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

Project ID LM012
AMD 703

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## Overview

### Timeline

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

### Barrier

- Design data & modeling tools
- Manufacturability
- 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
• The Minerals, Metals and Materials Society (TMS)
• ThermoCalc Inc
• MagmaSoft®
• Mississippi State University*
• Lehigh University*
• Oak Ridge National Lab*
• Pacific Northwest Labs*

China:
• Tsinghua University
• Northeastern University
• Central South University
• Shanghai JiaoTong University

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 $\beta$ 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.
Demonstration of ICME Tools

- Experimental set up at Center for Advanced Vehicle System (CAVS), Mississippi State University
Precipitation Kinetics Study with Phase Field

Crystal Structure  
Metastable Phase Equilibria  
Precipitate Microstructure  
Mechanical Properties (Yield Strength)

- $\Delta H, \Delta S$ of metastable phases
- Interfacial + strain energies + Mobilities
- Bulk (SS + Precipitate) Free Energies
- Precipitate Morphologies
- Yield Strength vs. Time (h)

First-Principles Calculations  
CALPHAD  
Phase-Field  
Micromechanical Models
Phase Field Modeling of $\beta$ in AZ91 system

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

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

- Local chemical free energy density$^{[1,2]}$:

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

- Growth of precipitates$^{[1,2]}$:

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

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


**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, $I4_3m$

$a=1.056$ nm

58 atoms
Characterization of Atomic Structure of Precipitates for DFT

$Z = [11\bar{2}0]$
Anisotropy of $\beta$ precipitates in Phase Field

- Interfacial energy from first principles*:

$$\gamma_{\alpha\beta}^c = 0.060 J / m^2 \quad \gamma_{\alpha\beta}^n = 0.300 J / m^2$$

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

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

- Stress-free strain tensor of $\beta$ precipitates:

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

- Elastic constants:

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

* Ford RIC, (unpublished)
Volume Fraction Determination of Continuous Precipitates

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

$Z = [11\overline{2}0]$  
Characterize thickness
Phase Field Prediction and TEM Measurement

Predicted $\text{Mg}_{17}\text{Al}_{12}$ precipitates

- TEM Measured Length
- Phase Field Simulated Length

Percent of precipitates vs. Length (nm)
Strengthening Modeling for AZ 91 alloy

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

**Grain size strengthening (Hall Petch)**

\[ \Delta \sigma_{gs} = k d^{-1/2} \]

**Solid solution strengthening**

\[ \sigma_{ss} = C X^{2/3} \]

**Orowan looping**

\[ \sigma_{Orowan} = \left( \frac{0.81 M G_m b}{2 \pi (1 - \nu)^{1/2}} \cdot \frac{1}{\lambda - d_p} \right) \ln \frac{d_p}{r_0} \]

**Parameters**

- \( d_p \) – mean diameter of precipitates (0.087µm)
- \( \lambda \) – 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**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number density</td>
<td>( 6.9 \times 10^{19} ) m(^{-3} )</td>
</tr>
<tr>
<td>Average length of ( \beta )</td>
<td>0.409µm</td>
</tr>
<tr>
<td>Average width of ( \beta )</td>
<td>0.076µm</td>
</tr>
<tr>
<td>Average thickness of ( \beta )</td>
<td>0.029µm</td>
</tr>
<tr>
<td>Average grain size of ( \alpha ) Mg</td>
<td>26µm</td>
</tr>
</tbody>
</table>

**Strengthening contribution**

<table>
<thead>
<tr>
<th>Contribution</th>
<th>MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain size</td>
<td>73</td>
</tr>
<tr>
<td>Solid solute</td>
<td>38</td>
</tr>
<tr>
<td>( \sigma_0 )</td>
<td>11</td>
</tr>
<tr>
<td>Experimental results</td>
<td>92</td>
</tr>
</tbody>
</table>

**Experimental results**

- As quenched: 92 MPa
- Heat treated: 151 MPa

**Dendrite Cell Size & Porosity**

**Cell Size**
- L1: 4.99 ± 2.26 µm
- L2: 4.17 ± 1.51 µm

**Porosity Area Fraction**
- L1: 4.18%
- L2: 1.75%

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**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
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;