structure-property relationships for Super Vacuum high pressure Die Cast (SVDC) Mg and integrate with Mfg simulation and constitutive models

Accomplishments:

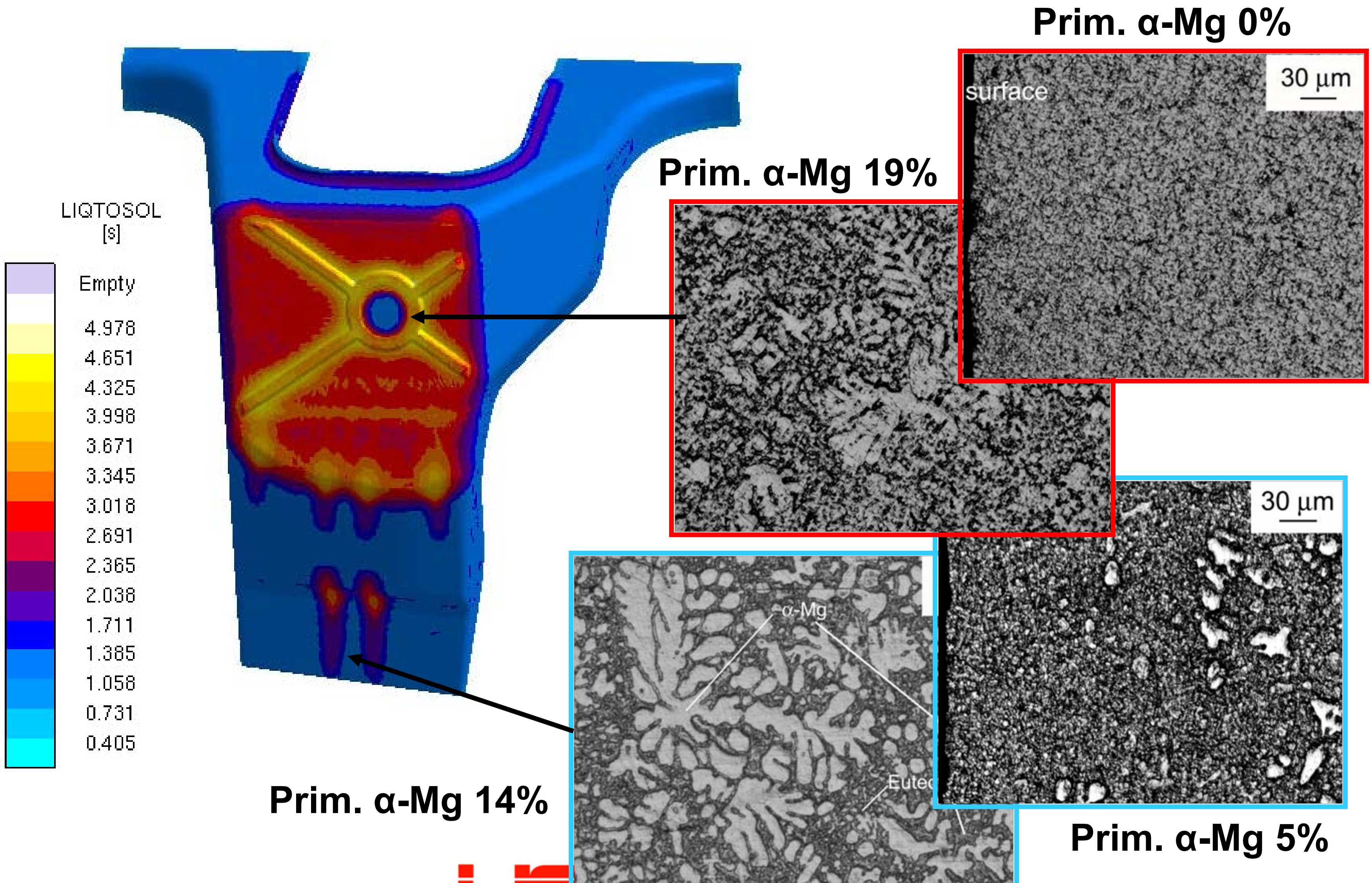
- Selected alloy and focal component
- *Developed robust models for heat transfer coefficents for casting simulation (Tsinghua U.)*
- Quantified the influence of solution treatment and aging on yield strength
- Demonstrated hybrid approach for prediction of precipitate evolution during aging
- Developed initial model for yield strength in heat treated die casting alloys

Mg Alloy: AZ91



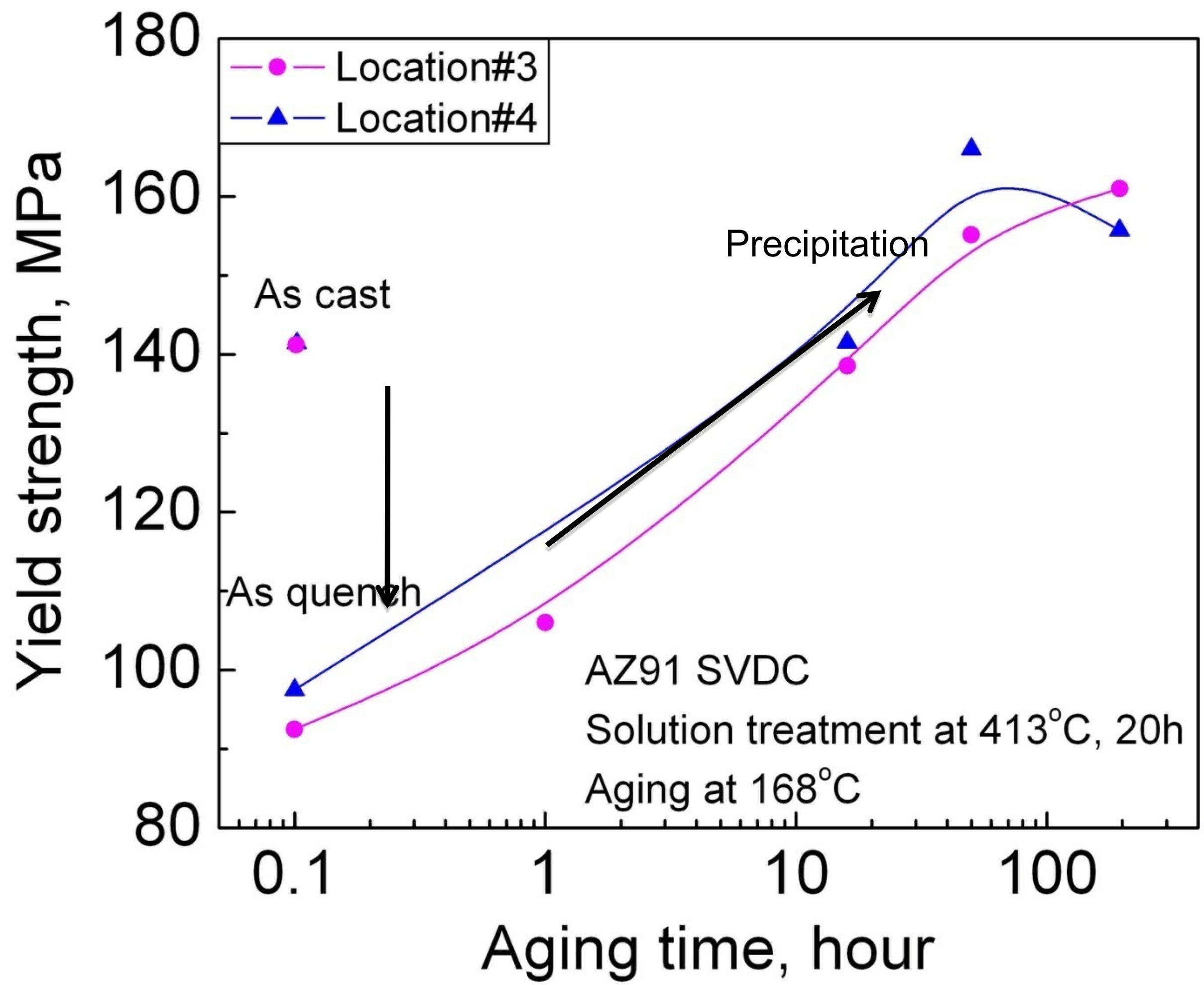
USAMP

Completed casting simulation on AZ91 SVDC shock tower



Ford & University of Michigan

Quantified influence of solution treatment and aging on yield strength



University of Michigan

USAMP

Collaboration and Coordination with Other Institutions

Extensive collaboration and coordination are implicit in this project and are occurring within all aspects of the project.

- Formal review & coordination workshops occur with entire team twice per year
- Task team meetings occur at least twice per year
- MSSt (Part 2) activity fully integrated with "Part 1"
- In addition to formal USAMP program participants, we have participants from PNNL and ORNL; China and Canada.
- Coordination also occurs with MFERD program (component production and simulation)

Future Work

- Develop models sufficient for MFERD Phase II demonstration (May 2011)

- Phase Equilibria & DFT Task Team
  - Upload Mg-Al-Zn DFT data into ESPEI & demonstrate automation
  - Complete first-principles calculations of precipitate or meta-stable phases other than AZ91, e.g., $MgZn_2$ or GP zones in Mg-Zn-Ca
  - Measure Mg, Zn tracer diffusivities in select Mg-Al-Zn alloys
  - Link with casting precipitation hardening model

- Sheet Task Team
  - Improve sheet thinning models
  - Implement dynamic recrystallization model into crystal plasticity and validate
  - *Develop new constitutive model formulation including adiabatic heating, damage, anisotropy, and kinematic hardening*

USAMP

Future Work (Continued)

- Casting Task Team
  - Calibrate the solution treatment kinetics model
  - Complete characterization of low cycle fatigue and quantify precipitate evolution during aging
  - Calibrate DFT-PF model using the precipitate measurements
  - Complete strength model and develop linkage with MSSt ISV models
- Cyberinfrastructure Task Team (MSSt) – Part 2 Presentation
  - *Demonstrate web-based ESPEI capability and DFT database*
  - *Assess informatics needs and enhance repository of experimental data and model calibration tools*
- Extrusion Task Team (MSSt) – Part 2 presentation
  - *Complete static / dynamic recrystallization experiments*
  - *Complete weld seam studies and develop weld seam models.*
  - *Enhance Crystal Plasticity Model to include temperature dependence, twinning, simple recrystallization model and damage.*
  - *Enhance ISV Model to include twinning & precipitation hardening.*

USAMP

Summary

- ICME represents a new approach for accelerating development of Mg for body applications
- An international consortia has been established to develop ICME tools for Mg
- Significant progress has been made in all task areas
- US and international collaborative efforts are on track
- Future plans & coordinated effort are well defined

USAMP