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: Feb 2012
- New project end date: Sept 2011
- Percent complete: 75%

#### Barrier

- Design data & modeling tools
- Manufacturability
- 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 MFED Phase II (September 2011):
  ➢ Demonstrate ability of ICME tools to link manufacturing and predict performance of MFED 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.*

Chemistry
Thermodynamics
Diffusion

Manufacturing Process Simulation
Quantitative Processing-Structure Relations
Quantitative Structure-Property Relations
Constitutive Models
Engineering Product Performance Analysis

• Process & product optimization
• Innovation
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

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
Mg Alloy: AZ31

Pan Die Geometry

Warm forming and Post-forming behavior
Predicted Thickness Strain vs. Measurements

Comparison of Experimental Results, panels formed under different conditions:

- Wrinkled
- Split
- Formed

Numbers, 227, 127, 102

Comparison of BCJ predictions:

- Wrinkled
- Split
- Formed

Numbers, 227, 127, 102

GM, University of Virginia and MSU
Predicted Solute Strengthening Map of Mg

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

GM

University of Virginia

2011 DOE Merit Review Presentation This presentation does not contain any proprietary, confidential or otherwise protected information
**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

Cell Size = 4.99 ± 2.26 µm
Porosity Area Fraction = 4.18%

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

- L1 As-Cast
- L2 As-Cast
- L1 T6
- L2 T6

\[ \varepsilon_a (\%) \quad N_f \]

University of Michigan
Disolution Kinetics of Eutectic Mg\textsubscript{17}Al\textsubscript{12}

- Dissolution kinetics model in Dictra

\[ g_{17\text{Al}_{12}} \text{ (wt\%)} \]

ST temperature
413°C

Solution Treatment Time (minutes)
DFT calculations on the Mg-alloy $\beta$-Mg$_{17}$Al$_{12}$ phase

**Inputs:** Experimental data from literature on $\alpha/\beta$ interface structure, orientation, …

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

$\beta$-Mg$_{17}$Al$_{12}$

BCC, $I43m$

$a=1.056$ nm

58 atoms

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


Ford
Precipitation Kinetics Study with Phase Field

Crystal Structure

Metastable Phase Equilibria

Precipitate Microstructure

Mechanical Properties (Yield Strength)

First-Principles Calculations

CALPHAD Phase-Field

Bulk (SS + Precipitate) Free Energies

ΔH, ΔS of metastable phases

Interfacial + strain energies + Mobilities

Precipitate Morphologies

Yield Strength

Time (h)
Simulated Precipitate Morphology

3D Simulation
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-strain 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