DOE Program Merit Review Meeting

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

May 12, 2011

Prime Recipient: Center for Advanced Vehicular Systems

Mississippi State University

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

PI: Professor Mark F. Horstemeyer, PhD

Presenter: Paul Wang, PhD, PE

DOE Manager: Carol Schutte, William Joost

SRCLID – Vision and Mission

- **Vision:** Develop and experimentally validate physics-based **multiscale material models** for **design optimization** of components, systems, and **lightweight** materials for applications critical to the southern automotive corridor of the U.S.
- **Mission:** Provide a robust **design methodology** which incorporates **uncertainty** to create **innovative solutions** for the automotive and materials industries. Integrate theory development, experimental characterization, large-scale computing, new material development, and math-based tools to design next-generation vehicles under various crash and high-speed impact environments.

SRCLID Tasks

Task 1: Multiscale Microstructure-Property Plasticity Considering Uncertainty (Solanki)
Task 2: CyberInfrastructure (Haupt)
Task 3: Fatigue Performance of Lightweight Materials (Jordon)
Task 4: Multiscale Modeling of Corrosion (Groh/Martin)
Task 5: High Strain Rate Impact Fracture Model (Gullett)
Task 6: Materials Design of Lightweight Alloys (Kim)
Task 7: Simulation-Based Design Optimization (Rais-Rohani)
Task 8: A Modified LENS Process (Felicelli)
Task 9: Structural Nanocomposite Design (Lacy, Tuskegee U)
Task 10: Natural Fiber Composite (Shi)
Task 11: Bio-Inspired Design (Williams)
Task 12: K-12 Program (Cuicchi)

Red: **Mg tasks**; Green: **Steel tasks**; Blue: **Composite tasks**; Black: **Education**

Multiscale Material and History Dependent Approach

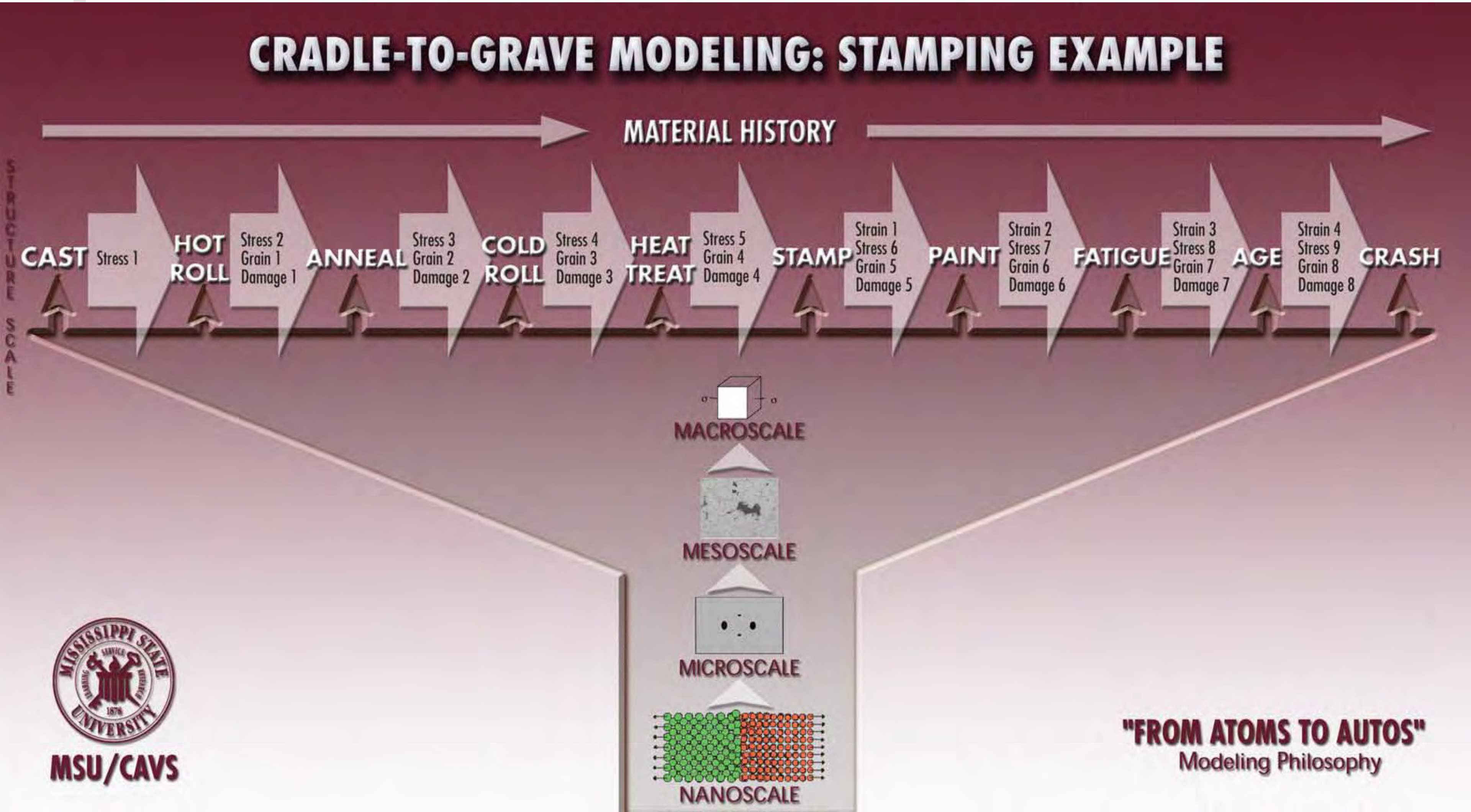
MISSISSIPPI STATE UNIVERSITY

JAMES WORTH BAGLEY COLLEGE OF ENGINEERING MISSISSIPPI STATE UNIVERSITY

CAVS

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.

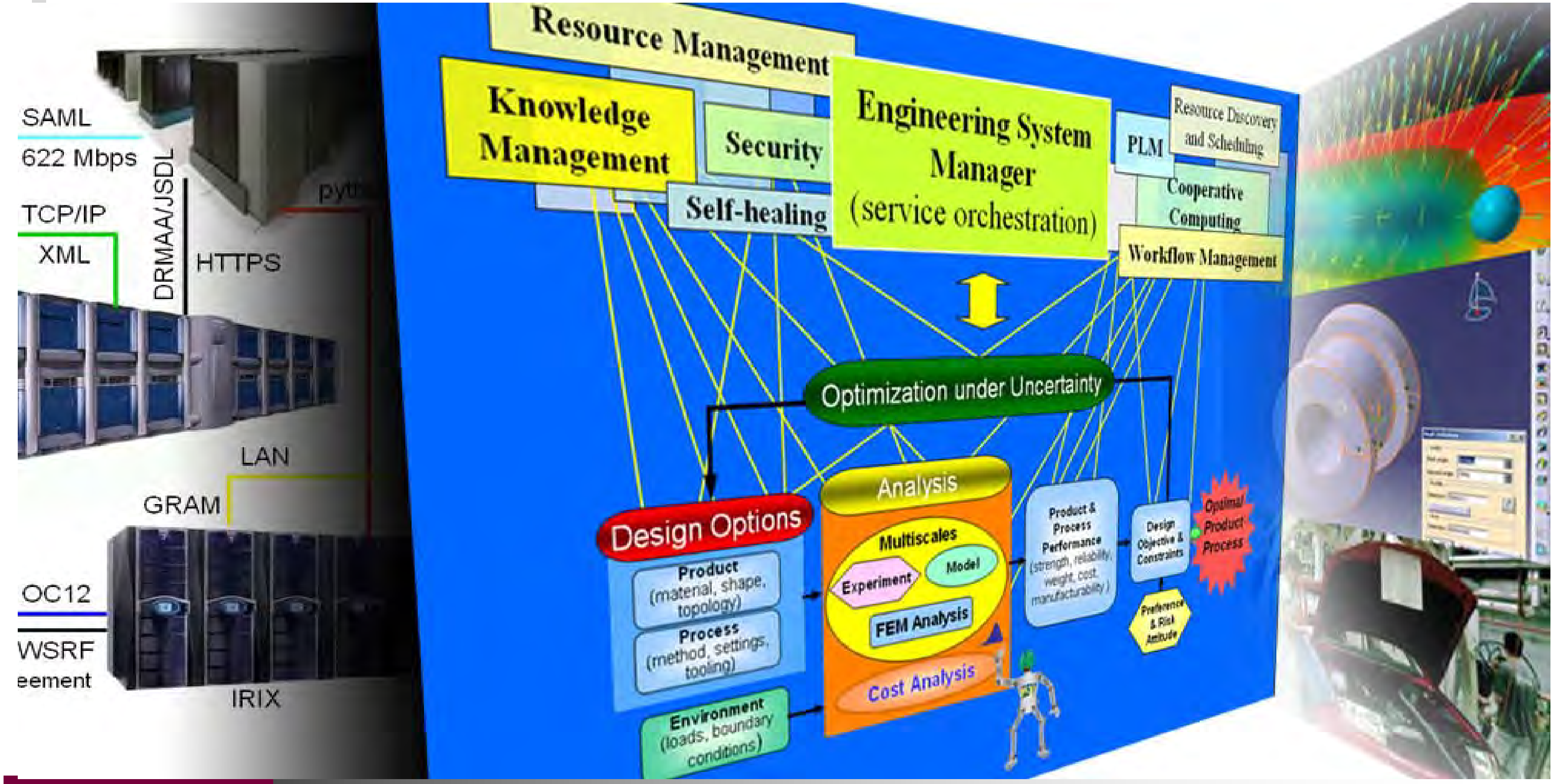


CyberInfrastructure

IT Technologies
(hidden from the engineer)

Conceptual Design Process
(user-friendly interfaces)

Engineering Tools
(CAD, CAE, etc.)



Magnesium Building Block Development

MISSISSIPPI STATE UNIVERSITY

JAMES WORTH BAGLEY COLLEGE OF ENGINEERING MISSISSIPPI STATE UNIVERSITY

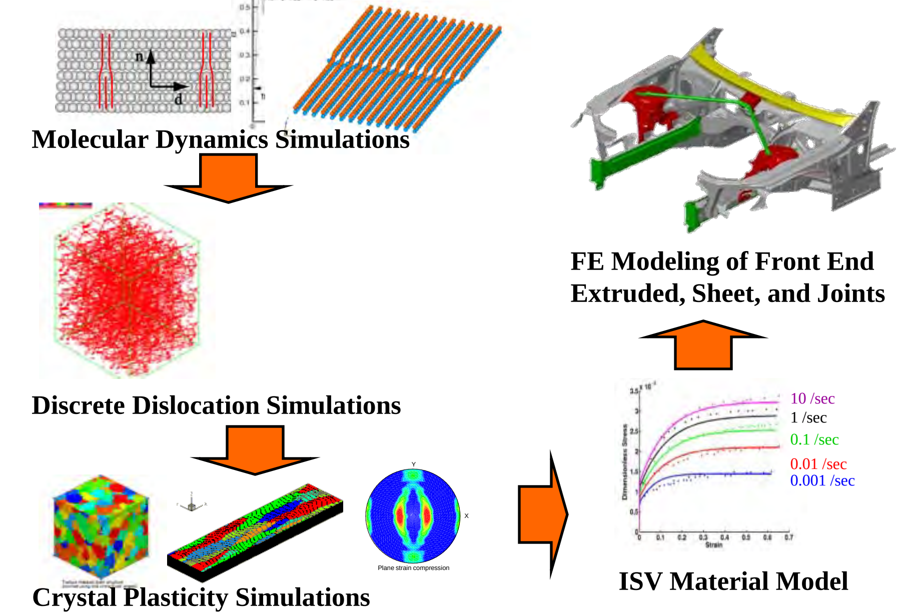
CAVS

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 LMRDC's 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



SWOT ANALYSIS

Strengths: Multiscale modeling of metallic materials; experimental capabilities for coupon testing, deformation processing and structural performance analysis; well-established, collaborative relationships with the automotive industry (Ford, GM); participation in ICME-MFERD.

Weaknesses: Additional investment in TEM and lab-scale modeling capabilities needed; limited access to material for testing.

Opportunities: Develop robust predictive numerical tools for thermo-mechanical processing of Mg alloys to improve their manufacturability. Industry is relying on university research to develop such predictive tools for the optimum design of lightweight auto components.

Threats: Lehigh University, GKSS (Europe).

MSU PERSONNEL

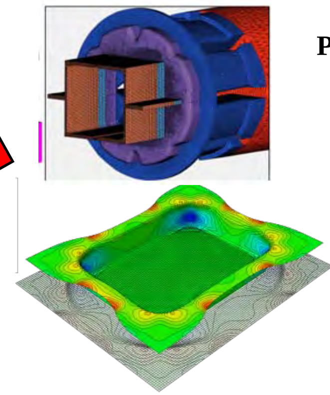
Antonyraj Arockiasamy (CAVS)
Doug Bammann (ME)
Clemence Bouvard (CAVS)
Haitham El Kadiri (ME)
Youssef Hammi (CAVS)
Mark Horstemeyer (ME)
Stephen Horstemeyer (CAVS)
Esteban Marin(CAVS)
Kiran Solanki (CAVS)
Paul Wang (CAVS)

PARTNERS

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

Roadmap: Simulation of Mg Processing

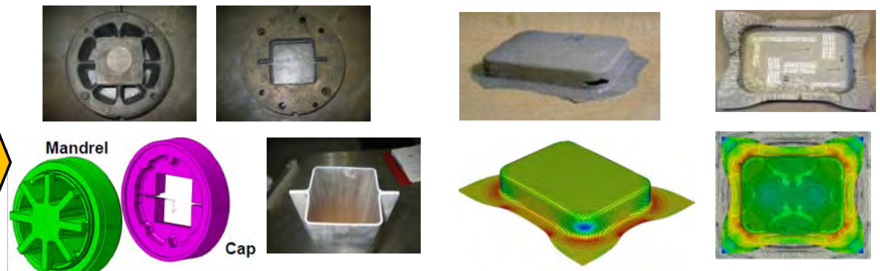
FEM Modeling of Materials Processing



Porthole Die Extrusion (Eulerian)

Pan Forming (Lagrangian)

Thermo-Mechanical Analysis of Materials Processing for Lightweight Alloys



Hollow Profile Extrusion

Warm Sheet Metal (Pan Forming)

Input Microstructure

- Composition
- Texture
- Grain size
- Precipitation
- Dislocations
- Phases

Output Microstructure

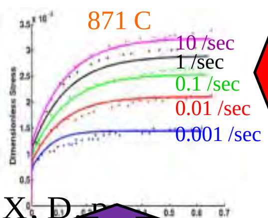
- Dislocations
- Recrystallization
- Grain size
- Texture
- Phases
- Precipitation
- Twinning

Properties

- Strength
- Ductility
- Extrudability
- Weldability
- Toughness
- Corrosion
- Fatigue

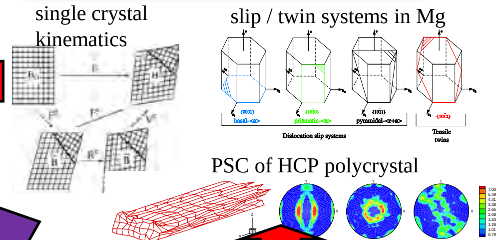
Macroscopic ISV Material Model

- Kinematics
- Elasticity
- Viscoplasticity:
- Recrystallization
- Anisotropy
- Twinning

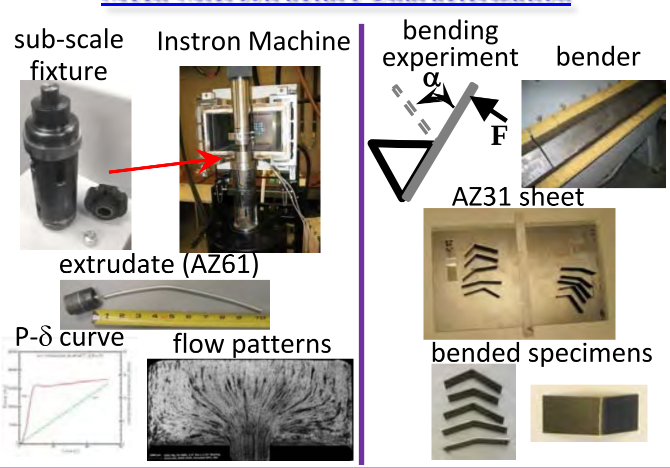


Some ISVs: ρ, φ, X, D, ...

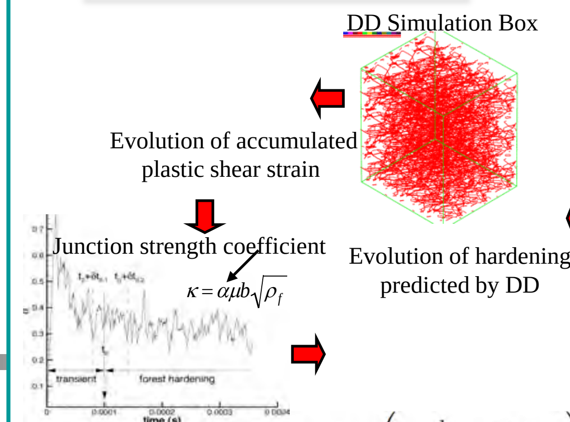
Crystal Plasticity Material Model



Sub-Scale Experiments Mech-Microstructure Characterization

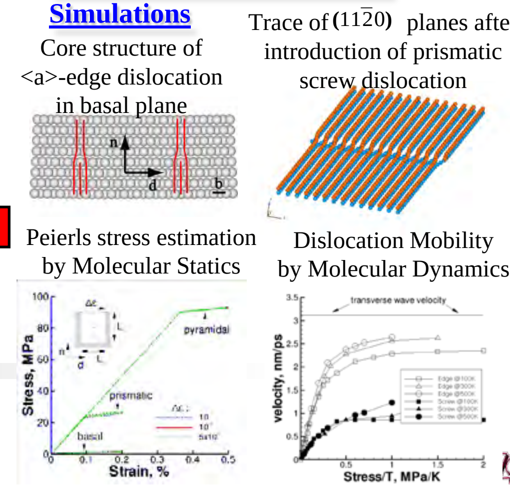


Discrete Dislocation Simulations



Hardening law used in CP: $\kappa = \kappa_s - (\kappa_s - \kappa_0) exp\left(-\frac{h_0}{\kappa_s - \kappa_0}\sum_{\alpha}|\dot{\gamma}^{\alpha}|t\right)$

Molecular Statics/Dynamics Simulations

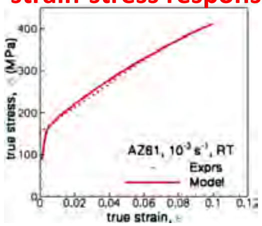


Processing Modeling & In-Service Models

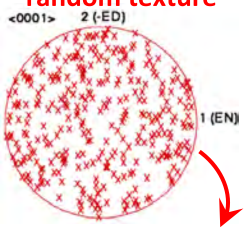
Processing Modeling
(FE Codes – Lagrangian, Eulerian
Matrerial Models: CP, ISV)

INPUT MICROSTRUCTURE/ PROPERTIES

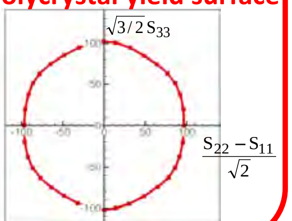
strain-stress response



random texture



polycrystal yield surface



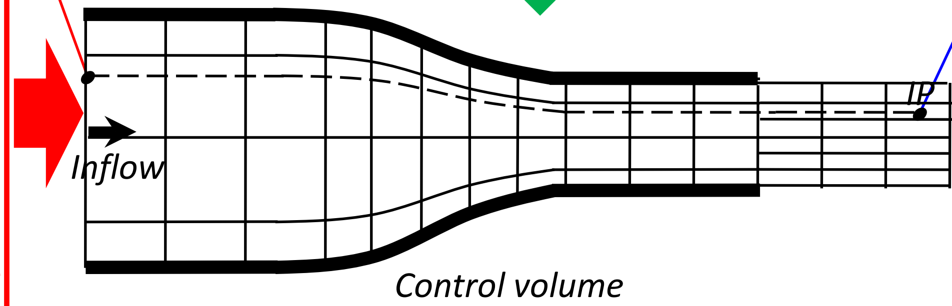
PROCESS MODELING

PROCESS PARAMETERS

- Billet temperature
- Ram speed
- Extrusion ratio

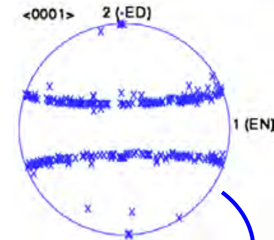
MODELING TOOLS

- FEM Technique (HX)
- Constitutive Models (ISV, Crystal Plasticity)

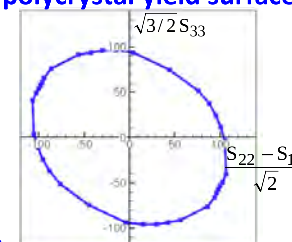


OUPUT MICROSTRUCTURE/ PROPERTIES

deformed texture



polycrystal yield surface



Crystal Plasticity → Continuum Model

ISV MATERIAL MODEL

Fitting material constants describing the anisotropy of yield response.

$$\chi = 1 + a_1 \cos\xi + a_2 \cos 2\xi + a_3 \cos 3\xi + a_4 \cos 4\xi$$

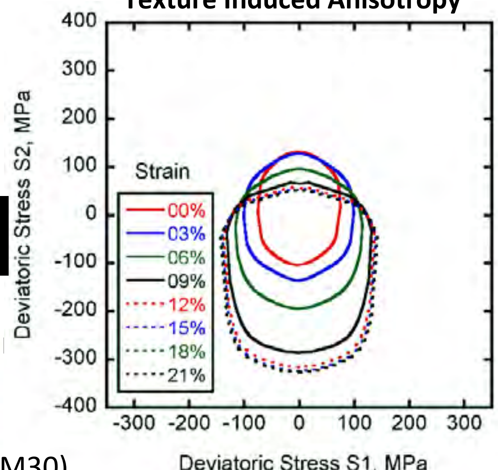
$$\cos\xi = \frac{\sigma_e}{\|\sigma_e\|} : \frac{A}{\|A\|}$$

$$w^p = c(Ad^p - d^p A)$$

$$\dot{A} + w^{eT}A + Aw^e = c_1(d_p A + Ad^p) + c_2 d^p - c_3(A : d^p)A$$

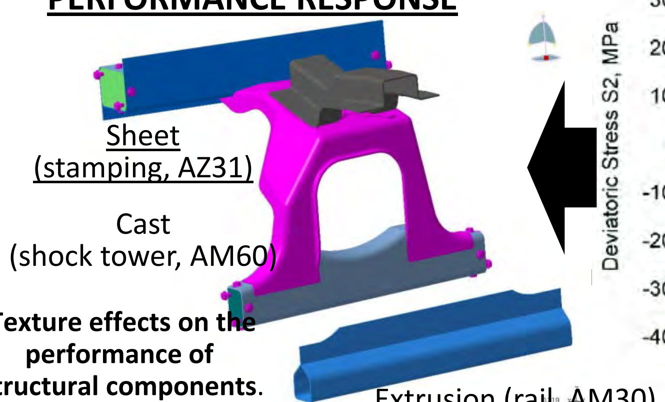
YIELD SURFACE EVOLUTION

Texture Induced Anisotropy



In-Service Models
(FE Codes – Lagrangian;
Matrerial Models: ISV)

PERFORMANCE RESPONSE

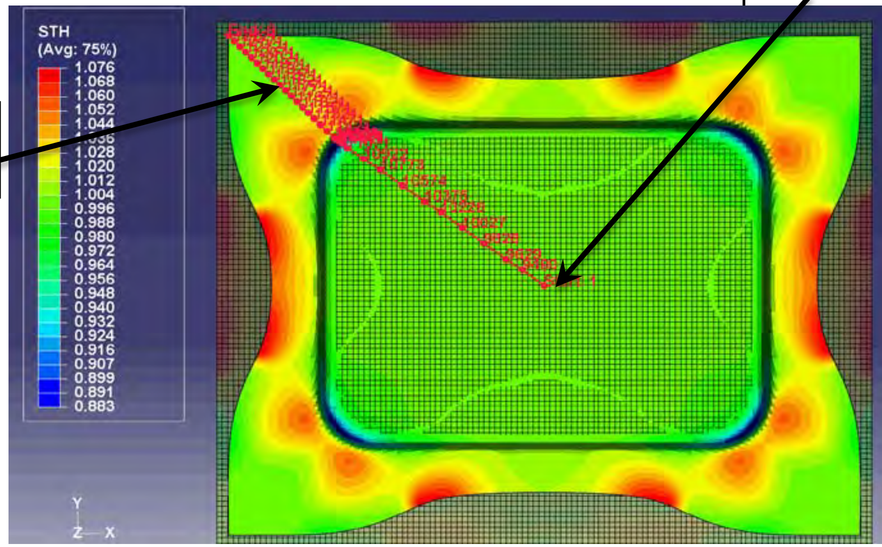


Texture effects on the performance of structural components.

Pan Forming: Prediction of Sheet Thickness Strains

path along which the thickness strain data is computed

the center or origin point in the plots



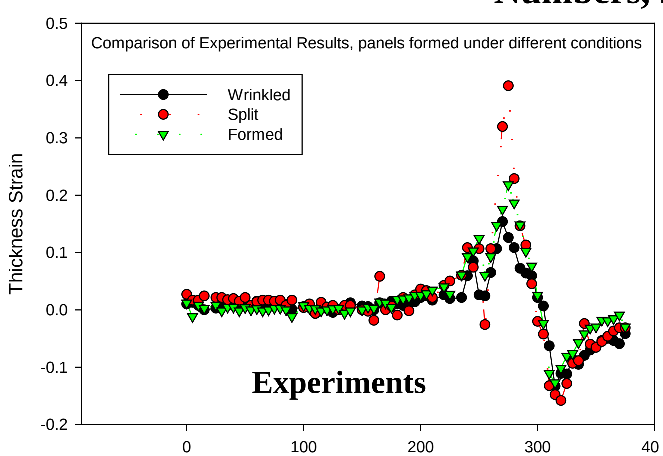
wrinkled

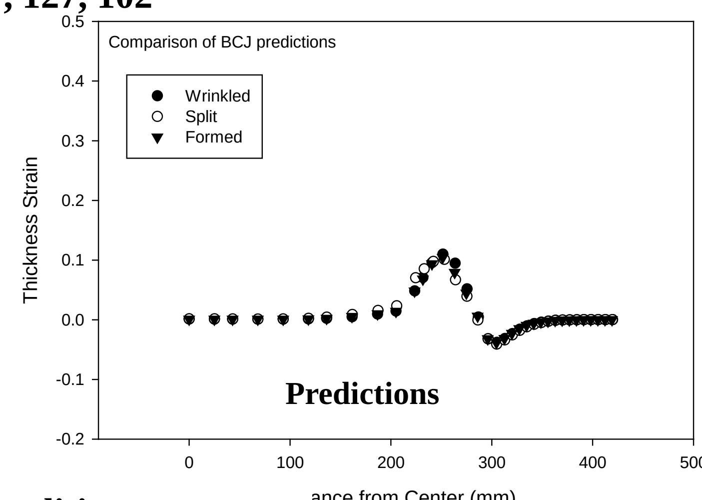
split

OK
Wrinkled
Split

Number	Pressure per Cylinder lbs -f	Temp °C
227	1000	350
26	1250	350
14	1500	350
132	1500	300
127	1500	275
92	1500	250
102	2000	225
191	2250	225
161	2500	200
164	2750	200
167	3000	200
36	3000	300
41	3000	325

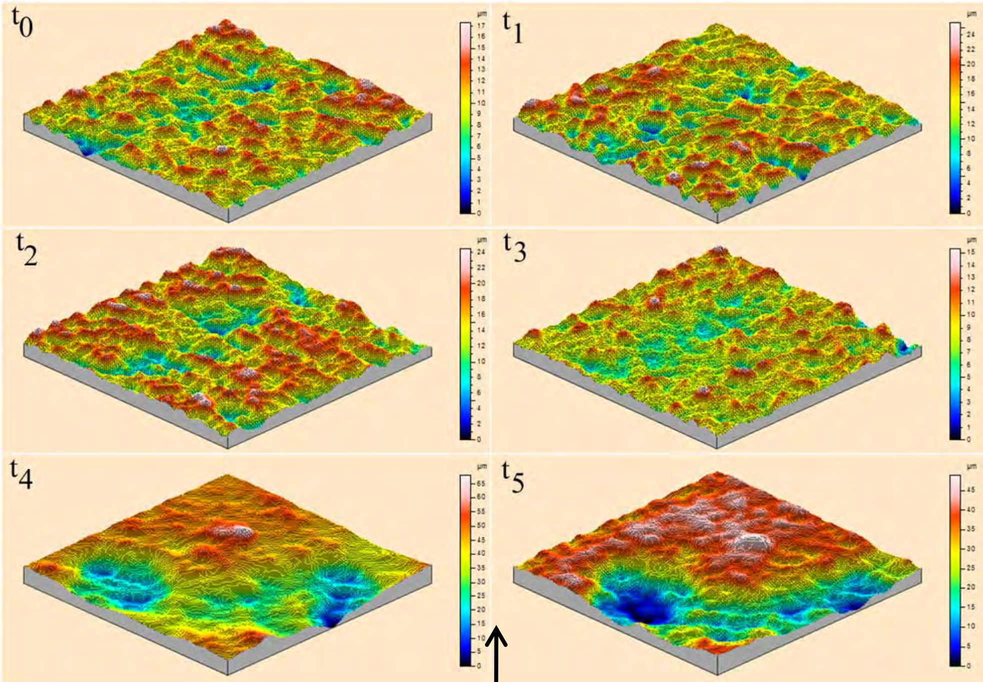
Numbers, 227, 127, 102





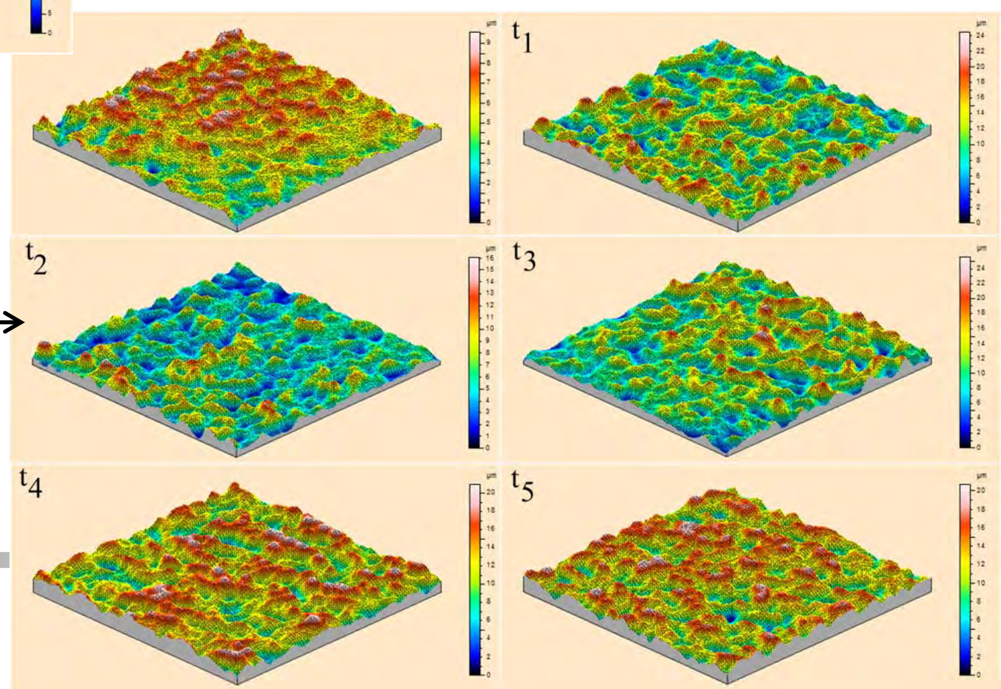
- ❑ Experimental results show differences in thinning under different conditions.
- ❑ ABAQUS / BCJ model show no differences in predicted thinning level for same 3 conditions.

Surface Profilometry–AZ61



- More pits present on the immersion surface at t_1
- Pits grew larger on the salt spray surface by t_5
  - Higher surface area
  - Higher volume
- Due to pit debris trapping chloride ions, pits allowed to grow

- Salt Spray Environment
- Immersion Environment



MISSISSIPPI STATE UNIVERSITY

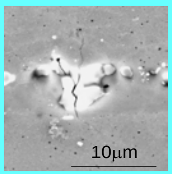
Multistage Fatigue Model for Ductile Materials

$$N_{total} = N_{INC} + N_{MSC/PSC} + N_{LC}$$

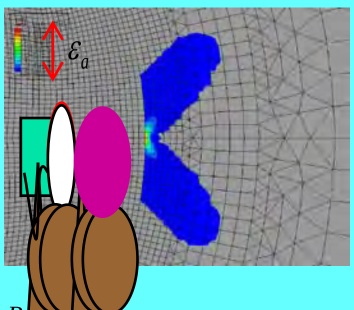
Microstructural Sensitive

Physics Based Model

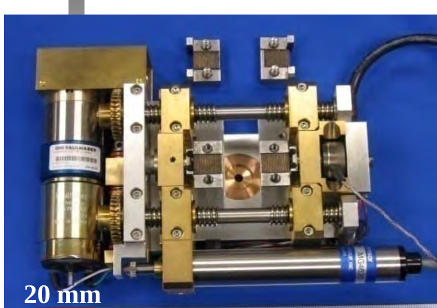
Incubation



Experiments

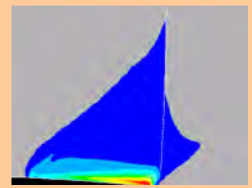


$$\beta = \frac{\Delta\gamma^{P}_{\max}}{2} = C_{inc} N_{inc}^{\alpha}$$

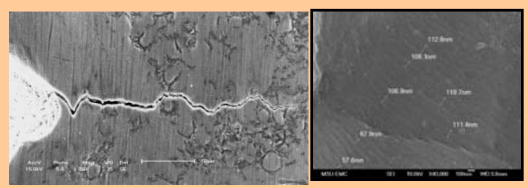


Small Crack Growth

Crystal Plasticity Modeling



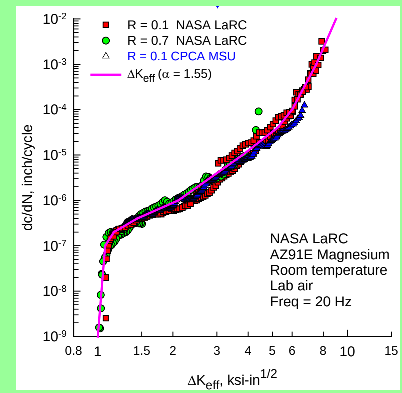
In-Situ SEM fatigue testing



$$\frac{da}{dN} \propto \Delta \mathrm{CTD}$$

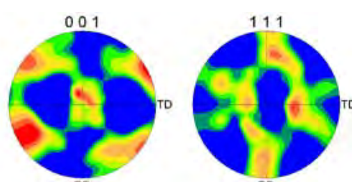
$$\propto \{inclusion(\text{size, density}), grain(size, orientation)\}\left(\frac{U\Delta\sigma}{S}\right)^{\varpi}$$

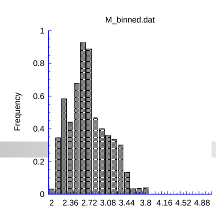
Long Crack Growth



$$\frac{da}{dN} \propto c\left(\Delta K_{\text{eff}}\right)^{m}$$

$$\frac{da}{dN} = \mathbf{Max}\left[\left.\frac{da}{dN}\right|_{MSC/PSC}, \left.\frac{da}{dN}\right|_{LC}\right]$$





BAGLEY COLLEGE OF ENGINEERING
MISSISSIPPI STATE UNIVERSITY

CAVS

Mg Fatigue: Milestones & Accomplishments

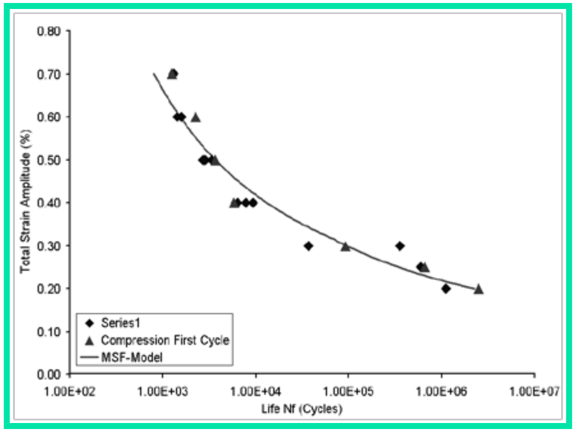
Subtask 3.9 – Develop a higher order MultiStage Fatigue models for the AZ31, AM30 and AZ61 extruded Mg alloys

Milestones:

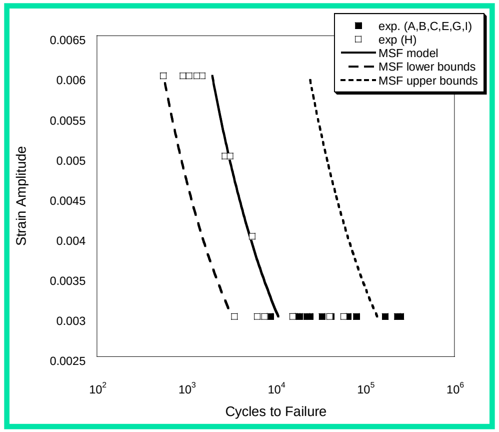
- ✓Develop a MultiStage Fatigue model for AZ61 Ford rail.
- ✓Incorporate structure-property relationships into the MultiStage Fatigue model to predict the scatter in the fatigue life for the AZ61 Ford rail
- ✓Quantify damage under monotonic loading for AZ61 Ford rail for additional modeling capabilities
- ✓Conduct small crack fatigue tests for purpose of modeling development

Accomplishments:

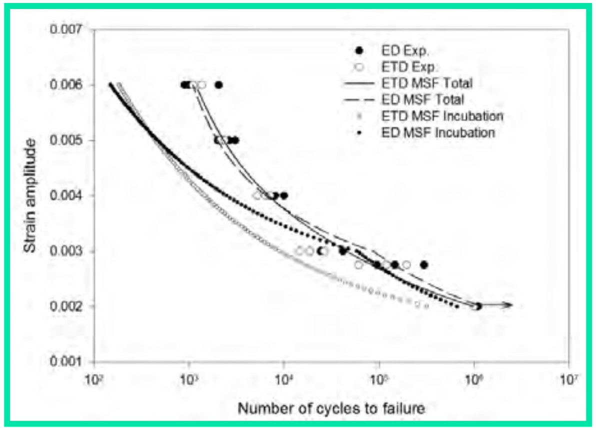
- ✓Developed multistage fatigue model for AZ61 Ford rail
- ✓Incorporating structure-property relationships into the MultiStage Fatigue model to predict the scatter in the fatigue life for the AZ61 Ford rail
- ✓Quantified damage under monotonic loading for AZ61 Ford rail for additional modeling capabilities
- ✓Conducted small crack fatigue tests for purpose of modeling development
- ✓Developed MultiStage Fatigue model for AM30 and AZ61 alloys
- ✓Incorporated structure-property relationships into the MultiStage Fatigue model to predict the scatter in the fatigue life
- ✓Generated fatigue life predictions based on specific microstructure information of Mg AM30 alloy



AZ31



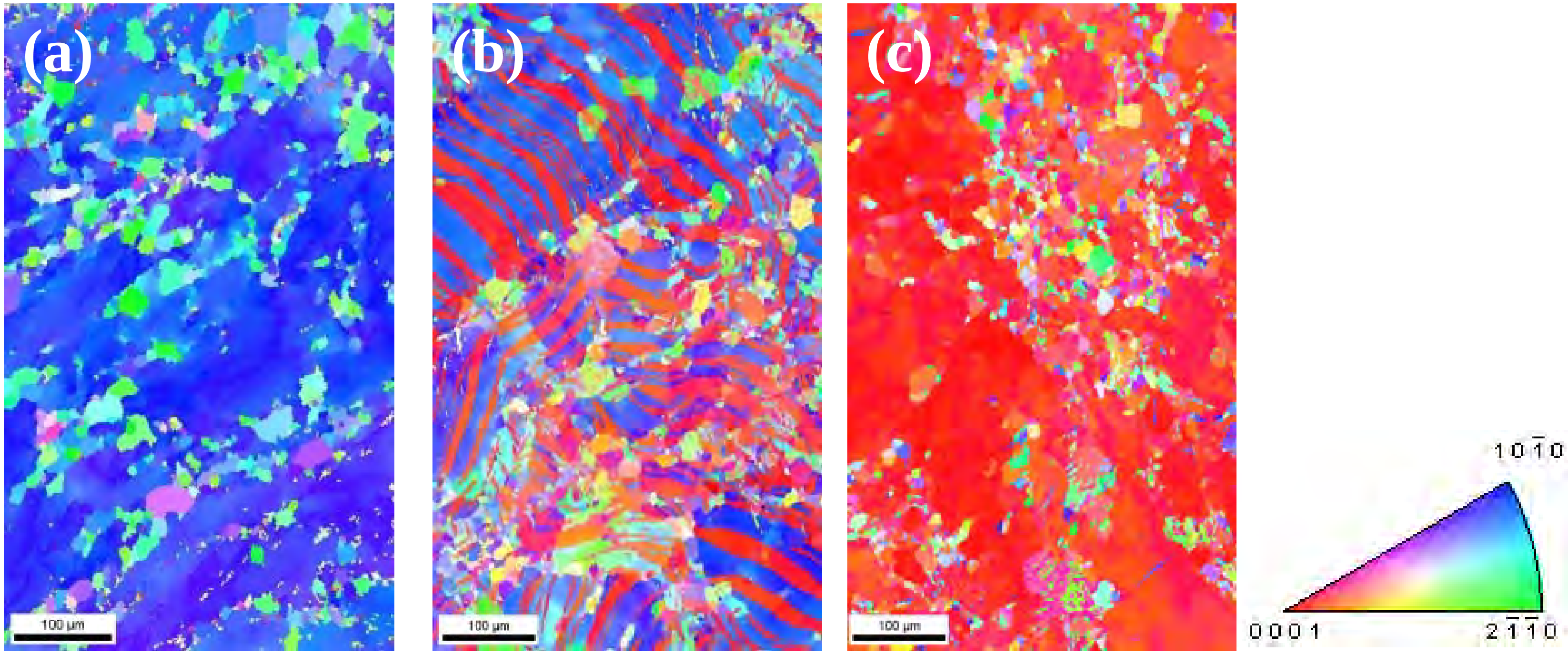
AM30



AZ61

Twinning Activated When Compressed Along Extrusion

EBSD IPF MAPS of ED

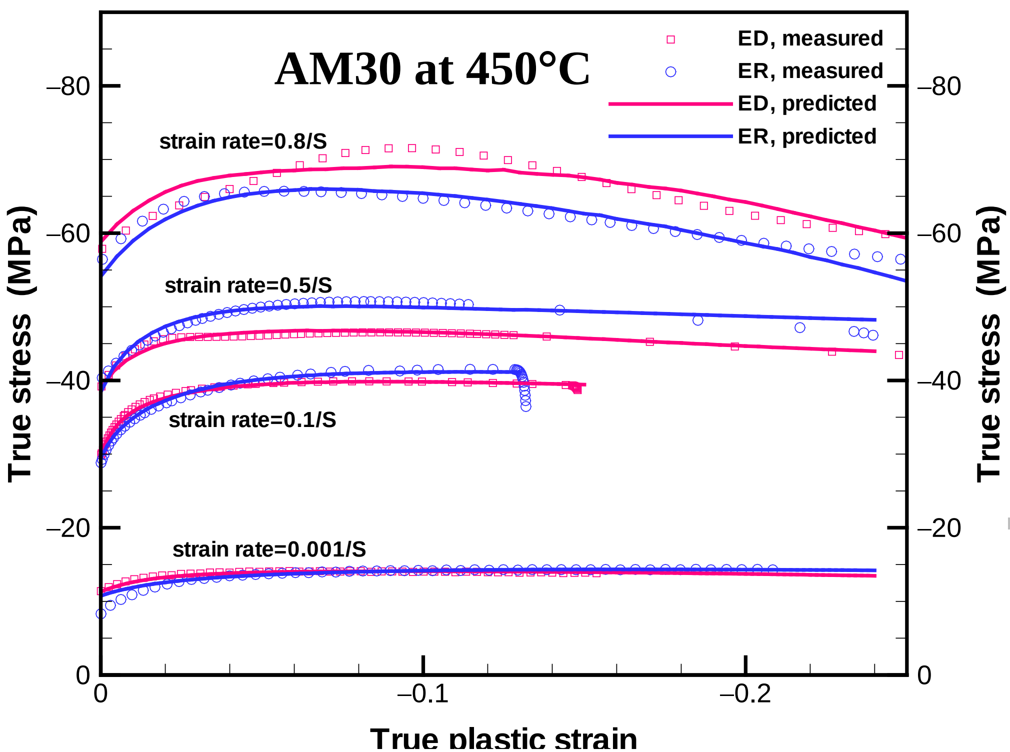


ε=0 **ε= -0.036** **ε= -0.088**

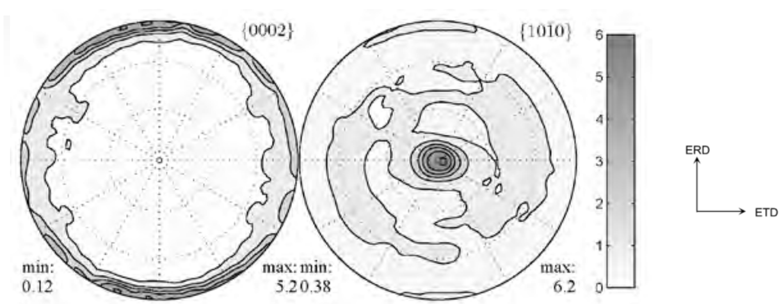
Very high hardening rate

EBSD IPF maps of ED at strain (a) 0; (b) -0.036; (c) -0.088 showing extension twin development. (The loading direction is out of paper. Inverse pole figure represents the ED direction.)

Predicted Stress-Strain Curves of AM30 at High Temperature and Various Strain Rates



Measured and VPSC predicted AM30 stress-strain curves of ED and ER at 450°C and various strain rates.



AM30 initial texture by XRD

Table 1. VPSC best fitting parameters

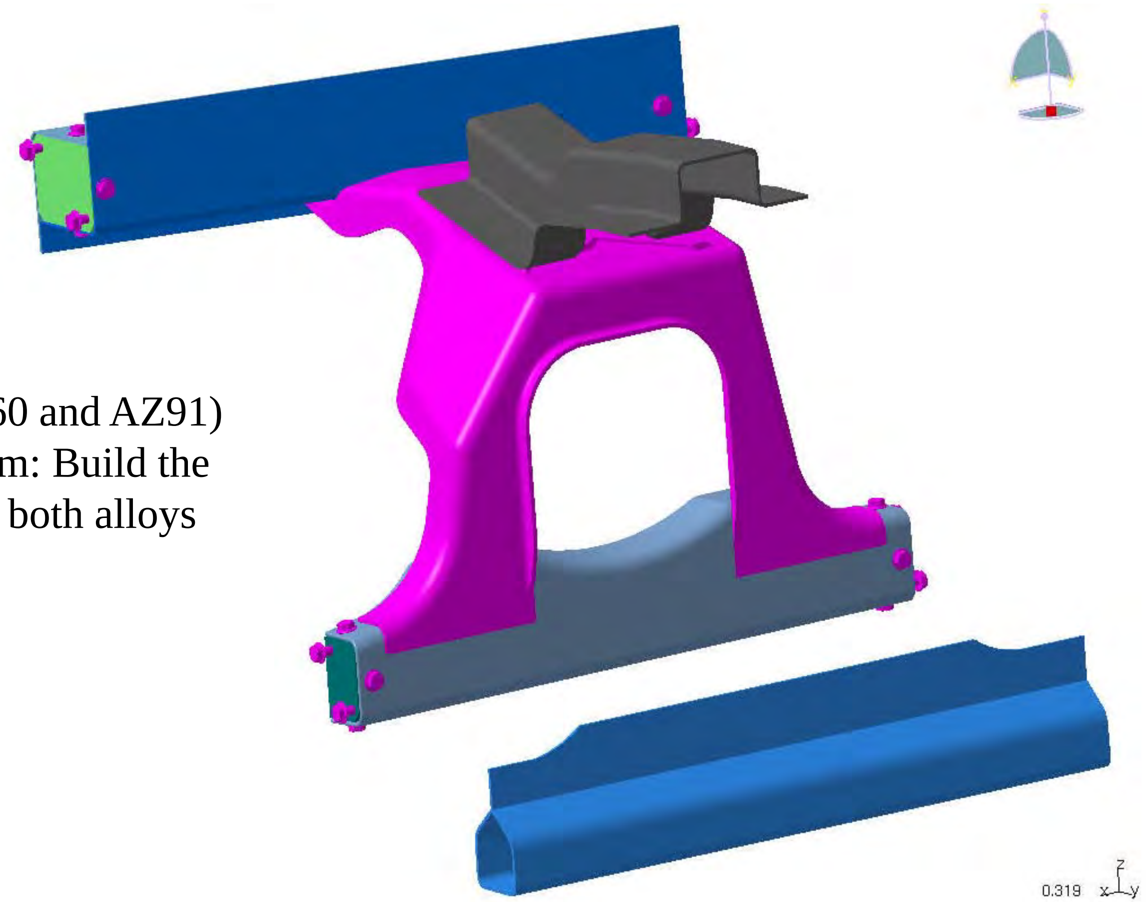
Strain rate	Deformation modes	τ_0	τ_1	θ_0	θ_1
0.001/S	prismatic <a>	7	2	78	-2
	basal <a>	4	7	42	-2
	2nd <c+a>	8	3	0	-2
0.1/S	prismatic <a>	17	4	421	-2
	basal <a>	11	11	131	-2
	2nd <c+a>	24	5	151	-2
0.5/S	prismatic <a>	22	1	77	-5
	basal <a>	12	15	244	-5
	2nd <c+a>	40	0	1119	-5
0.8/S	prismatic <a>	37	7	149	-15
	basal <a>	14	8	64	-15
	2nd <c+a>	70	3	0	-15

*Tensile twinning CRSS was fixed at 55 MPa. h^{ss}=1 and $h^{ss'}$=1.2 for $\dot{\varepsilon}$=0.001,0.1,0.5 and $h^{ss'}$=5 for $\dot{\varepsilon}$=0.8 due to latent hardening by twinning on slip.

JAMES WORTH BAGLEY COLLEGE OF ENGINEERING MISSISSIPPI STATE UNIVERSITY

CAVS

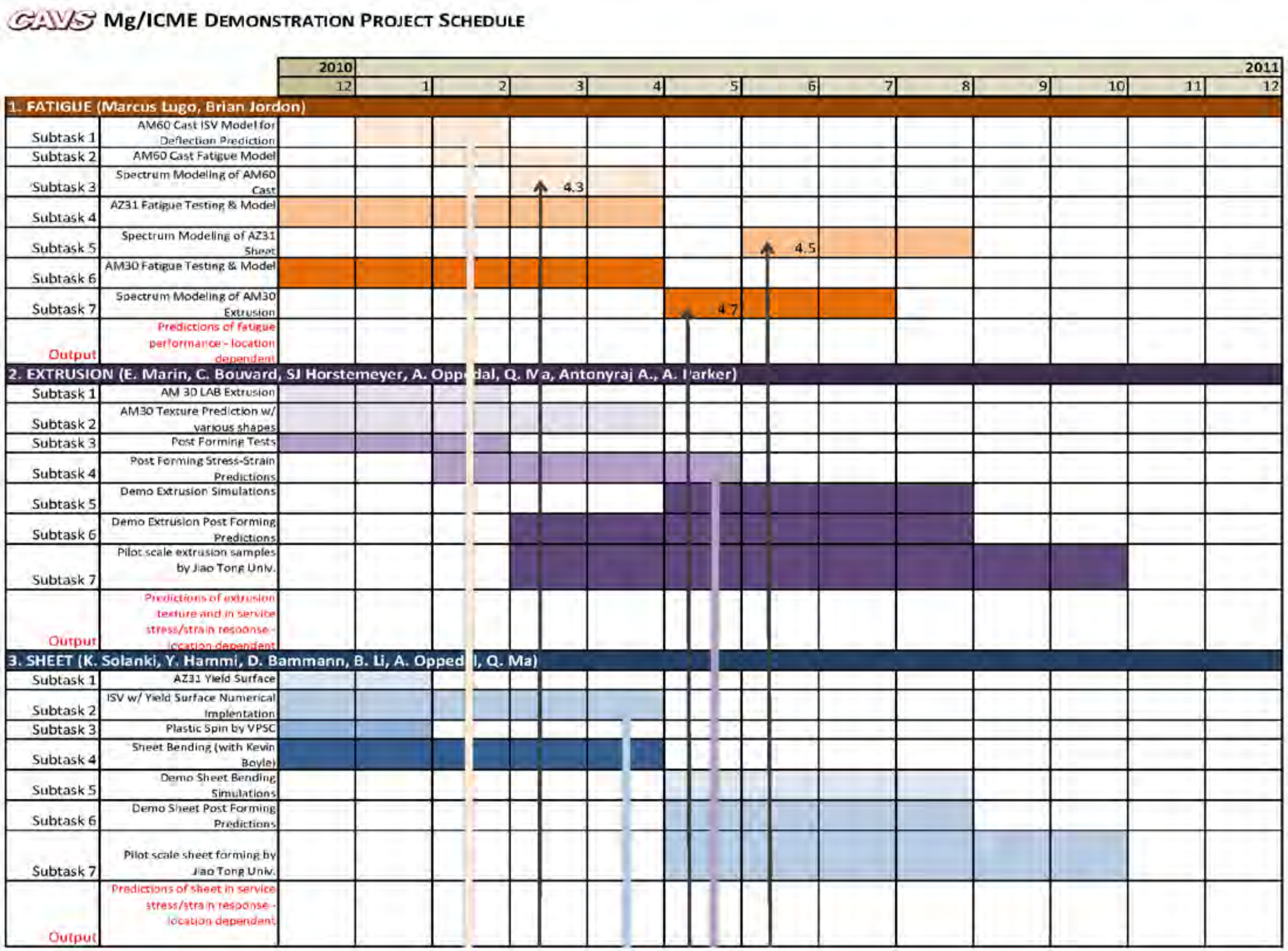
Mg Demo Project - USAMP



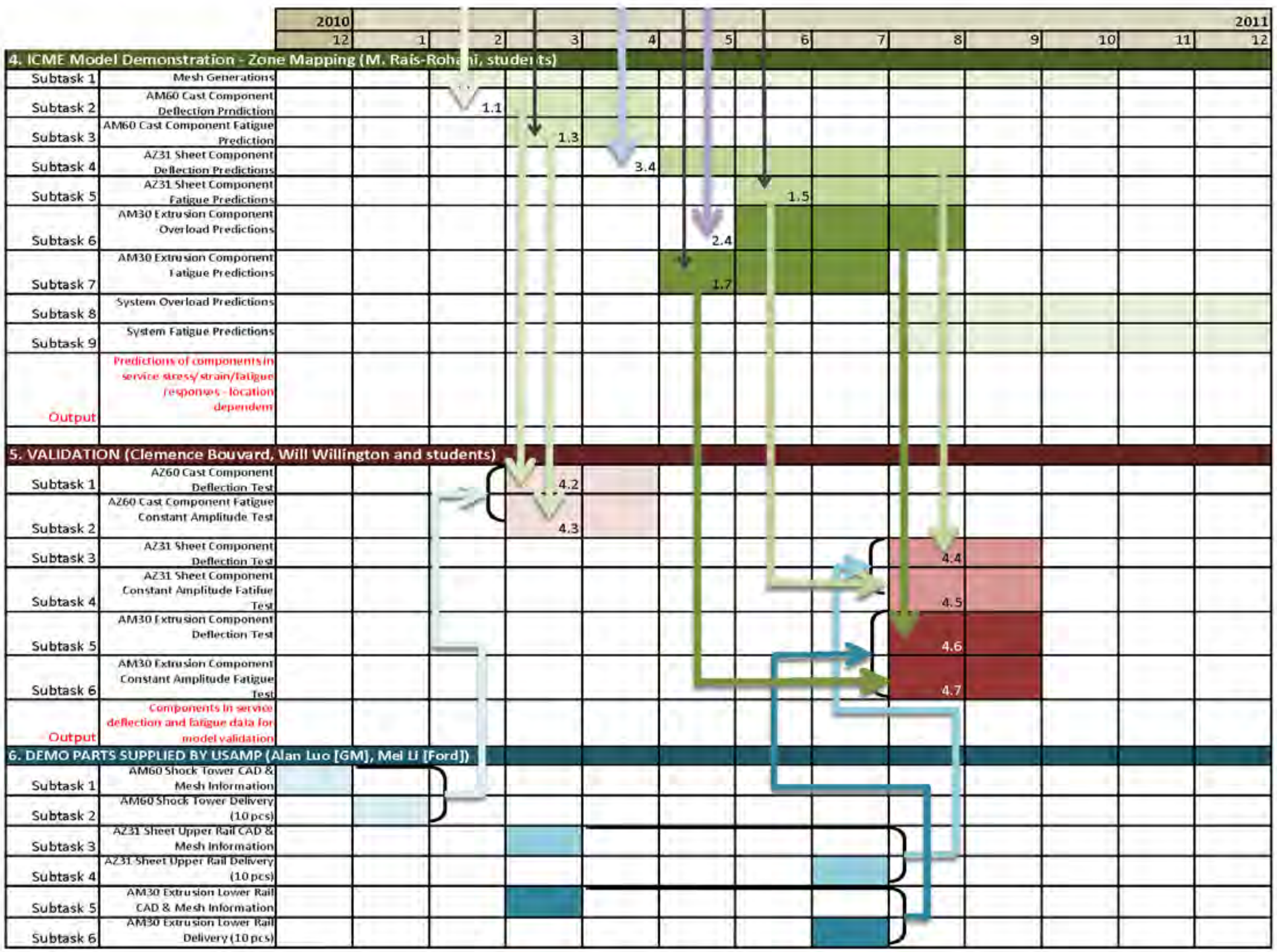
- ***Casting*: shock tower**
  - Alloys (casting team: AM60 and AZ91)
  - Suggestion from ICME team: Build the demo with shock towers of both alloys
- ***Extrusion*: rail**
  - Alloy: AM30
- ***Stamping*: sheet**
  - Alloy: AZ31

Work with GM and Ford casting, sheet and extrusion teams to implement the local property using zone methods

Demo Project Schedule



Demo Project Schedule (cont'd)



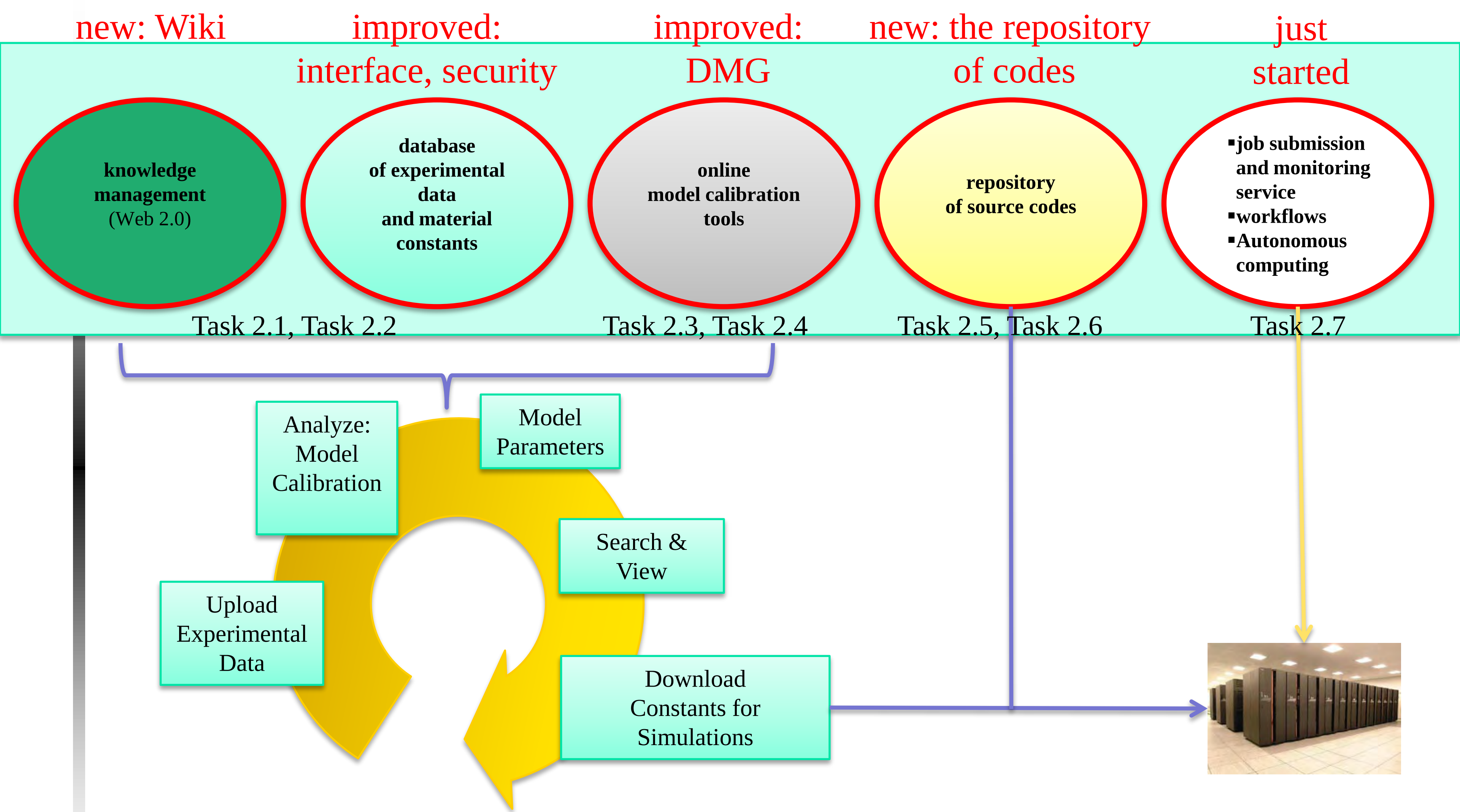
CyberInfrastructure

MISSISSIPPI STATE UNIVERSITY

JAMES WORTH BAGLEY COLLEGE OF ENGINEERING MISSISSIPPI STATE UNIVERSITY

CAVS

Progress Report of CyberInfrastructure



Knowledge Management

Community Portal: Wiki—http://ccg.hpc.msstate.edu

How to

Community Knowledge

Repositories

Projects

Haupt | my talk | my preferences | my watchlist | my contributions | log out

page | discussion | edit | history | delete | move | protect | watch

home
- Home
- About
- Help with Wiki

materials
- Metals
- Ceramics
- Polymers
- Biomaterials

material models
- Models Home
- Structural Scale
- Macroscale
- Mesoscale
- Microscale
- Nanoscale
- Electronic Scale

services
- Repository of Codes
- Experimental Data
- Model Calibration

projects
- ICME
- SRCLID
- Mission Eggcellence

search

Go | Search

toolbox
- What links here
- Related changes

Engineering Virtual Organization for CyberDesign

USAMP's Integrated Computational Material Engineering (ICME) and Southern Regional Center for Innovative Lightweight Design (SRCLID) supported by the Department of Energy (DOE)

Welcome! [edit]

Welcome to our Materials CyberSpace! Included in this CyberSpace is a collection of materials databases and multiple size scale codes so that one can design and develop the next generation materials and structural components. Our hope is that the creation of this cyberinfrastructure will result in the development of the "community of practice" portal that allows development and integration of multiscale physics-based materials models for selected properties and processes, in the context of United States Automotive Materials Partnership (USAMP) three-nation Magnesium Front-End Research and Development pilot project (MFERD), in particular task 1.9: Cyberinfrastructure for Integrated Computational Material Engineering (ICME).

There are separate web sites that provide more information on the MFERD and ICME projects. If you have any questions or comments regarding this website, please feel free to contact us at haupt@cavs.msstate.edu. Thanks and have fun lightweighting your designs using our tools.

Sincerely,

Dr. Tomasz Haupt, CAVS Professor at Mississippi State University (MSU)

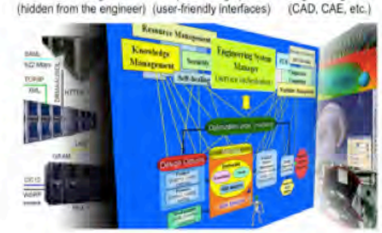
Dr. Mark Horstemeyer, CAVS Chair Professor at Mississippi State University (MSU)

This effort is funded by the Center for Advanced Vehicular Systems (CAVS) at MSU, the U.S. Department of Energy under contract 4000054701, and the NSF grant Virtual Organization for CyberDesign (Award ID: 0742730).

Material Models at different length scales

Click on image to enter

Cyberinfrastructure



Click on image to enter

Call for Participation [edit]

The Cyberinfrastructure team created the infrastructure for web-based collaborative efforts. The success of this effort critically depends on the participation of the community towards the generation of the contents that will aid the research in Materials Science and lightweight innovative design. The expected community contributions are:

- Creating and updating pages in this Wiki. Please, refer to Help with Wiki tutorial on how to create and edit Wiki pages.
- Experimental data, material models, material constants, and codes at any length scale. Please refer to help sections available from *services* toolbox.
- Specifications for the requirements of the Cyberinfrastructure by adding to the *projects* pages.

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,

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

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

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

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

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

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

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

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

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

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

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

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.

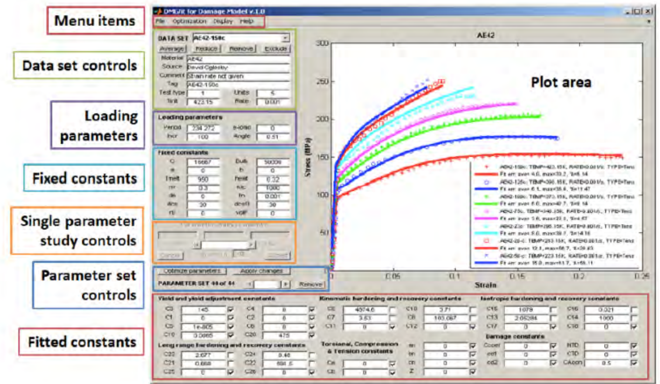
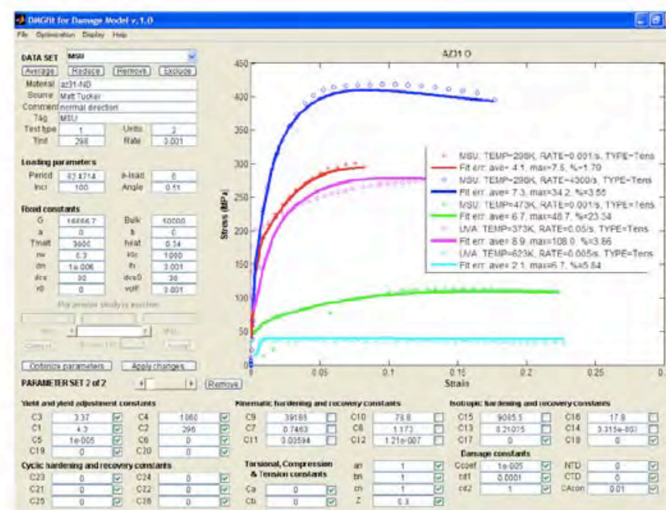


Figure 3. The logical groupings of controls in the DMGfit GUI.

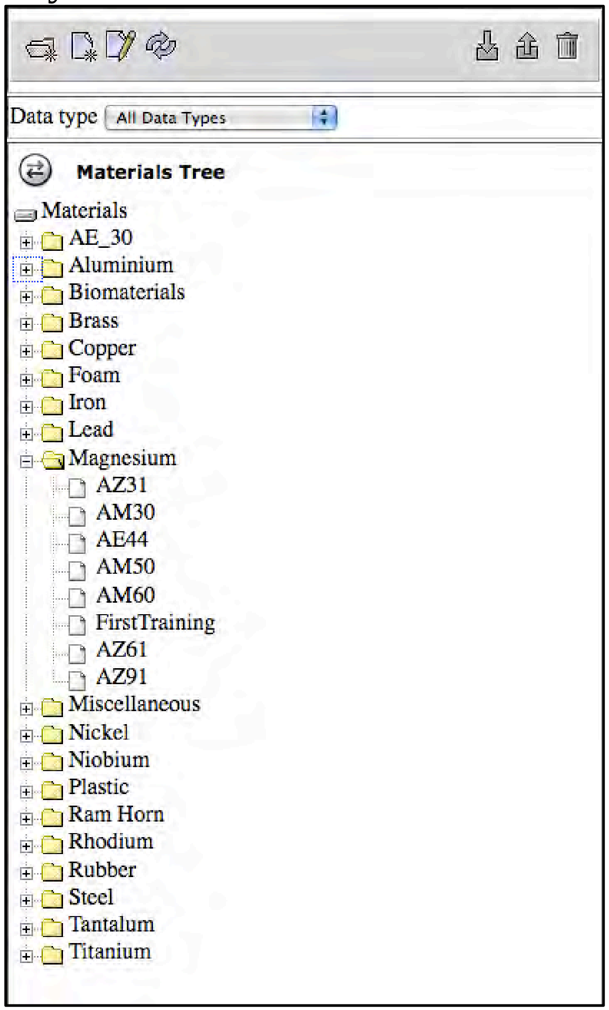


B43. AZ31 Mg alloy: temperature and strain rate model correlation

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

Synthetic and Natural Composite Program

Highlights of Natural Fiber Research

Chemical Fiber Retting and Inorganic Nanoparticle Impregnation

MSU North Farm

Bast & Core

Bast

Cut into 2” Length

Chemical Compositions Analysis

Chemical retting With 5% NaOH At 160°C for 1h.

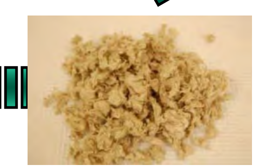
Adjust pH value to 7.0 And wash out chemical

Impregnate with Na_2CO_3

Impregnate with $CaCl_2$

$$Na_2CO_3 + CaCl_2 \xrightarrow[\text{Na}_2\text{CO}_3\text{:CaCl}_2\text{=1:1, 1:2 (mol:mol)}]{100^\circ C,\ 130^\circ C,\ 160^\circ C} CaCO_3$$

Freeze Dried



Oven dried

- Fiber mechanical properties
- Surface Roughness
- Surface Morphology & Topography

Composite fabrications

Composites properties

MISSISSIPPI STATE UNIVERSITY

BAGLEY COLLEGE OF ENGINEERING MISSISSIPPI STATE UNIVERSITY

CAVS

Properties of LSMC Treated Kenaf Fiber Unsaturated Polyester Composites in 2010

SMC Sample

PROPERTIES	Kenaf/UPE*[1]	Commercial Glass/UPE*[2]
Density, g/cm^3	1.2-1.4	1.9
Flexural Modulus, GPa	8.0-10.0	10.0
Flexural Strength, MPa	80-100	167
Tensile Modulus, GPa	6.0-13.7	10
Tensile Strength, MPa	50-70	74
24 hr WA, %	1.5-6.0	0.7

*[1]**Kenaf fiber + $CaCO_3$ content**: 60 wt%

*[2]**Glass fiber content**: 25%; **$CaCO_3$ content**: 40 wt% EpicBlendSMC (Magna Auto)

Key Actions and Deliverables

- **Received additional cost share support from industry: MSC, Alpha Star, SAC, POSCO, Mitsubishi Motors, and USAMP.**
- **Organized a symposium at MsSt in June 2010 – *Symposium of Predictive Science & Technologies in Mechanics and Materials*.**
- **Actively participate in MFERD Phase II Demo program, due Sept. 2011.**
- **Established and validated process-structure-property (PSP) relationships, material models (ISV) and uncertainty for aluminum and steel , and continued the development of PSP and ISV as well as the validation for Mg alloys.**
- **At the atomistic scale, a number of atomistic potentials (i.e., Fe, C, Si, Al, Mg) established for alloy design purposes.**
- **Initiated design/optimization methods to include ISV and PSP with finite element analyses.**
- **Natural fiber: SMC panel delivered to ACC for review – results encouraging.**
- **CyberInfrastructure integrates our software and experimental information in Wiki and has garnered high recognition from TMS.**

Future Work

- Develop and validate material models and deploy them for use—MFERD Phase II demo project (Sept. 2011).
- Establish Mg alloy design methodology using lower-length scale models.
- Composite, biomechanics and natural fiber research teams will move forward to develop material-specific multiscale models, validated by critical experiments, and produce demo cases.
- Update the CyberInfrastructure and further establish a national and an international user base.

Thank You !!