DOE Program Merit Review Meeting

Southern Regional Center for Lightweight Innovative Design (SRCLID)
Project ID: LM037

May 17, 2012

Prime Recipient: Center for Advanced Vehicular Systems

Mississippi State University

Agreement Number: (# DE-FC-26-06NT42755)

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Presenter: Paul T. Wang, PhD, PE

DOE Manager: Carol Schutte, William Joost

DOE SRCLID Programs

Lightweight Metals | **Steel Materials** | **Polymeric Materials**

Vision: Develop **multiscale physics-based material models** for **design optimization** of components and systems made of **lightweight** materials in automotive applications.

Mission: (1) Provide a design methodology that includes physics-based material models that include **uncertainty** in consideration of the material history;

(2) Develop **new materials and math-based tools** for use in next-generation vehicles under various crash and high-speed impact environments.

Goals: (1) an experimentally validated **cradle-to-grave** modeling and simulation effort to optimize automotive and truck components for various materials;

(2) a multiscale ("From Atoms to Autos") modeling philosophy with characterization of the **microstructure-property relations** by evaluating various length scales;

(3) an integrated K-PhD **educational program** to educate students on lightweight designs and impact scenarios.

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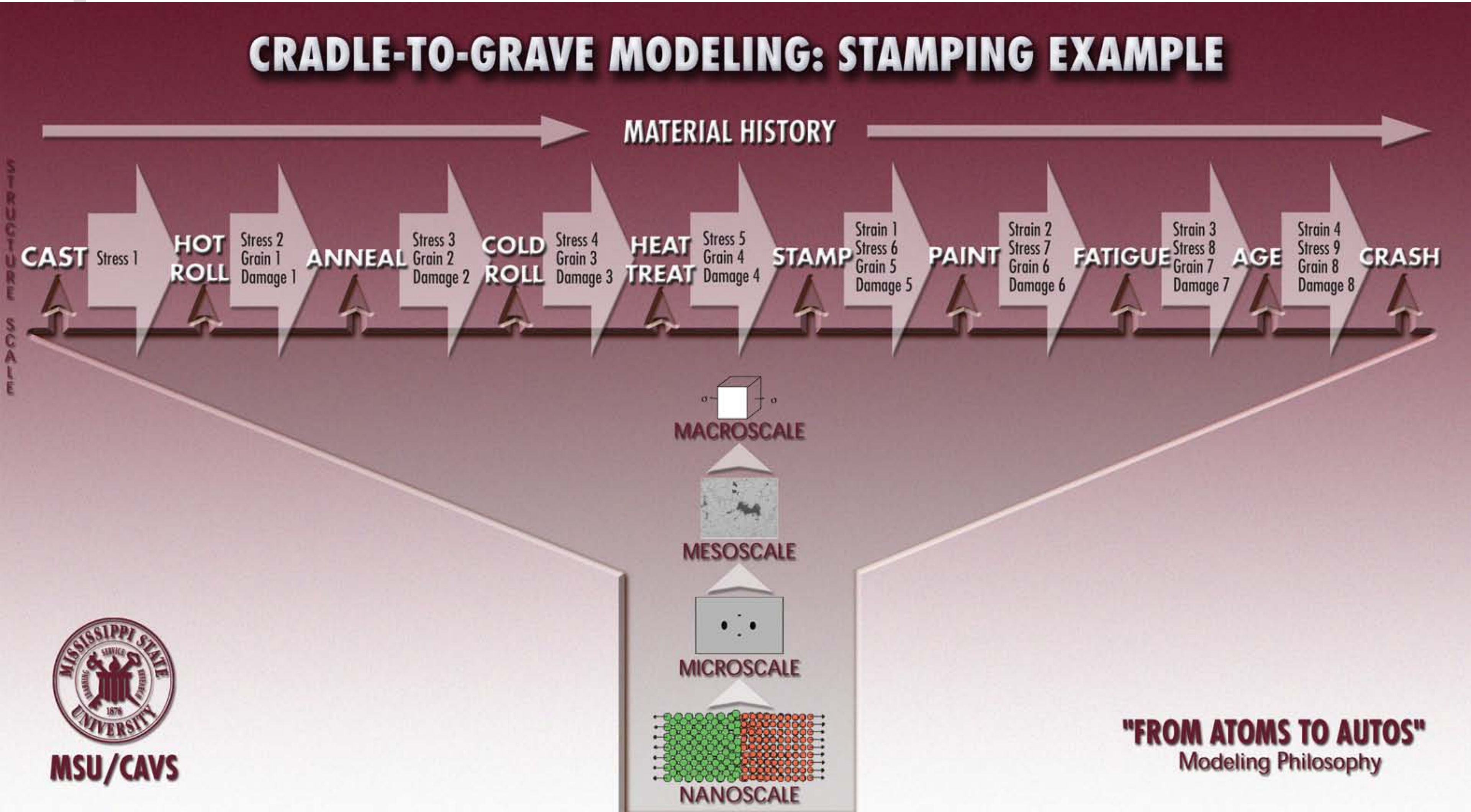
Approach/Strategy

Development and Deployment
of
Multiscale Lightweight Material Program

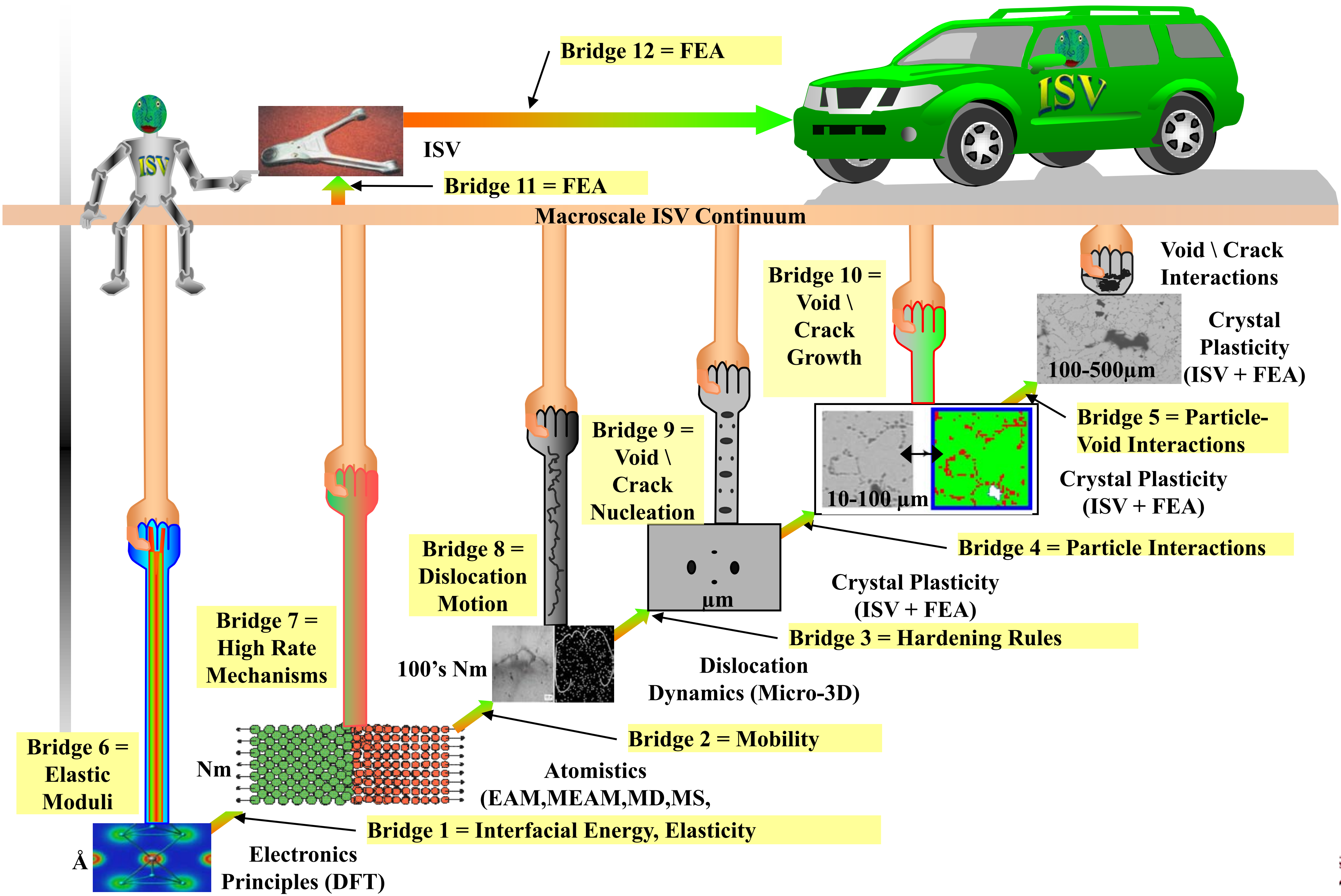
1. Quantify history dependent process-structure-property relationship
2. Repository material data base and model in cyberinfrastructure
3. Verification, validation and demonstration
4. Establish close relationship with industrial partners

Computational Manufacturing and Design

Mission: To optimize design and manufacturing processes, we integrate multidisciplinary research of solid mechanics, materials, physics, and applied mathematics in three synergistic areas: theoretical modeling, experimentation, and large scale parallel computational simulation.



Multiscale Modeling

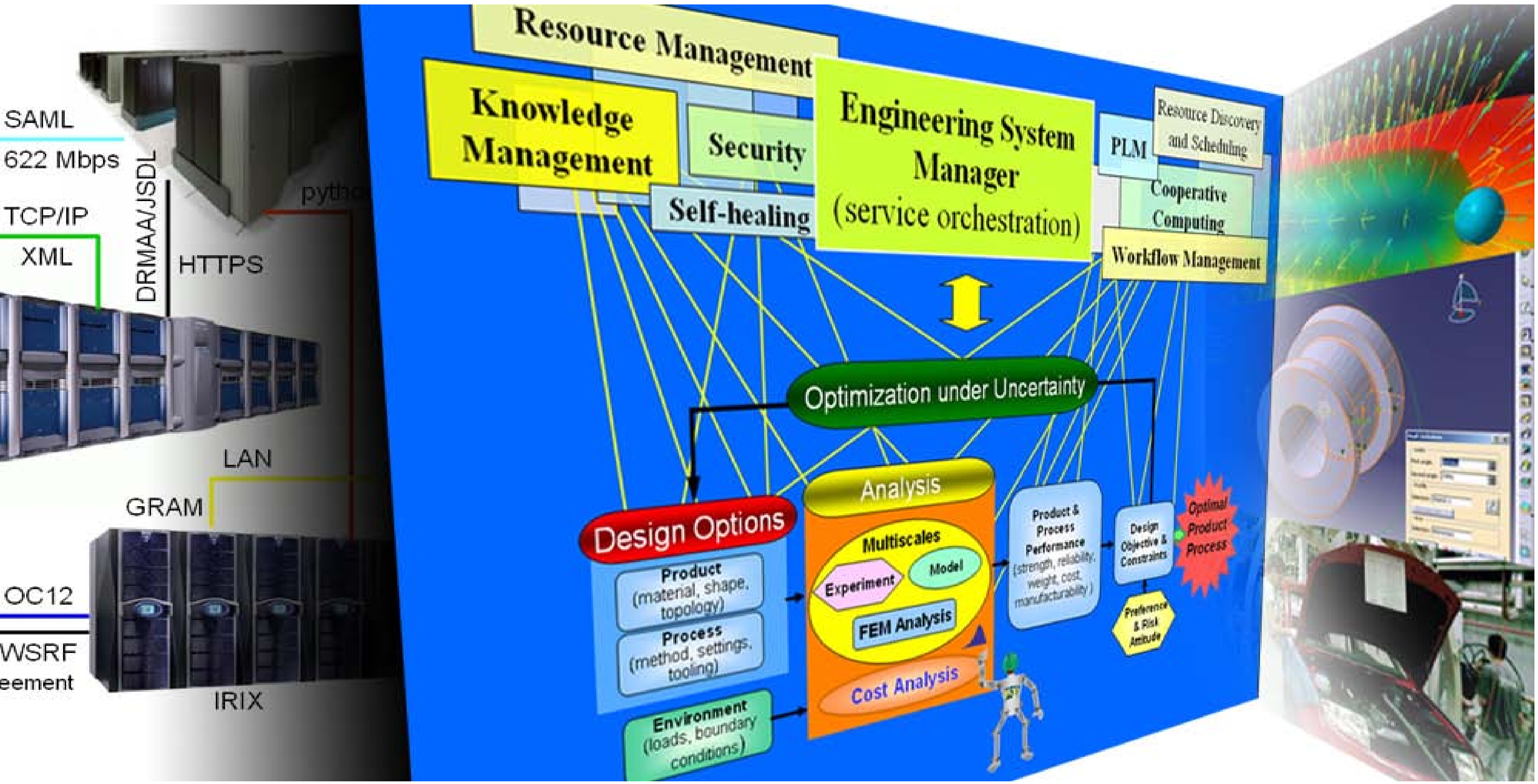


CyberInfrastructure

IT Technologies (hidden from the engineer)

Conceptual Design Process (user-friendly interfaces)

Engineering Tools (CAD, CAE, etc.)

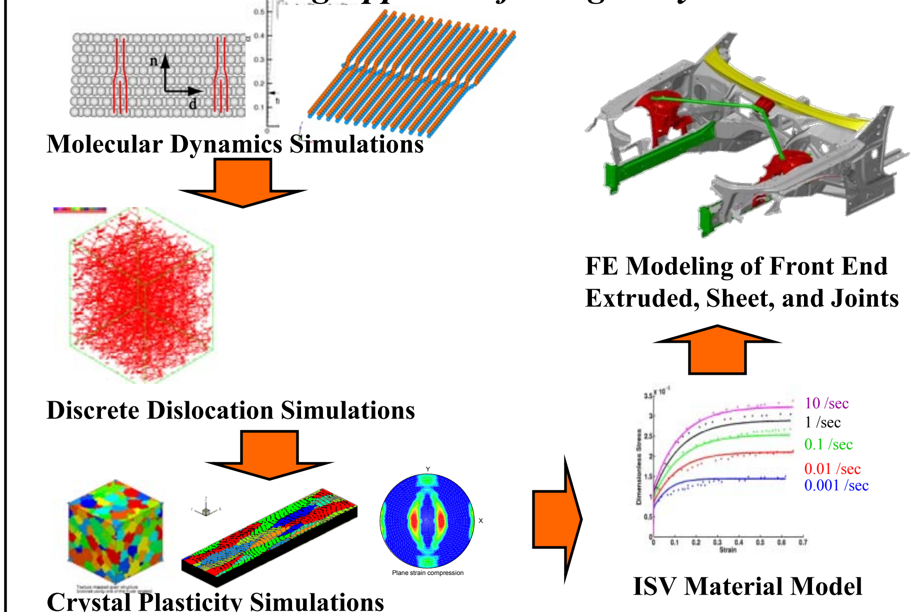


Lightweight Metal - Magnesium Overview

Goals

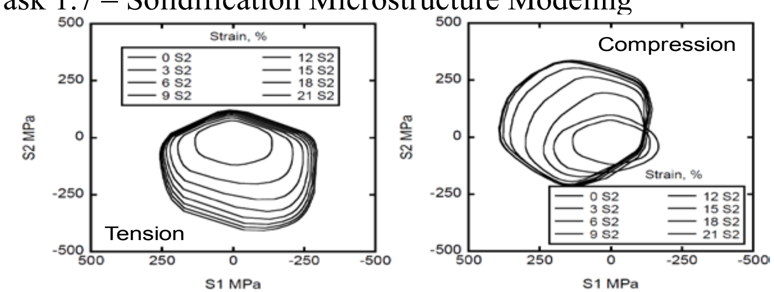
- ❑ Deploy and adapt current capabilities developed at CAVS in materials characterization and multiscale modeling approaches to establish a Lightweight Materials Research and Development Center.
- ❑ Drive the advanced modeling and experimental capabilities to reduce the manufacturing cost of Mg alloy vehicle components, and enhance the use of Mg in the automotive industry.
- ❑ Impact the growth of the regional economy and draw regional/national/international company participation into education, services and research on Magnesium alloys.

Multiscale Modeling Approach for Mg Alloys



Tasks and Accomplishment:

Task 1.1 – Internal State Variable Material Models
Task 1.2 – Cyberinfrasstructure
Task 1.3 -- Fatigue Performance
Task 1.4 – Corrosion
Task 1.5 – Material Design
Task 1.6 – Simulation-Based Design Oprimization
Task 1.7 – Solidification Microstructure Modeling



Cost Share

Abaqus
Altair
ESI
Simufact-America
F-Tech
Genesis System

Partners

Ford (MI)
GM (MI)
DOE
Lehigh Univ
Virginia Tech
USAMP-HIMAC Team
USAMP-MFERD Team

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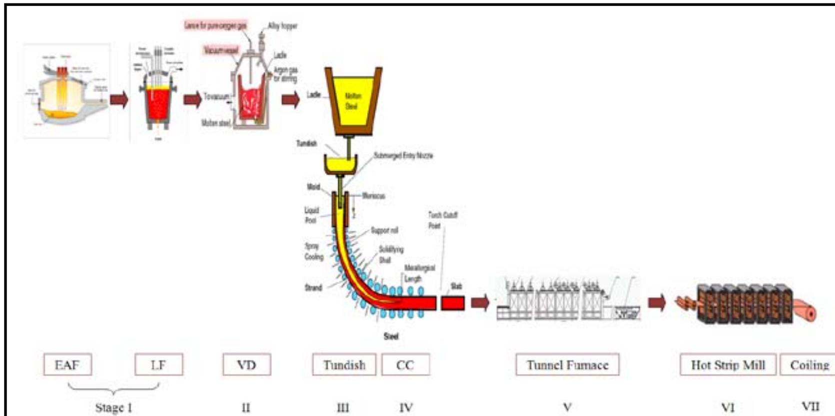
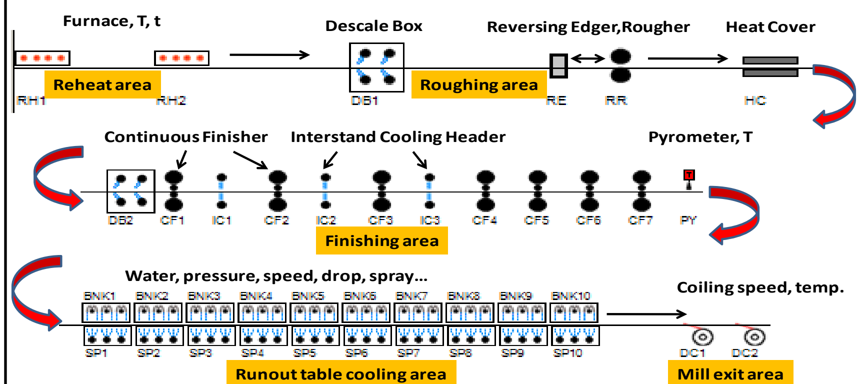
Steel Program Overview

Goal:

Deploy and adapt current enhanced capabilities developed at CAVS in multiscale materials modeling and characterization to steel manufacturing, process optimization, and alloy design impacting the growth of regional economy and drawing regional/national/international company participation into education, services, and research on ferrous alloys.



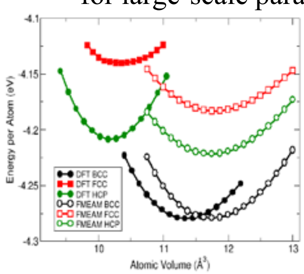
Steel Manufacturing Process (Cradle to Grace Concept)



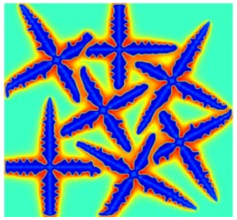
Hot Strip Mill Simulation

Tasks and Accomplishment:

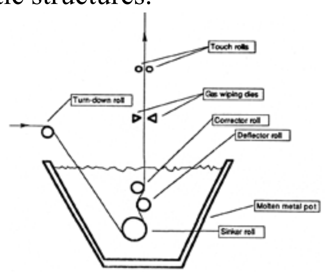
- **Task 2.1** – Materials Design of Lightweight Alloys
  - Design a novel high strength steel alloy with improved formability and strength for automotive use.
- **Task 2.2** – Solidification and Phase Transformation in Steel Alloys
  - Explore the feasibility of an all-local approach to solidification microstructure modeling in steel alloys with potential for large-scale parallel simulations of dendritic structures.



DFT Fe-X interatomic potential



Dendrite Growth in Cubic Systems



Zinc Bath Coating

Cost Share / Corporate Partners:

Severstal (MS), Nucor Steel (MS), Schultz (MS), Optomec (NM), Ice Prototyping (TX), POSCO (Korea), SAC, (Korea), KITECH (Korea), Dayou Smart Aluminum (Korea), International Zinc Association

Polymer Program Overview

Goal: Establish high fidelity predictive tools for polymeric materials to be used for fabrication/manufacturing, design, and optimization of complex engineering boundary value problems and structural components. This research focuses on the development of multiscale material models which are experimentally validated to obtain process-structure-property relationships for polymers.

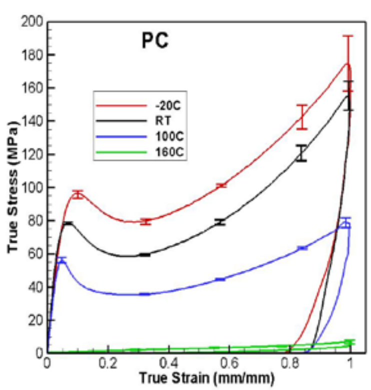
Tasks and Accomplishment:

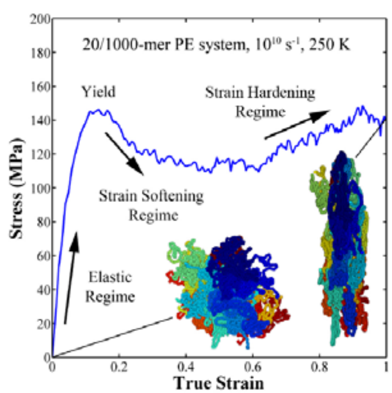
Task 3.1 – Polymers

- Develop a microstructure based ISV model capable of describing structure-property relationship to predict the mechanical behavior of polymers.

- **Task 3.2 – Carbon Fiber Composites and Nanocomposites**
  - Design low-cost nanoreinforced and continuous composite systems ; Develop a multiscale modeling methodology for predicting evolution and failure of structural nanocomposites and continuous fiber composites.

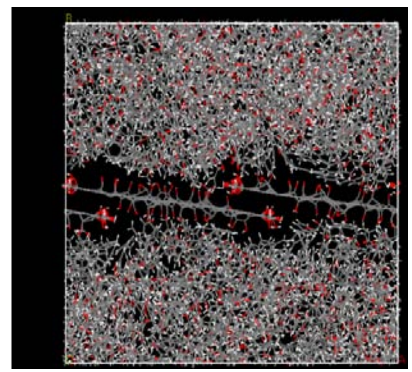
Stress-Strain Responses by ISV and Low-scale Models



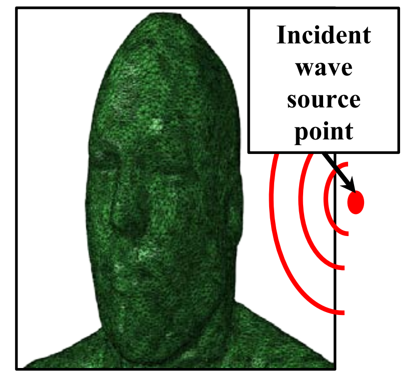


- **Task 3.3 – Biodegradable composites**
  - Refine the processes in lab-scale on fiber retting/treatment process, natural fiber composite products from kenaf bast fiber, with a potential to scale up the process; Develop predictive tools on the developed natural fiber.
- **Task 3.4 – Biomaterials**
  - Determine the structure-property relationships of both soft biological tissues and animal outer armor. Use the relationships to develop material models for implementation into finite element codes.

Nano-fiber Interface Model



Human Head/Brain Model



Cost Share / Corporate Partners:

American Chemistry Council, Mitsubishi Motors, Kengro, Louisiana Pacific, MIMICS, Alpha Star

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Magnesium Building Block Development & Demonstration

1. Internal state variable (ISV) material model with twinning, texture, damage, ..
2. Lower-scale modeling effort - DFT, molecular dynamics, crystal plasticity, twinning and dislocation mechanisms, leading to **Alloy Design concepts**
3. In-house lab-scale experimentation - extrusion, sheet bending, post forming, fatigue, corrosion, casting, recrystallization,…
4. USAMP/ICME Mg demo project

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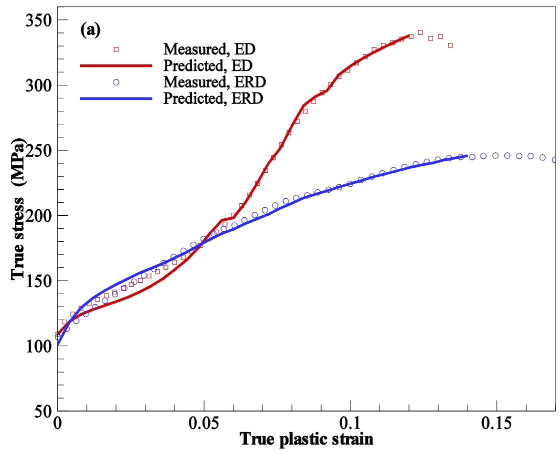
ISV Material Model Development



$$\dot{\boldsymbol{\alpha}} = -\left[\frac{m_\phi}{\mu(\phi)}\dot{\phi} + \frac{m_\theta}{\mu(\theta)\theta_M}\dot{\theta}\right]\boldsymbol{\alpha} + \tilde{\boldsymbol{w}}^e\boldsymbol{\alpha} - \boldsymbol{\alpha}\tilde{\boldsymbol{w}}^e + c_\alpha\mu(\phi,\theta)h\boldsymbol{d}^p - \frac{r_d(\theta)}{c_\alpha\mu(\phi,\theta)}\frac{2}{3}\|\boldsymbol{d}^p\|\|\boldsymbol{\alpha}\|\boldsymbol{\alpha}$$

(Kinematic hardening)

$$\dot{\kappa} = -\left[\frac{m_\phi}{\mu(\phi)}\dot{\phi} + \frac{m_\theta}{\mu(\theta)\theta_M}\dot{\theta}\right]\kappa + \left[c_\kappa\mu(\phi,\theta)H - R_d(\theta)\kappa\right]\sqrt{\frac{2}{3}}\|\boldsymbol{d}^p\| - R_s(\theta)\kappa\sinh\left(\frac{c_{10}}{c_\kappa\mu(\phi,\theta)}\kappa\right)$$

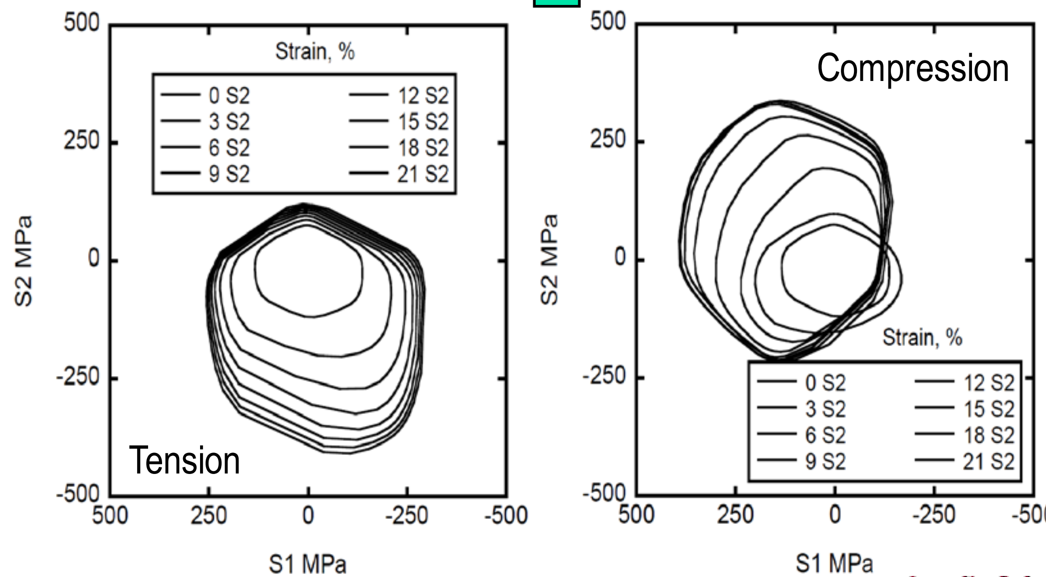
(Isotropic hardening)

$$\dot{\boldsymbol{A}} = \boldsymbol{w}\boldsymbol{A} - \boldsymbol{A}\boldsymbol{w} + \frac{\lambda_g}{7}(3+4f)\left[\boldsymbol{A}\boldsymbol{d}^p + \boldsymbol{d}^p\boldsymbol{A} - \frac{2}{3}(\boldsymbol{A}:\boldsymbol{d}^p)\,\mathbf{1}\right] + 2\frac{\lambda_g}{15}(3+2f)\boldsymbol{d}^p - 2\lambda_g f(\boldsymbol{A}:\boldsymbol{d}^p)\,\boldsymbol{A}$$

$$f = 1 - 27\det\left(\boldsymbol{A} + \frac{1}{3}\mathbf{1}\right)$$

(Structure tensor)

Twinning impacts yield surface evolution

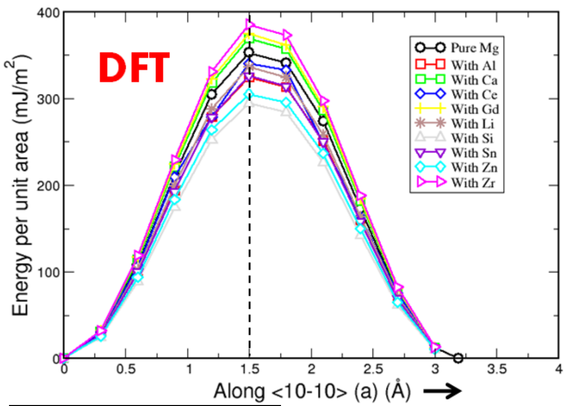


DFT-guided alloy design

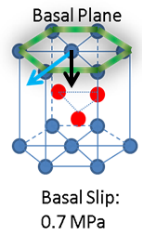
c/a, structural parameter

Alloying Effects on Properties

What effect do alloying elements have on stacking fault energies?



Zr
Gd
Ca
Mg
Ce
Li
Sn
Al
Zn
Si



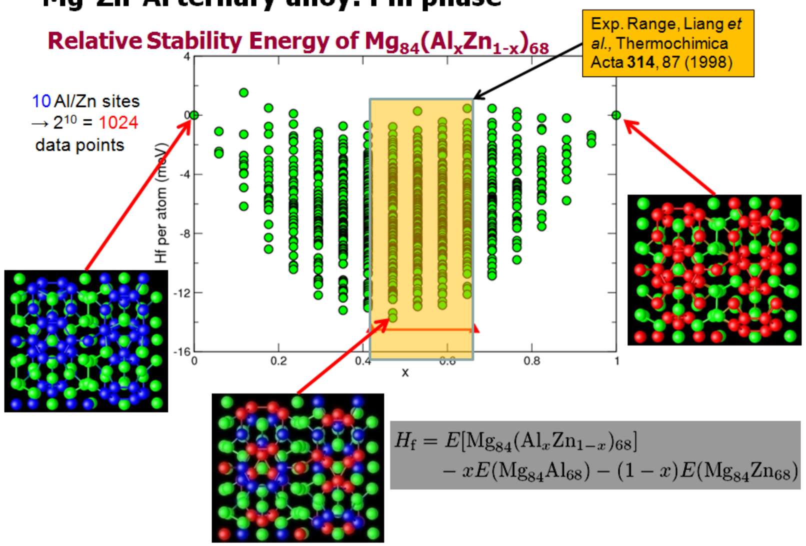
Order of effect of impurities on Mg SFE

A. Moitra et al.

Substitutional Element Effects on Stacking Fault Energies

Mg-Zn-Al ternary alloy: Phi phase

Relative Stability Energy of $Mg_{84}(Al_xZn_{1-x})_{68}$



$$H_f = E[Mg_{84}(Al_xZn_{1-x})_{68}] - xE(Mg_{84}Al_{68}) - (1-x)E(Mg_{84}Zn_{68})$$

The Tau phase - $Mg_{32}(Al,Zn)_{49}$

- Icosohedral quasicrystal
- – Structure determined – 1957 – Bergman et. al.
- Cubic – space group $\bar{I}m3$
- Unit – Bergman atom cluster
- Exists in a wide compositional range

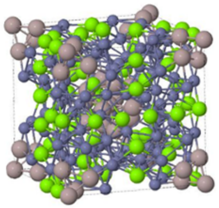


Image from - http://cst-www.nrl.navy.mil/lattice

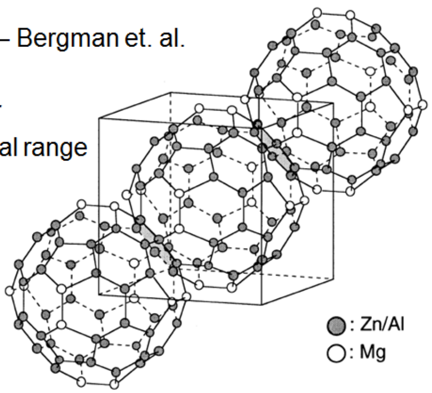


Image from - Sun, W., et.al., *Mat. Sci. Eng. - Lausanne- A. 294-296 (2000): 327-330*

Structure and Properties of Intermetallics

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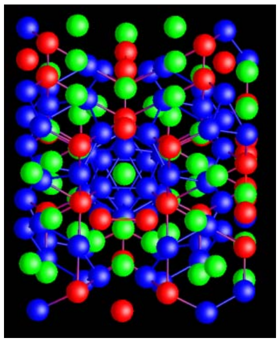
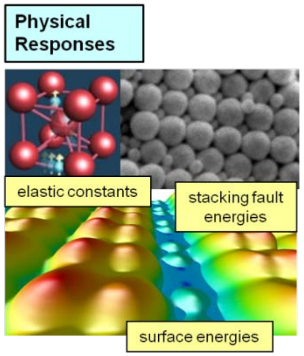
Alloy Design: Multiscale Strategy for Twinning

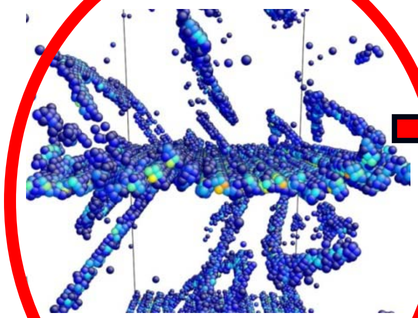
MAGNESIUM



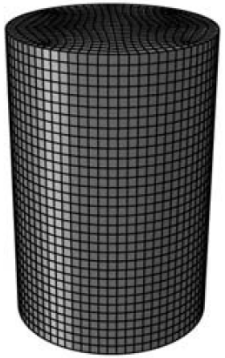
DFT



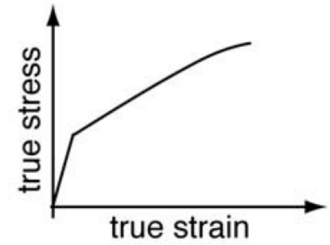
DFT-MD



Molecular Dynamics

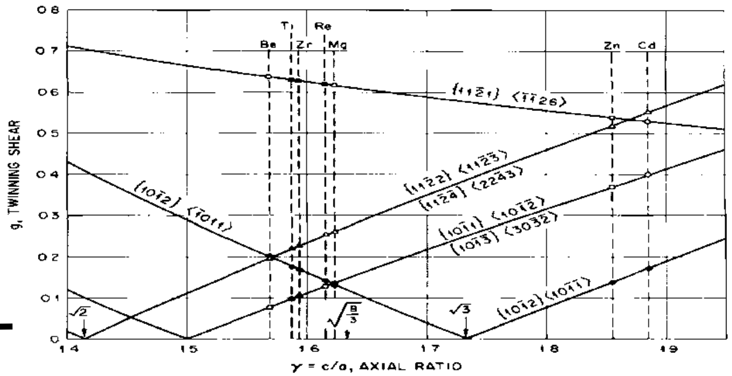


Crystal Plasticity



Design of new material

Twinning Nucleation,
Nanoscale Plasticity,
Grain Boundaries



Alloying Element Effects, Intermetallics,
DFT Properties (c/a)

In-house Lab-scale Experimentation

(Stage I & II) | (Stage III &IV) | (Stage V) | (Stage VI)

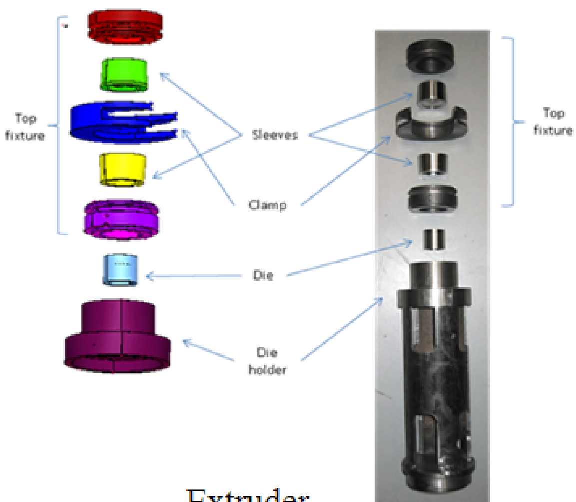
Induction Melting Furnace & Ladle

Ladle & Ingot Casting

High Temperature Re-Heat Furnace

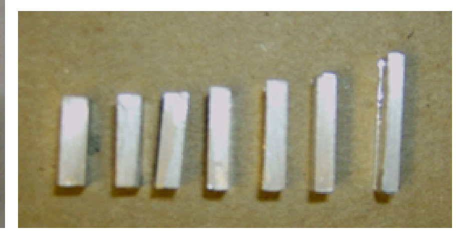
Rolling Mill

Materials/Mechanical Properties Characterization



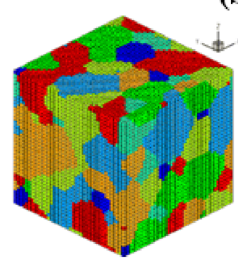
Extruder

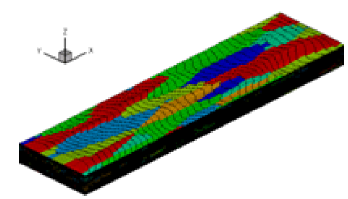
Channel Die



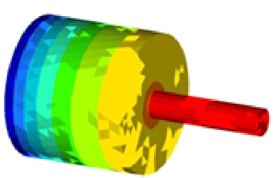
Deformed sheet samples

(Stage VI)





Structure/Texture Research



FEA Simulation Research

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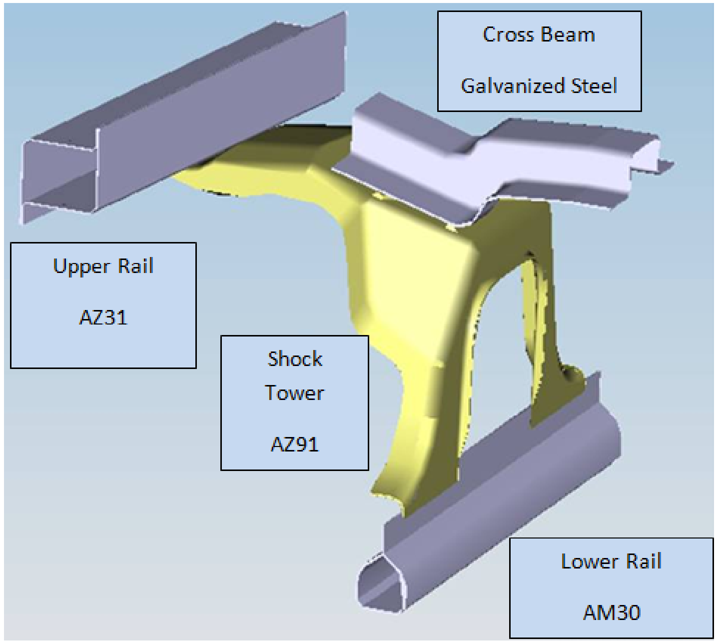
USAMP/ICME Mg Demo Project

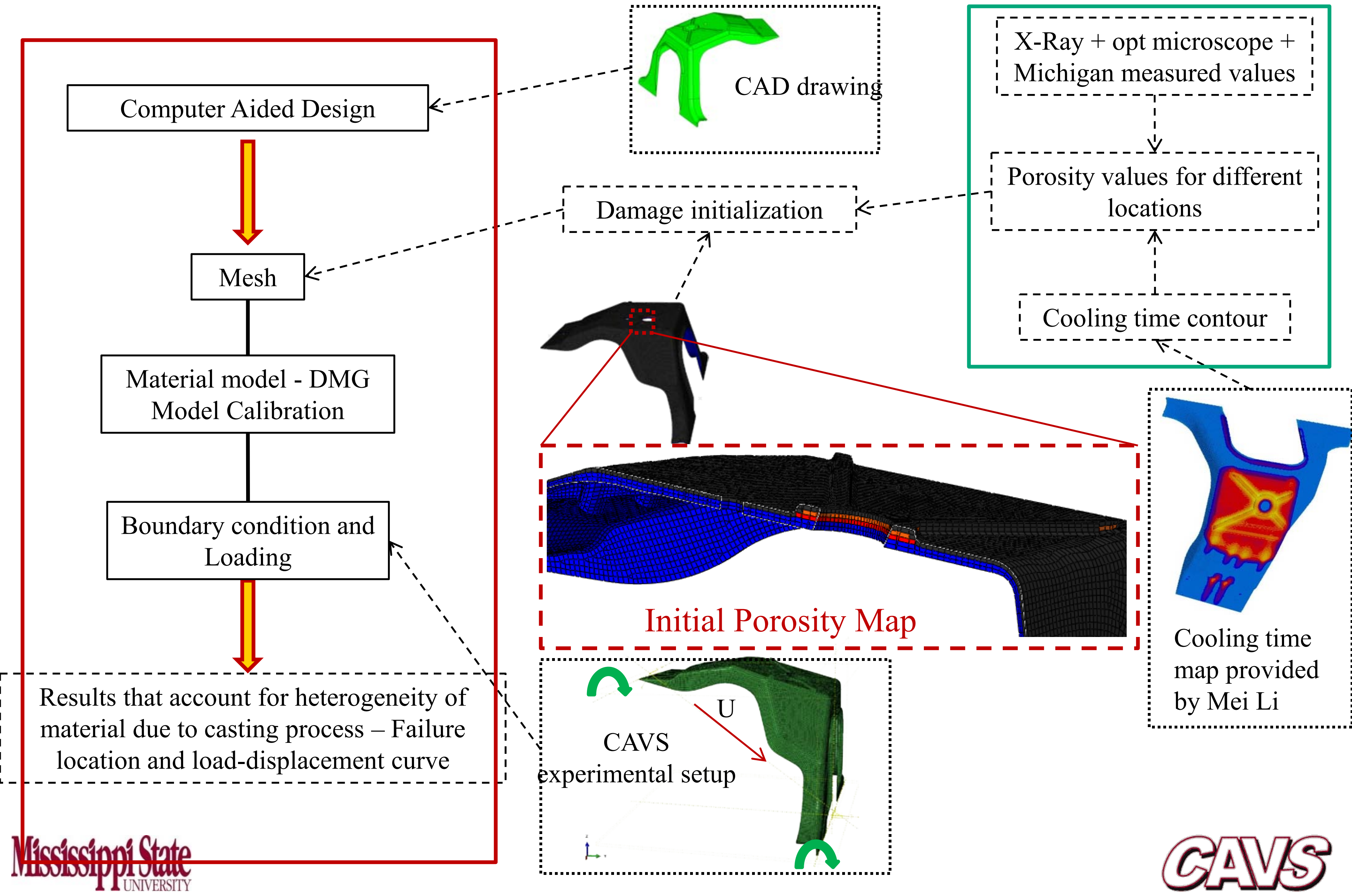
Objectives:

Predict component's mechanical responses and process-structure-property relationship using methodology developed by ICME building block program.

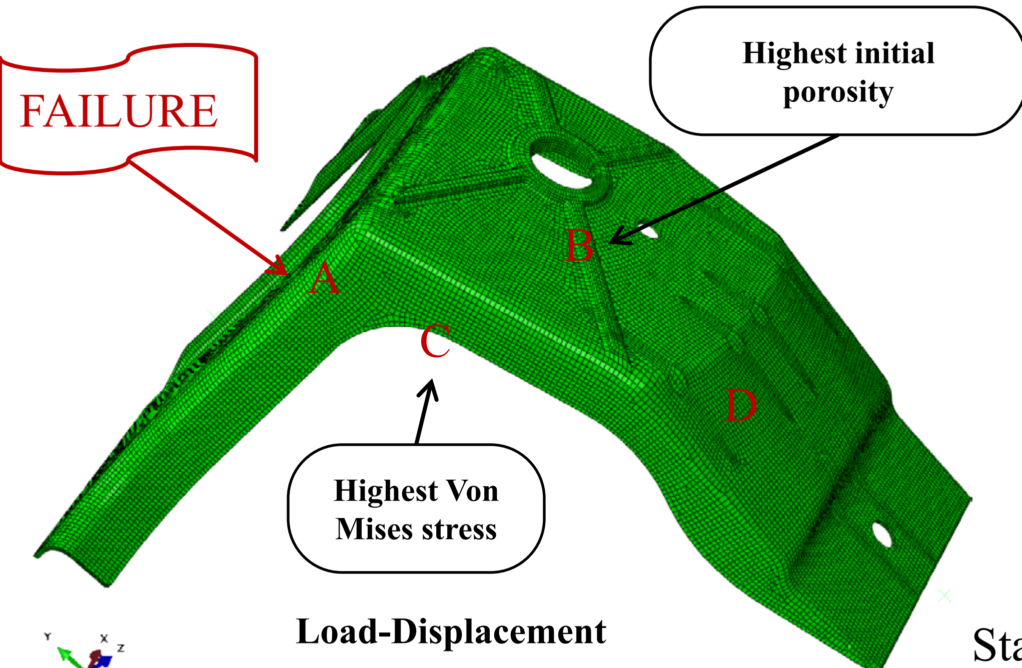
- **Cast/Shock Tower: failure location and load-displacement curve under monotonic and fatigue loading.**
- **Extrusion/Lower Rail: texture at different locations in a section profile after extrusion and yield strength at room temperature.**
- **Sheet/Upper Rail: texture after bending.**



Validation Effort for Mg Shock Tower: Zone Mapping Method



ICME-Demo Shock Tower – Validation Result

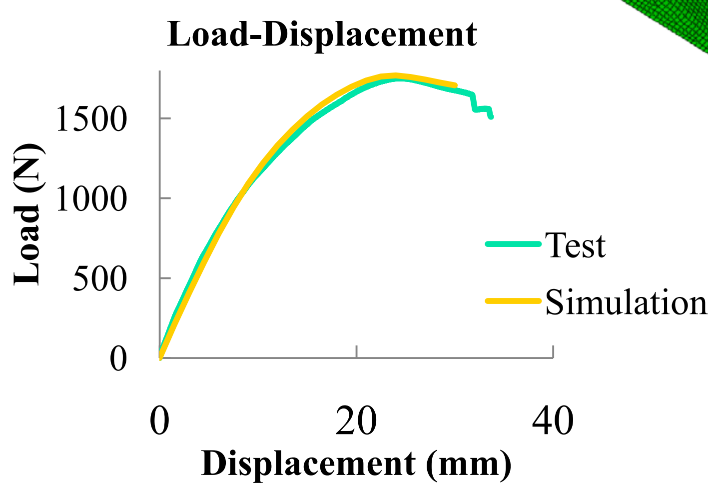


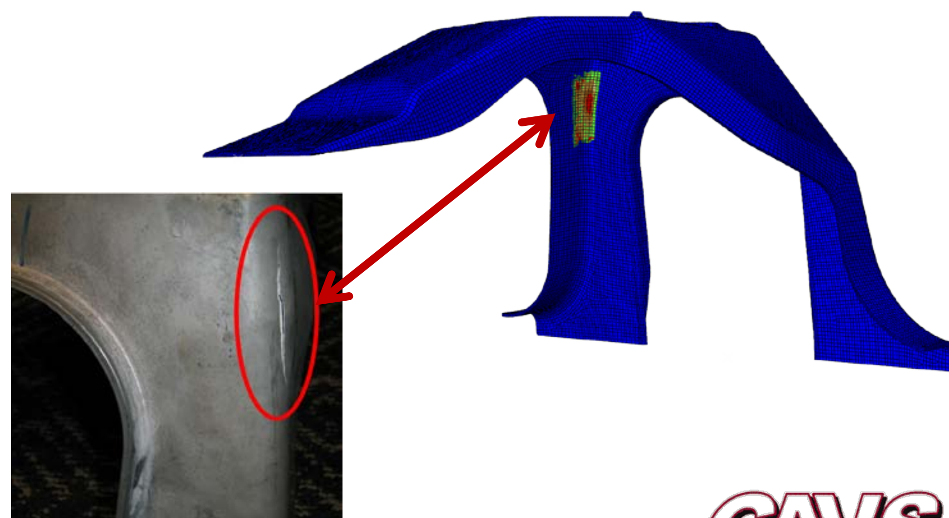
	Mises Stress	Initial Porosity	Damage
Highest	C	**B**	A
	A	D	C
	B	A	D
Lowest	D	C	B

Standard FEA answer (Mises Stress)

Standard Materials Science answer (Initial Porosity)

ISV Prediction (Damage)

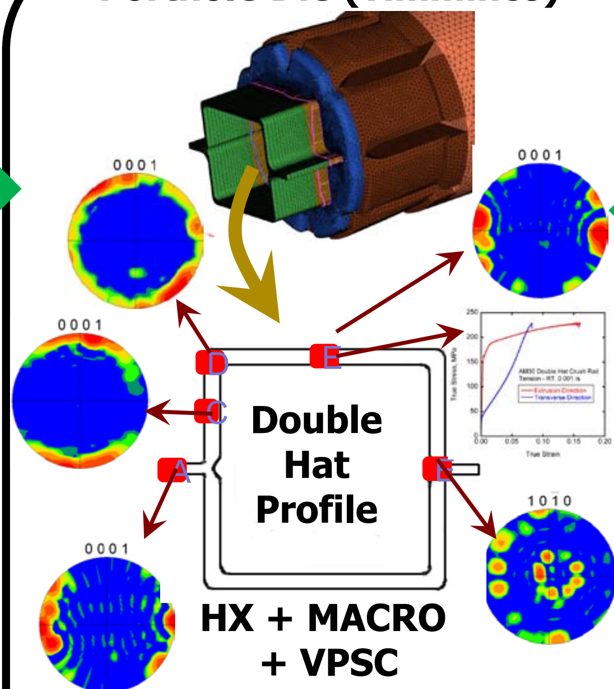




Integration of Extrusion Work

INDUSTRY-TYPE EXTRUDED PROFILE

Porthole Die (Timminco)



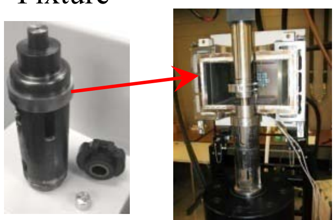
HX + MACRO + VPSC

Texture Prediction during Extrusion (T-M Problem) & Post-Forming Structural Performance

I

Sub-Scale Indirect Extrusion Experiments

Sub-Scale Fixture — Instron Machine



Data Recorded
- Load-time
- Temperature-time
- Texture

II

FEM Modeling of Extrusion Process

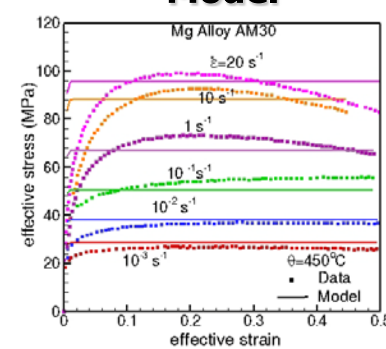
HyperXtrude (HX)

Eulerian-ALE Mesh

Numerical Analysis
- Validate T-M problem
- Streamline data
- Simple material model

III

Macroscopic Material Model

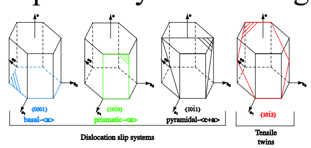


Material Modeling
- $Sinh^{-1}$ () model for T-M problem
- HX being modified to add ISV material models

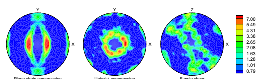
IV

Crystal Plasticity Material Model

slip/twin systems in Mg



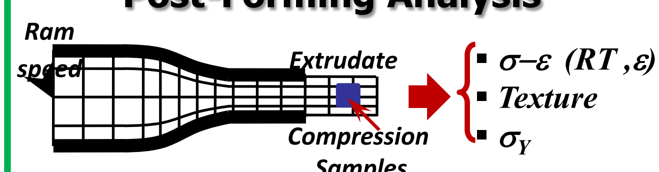
Texture Predictions



Texture Predictions
- VPSC Code
- Voce hard law
- Dislocation-based hard law

V

Post-Forming Analysis



- σ–ε $(RT, \dot{\varepsilon})$
- *Texture*
- σ_Y

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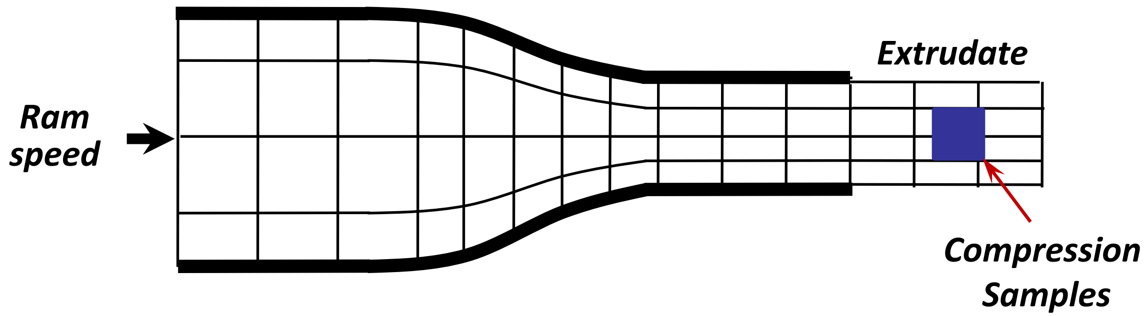
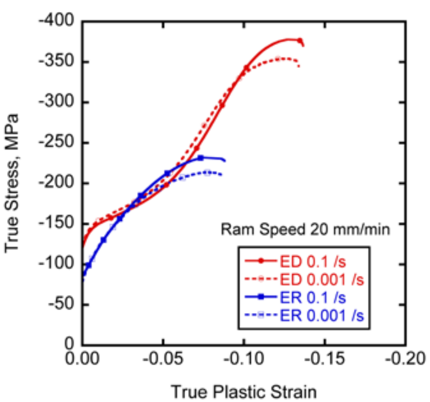
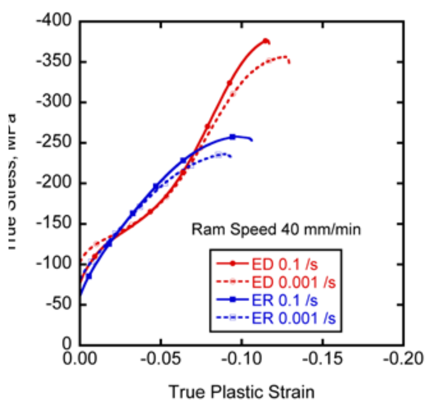
Post-Forming Analysis

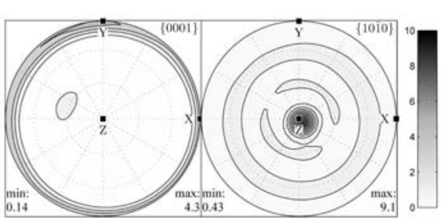


- $\sigma\!-\!\varepsilon$ *at RT & diff rates*
- *Microstructure (texture)*
- *Yield strength*

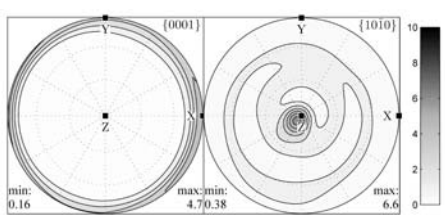
1/2 " extrudate





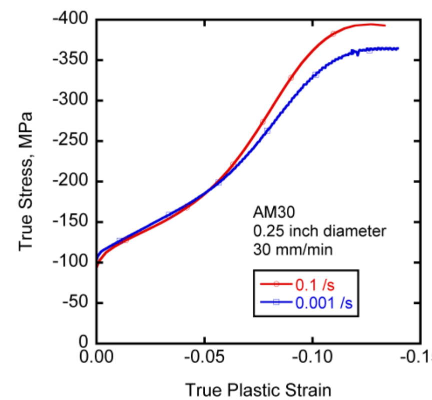


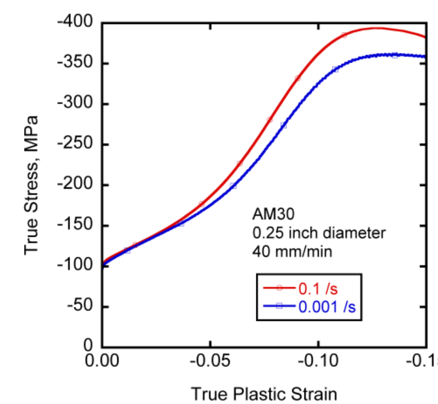
Initial Texture: am30_20mm

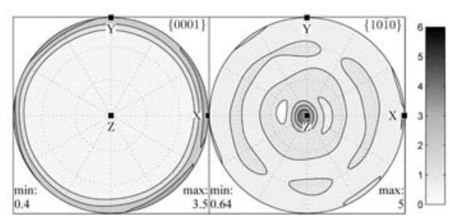


Initial Texture: am30_40_mm

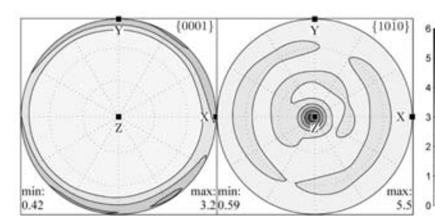
1/4 " extrudate







Initial Texture: am30_30mm



Initial Texture: am30_40_mm

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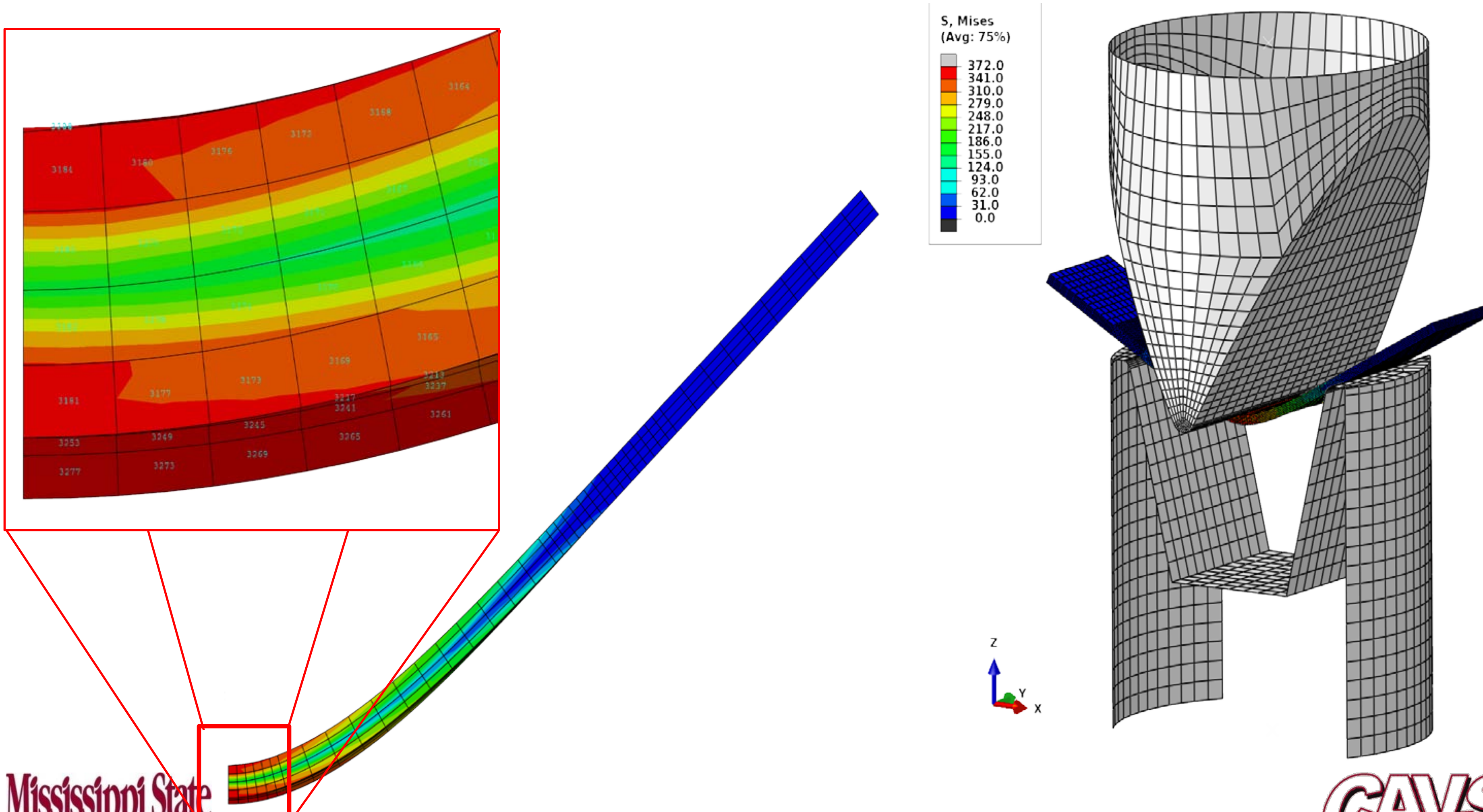
Sheet Bending FE Analysis

Perform bending simulation using a plasticity Abaqus *Plastic and Umat plasticity subroutine (no damage).
Post-process results into VPSC for texture prediction



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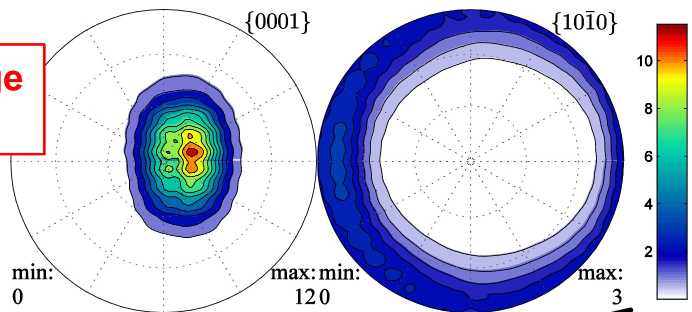
Texture/Twinning Prediction of AZ31 Sheet during Bending

3165

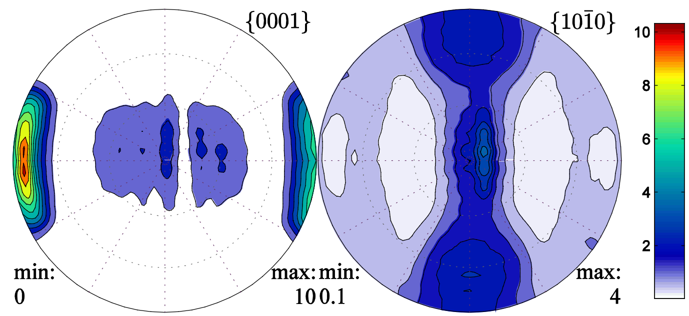
Slight change in texture



ε=0.043

3184

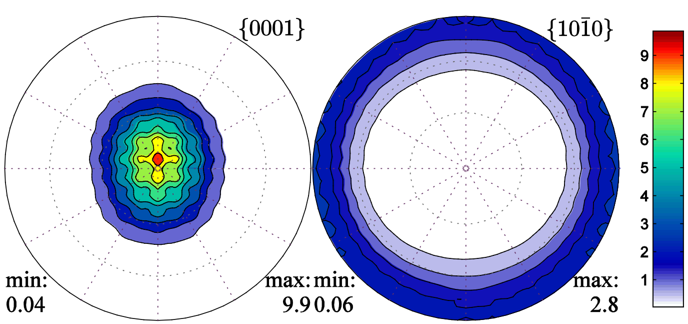
Appearance of twinning

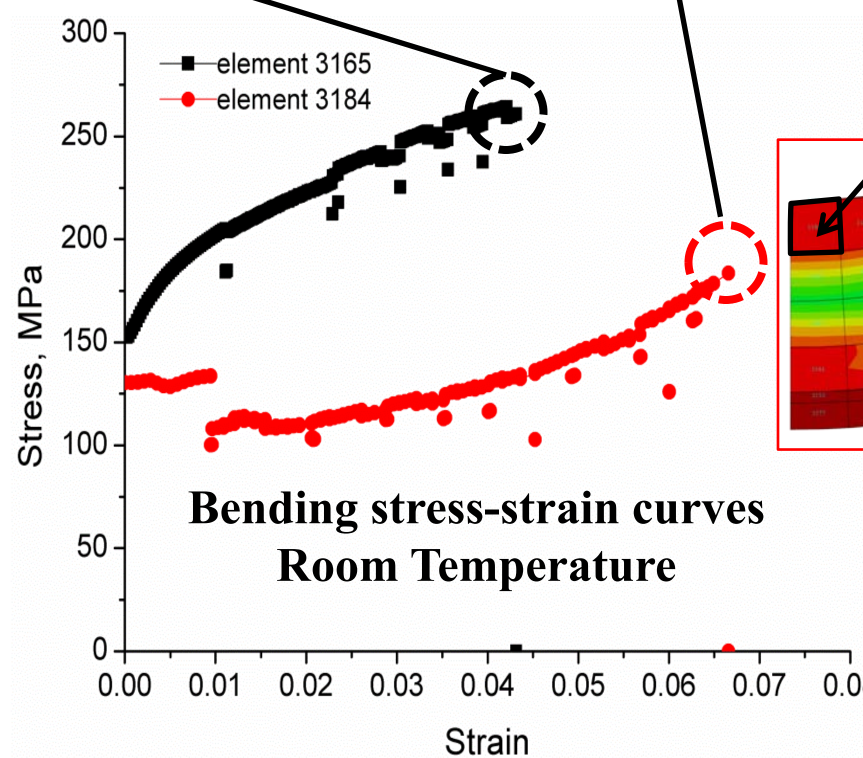


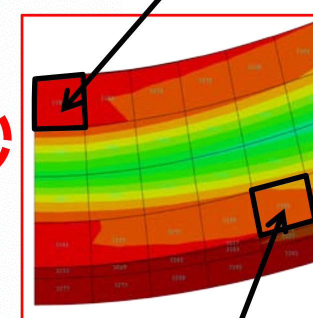
ε=0.076.

RD
TD

Initial texture



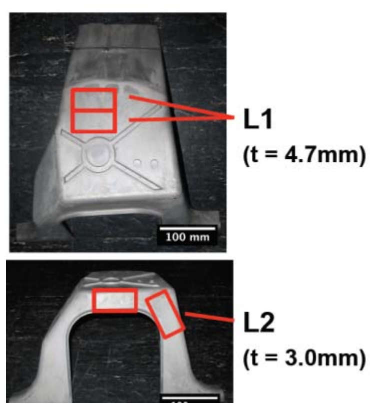




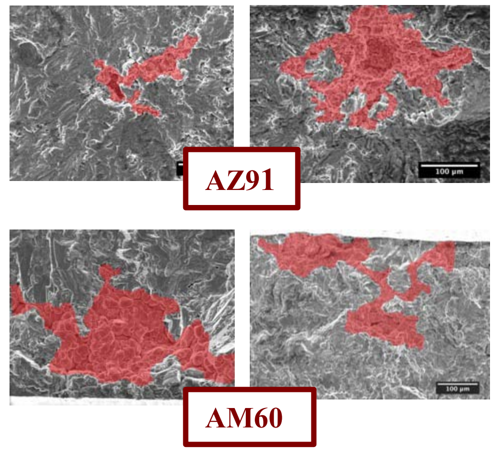
Microstructure-Sensitive Fatigue Modeling of Cast Mg AM60 and AZ91 Shock Tower

Accomplishments

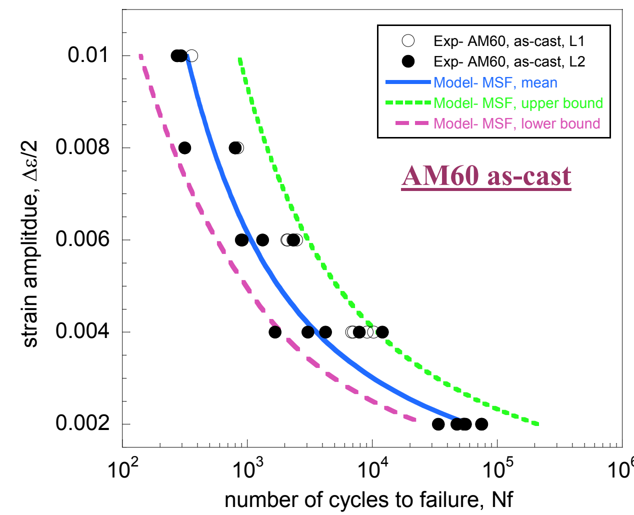
- ❑Variation in AM60 and AZ91: DCS, porosity, pore size, and cyclic hardening parameters
- ❑Cracks initiated from casting pores
- ❑The MultiStage fatigue (MSF) model correlated to fatigue results AM60 and AZ91 shocktower.
- ❑MSF model captured the upper and lower bounds of fatigue data based on:
  - ▪microstructural
  - ▪max inclusion size
  - ▪cyclic hardening

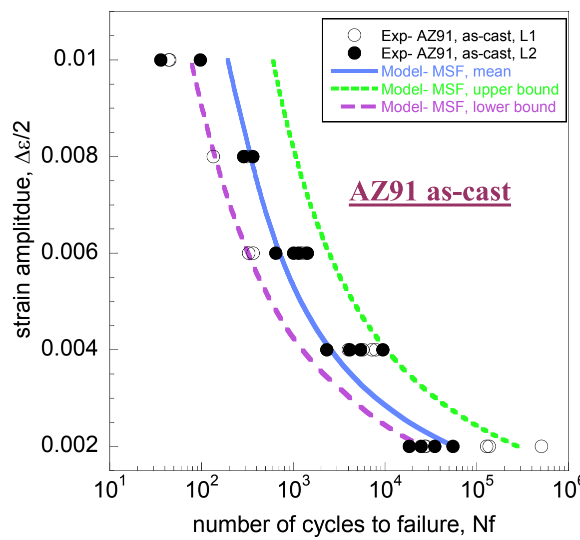


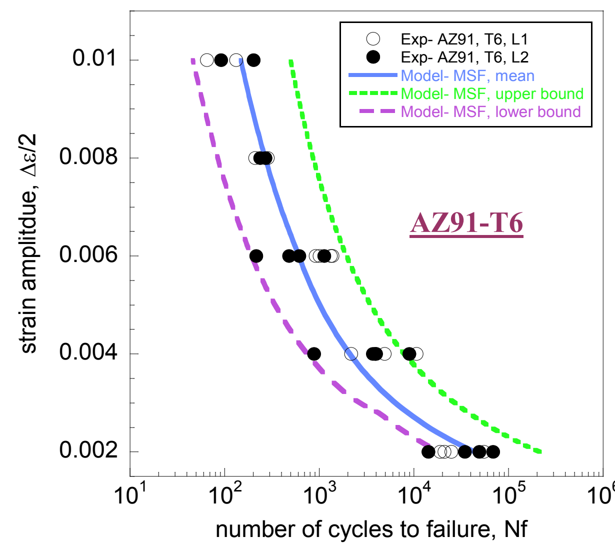
AM60 and AZ91 Shock Tower



Typical Initiation sites







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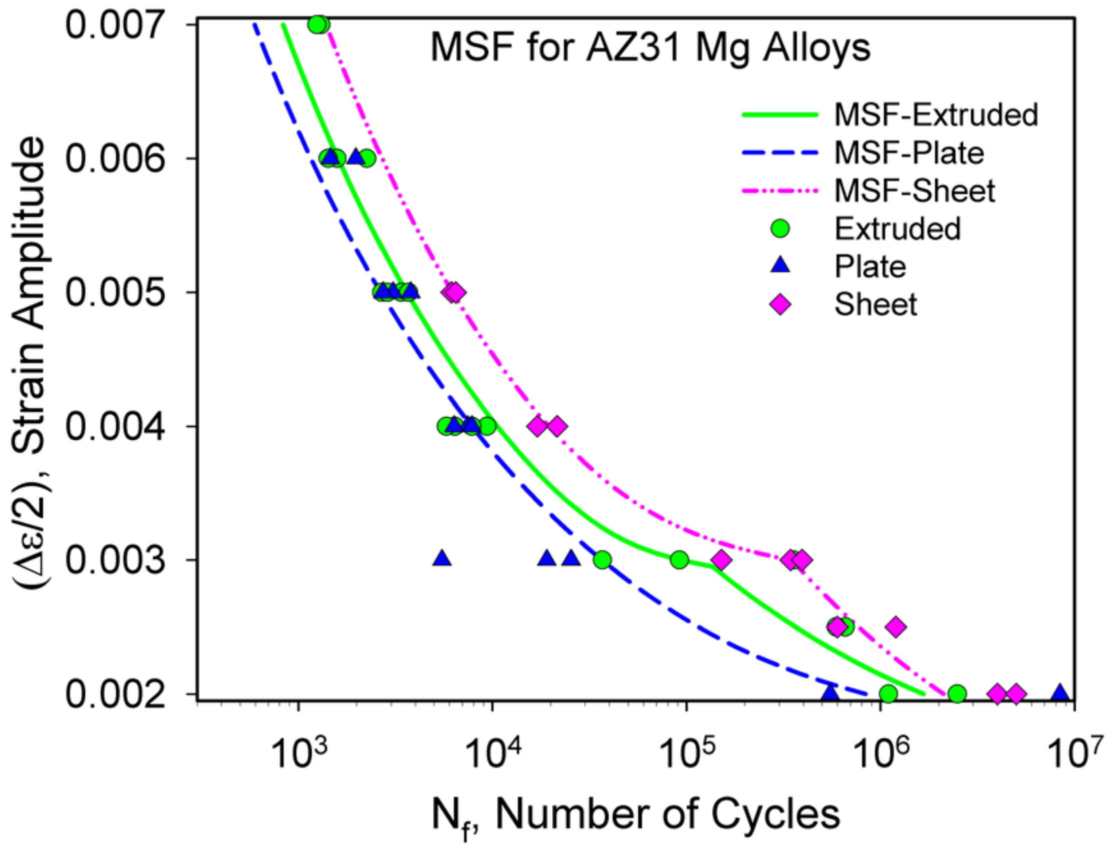
Multi-Stage Fatigue (MSF) Modeling of AZ31 Products



A MSF model was developed for each of the three product forms of AZ31 alloy along with strain-life fatigue data

MultiStage Fatigue-Joints Model (MSF-J) Overview

Synergy with other research trusts

Thermo-mechanical simulations

Macroscale Finite element analysis of structure

Inputs

Microstructure and joint geometry:

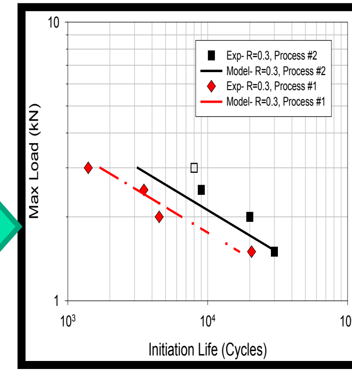
Loading type (structural stress components)

Model

MSF-J

A physically motivated and mechanics-based approach: ***incubation*** and ***crack growth***

Output



Capture process induced variation in fatigue performance

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CyberInfrastructure

https://icme.hpc.msstate.edu/

Progress Report of CyberInfrastructure

new: Wiki

knowledge management (Web 2.0)

improved: interface, security

database of experimental data and material constants

Task 2.1, Task 2.2

improved: DMG

online model calibration tools

Task 2.3, Task 2.4

new: the repository of codes

repository of source codes

Task 2.5, Task 2.6

just started

- **job submission and monitoring service**
- **workflows**
- **Autonomous computing**

Task 2.7

Analyze: Model Calibration

Model Parameters

Search & View

Upload Experimental Data

Download Constants for Simulations

https://icme.hpc.msstate.edu

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Repository of Codes

Example: Internal State Variable Plasticity-Damage Model—Documentation

Appendix A. MSU ISV DMG 1.0 Production Model Equations

The MSU ISV DMG 1.0 production material model is given by the following equations. The pertinent equations in this model are denoted by the rate of change of the observable and internal state variables. The equations used within the context of the finite element method are given by,

$$\overset{\circ}{\underline{\sigma}} = \dot{\underline{\sigma}} - \underline{W}^e \underline{\sigma} - \underline{\sigma}\underline{W}^e = \lambda(1-D)tr(\underline{D}^e)\underline{I} + 2\mu(1-D)\underline{D}^e - \frac{\dot{D}}{1-D}\underline{\sigma} \qquad \text{Equation A.1}$$

$$\underline{D}^e = \underline{D} - \underline{D}^{in} \qquad \text{Equation A.2}$$

$$\underline{D}^{in} = f(T)\sinh\left[\frac{\|\underline{\sigma}' - \underline{\alpha}\| - \{R+Y(T)\}\{1-D\}}{V(T)\{1-D\}}\right]\frac{\underline{\sigma}'-\underline{\alpha}}{\|\underline{\sigma}'-\underline{\alpha}\|} \qquad \text{Equation A.3}$$

$$\overset{\circ}{\underline{\alpha}} = \dot{\underline{\alpha}} - \underline{W}^e\underline{\alpha} + \underline{\alpha}\underline{W}^e = \left\{h(T)\underline{D}^{in} - \left[\sqrt{\frac{2}{3}}r_d(T)\|\underline{D}^{in}\| + r_s(T)\right]\|\underline{\alpha}\|\underline{\alpha}\right\}\left[\frac{DCS_0}{DCS}\right]^z \qquad \text{Equation A.4}$$

$$\dot{R} = \left\{H(T)\underline{D}^{in} - \left[\sqrt{\frac{2}{3}}R_d(T)\|\underline{D}^{in}\| + R_s(T)\right]R^2\right\}\left[\frac{DCS_0}{DCS}\right]^z \qquad \text{Equation A.5}$$

$$\dot{D} = [\dot{\phi}_{particles} + \dot{\phi}_{pores}]c + [\phi_{particles}+\phi_{pores}]\dot{c}, \qquad \text{Equation A.6}$$

$$\dot{\phi}_{particles} = \dot{\eta}v + \eta\dot{v} \qquad \text{Equation A.7}$$

$$\dot{\eta} = \|\underline{D}^{in}\|\frac{d^{1/2}}{K_{IC}f^{1/3}}\eta\left\{a\left[\frac{4}{27}-\frac{J_3^2}{J_2^3}\right] + b\frac{J_3}{J_2^{3/2}} + c\left\|\frac{I_1}{\sqrt{J_2}}\right\|\right\}\exp\left(-\frac{C_{\eta T}}{T}\right) \qquad \text{Equation A.8}$$

$$\dot{v} = \frac{3}{2}v\left[\frac{3}{2}\frac{V(T)}{Y(T)}\frac{\sigma_H}{\sigma_{vm}} + \left(1-\frac{V(T)}{Y(T)}\right)(1+0.4319)\right]^{Y(T)/V(T)}\underline{D}^{in} \qquad \text{Equation A.9}$$

$$\dot{c} = C_{coal}[\eta\dot{v}+\dot{\eta}v]\exp(C_{cT}T)\left(\frac{DCS_0}{DCS}\right)^z \qquad \text{Equation A.10}$$

$$\dot{\phi}_{pores} = \left[\frac{1}{(1-\phi_{pores})^m} - (1-\phi_{pores})\right]\sinh\left\{\frac{2\left(2^{V(T)/Y(T)}-1\right)}{\left(2^{V(T)/Y(T)}+1\right)}\frac{\sigma_H}{\sigma_{vm}}\right\}\|\underline{D}^{in}\| \qquad \text{Equation A.11}$$

Graphical User Interface

The remainder of this report describes the user interface of the stand-alone version of DMGfit. The documentation for the Web version of DMGfit is online at **http://ccg.hpc.msstate.edu/ccgportlets/apps/cmd/html/help/Help.htm**.

A snapshot of the DMGfit GUI in operation, annotated to highlight the logical groupings of the controls, is shown by Figure 3.

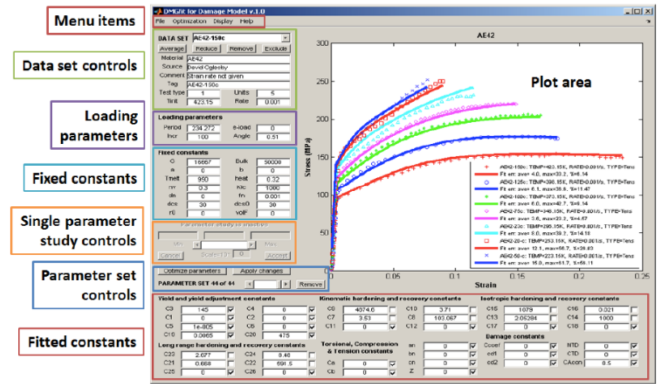
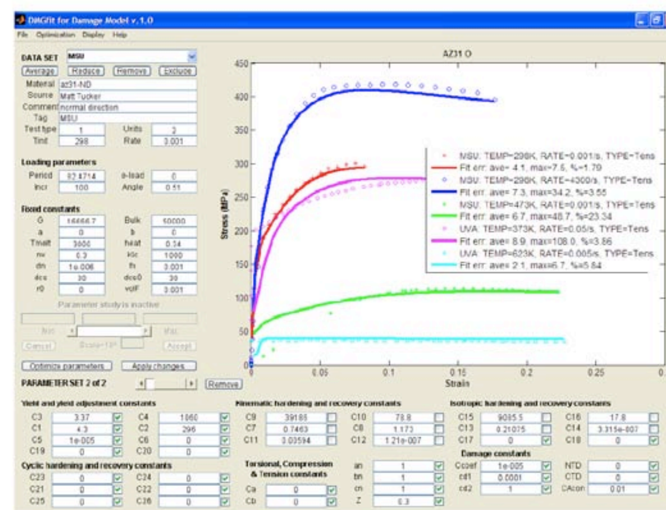


Figure 3. The logical groupings of controls in the DMGfit GUI.



B43. AZ31 Mg alloy: temperature and strain rate model correlation

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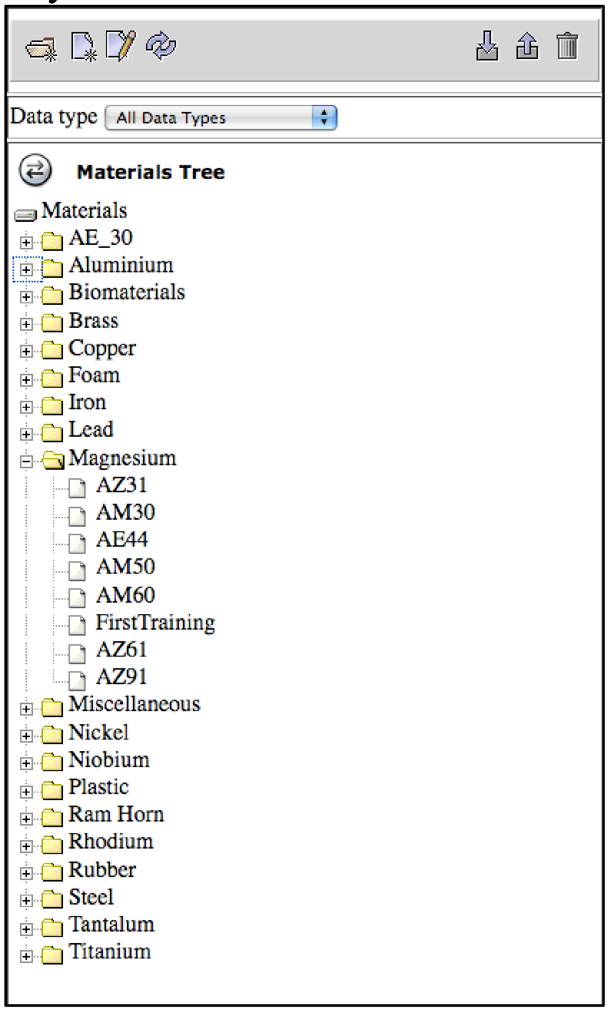
Repository of Materials Database

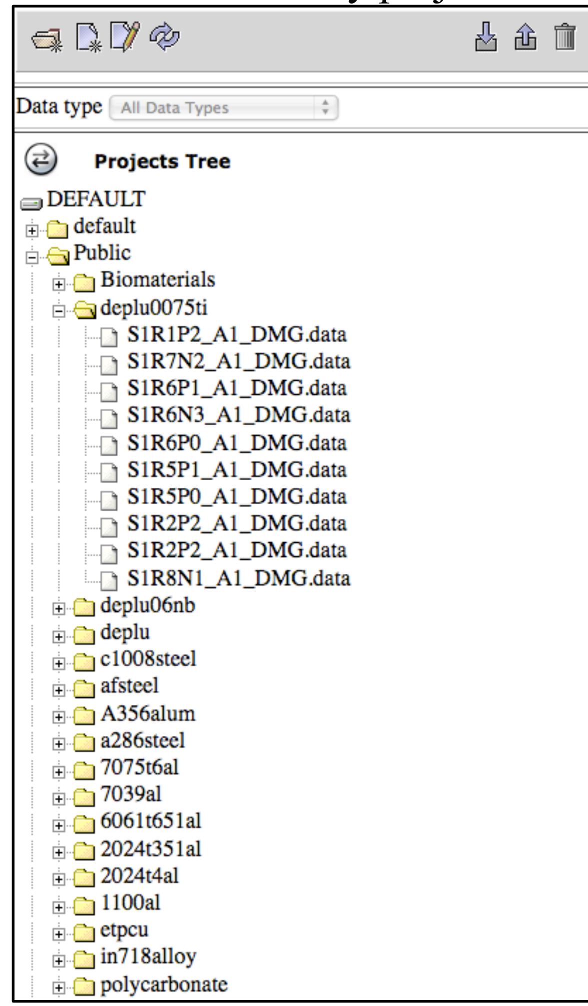
Two Views of the Same Database

by material



Consistency
the same organization and appearance for the repository and model calibration tools

by project/user



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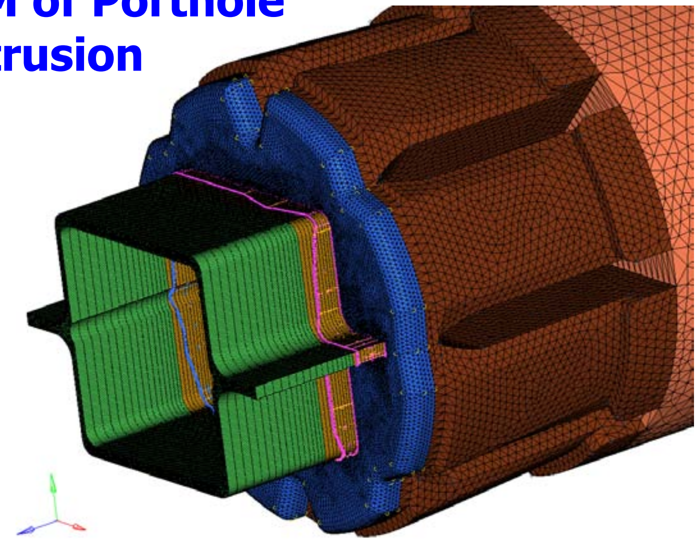
Future Work

- **Develop and validate material and process models for Mg alloys and deploy tools for use, i.e., MFERD Phase II demo project.**
- **Establish Mg alloy design methodology and verification by using lower-length scale simulation tools and lab experimentation.**
- **Establish close partnership with steel and plastic industries so as to direct R&D&A in steel and polymer programs.**
- **Continue the CyberInfrastructure effort and establish a national and an international user base.**

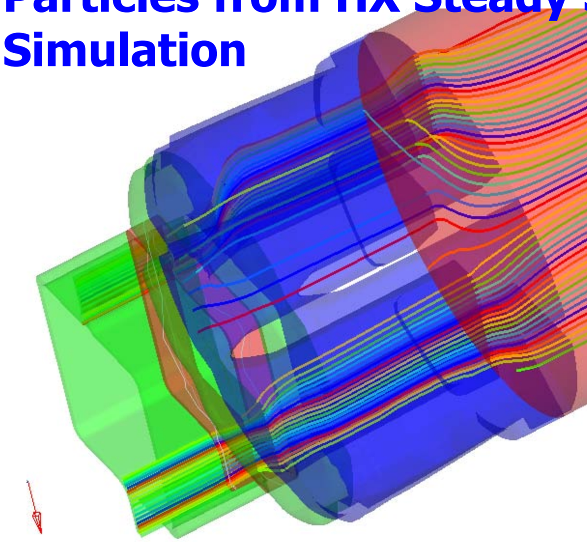
Technical Back-Up Slides

Points/Streamlines for Texture Predictions

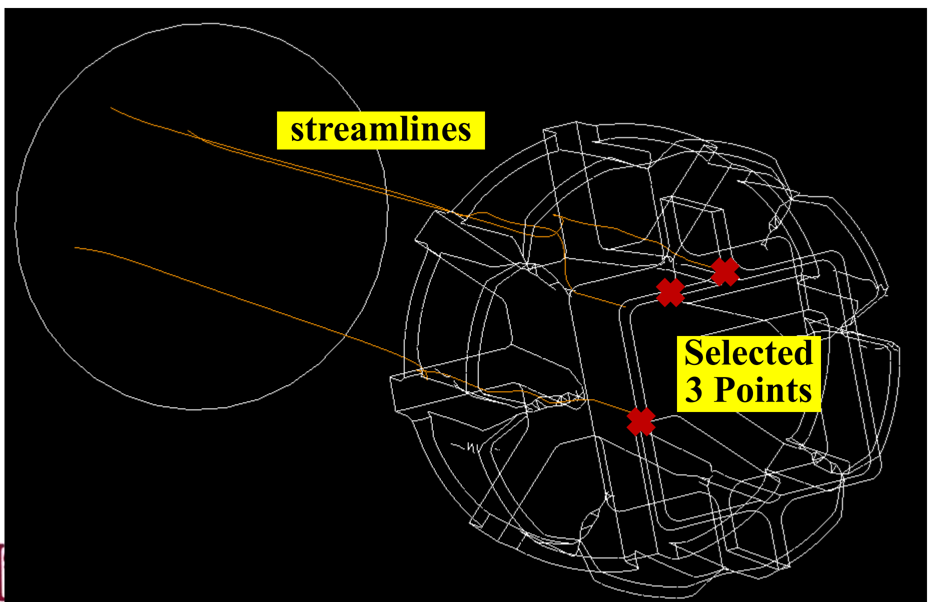
HX-FEM of Porthole Die Extrusion



Streamline Traces of Material Particles from HX Steady State Simulation



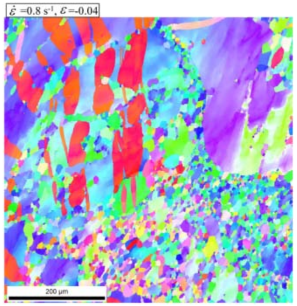
Selected Point Locations on Profile



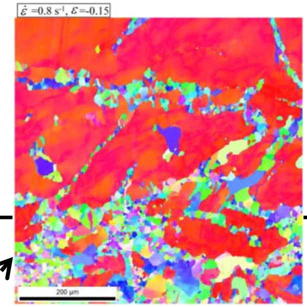
<u>Current Issues with HX Particle Tracer:</u>

- HX particle tracer writes HUGE files for TET elements.
- HX developers are working on a improved version of the particle tracing capability to:
  - Reduce the size of the file for TETs
  - Check tr(L)=0
- Altair is also working on other more efficient tools for particle tracing.

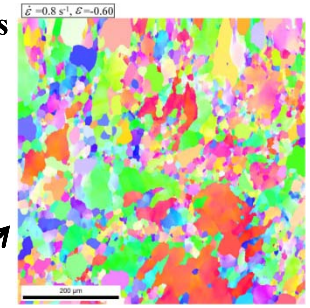
Need of DRX Models for Mg



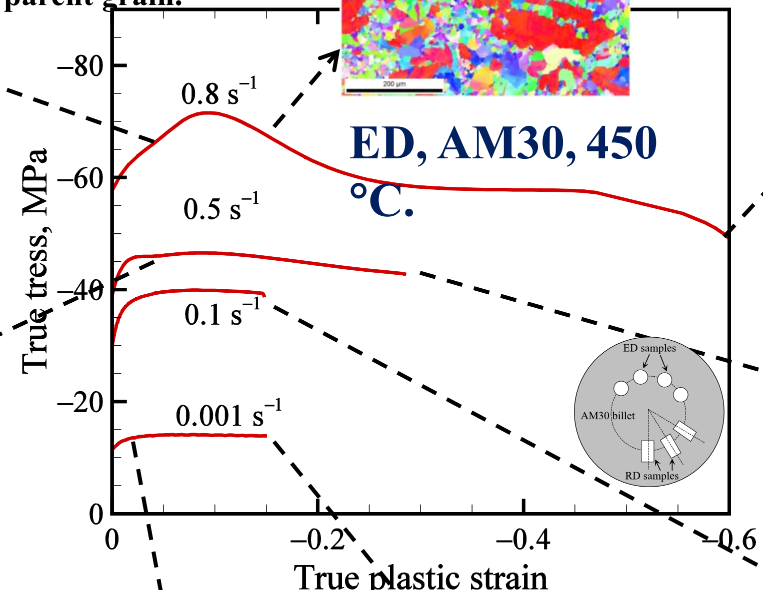
Profuse twinning activates and necklace DRX grains nucleate around parent grain.

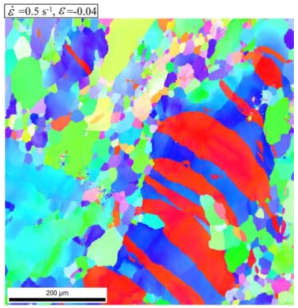


Twinning sweeps parent grains.

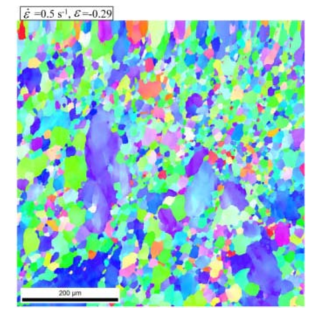


DRX grains invade twinned parent grains.

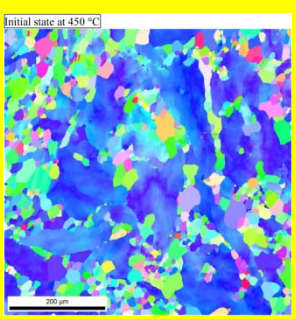




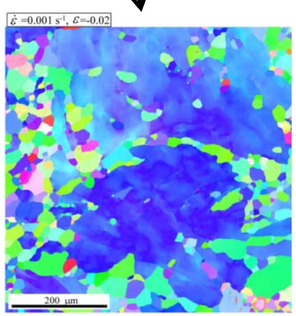
Twinning originates in parent grains and DRX grains grow along twin boundaries.



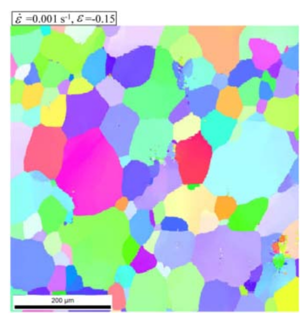
Twins totally eliminated by DRX grain growth.



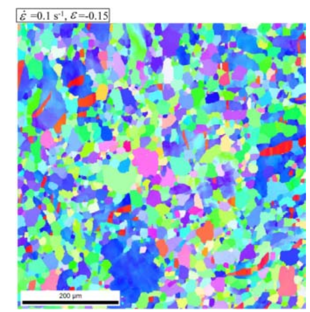
Initial microstructure at 450 °C.



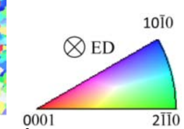
Grain boundaries begin to migrate.



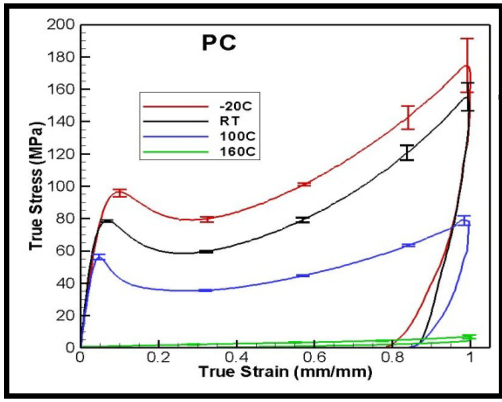
Grains impinge and ripen.



Thin lenticular {10-12} twins (in red) appear.



Methodology Applied to Model Mechanical Response of Polymers

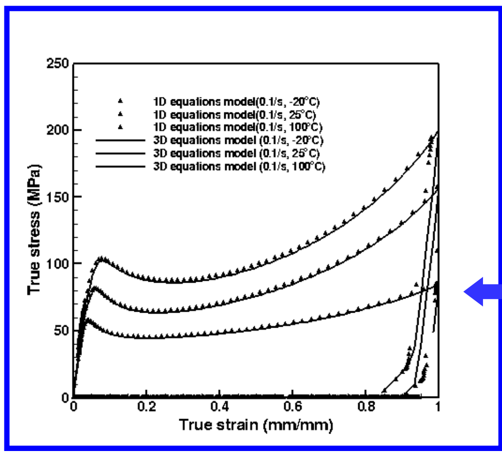


EXPERIMENTAL DATA

ISV MODEL

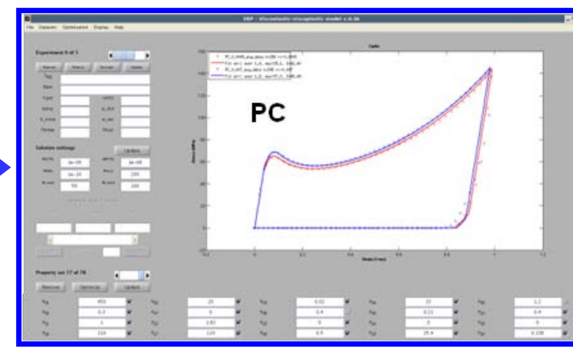
3-D Constitutive Equations
+ Numerical Integration Procedure

fitting algorithm developed for MATLAB

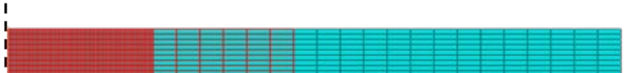


1-D Constitutive Equations

MODEL PARAMETERS CALIBRATION TOOL



Impact Problem (ABAQUS Explicit)



FEA

Numerical Implementation in FEM Codes

Highlights of Natural Fiber Research

Chemical Fiber Retting and Inorganic Nanoparticle Impregnation