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

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Project ID
LM012
Overview

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

Barriers
• Barriers addressed:
  - Design data & modeling tools
  - Manufacturability
  - Performance
  - Cost

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

Partners
• 3 US Universities
• 3 US Companies
• TMS
• Lead: 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.
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/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
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.*

* NAE ICME Report, 2008
Program Integration

USAMP (Three Countries)
MFERD Project LM008

Three Countries
ICME for Mg Project

Canada, China, PNNL,
ORNL

MSSt
CAVS/SCRLID
Project LM013

Project LM012
$1M/$1M

MSSt/USAMP Project B
$2.4M/$600K

Project LM013
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
International Partners – China*

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

International Partners – Canada*

- CANMET-MTL

*Not funded in this project LM012
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
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

![Graph showing phase diagram and diffusion characteristics](image-url)
**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

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

Northwestern Univ
**Goal:** 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

![Pan Die Geometry Image](Image)

Mg Alloy: AZ31
Sheet Metal Forming Simulation @ 473K

MissSt ISV Model
Thickness (mm)

Sellars –Tegart Model (UVA)

Univ of Virginia, GM, MSSf
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 coefficients 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
Completed casting simulation on AZ91 SVDC shock tower

Prim. α-Mg 19%

Prim. α-Mg 14%

Prim. α-Mg 0%

Prim. α-Mg 5%

Ford & University of Michigan
Quantified influence of solution treatment and aging on yield strength

![Graph showing the quantified influence of solution treatment and aging on yield strength.](image)

- **Yield strength, MPa**
- **Aging time, hour**
- **Location#3**
- **Location#4**

- **As cast**
- **As quench**
- **AZ91 SVDC**
- **Solution treatment at 413°C, 20h**
- **Aging at 168°C**

*University of Michigan*
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., MgZn2 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
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.
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