Integrated Computational Materials Engineering for Light Metals Applications

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Outline and Acknowledgements

- USCAR Mg-intensive front end & integrated computational materials engineering (ICME) projects
  - Department of Energy (DOE) for finanical support
  - Mei Li, Ford Research and Advanced Engineering
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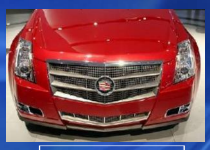
  - Chris Wolverton, Northwestern University
  - Sean Agnew, University of Virginia
- Diffusion data needs for ICME
  - Kaustubh Kulkarni, General Motors India
  - Chuan Zhang and Fan Zhang, CompuTherm LLC

USCAR Mg-Intensive Front End Project

Cadillac CTS



Steel baseline design
110 Parts & 99.6 kg

Mg-intensive design
47 Parts & 55.3 kg

44.3 kg mass reduction (44.5%)
63 part reduction (57.3%)

CHRYSLER Ford General Motors

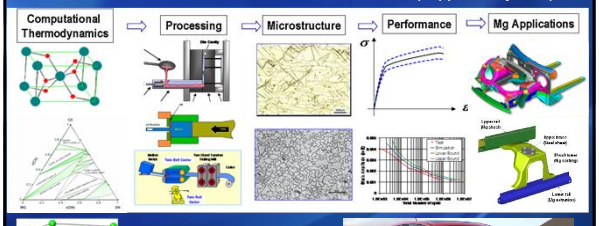
Integrated Computational Materials Engineering (ICME)

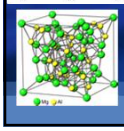
Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.

"Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security", National Research Council, 2008, The National Academies Press, Washington, DC.

USCAR Integrated Computational Materials Engineering (ICME) Task on Magnesium-Intensive Front End

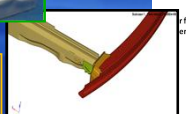
- USA-Canada-China Collaboration in ICME since 2007 (supported by DOE)

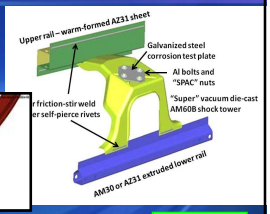




Atoms to Autos

Mg ICME Challenges

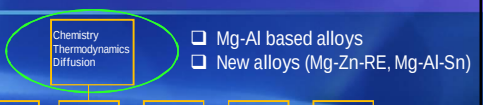




- Mg-Al alloys
- New alloys

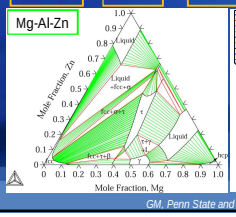
- Casting
- Extrusion
- Sheet Forming
- Stress-Strain Response
- YS (& Anisotropy)
- Ductility (& Anisotropy)
- Fatigue
- Crash Response
- Durability

Calculated Phase Equilibria & Diffusion

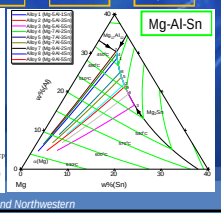


- Mg-Al based alloys
- New alloys (Mg-Zn-RE, Mg-Al-Sn)

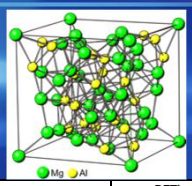
Mg-Al-Zn

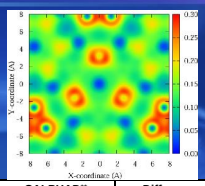


Mg-Al-Sn



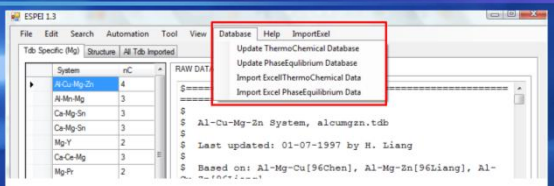
Density Functional Theory & CALPHAD Modeling of γ-$Mg_{17}Al_{12}$





ΔH_f	DFT* (kJ/mol)	CALPHAD** (kJ/mol)	Difference (kJ/mol)
$Mg_{17}Al_{12}$ (Mg:Mg:Al)	-3500	-3597	-97
Mg_{29} (Mg:Mg:Mg)	4490	4806	316
Mg_5Al_{24} (Mg:Al:Al)	802	288	-514
$Mg_{17}Al_{12}$ (Mg:Al:Mg)	6167	6226	59

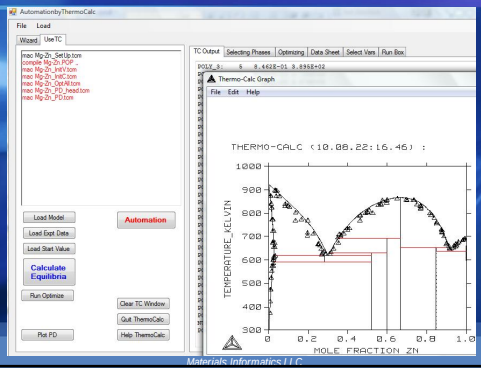
ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure for Magnesium Alloys



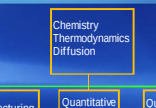
Updates:

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

Example: Automation by ThermoCalc



ICME for Casting (SVDC)



Mg Alloy: AZ91

Need to model – Development / Influence of

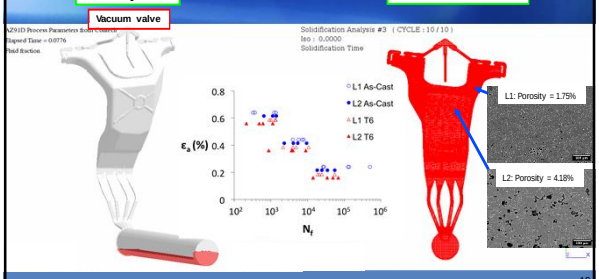
- Turbulent Flow & solidification
- Eutectic Phases
- Precipitate Phases

SVDC Process Simulation and Optimization

- Fatigue properties vs. porosity simulation

Cavity fill

Solidification



Precipitation Simulation

Crystal Structure

Metastable Phase Equilibria

ΔH, ΔS of metastable phases

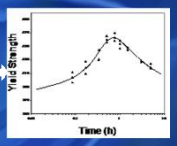
Bulk (SS + Precipitate) Free Energies

Precipitate Microstructure

Interfacial + strain energies + *Mobilities*

Precipitate Morphologies

Mechanical Properties (Yield Strength)



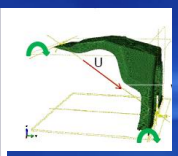
First-Principles Calculations

CALPHAD

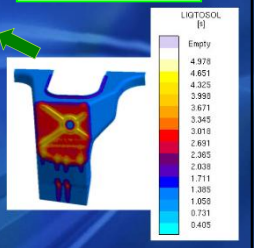
Phase-Field

Micromechanical Models

ICME for Casting (SVDC): Validation



Porosity data from MAGMAsoft simulation



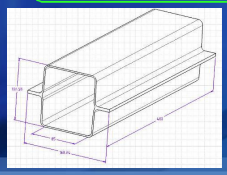
ABAQUS simulation that accounts for heterogeneity of the material due to casting process

ICME for Extrusion

Chemistry Thermodynamics Diffusion

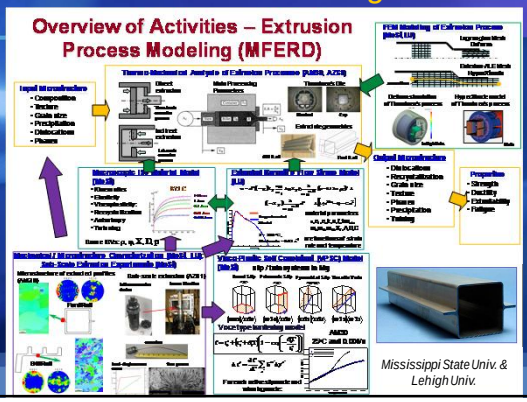
Mg Alloys: AM30 & AZ61

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



Need to model – Development/ Influence of
- Texture
- Twinning
- Dynamic Recrystallization
- Precipitate Phases (Age Hardening)

Extrusion Process Modeling



Mississippi State Univ. & Lehigh Univ.

ICME for Sheet

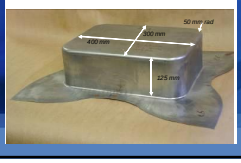
Chemistry Thermodynamics Diffusion

Mg Alloy: AZ31

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

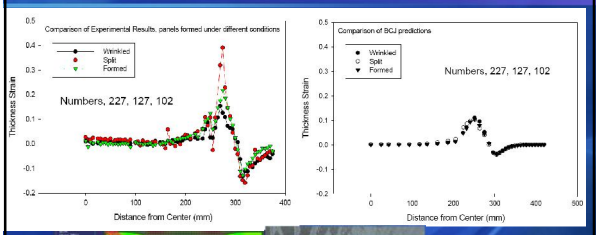
Warm forming and Post-forming behavior

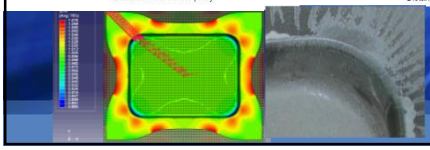
Pan Die Geometry



Need to model – Development/Influence of
- Texture
- Twinning
- Dynamic Recrystallization

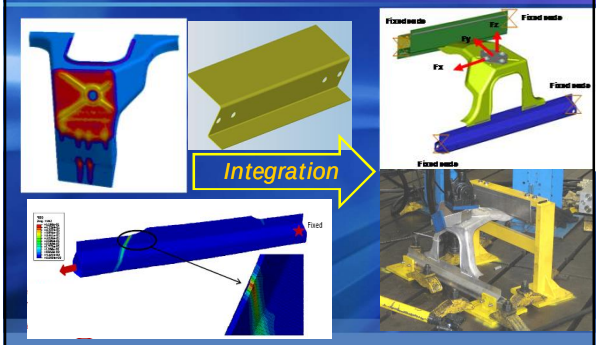
Sheet Forming Process Simulation





GM, Mississippi State Univ. & Univ. of Virginia

Ongoing Work: ICME for "Demo" Testing



Al and Mg Alloy Development Needs

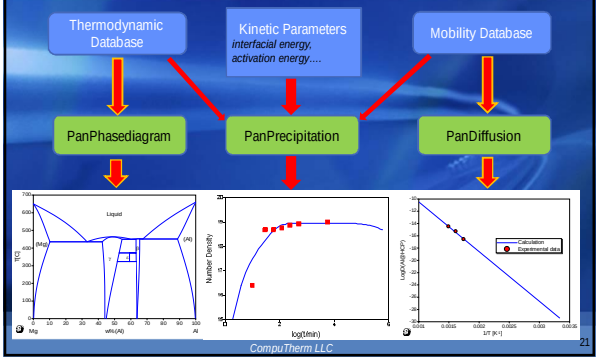
Al alloy development

- High-temperature alloys due to increased horsepower, power density and warranty
- New high-temperature alloys containing Si, Mg, Cu, Sc, Zr, Y, etc.

Mg alloy development

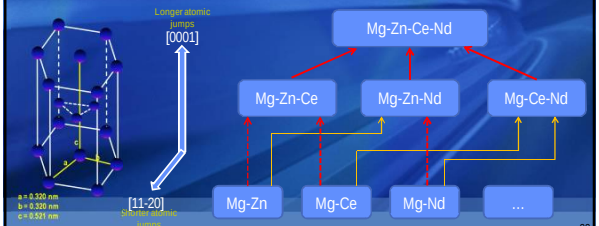
- High-strength alloys due to high static & fatigue loading
- Precipitation-hardening alloys containing Al, Zn, Sn, RE etc.

Diffusion Data: CALPHAD Approach



Diffusivity Data Needed for Mg Alloys

- Chemical diffusivities of Mg-Al based alloys (such as Mg-Al-Sn, Mg-Al-Ca…)
- Chemical diffusivities of Mg-Zn based alloys (such as Mg-Zn-Ce, Mg-Zn-Nd…)
- Impurity diffusivity of REs (rare earth) in the pure Mg (such as Nd, Gd..)
- Mg (HCP): atomic jump frequencies & diffusion kinetics maybe different in [0001] direction & [11-20] direction – need to consider texture effect in diffusion?



Opportunities: Advanced Manufacturing Initiative (AMI) & Materials Genome Initiative (MGI)

SUMMARY OF RECOMMENDATIONS

RECOMMENDATION 1: LAUNCH THE ADVANCED MANUFACTURING INITIATIVE

The Federal Government should launch an Advanced Manufacturing Initiative for America's Future (AMI). AMI should be a concerted, whole-of-government effort, spearheaded by the Department of Commerce, Department of Defense, and Department of Energy and coordinated by the Executive Office of the President (EOP).

The coordinating body of AMI should prepare a biennial report to the President on the most important needs for Federal investments, including:

- Coordinated Federal support to academia and industry for applied research on new technologies and design methodologies
- Public-private partnerships (PPPs) to advance such technologies through pre-competitive consortia that tackle major-cross-cutting challenges
- Development and dissemination of design methodologies that dramatically decrease the time and lower the barrier for entrepreneurs to make products
- Shared facilities and infrastructure to help small and medium-sized firms improve their products to compete globally.

The report should also identify the most pressing technological challenges that merit focused attention for these activities.

AMI should also report on the availability of financing for pilot plants and early-stage activities within these technology areas.

It is crucial that this whole-of-government effort be complemented by parallel initiatives in the industry and academia. AMI should develop mechanisms to involve these sectors and to draw on their expertise in identifying technological opportunities. An external advisory board that has access to advanced manufacturing expertise should help guide this work.

Summary: Take-Away Message

- "Atoms to Autos" – Integrated Computational Materials Engineering (ICME) & Materials Genome Initiative (MGI) are great opportunities for the materials community.
- ICME and MGI require close industry-academia collaboration and public-private partnerships: everyone has a role to play…
- Diffusivity study and data are key to accelerated development of materials, processes and engineering products.

DOE/USAMP Disclaimer

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Thank You…Questions?