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

Project ID LM012

AMD 703

Mei Li

Ford Motor Company

May 17, 2012

Overview

Timeline

- Project start date: Feb 2007
- Project end date: March 2012
- Percent complete: 100%

Barrier

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

Budget

- Total project funding
  - DOE share: $853K
  - Contractor share: $853K
- Funding received in FY11
  - $240K
- Funding for FY12
  - $46K

Partners

- 3 US Universities
- 3 US Companies
- TMS
- Lead: USAMP
- International Partners from China & Canada (Partners are shown on next slide)

US Mg ICME Team

- Ford
- GM
- McCune & Associates
- Northwestern University
- University of Michigan
- University of Virginia
- Materials Informatics Inc

China:

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

- The Minerals, Metals and Materials Society (TMS)
- ThermoCalc Inc
- MagmaSoft®
- Mississippi State University*
- Lehigh University*
- Oak Ridge National Lab*
- Pacific Northwest Labs*

Canada:

- CANMET-MTL

Project Objectives

- 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

Deliverables

- **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

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

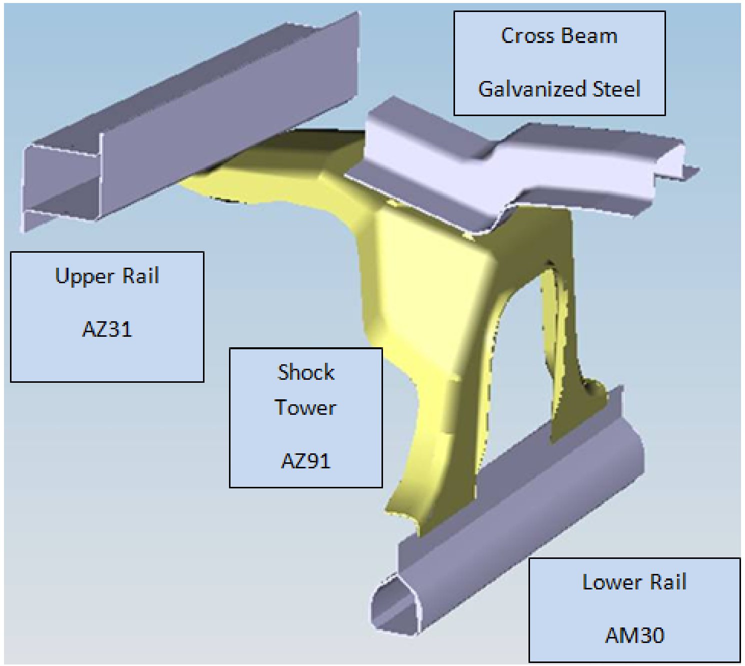
- Milestone 3: Application to MFERD Phase II (March 2012):
  - Demonstrate ability of ICME tools to link manufacturing and predict performance of MFERD demonstration structure

Demonstration of ICME Tools

Goal: Predict component performance based on local microstructures and properties vs. traditional nominal values

Accomplishments:

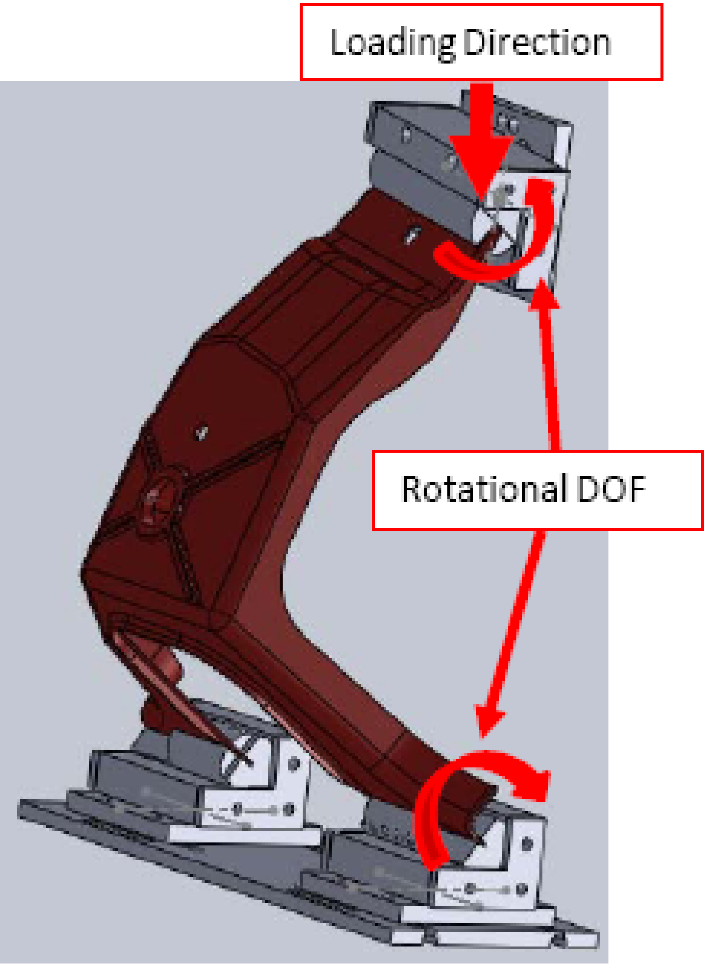
- Developed and validated the hybrid methodology of Phase field model/TEM characterization to predict the precipitation kinetics of β in AZ91.
- Developed the strengthening model for AZ91.
- Mapped local porosity distribution onto AZ91 shock tower performance model based on casting process simulation and porosity characterization using SEM and x-ray tomography.
- Predicted failure location and load-displace curve under monotonic loading

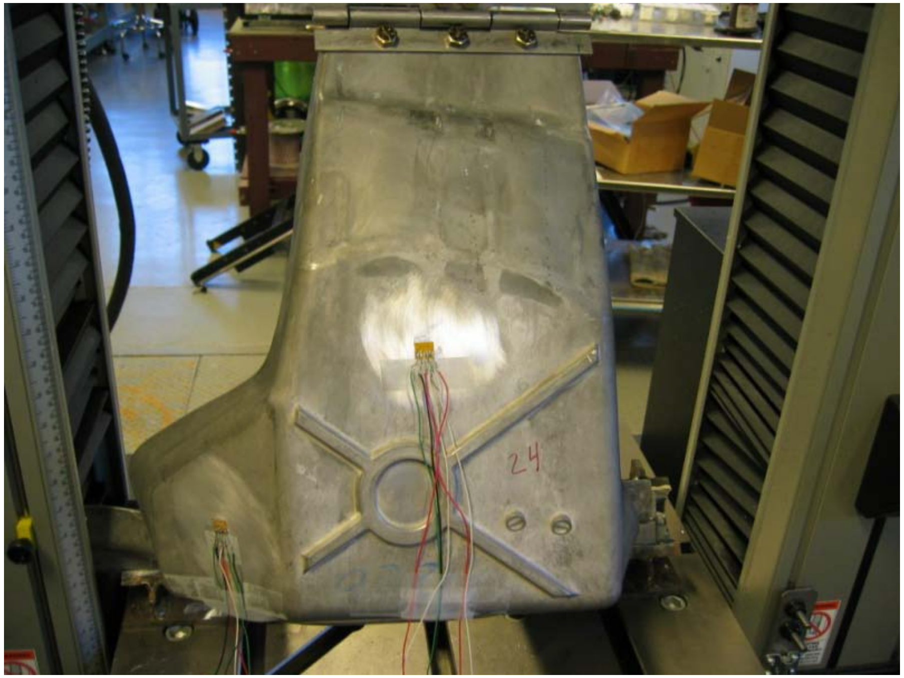


MFERD demo structure assembly

Demonstration of ICME Tools

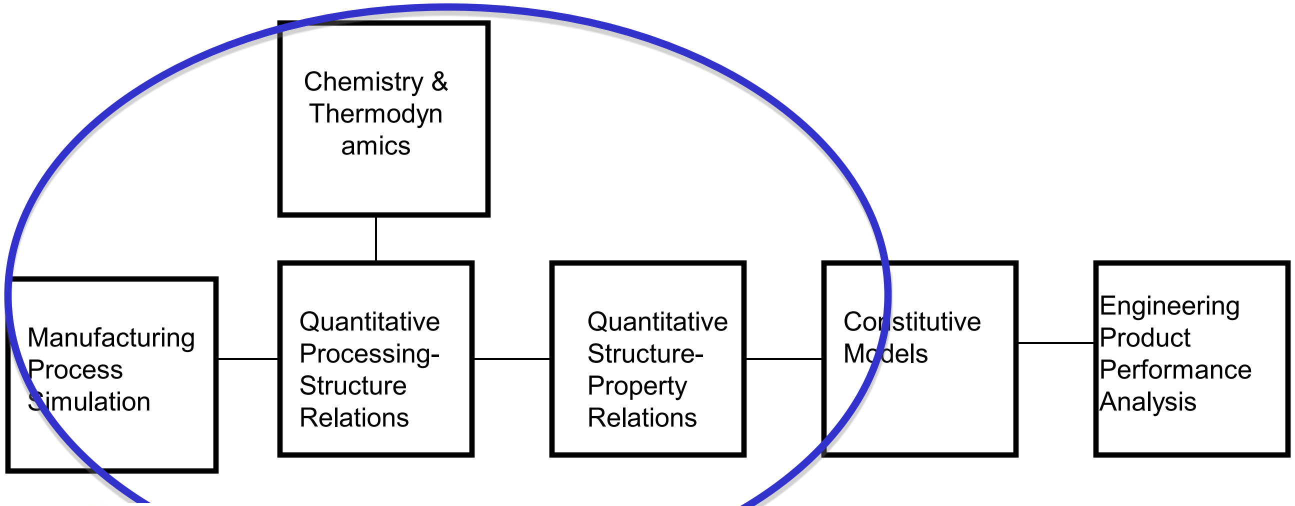
- Experimental set up at Center for Advanced Vehicle System (CAVS), Mississippi State University





ICME for Super Vacuum HPDC (SVDC)

Mg Alloy: AZ91



Chemistry & Thermodynamics

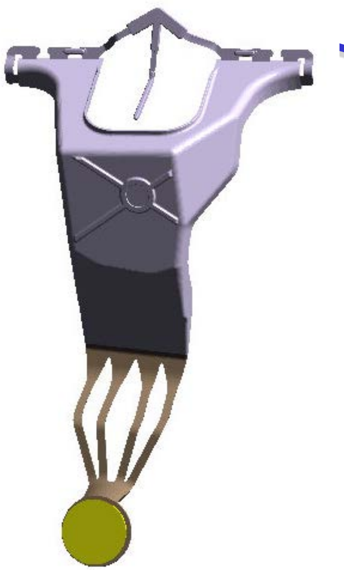
Manufacturing Process Simulation

Quantitative Processing-Structure Relations

Quantitative Structure-Property Relations

Constitutive Models

Engineering Product Performance Analysis



Precipitation Kinetics Study with Phase Field

Crystal Structure

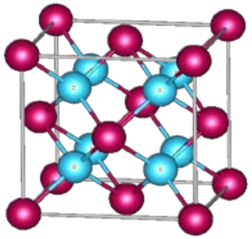
Metastable Phase Equilibria

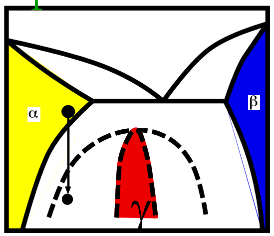
Precipitate Microstructure

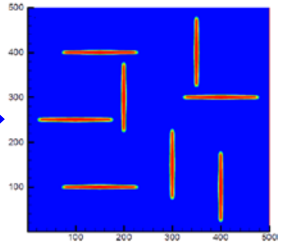
Mechanical Properties (Yield Strength)

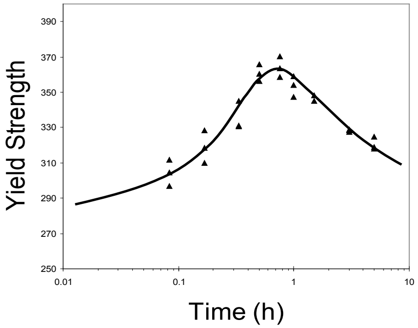
ΔH, ΔS of metastable phases

Interfacial + strain energies + *Mobilities*









Bulk (SS + Precipitate) Free Energies

Precipitate Morphologies

First-Principles Calculations

CALPHAD

Phase-Field

Micromechanical Models

Phase Field Modeling of β in AZ91 system

- Total Free energy of Mg-Al-Zn alloy system[1,2]:

$$F(c_{Al},c_{Zn},\eta_i,T)=\int_V\left[\frac{1}{V}G(c_{Al},c_{Zn},\eta_i)+\sum_{i=1}^{3}\frac{\kappa(\theta_i)^2}{2}\left|\nabla\eta_i\right|^2+E^{elast}\right]dv$$

- Local chemical free energy density[1,2]:

$$G(c_{Mg},c_{Al},c_{Zn},\eta_i)=h(\eta_i)f^{\beta}(c^{\beta}_{Mg},c^{\beta}_{Al})+\left[1-h(\eta_i)\right]f^{\alpha}(c^{\alpha}_{Mg},c^{\alpha}_{Al},c^{\alpha}_{Zn})+wg(\eta_i)$$

- Growth of precipitates[1,2]:

$$\frac{\partial\eta_i}{\partial t}=L(\theta_i)\left[-\frac{1}{V_m}\frac{\partial G}{\partial\eta_i}-\frac{\partial}{\partial\eta_i}\left(\frac{\kappa(\theta_i)^2}{2}\left|\nabla\eta_i\right|^2\right)-\frac{\partial E^{elast}}{\partial\eta_i}\right]$$

$$\frac{\partial C_i}{\partial t}=\nabla\left[\frac{D(\eta_1,\eta_2,\eta_3,T)}{G_{cc}}\nabla\left(\frac{\partial G}{\partial C_i}\right)\right]$$

[1] Hu SY, Murray J, Weiland H, Liu ZK, Chen LQ. Calphad 2007;31:303.

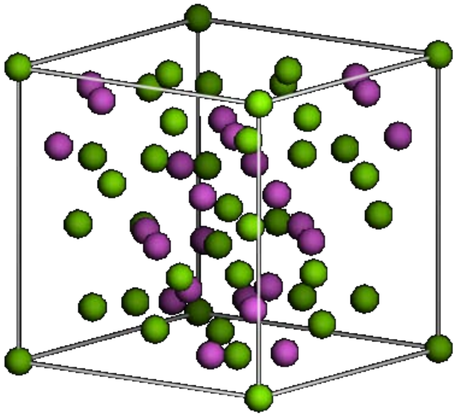
[2] Chen LQ. Annu Rev Mater Res 2002;32:113.

DFT calculations on the β Phase

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

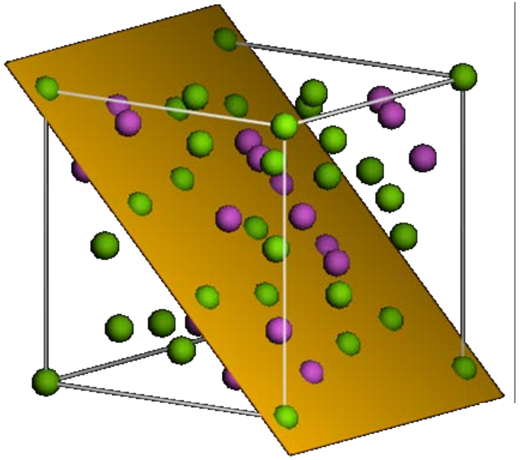
Outputs: Low-energy interface structures, interfacial energies, strain energies, lattice parameters and elastic constants for the phase field model

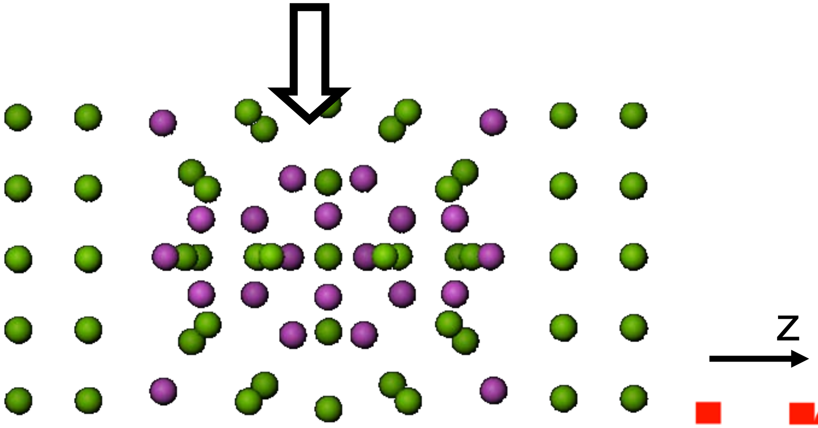
β-$Mg_{17}Al_{12}$



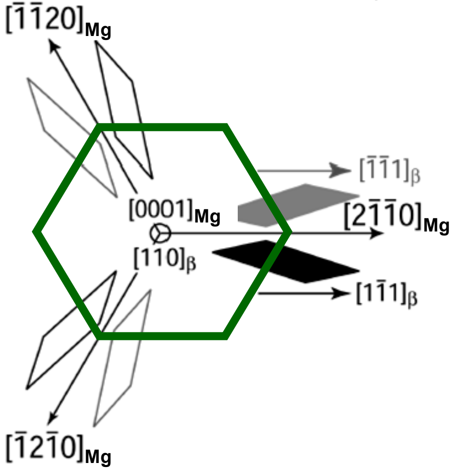
BCC, *I43m*
a=1.056 nm
58 atoms

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

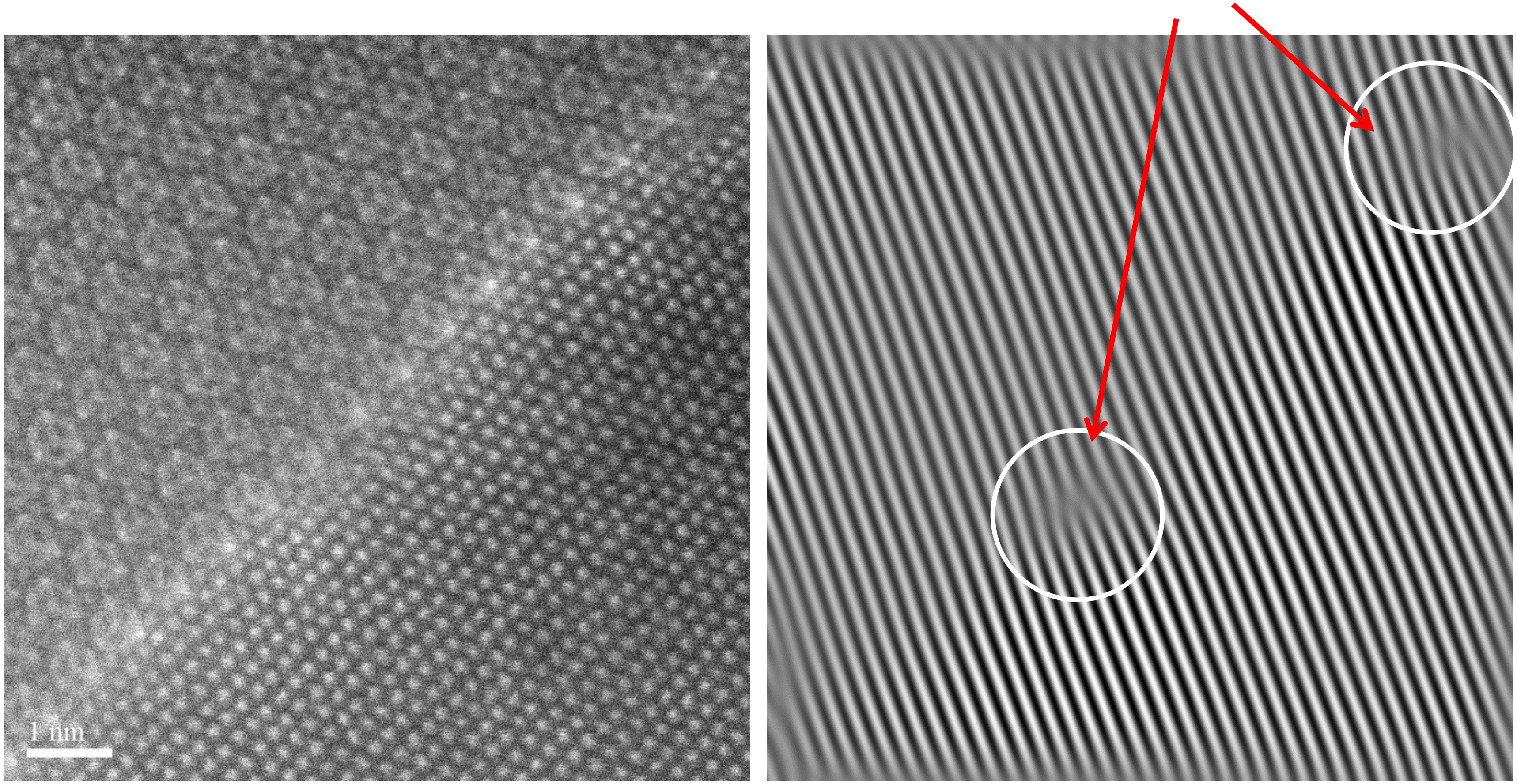




$[1\text{-}210]_\alpha \parallel [1\text{-}11]_\beta$



Characterization of Atomic Structure of Precipitates for DFT



Misfit dislocation

$Z = [11\bar{2}0]$

IFFT

Anisotropy of β precipitates in Phase Field

- **Interfacial energy from first principles*:**

$$\gamma^c_{\alpha\beta} = 0.060 J/m^2 \qquad \gamma^n_{\alpha\beta} = 0.300 J/m^2$$

- **Anisotropy of interfacial energy $\gamma(\theta)$ and Mobility coefficient $L(\theta)$ similar angular:**

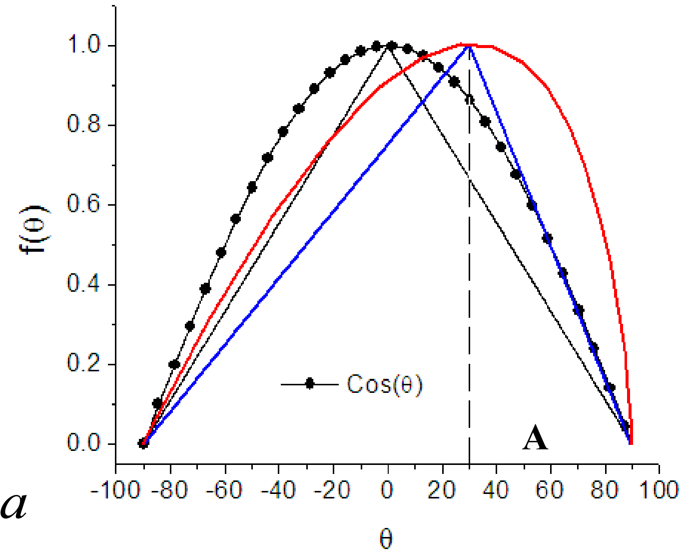
$$\gamma(\theta_i) = \begin{cases} \gamma^c_{\alpha\beta} + \Delta\gamma_{\alpha\beta}\cos(\theta_i) & \theta_i \le \pi/2 - \theta_0 \\ \gamma^c_{\alpha\theta} + \Delta\gamma_{\alpha\beta}(\tan(\theta_0) - \sin(\theta_i)/\sin(\theta_0)) & \pi/2 - \theta_0 < \theta_i \le \pi/2 + \theta_0 \\ \gamma^c_{\alpha\beta} - \Delta\gamma_{\alpha\beta}\cos(\theta_i) & \theta_i \ge \pi/2 + \theta_0 \end{cases}$$

- **Stress-free strain tensor of β precipitates:**

$$\varepsilon^{order}_{ij[110]_\beta \| [0001]_{\alpha-Mg}} = \begin{pmatrix} 0.00914 & 0 & 0 \\ 0 & 0.039 & 0 \\ 0 & 0 & 0.039 \end{pmatrix}$$

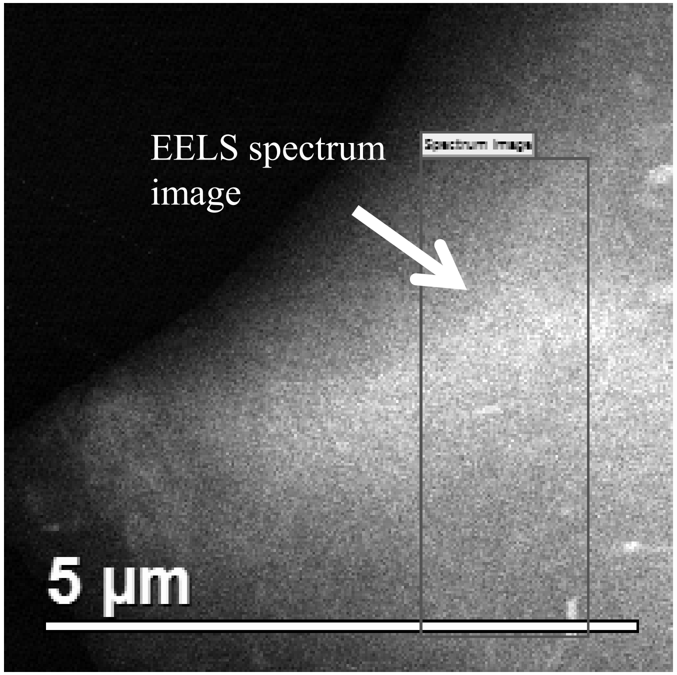
- **Elastic constants:**

$$C_{11} = 108.64GPa, \; C_{12} = 61.88GPa, \; C_{44} = 28GPa$$

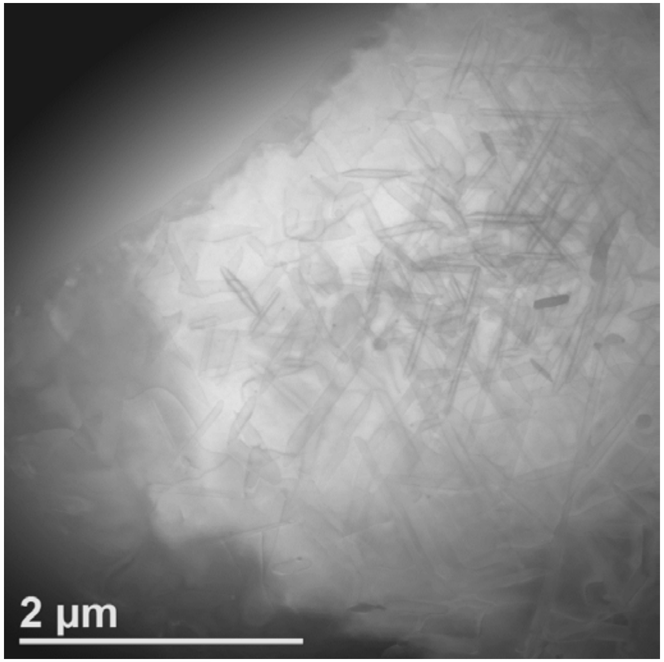


* Ford RIC, (unpublished)

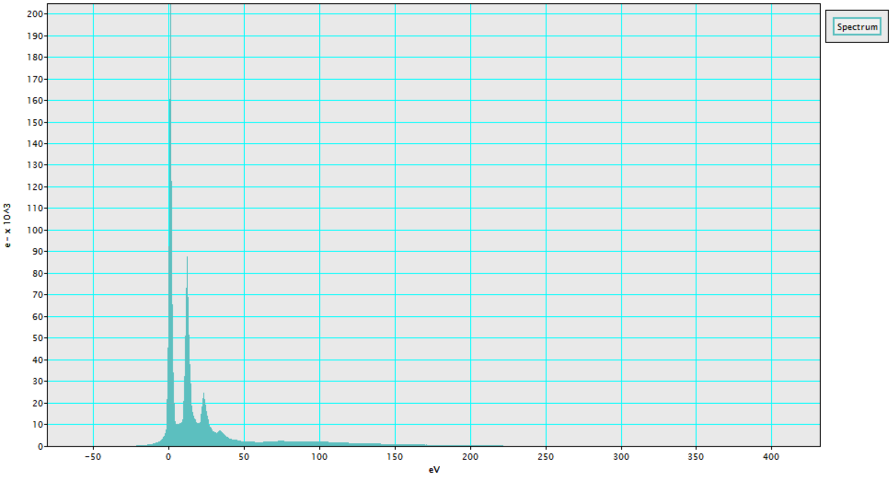
Volume Fraction Determination of Continuous Precipitates



STEM-DF



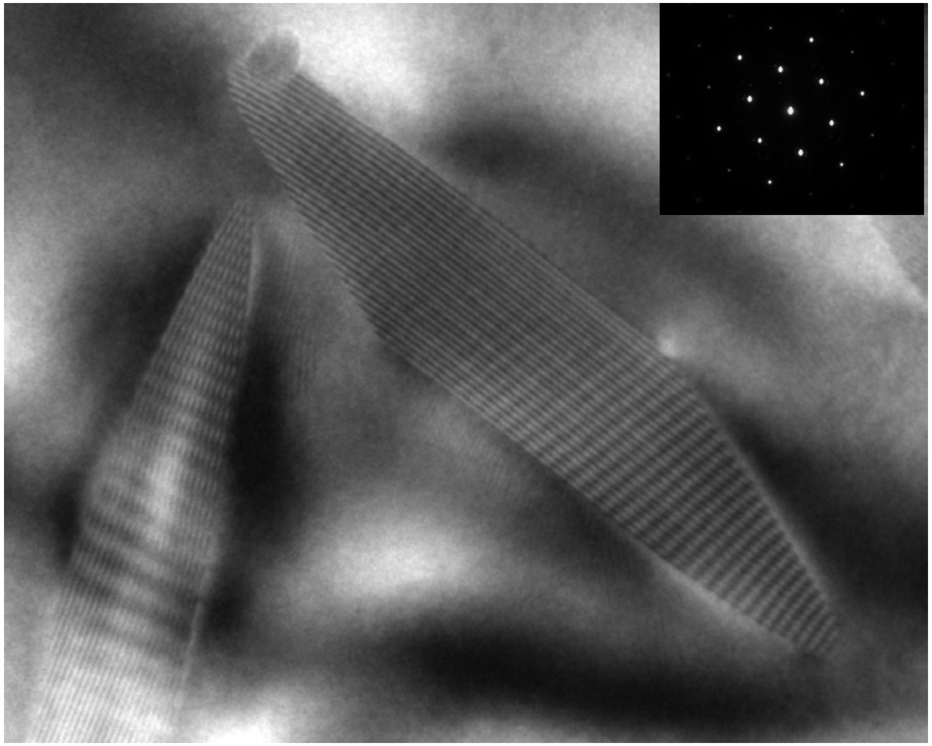
STEM-BF



EELS spectrum

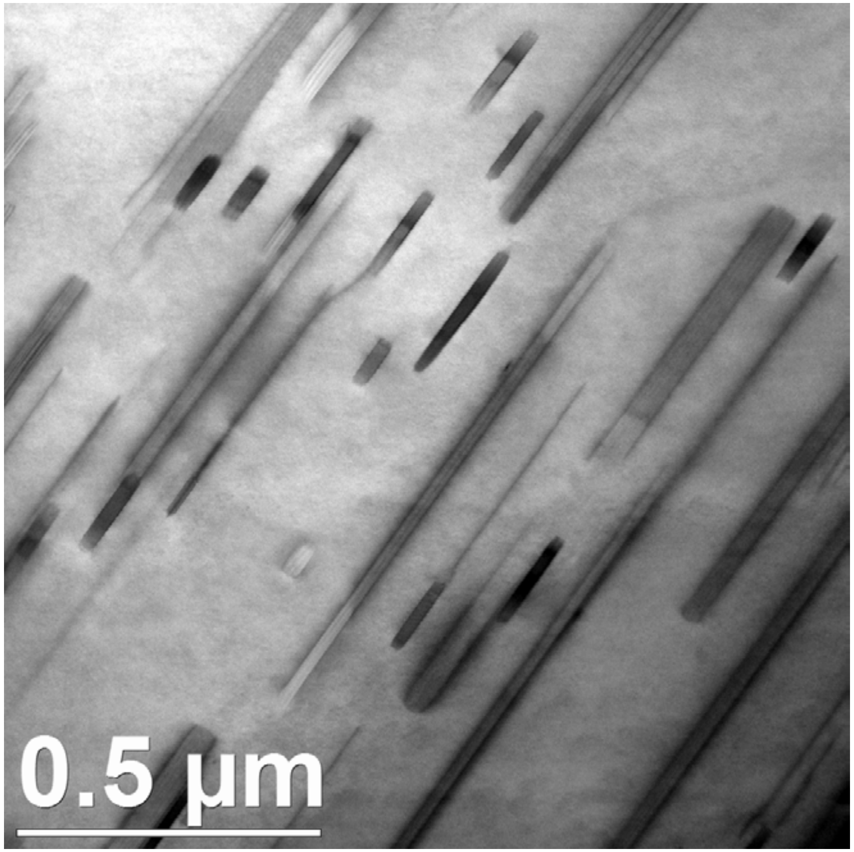
- ➢ EELS spectrum image was collected from areas where precipitate number density was measured.
- ➢ Foil thickness was measured using EELS spectrum.
- ➢ Grains were tilted to [0001] zone axis for number density measurement.

Quantitative Characterization of Precipitate Morphology



$Z= [0001]$

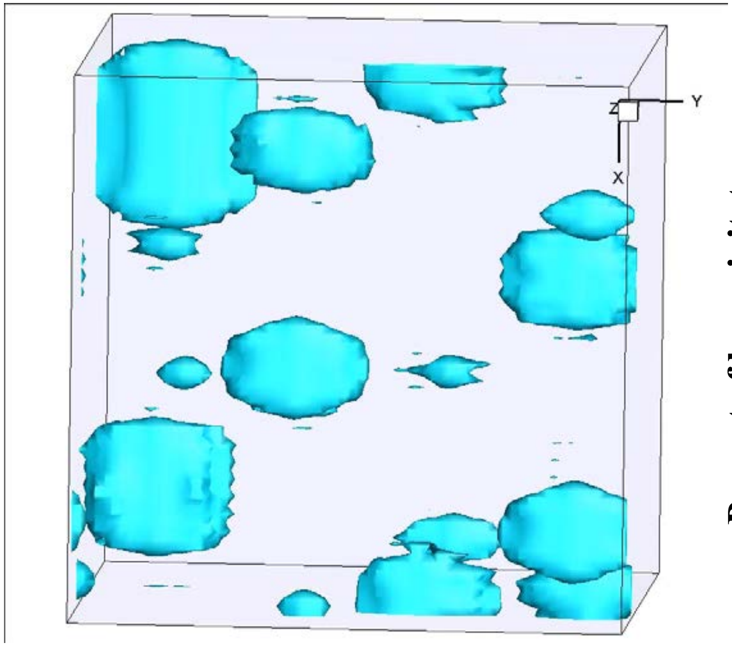
Characterize length and width



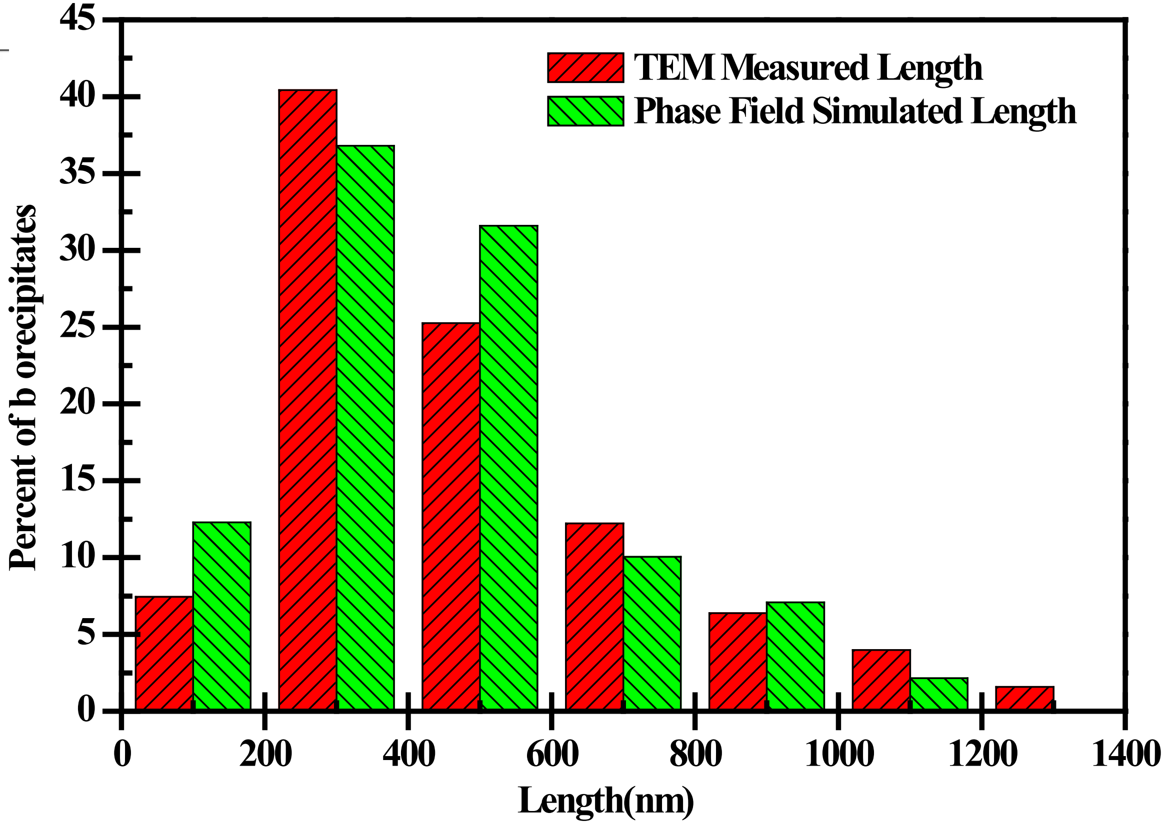
$Z = [1\,1\bar{2}0]$ STEM-BF

Characterize thickness

Phase Field Prediction and TEM Measurement



Predicted $Mg_{17}Al_{12}$ precipitates



Strengthening Modeling for AZ 91 alloy

$$\sigma_S = \sigma_0 + \Delta\sigma_{gs} + \sigma_{ss} + \sigma_{Orowan}$$

$$\Delta\sigma_{gs} = kd^{-1/2}$$ Grain size strengthening (Hall Petch)

$$\sigma_{ss} = CX^{2/3}$$ Solid solution strengthening

X – atomic fraction of solute

$$\sigma_{Orowan} = \left(\frac{0.81MG_m b}{2\pi(1-\nu)^{1/2}} \cdot \frac{1}{\lambda - d_p}\right) \ln\frac{d_p}{r_0}$$ Orowan looping

$$\lambda = \frac{d_p}{2}\left(\frac{3\pi}{2f_v}\right)^{½}$$

d_p – mean diameter of precipitates (0.087μm)

λ - mean spacing of precipitates (0.48μm)

M – Taylor factor (5).

G_m- shear modulus (27.2GPa)

b = r_0 = Burger vector (0.32nm)

Experimental Microstructure parameters	
Number density	6.9×10^{19} m^{-3}
Average length of β	0.409μm
Average width of β	0.076μm
Average thickness of β	0.029μm
Average grain size of α Mg	26μm

Strengthening contribution	MPa
Grain size	73
Solid solute	38
σ_0	11
Experimental results	92

As quenched

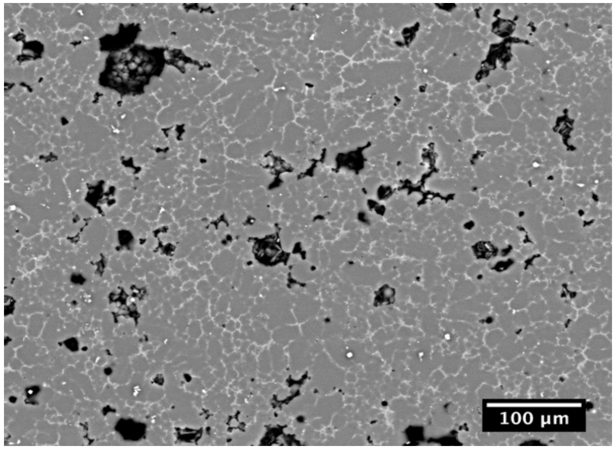
Strengthening contribution	MPa
Orowan looping	99
Solid solute	16.8
σ_0	11
Experimental results	151

Heat treated

*Modeling the precipitation processes and strengthening mechanisms in a Mg-Al-(Zn) AZ91 alloy, C.R.Hutechinson, et al., Metallurgical and materials transactions A, Vol 36A, 2005, p2093-2105.

*L.M. Brown, P.k.Ham, Strengthening methods in Crystals, A. Kelly and R.B. Nicholson, 1971, p10-15

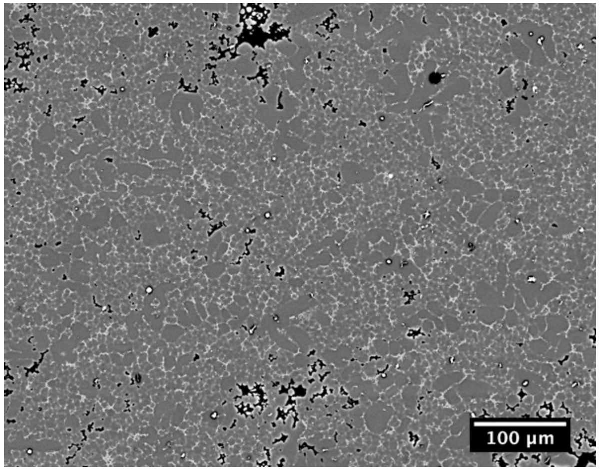
Dendrite Cell Size & Porosity



L1

Cell Size = 4.99 ± 2.26 µm

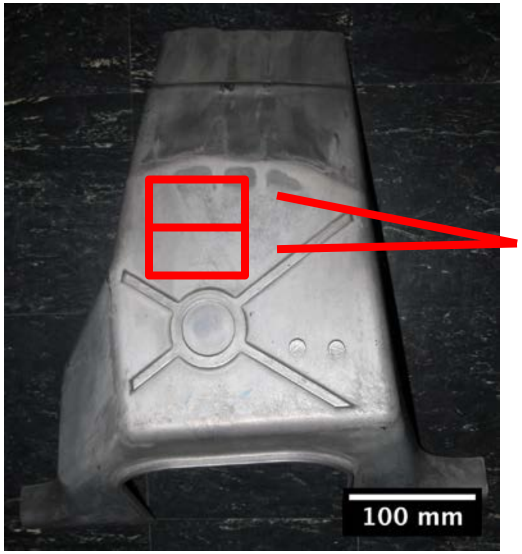
Porosity Area Fraction = 4.18%



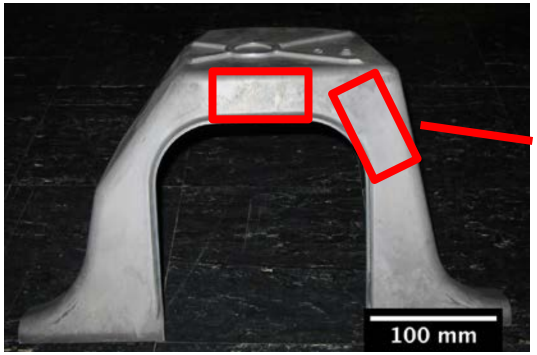
L2

Cell Size = 4.17 ± 1.51 µm

Porosity Area Fraction = 1.75%



L1
(t = 4.7mm)

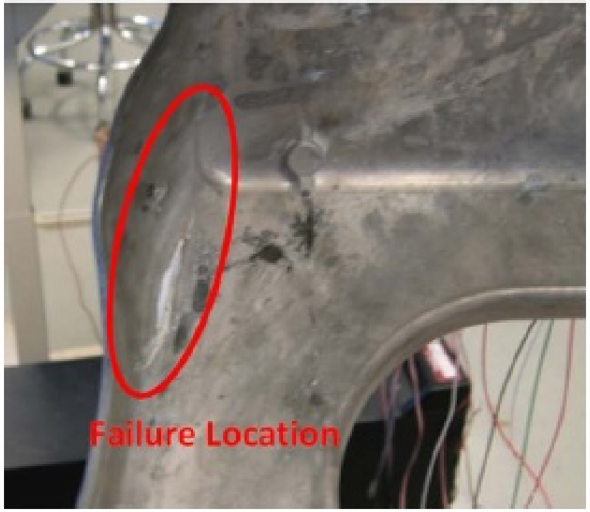


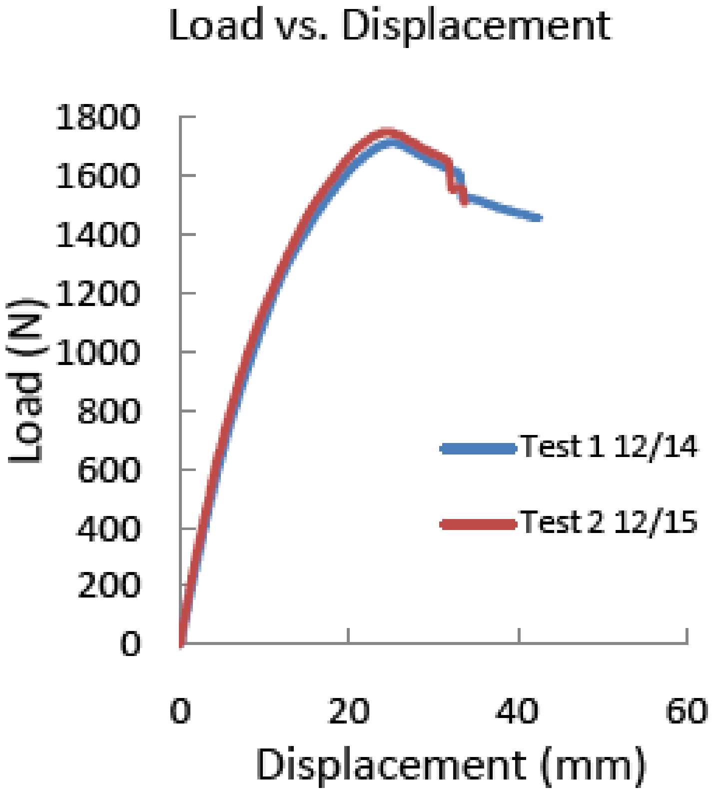
L2
(t = 3.0mm)

University of Michigan

Demonstration of ICME Tools

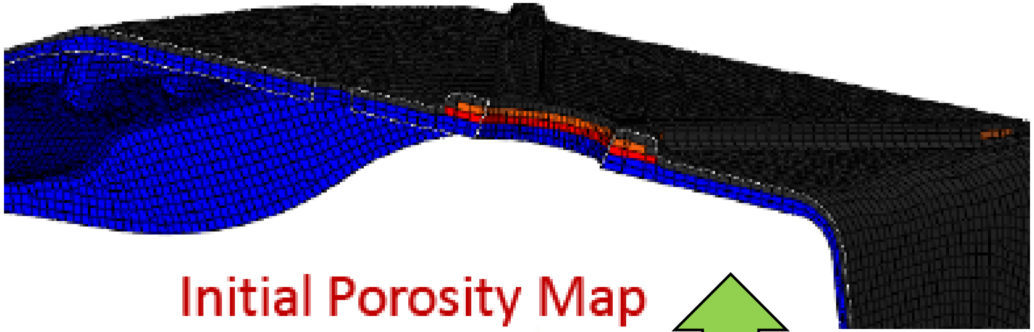
- Failure locations AND load displacement curves



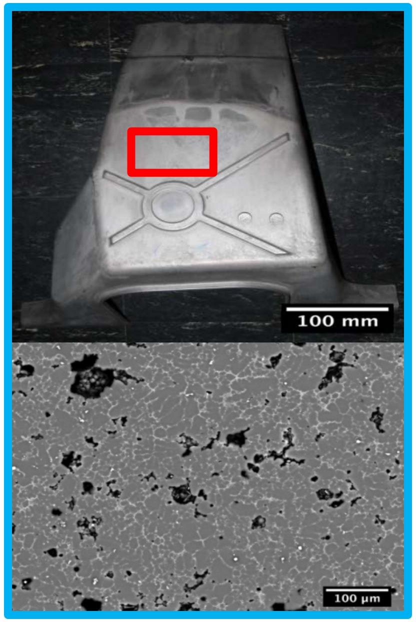


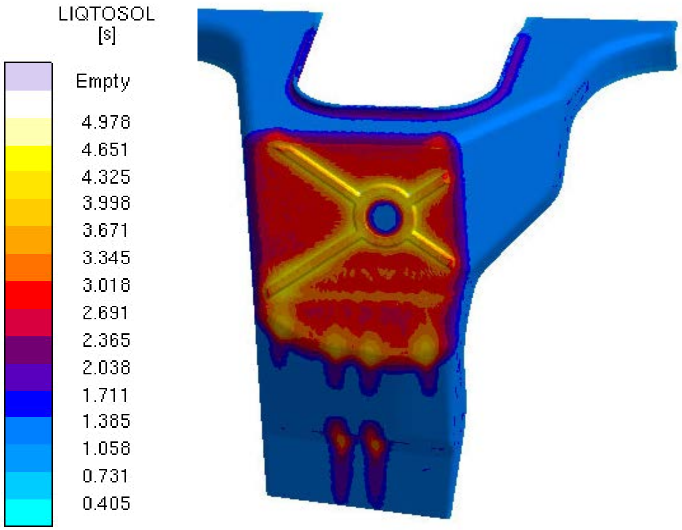
Demonstration of ICME Tools

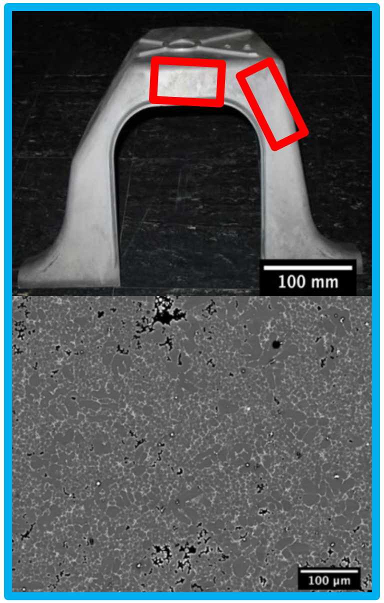
- Mapped local porosity distribution onto AZ91 shock tower



Initial Porosity Map

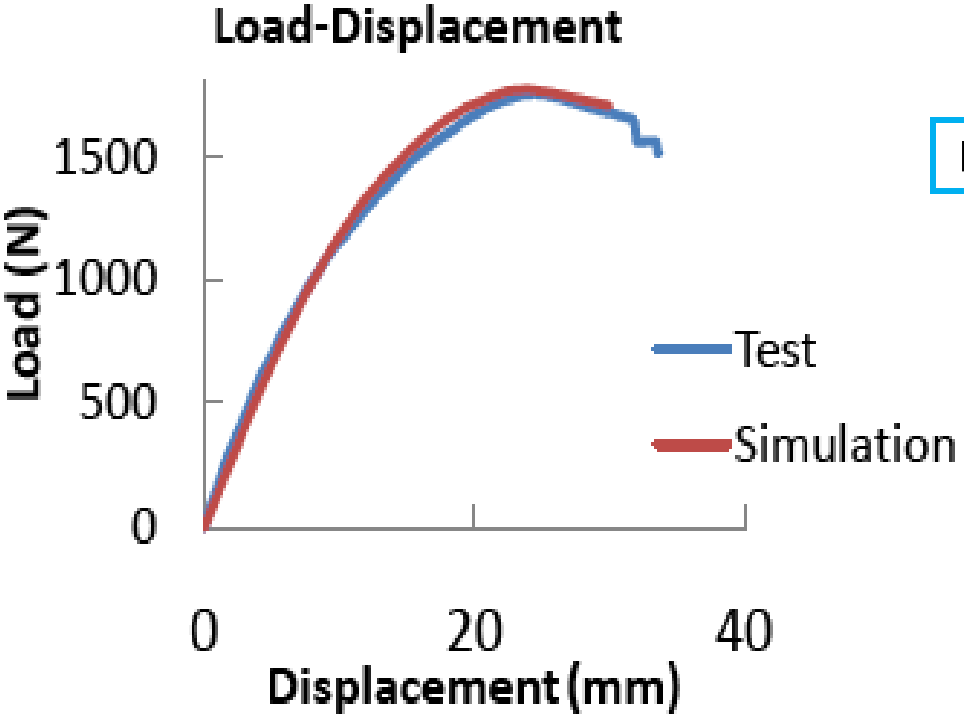


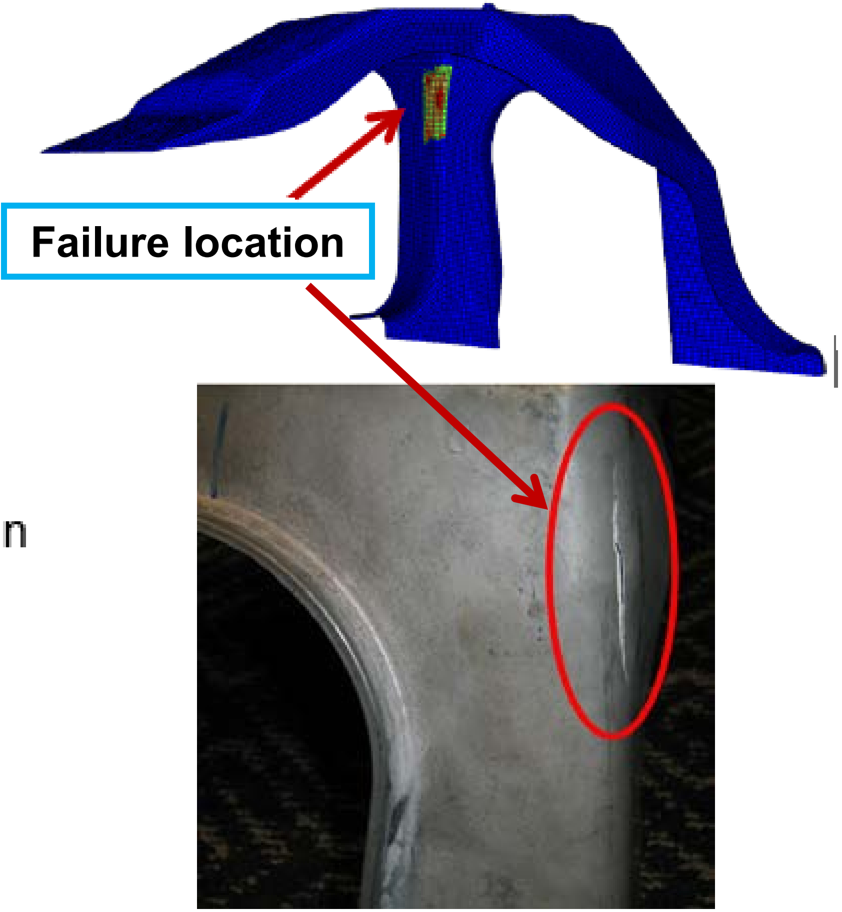




Demonstration of ICME Tools

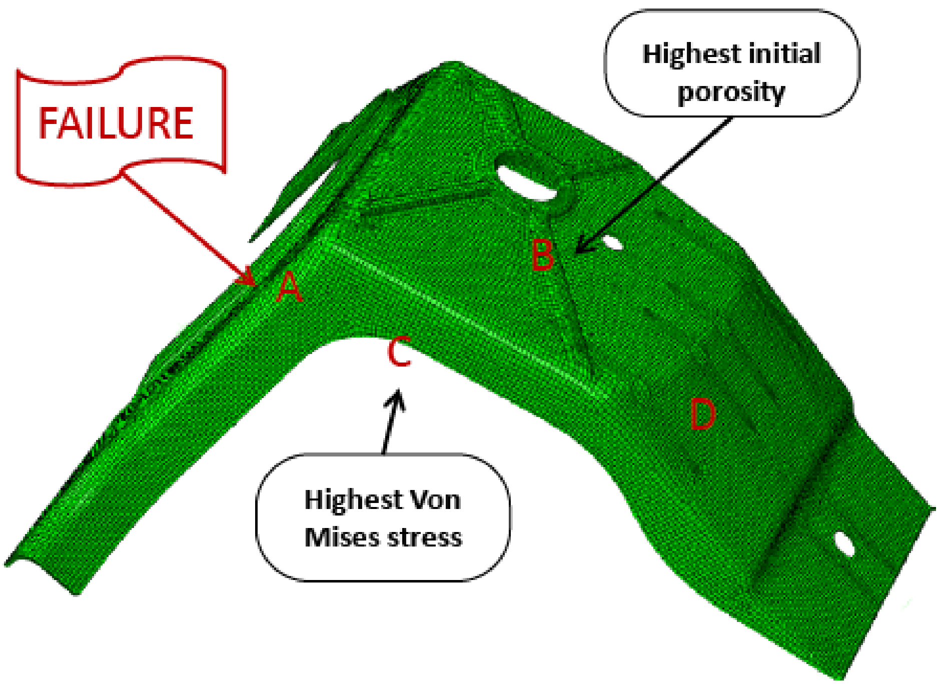
- Accurately predicted load-displace curve and failure location





Demonstration of ICME Tools

- Traditional FEA analysis will predict C as failure location;
- Standard materials science and engineering will predict B as failure location;
- ICME approach predicted accurately A as the failure location



Summary

- Integrated Computational Materials Engineering (ICME) for Mg project has successfully delivered on all task areas;

- The project has demonstrated the power of ICME approach compared with traditional FEA analysis in predicting the failure;

- ICME links the impact of manufacturing process on local properties with the performance analysis, providing a unprecedented insight and accuracy

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