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

Project ID LM012

AMD 703

Mei Li

Ford Motor Company

Overview

Timeline

- Project start date: Feb 2007
- ~~Project end date: Feb 2012~~
- New project end date: Sept 2011
- Percent complete: 75%

Barrier

- Design data & modeling tools
- Manufacturabiity
- Performance
- Cost

Budget

- Total project funding
  - DOE share: $1M
  - Contractor share: $1M
- Funding received in FY10
  - $224,714
- Funding for FY11
  - $398,816

Partners

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

Relevance to Materials Technologies Lightweight 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.

Goals –What we are trying to do

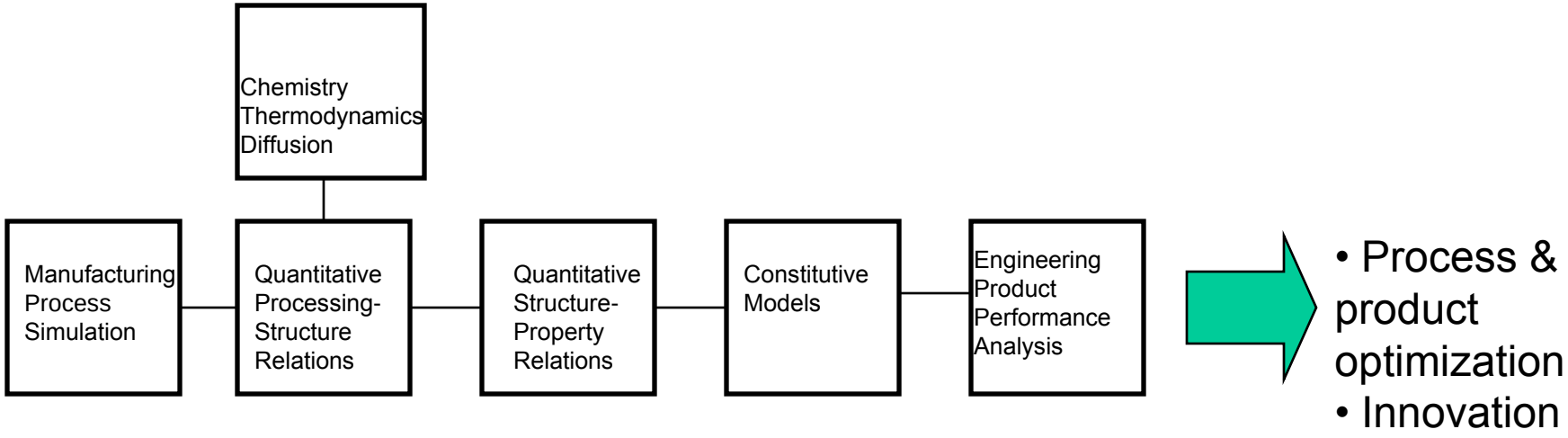
- Establish, demonstrate and utilize an ICME knowledge infrastructure for magnesium in body applications for:
  - Microstructural engineering
  - Process and product optimization
  - Future alloy development
- Attract materials researchers into Mg field & leverage their efforts by providing a collaboration space for coupling high quality data and models.
- Identify and fill technical gaps in fundamental knowledge base

Milestones

- Milestone 1: Infrastructure Demonstration (March 2009):
  - ➢ Demonstrate a cyber-infrastructure data to enable integration and collaboration
- Milestone 2: ICME Progress Demonstration (March 2010):
  - ➢ Demonstrate substantial progress in all task areas
  - ➢ Demonstrate integration with manufacturing simulation
- Milestone 3: Application to MFERD Phase II (September 2011):
  - ➢ Demonstrate ability of ICME tools to link manufacturing and predict performance of MFERD demonstration structure ~~& validate the results (Dec 2012)~~

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.*



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*

International Partners

China:

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

Canada:

- CANMET-MTL

ICME for Mg Program Task Goals

- **Task 1 Cyberinfrastructure (CI):** Establish a Mg ICME 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

Task 2: Calculated Phase Equilibria & Diffusion

Goal: Establish a Phase Diagram and Diffusion infrastructure (within Cyberinfracture)

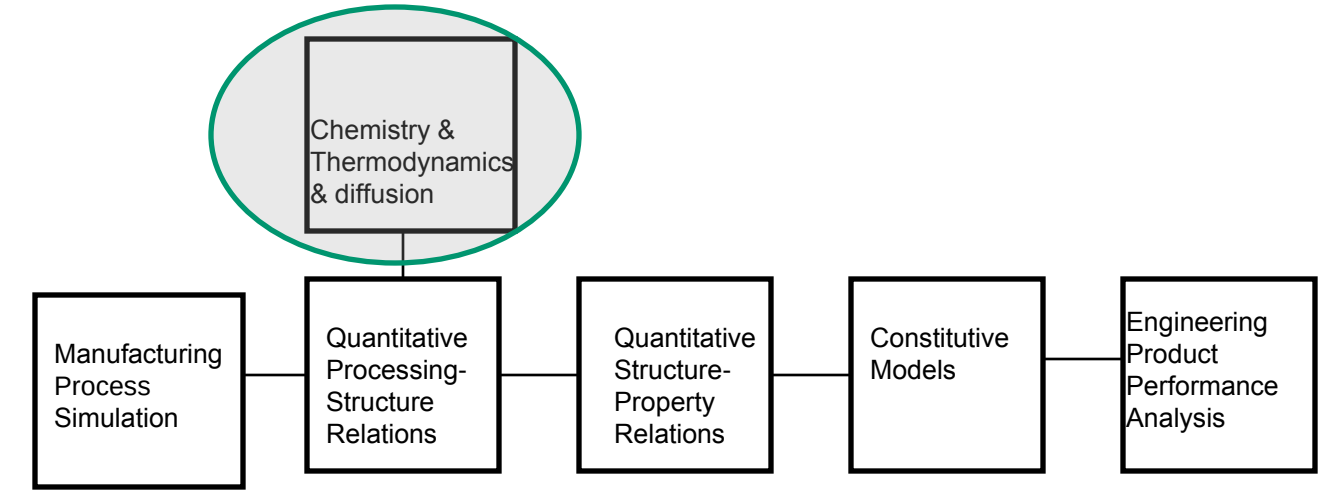
Accomplishments:

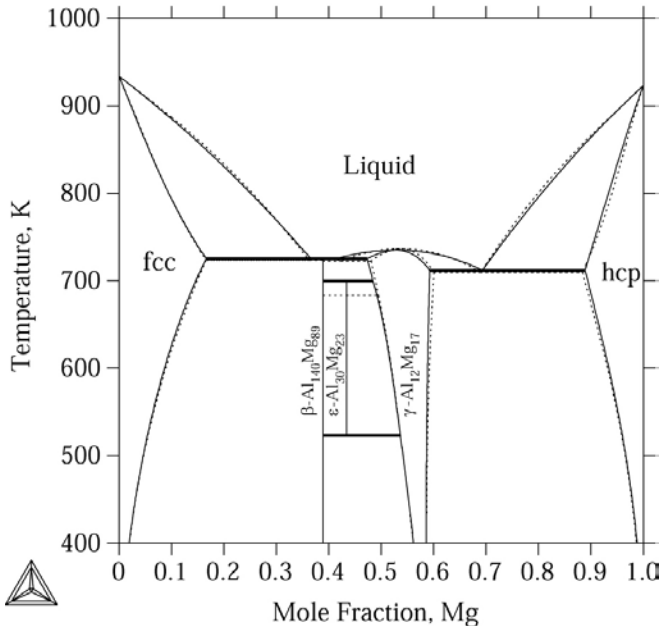
• Established Extensible, Self-Optimizing Phase Equilibria Infrastructure (ESPEI) framework on CI.

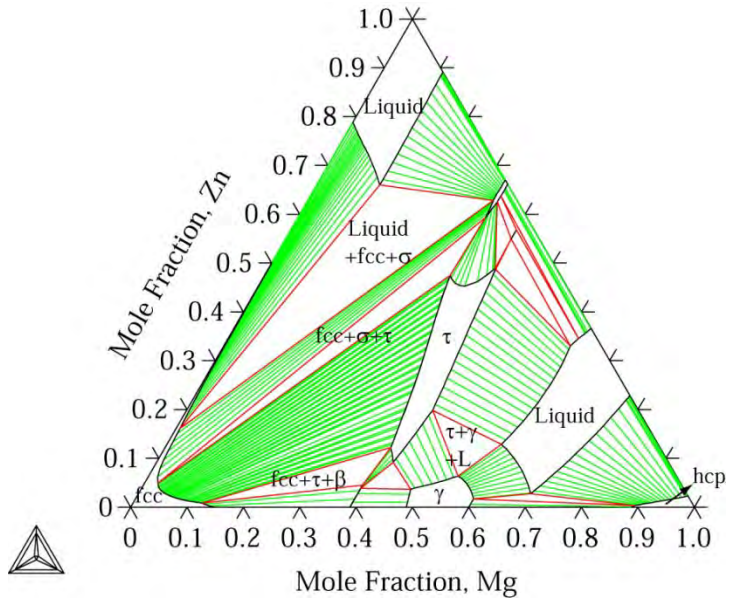
• Extended and demonstrated GUI for automation of thermodynamic modeling for selected binaries (Al-Mg, Mg-Ni, Mg-Zn) and ternary (Mg-Al-Zn). Completed the user manual.

• DFT results was successfully downloaded to ESPEI (via CI).

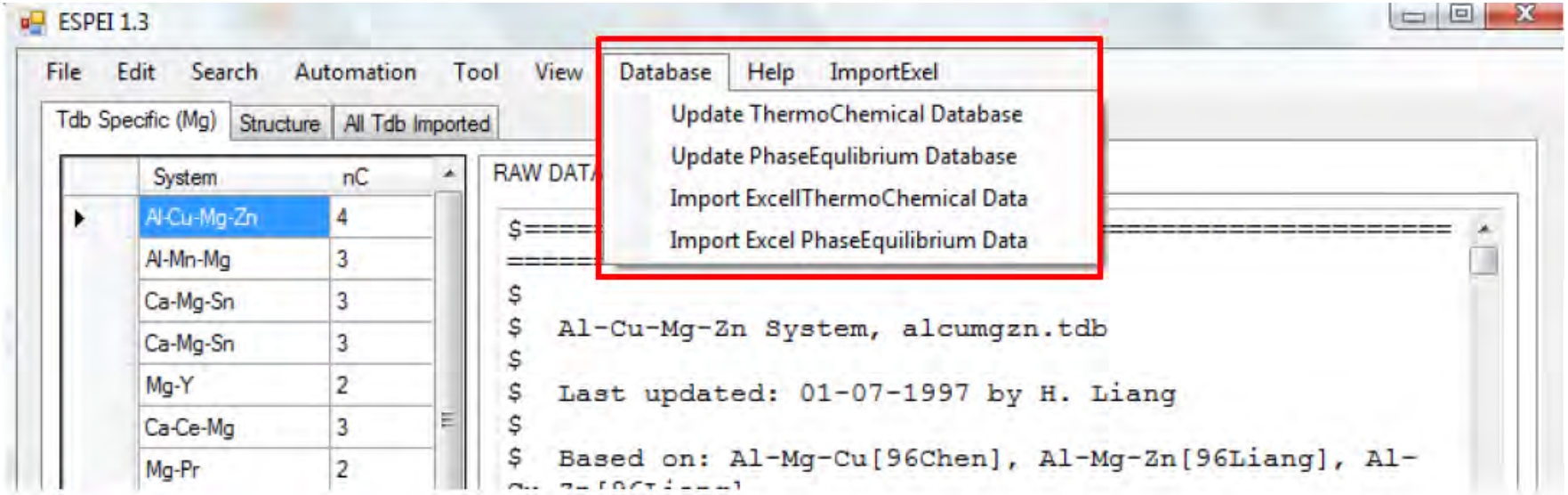
Task 2: Calculated Phase Equilibria & Diffusion







ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure for Magnesium Alloys



Updates:

- Download database from Internet
- Import database from Excel file (with detailed template and manual)
- The needed thermodynamic data for automation

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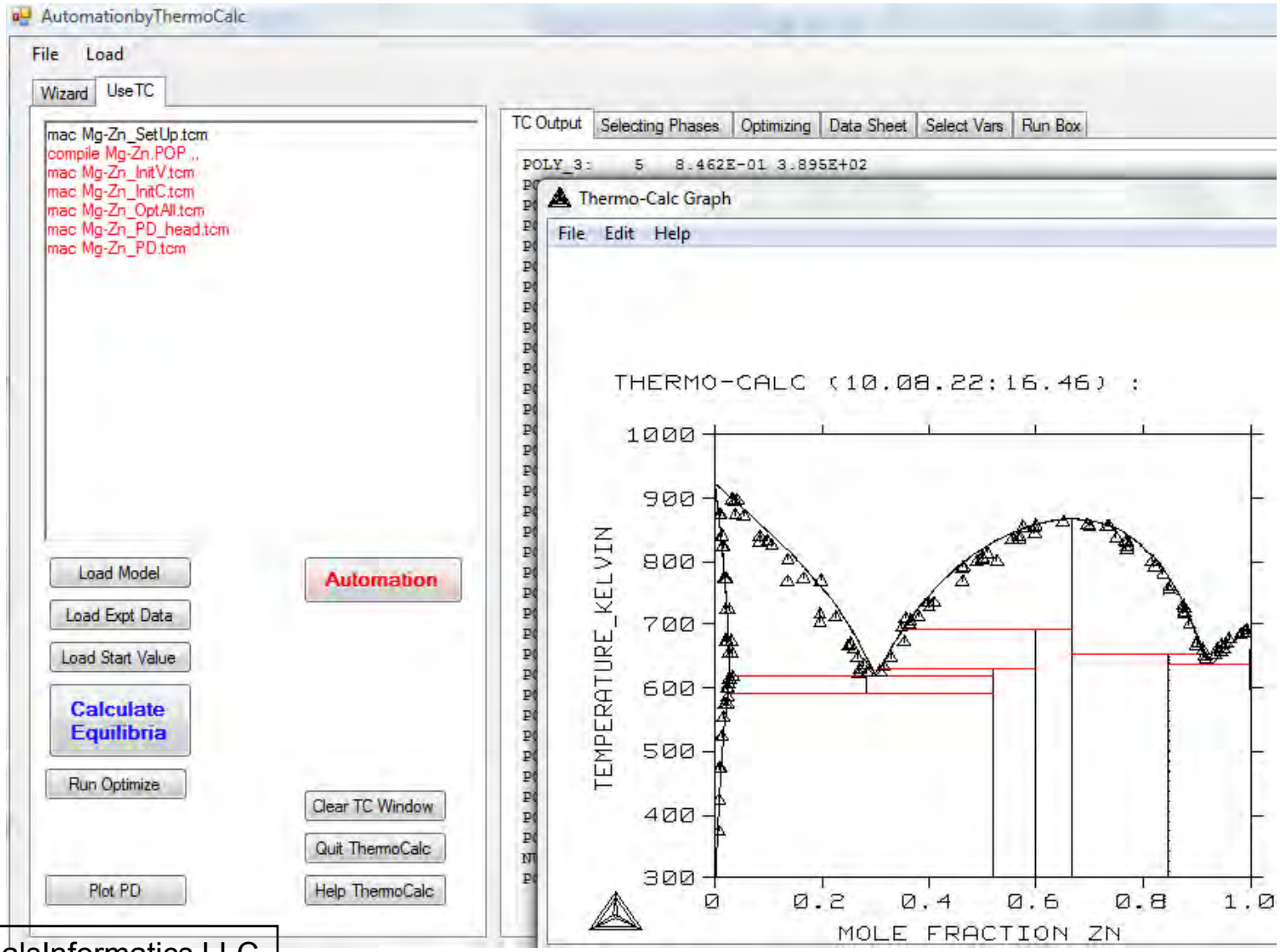
MaterialsInformatics LLC

Automation by ThermoCalc



MaterialsInformatics LLC

Task 3: ICME for Sheet

Goal: Establish quantitative processing-structure-property relationships for sheet Mg and integrate with Mfg simulation and constitutive models.

Accomplishments:

- Completed warm sheet stamping FEM simulations (with and without adiabatic heating) with BCJ model.

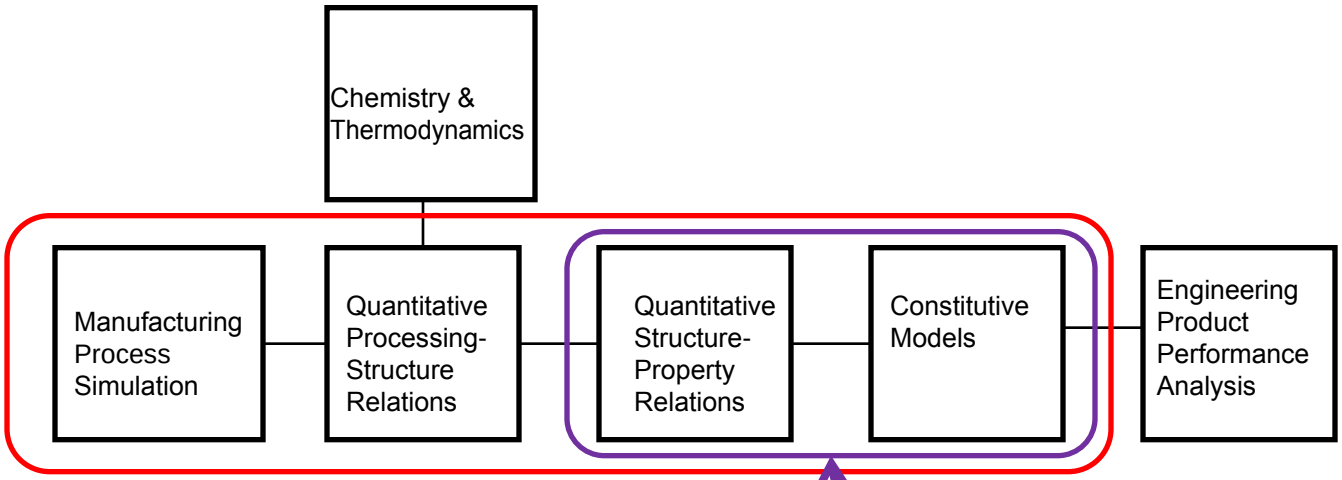
- Developed capability of simulating sheet stamping in new version of PamStamp2G with material model in numerical format.

- Developed solute strengthening map of Mg from first principles+Fleischer model

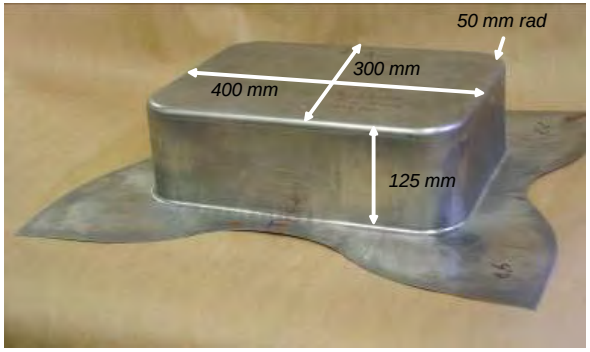
- Continue to develop the detwinning model that uses tension/compression test results

Task 3: ICME for Sheet

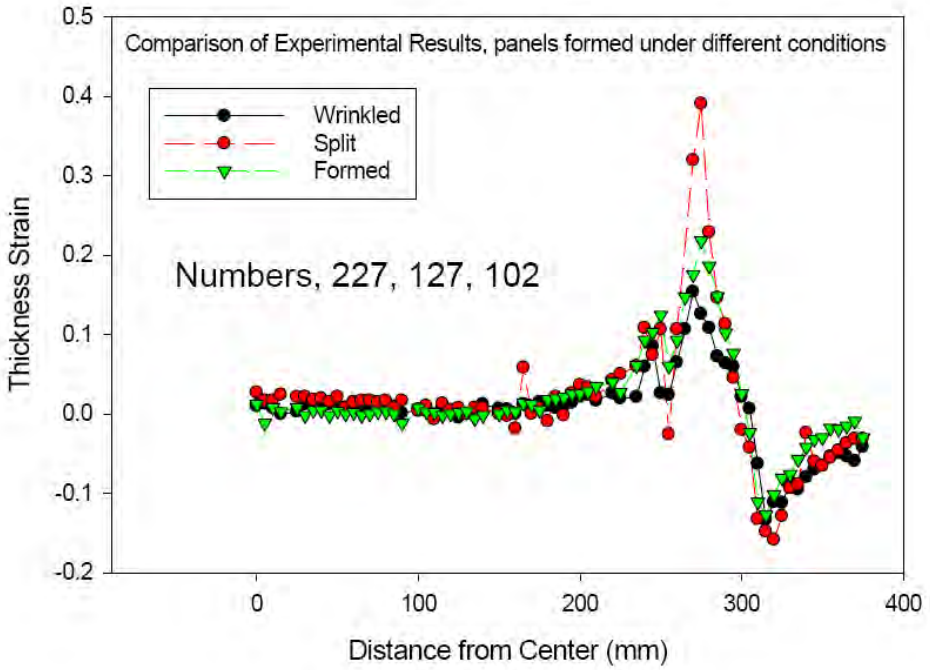
Mg Alloy: AZ31

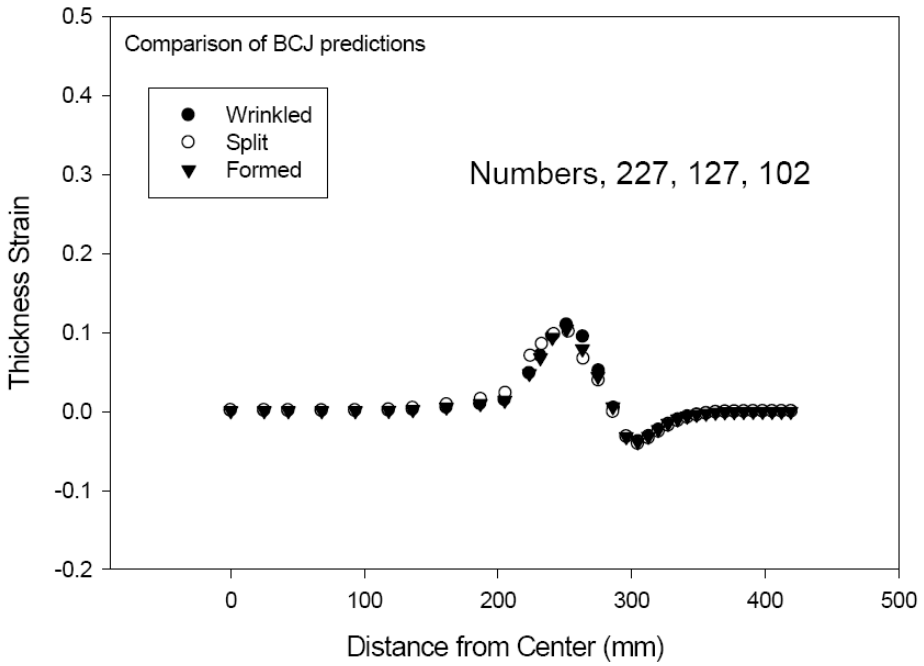


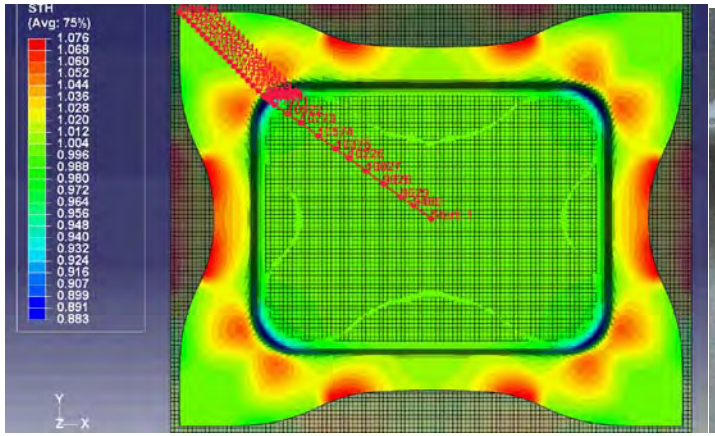
Pan Die Geometry



Predicted Thickness Strain vs. Measurements

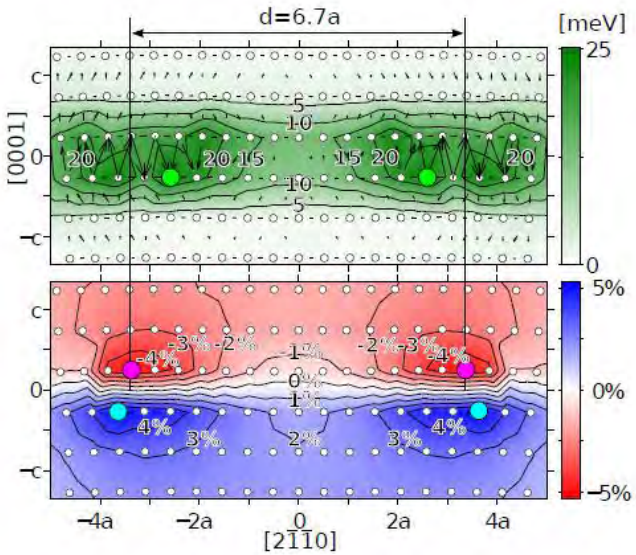


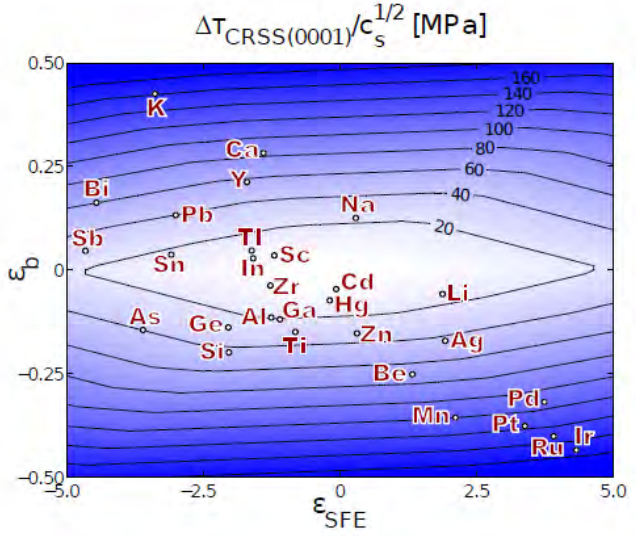




GM, University of Virginia and MSU

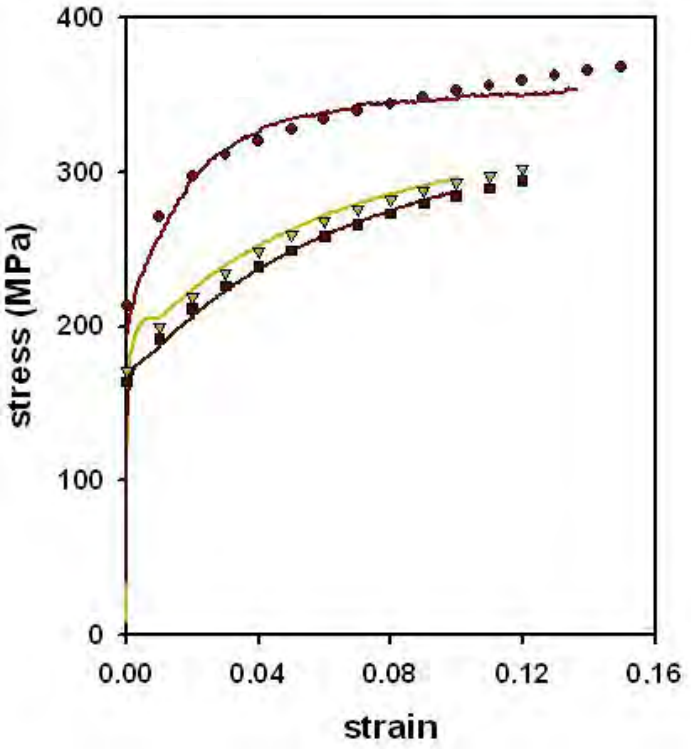
Predicted Solute Strengthening Map of Mg





GM

- Alloy AZ31 (0.4 at% Zn, 2.7 at% Al) simulated using the viscoplastic self-consistent (VPSC) model.



University of Virginia

Task 5: ICME for Super Vacuum HPDC (SVDC)

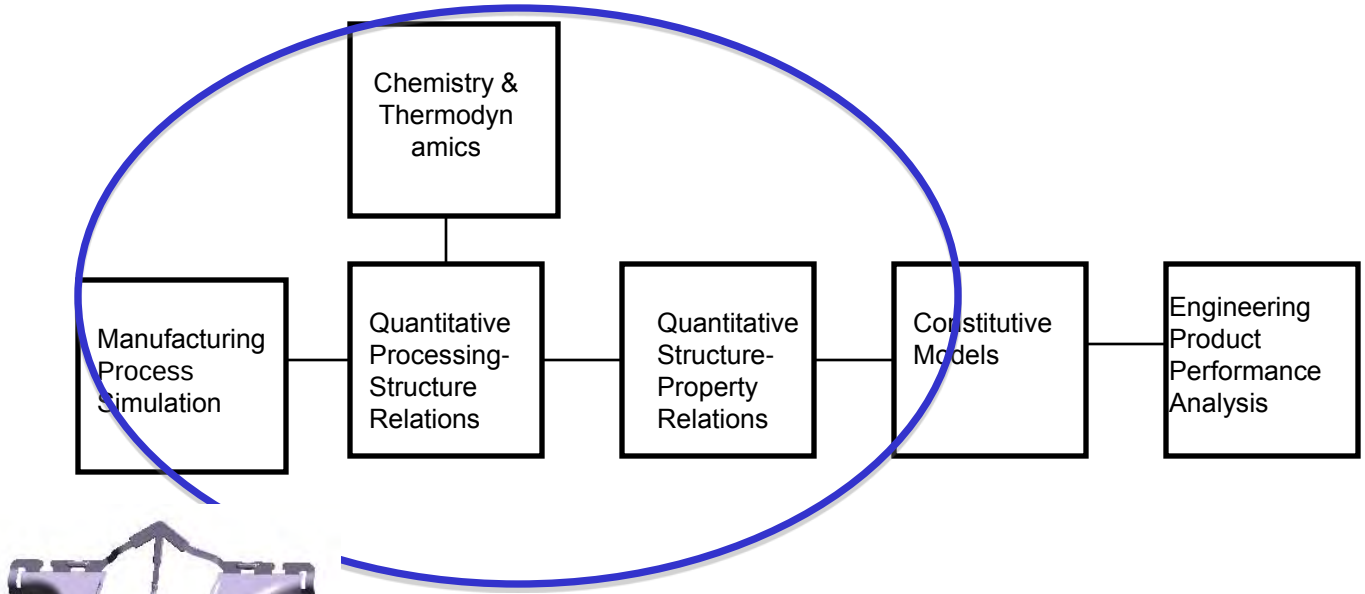
Goal: Establish quantitative processing-structure-property relationships for Super Vacuum high pressure Die Cast (SVDC) Mg and integrate with Mfg simulation and constitutive models

Accomplishments:

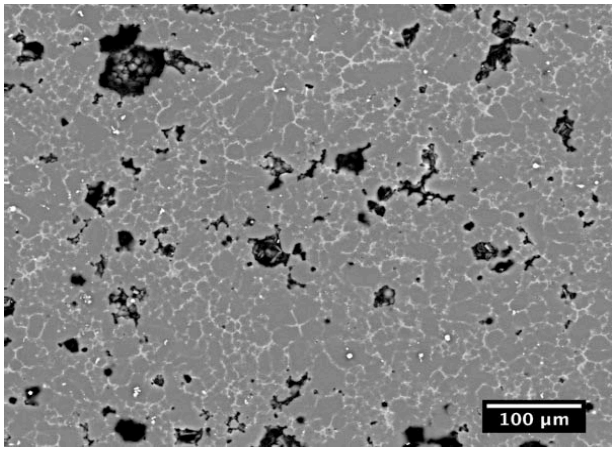
- Characterized the low-cycle fatigue properties of AZ91.
- Determined that fatigue life is primarily limited by porosity.
- Established 3D Phase Field to be calibrated with experimental data for lathes in Mg.
- Developed the dissolution kinetics model in Dictra.
- Made progress on first-principle calculation of interfacial energies, strain energies, lattice parameters and elastic constants.

Task 5: ICME for Super Vacuum HPDC (SVDC)

Mg Alloy: AZ91



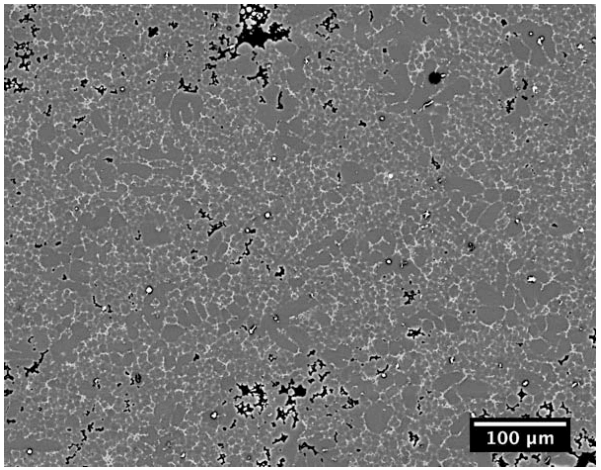
Dendrite Cell Size & Porosity



L1

Cell Size = 4.99 ± 2.26 µm

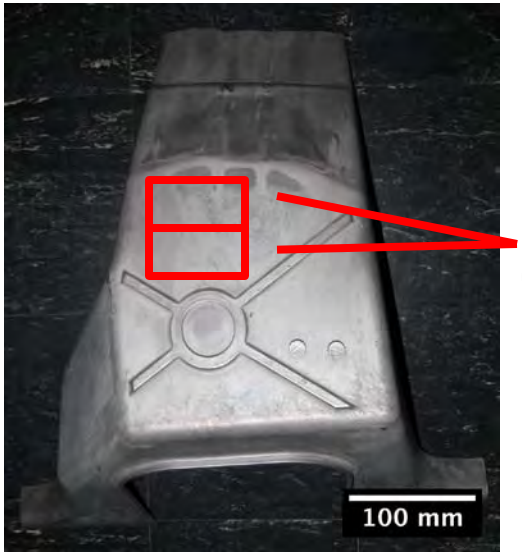
Porosity Area Fraction = 4.18%



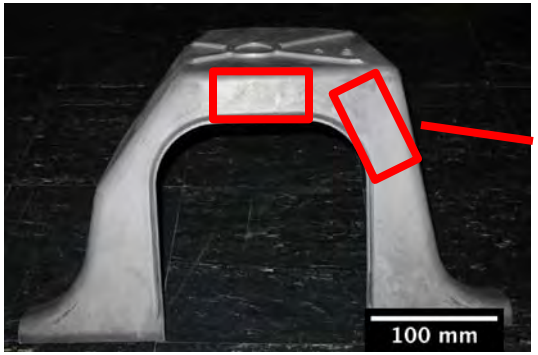
L2

Cell Size = 4.17 ± 1.51 µm

Porosity Area Fraction = 1.75%



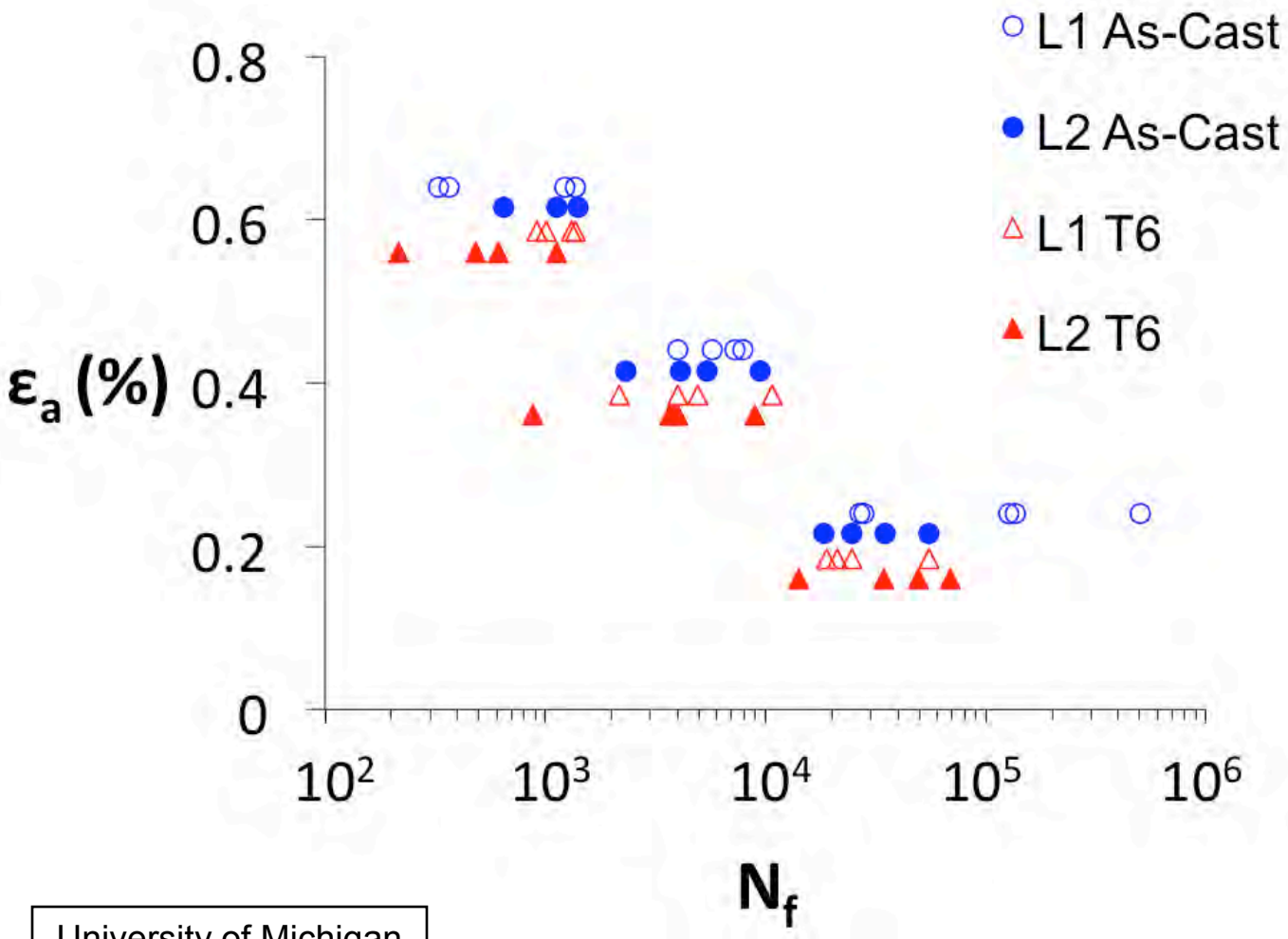
L1
(t = 4.7mm)



L2
(t = 3.0mm)

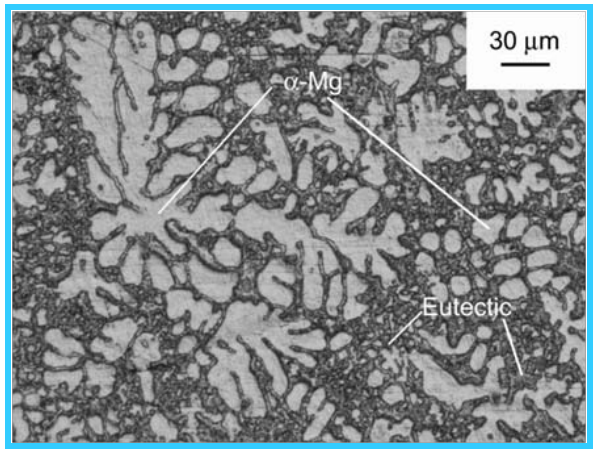
University of Michigan

Low-Cycle Fatigue of Die-Cast AZ91

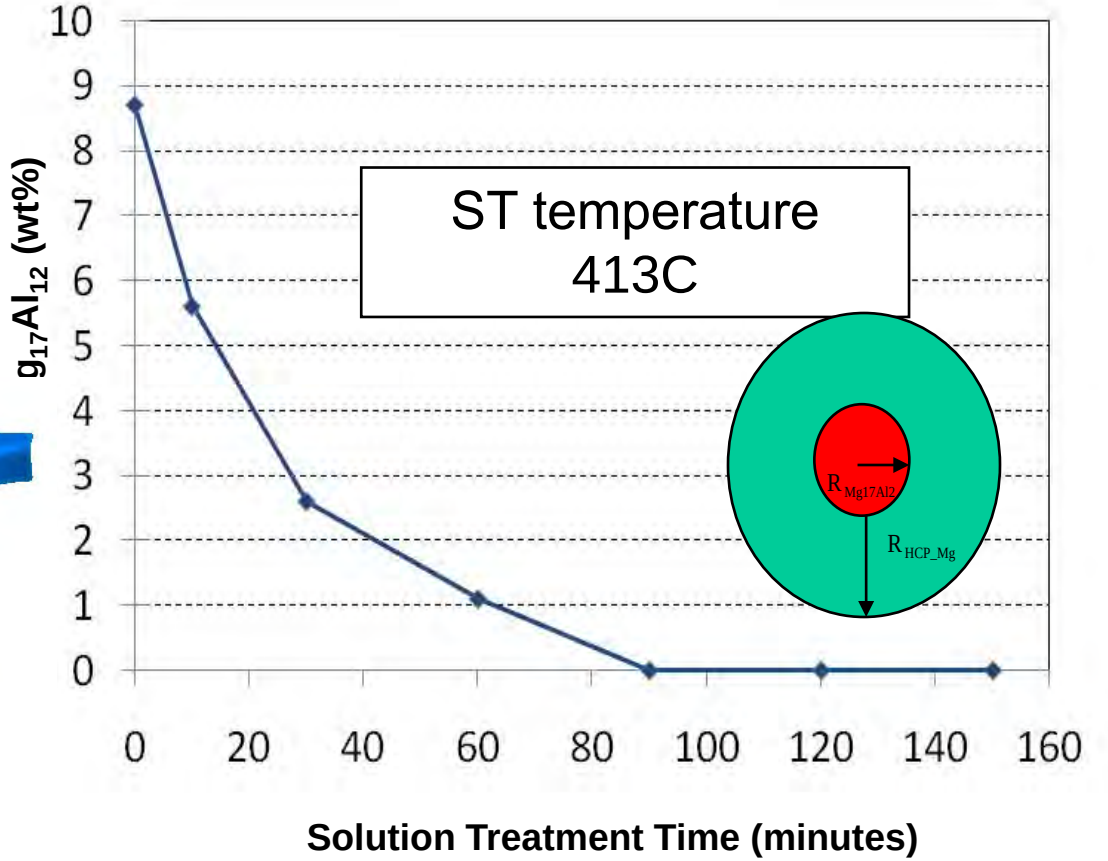


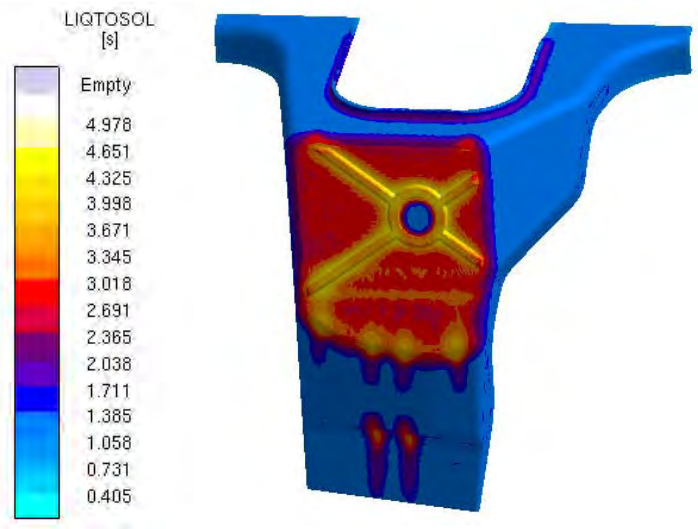
University of Michigan

Disolution Kinetics of Eutectic $Mg_{17}Al_{12}$



- Dissolution kinetics model in Dictra





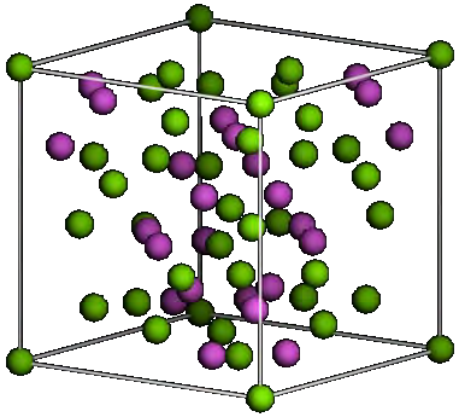
Ford

DFT calculations on the Mg-alloy β-$Mg_{17}Al_{12}$ phase

Inputs: Experimental data from literature on α/β interface structure, orientation, …

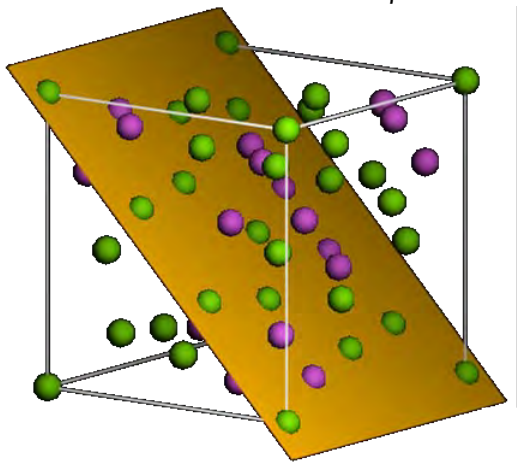
Outputs: Low-energy interface structures, interfacial energies, strain energies, lattice parameters and elastic constants for the phase field model

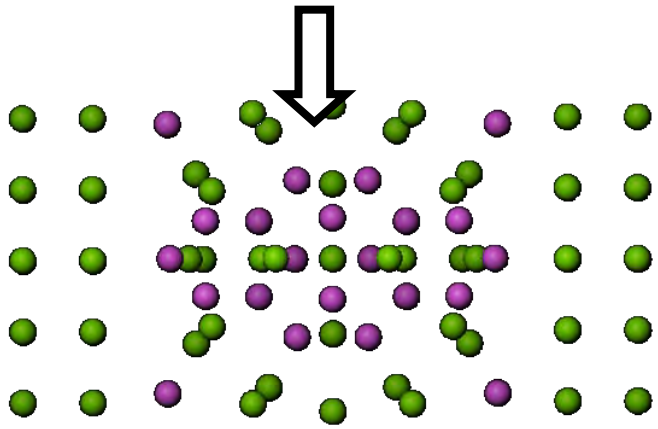
β-$Mg_{17}Al_{12}$



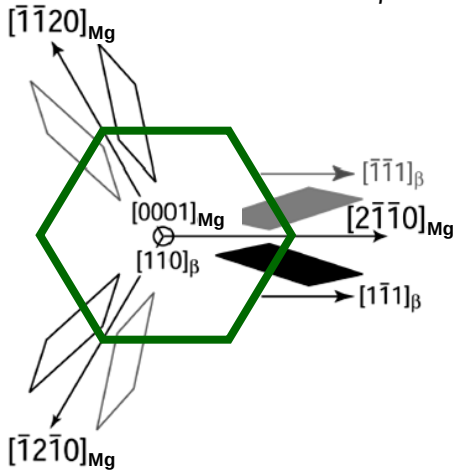
BCC, *I43m*
a=1.056 nm
58 atoms

$(0001)_\alpha$ || $(110)_\beta$





[1-210] $_\alpha$ || [1-11]$_\beta$



Z

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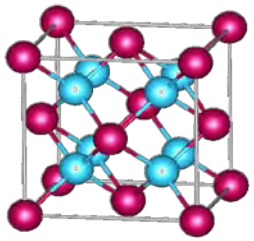
Precipitation Kinetics Study with Phase Field

Crystal Structure

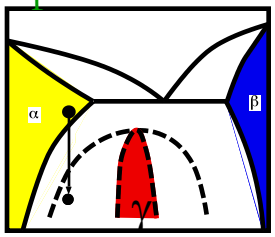
Metastable Phase Equilibria

Precipitate Microstructure

Mechanical Properties (Yield Strength)

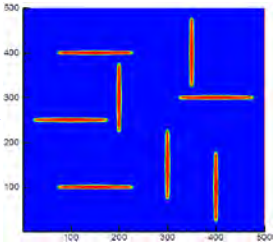


ΔH, ΔS of metastable phases

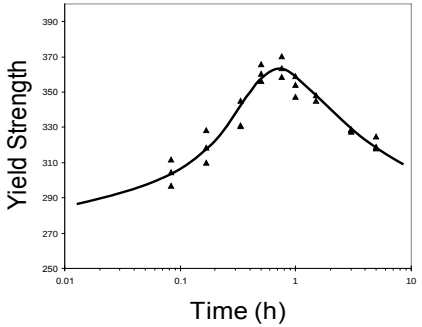


Bulk (SS + Precipitate) Free Energies

Interfacial + strain energies + *Mobilities*



Precipitate Morphologies



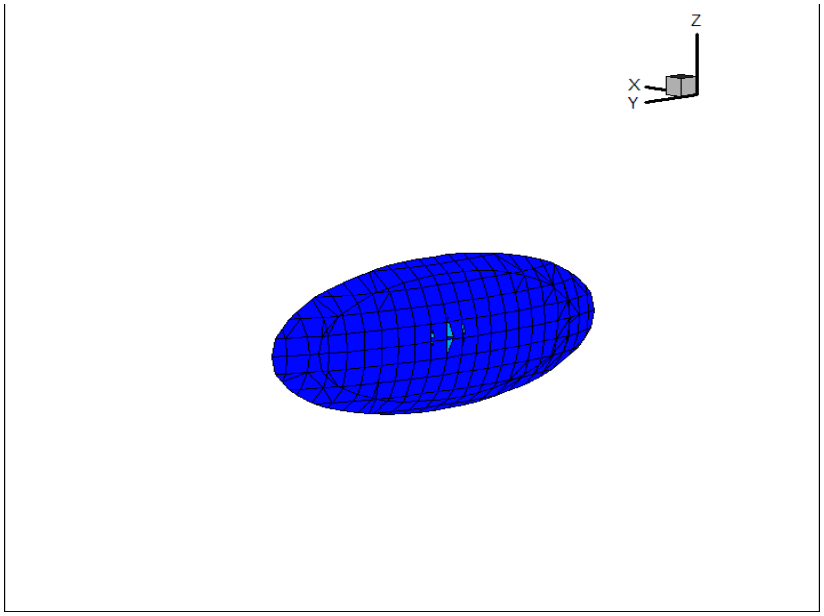
First-Principles Calculations

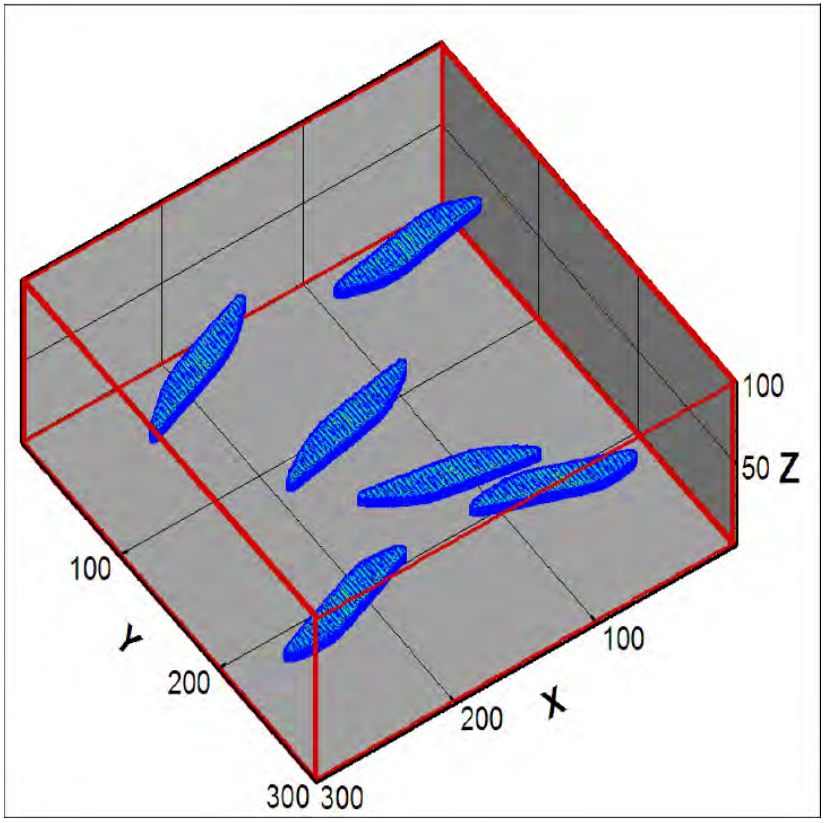
CALPHAD

Phase-Field

Micromechanical Models

Simulated Precipitate Morphology





3D Simulation

Ford

Future Work

- **Work with MFERD CAE demo team to implement the local properties (Zone method, no anisotropy capability for CAE analysis)**
- **Develop user-subroutine to implement the ICME predictions on element level (MSU)**
- **Casting Team:**
  - Process to properties models (yield strength and fatigue strength)
  - Casting process simulation (Ford and Tsinghua University)
  - Casting microstructure models (Tsinghua University)
  - Link MicroModel with Solution Treatment Mode (Ford)
  - Aging Model (Ford and University of Michigan)
  - Yield strength model (Ford, UofM and Tsinghua University)
  - Fatigue strength model (UofM)

Future Work (Continued)

- **Extrusion Team:**
  - Process to properties to FEA model (post-forming yield strength, fatigue and stress-strain curves)
  - Extrusion process simulation (MSU)
  - Texture prediction using VPSC model in Hyper-extrude (MSU)
  - Develop the stress-strain relationship and yield strength (MSU)
  - Post-forming fatigue strength model (MSU)
- **Sheet Team:**
  - Processing to properties to FEA model (localization, post-forming stress-train curves)
  - Stamping (bending) process simulation (MSU)
  - Texture prediction using VPSC model (MSU)
  - Develop the stress-strain relationship for AZ31(MSU and CANMET)
  - Post-forming fatigue strength model (MSU)

Summary

- ICME represents a new approach for accelerating development of Mg for body applications

- An international consortia has been working together to develop ICME tools for Mg

- Significant progress has been made in all task areas

- Future plans & coordinated effort are well defined