DOE Program Merit Review Meeting
Southern Regional Center for Lightweight Innovative Design (SRCLID)

Magnesium Projects

June 7-11, 2010

Prime Recipient: Center for Advanced Vehicular Systems
Mississippi State University
Agreement Number: (# DE-FC-26-06NT42755)
MSU Principal Investigators: Mark Horstemeyer, Paul Wang
DOE EE Manager: Carol Schutte, William Joost
NETL Program Manager: Magda Rivera

Project ID LM014

SRCLID – Vision and Mission

- **Vision:** Develop **multiscale** physics-based **material models** experimentally validated to be used for **design optimization** of components, systems, and **lightweight** materials for the southern automotive corridor of the U.S.

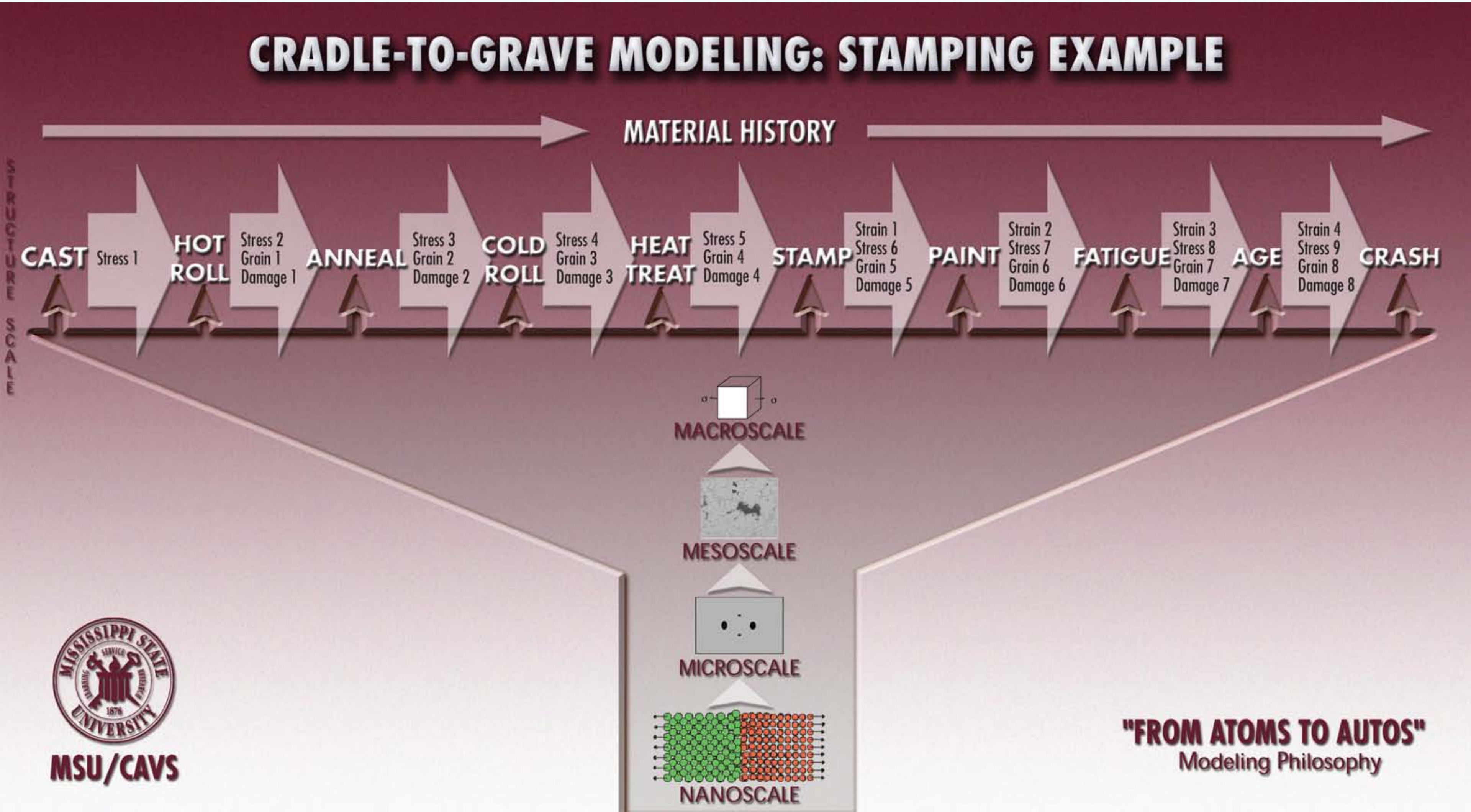
- **Mission:** Provide a robust **design methodology** including **uncertainty** to create **innovative solutions** for the automotive and materials industries. Theory development, experimental characterization, large-scale computing, new material development, and math-based tools are sought for use in designing next-generation vehicles under various crash and high-speed impact environments.

SRCLID Tasks

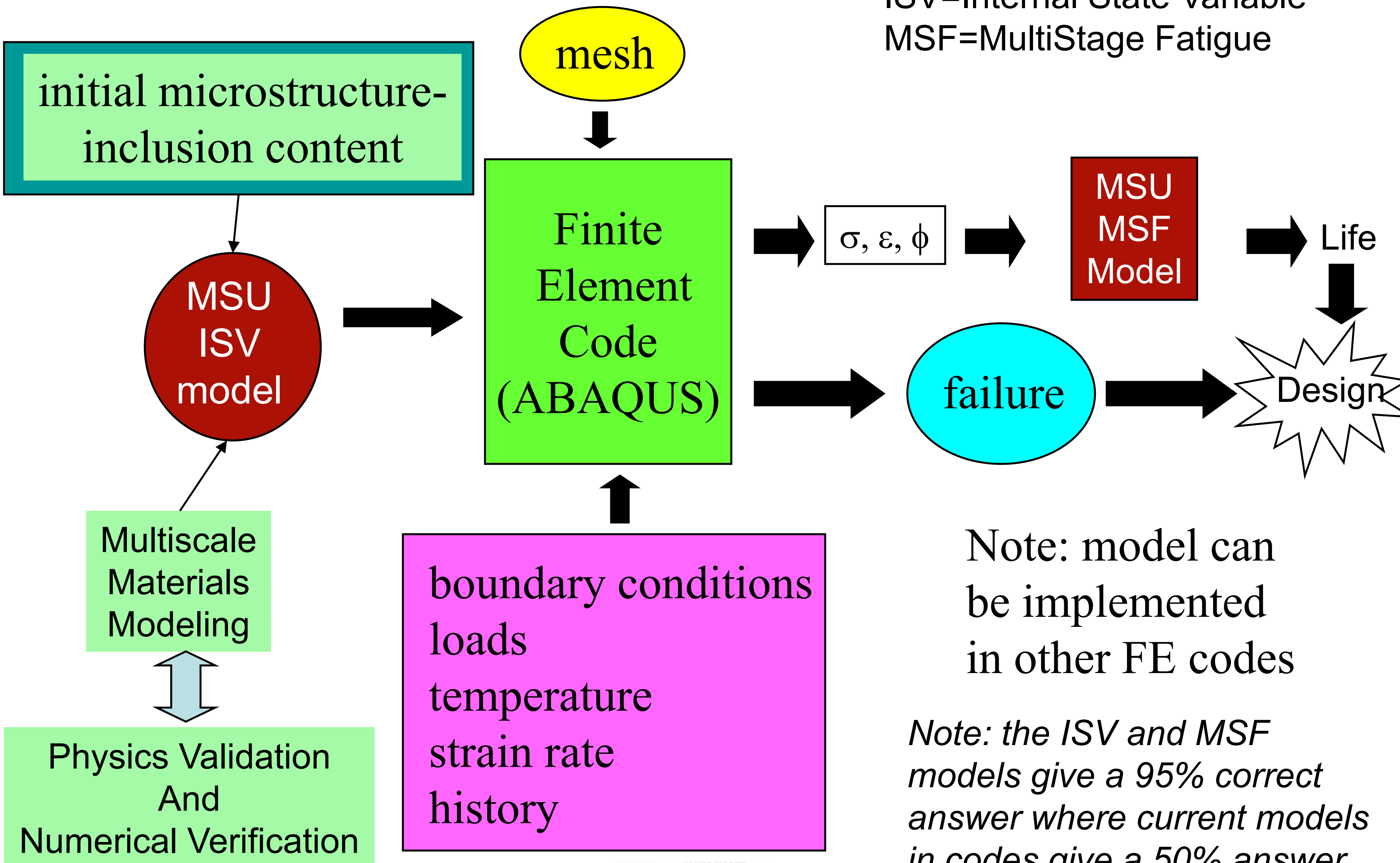
Task 1: Multiscale Microstructure-Property Plasticity Considering Uncertainty (Solanki)
Task 2: Cyberinfrastructure (Haupt)
Task 3: Fatigue Performance of Lightweight Materials (Jordon)
Task 4: Multiscale Modeling of Corrosion (Groh/Martin)
Task 5: High Strain Rate Impact Fracture Model (Gullett)
Task 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)

Computational Manufacturing and Design

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



Models Implementation/Use

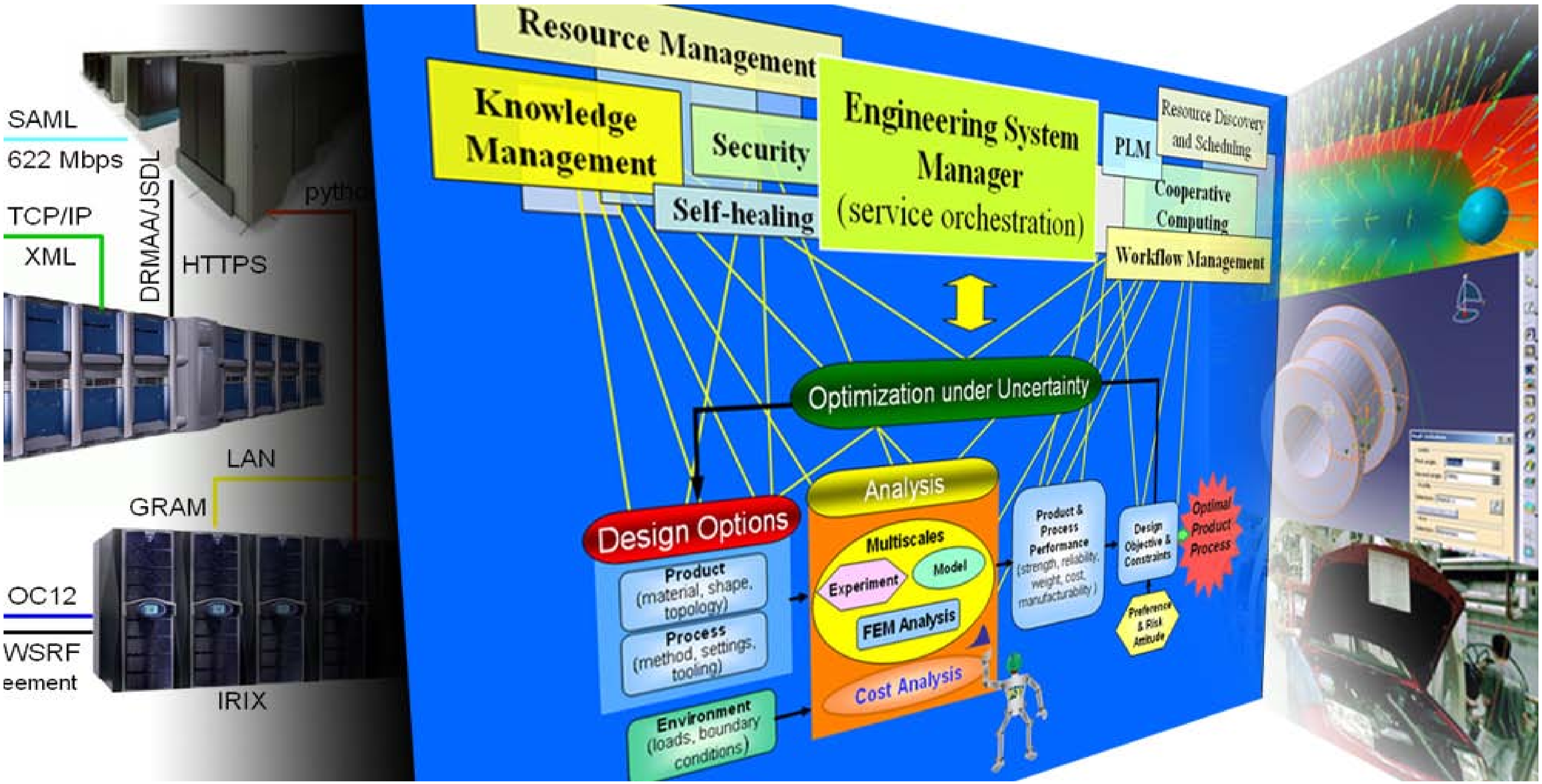


Note: model can be implemented in other FE codes

Note: the ISV and MSF models give a 95% correct answer where current models in codes give a 50% answer

CyberInfrastructure

IT technologies (hidden from the engineer) | Conceptual design process (user-friendly interfaces) | Engineering tools (CAD, CAE, etc.)

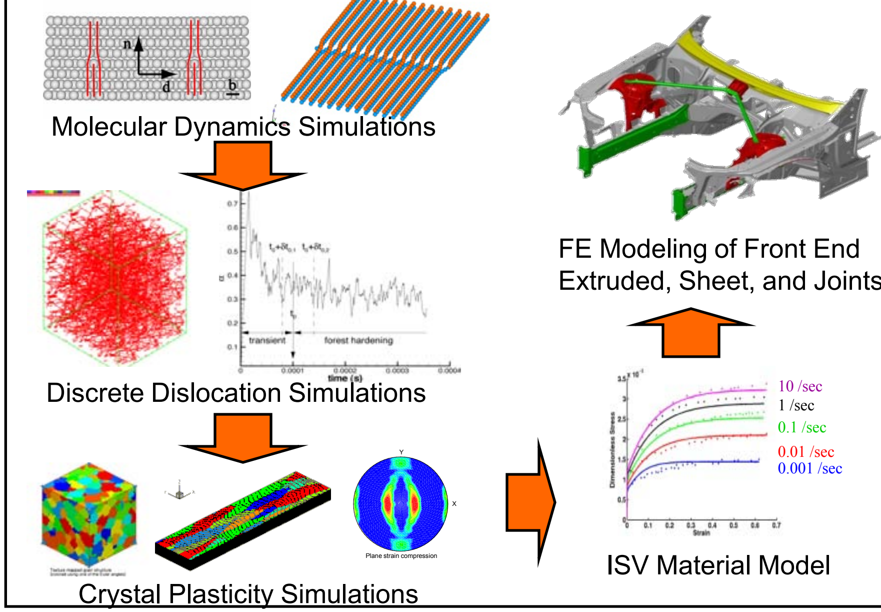


Magnesium Overview

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 center'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, good experimental capabilities for coupon testing, deformation processing and structural performance analysis, good relations with the automotive industry (Ford, GM), participation in ICME-MFERD.

Weaknesses: Needs additional investment of TEM and lab-scale modeling capabilities. 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 developed such predictive tools for the optimum design of lightweight auto components.

Threats: Lehigh University, GKSS (Europe).

MSU Personnel:

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

Partners:

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

Lab-Scale Extrusion Experiments

Fixture Design / Test matrix

Indirect Extrusion Fixture

Parametric Study of the Extrusion Process

- ❖ Lab-scale extrusion defined by 3 processing parameters:
  - billet temperature,
  - ram speed (cross-head speed of Instron),
  - extrusion ratio (die orifice)
- ❖ Specimen size: 1 ¼” diameter x 1” length
- ❖ Bearing Lengths: 1/16”, 1/32”

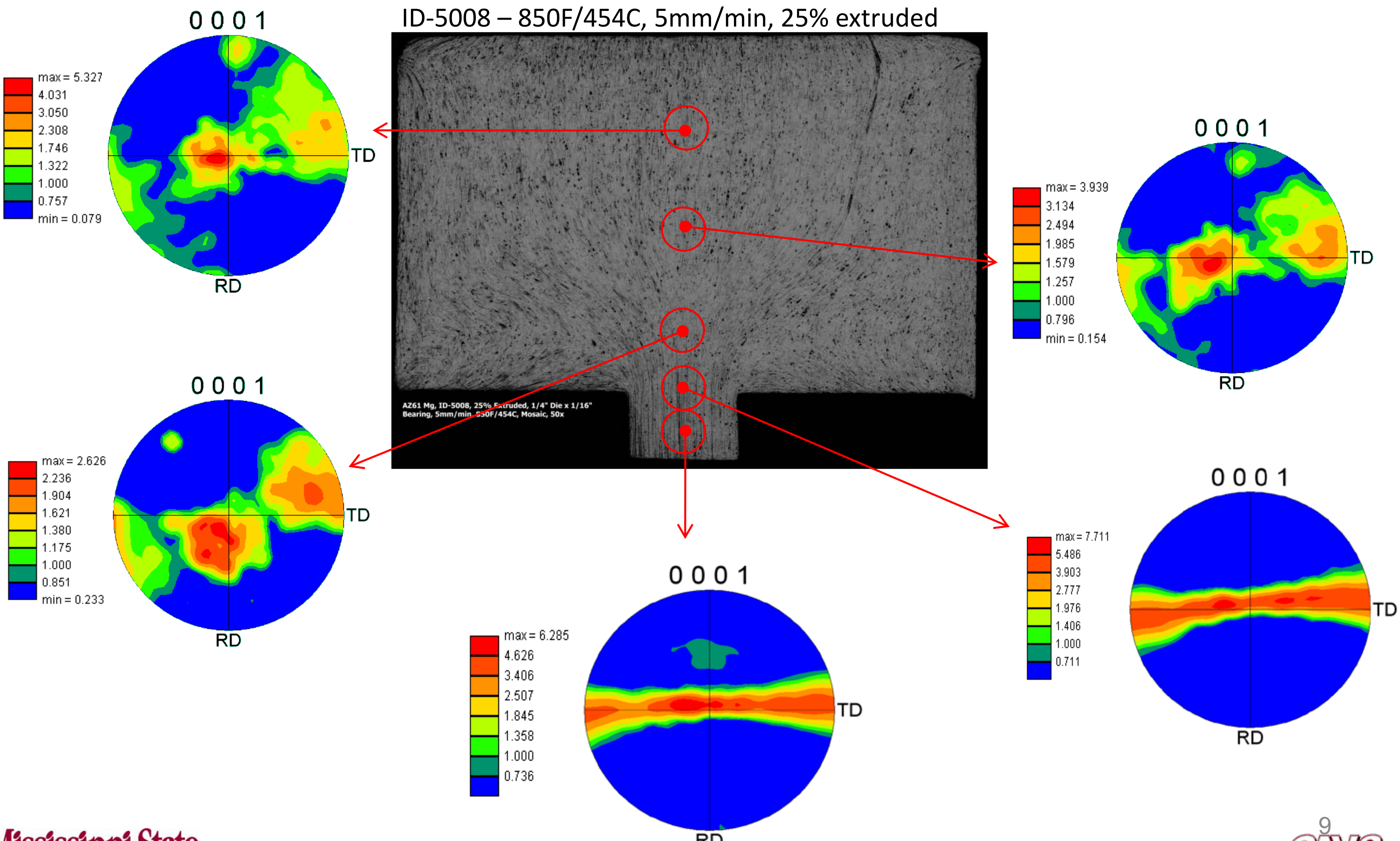
General Test Matrix: Lab-Scale Extrusion Parameters

Billet Temperature, θ_b,°C (°F)	**Ram Speed V, mm/min**	**Extrusion Ratio, ER (Orifice Diameter, D_d, in)**
454 (850)	5, 10	25, 100 (1/4, 1/8)
482 (900)	5, 10	25, 100 (1/4, 1/8)
510 (950)	5, 10	25, 100 (1/4, 1/8)

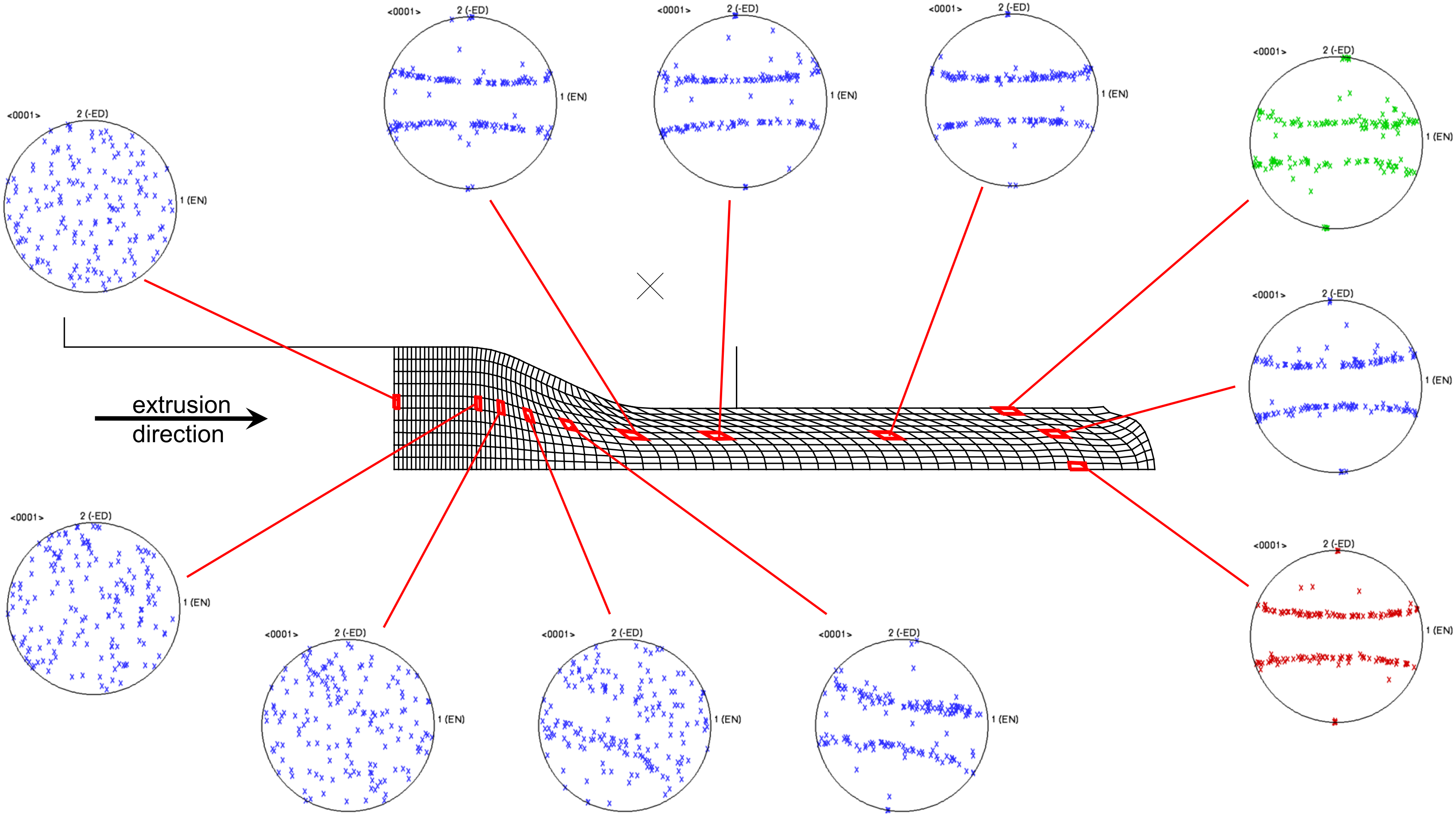
- ❖ Perform microstructure / mechanical characterization:
  - metal flow pattern
  - texture development and grain morphology
  - mechanical properties of extrudate
- ❖ Use: OIM, SEM-EBSD, Instron loading frame

Lab-Scale Extrusion Texture Measured

Data from Experiments: Texture along flow lines



Evolution of Texture during Direct Extrusion



REMARKS:

- Simulations run with ABAQUS/Standard.
- Trends to form ‘rod’-type texture predicted by simulations.
- Texture evolution is greatly influenced by the presence of dynamic recrystallization.

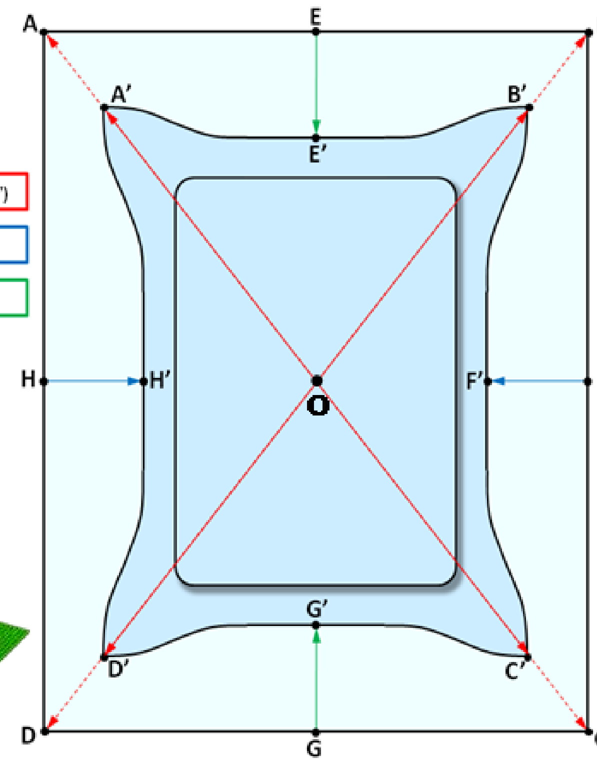
Pan Forming - Dimensions and Thickness Profiles
Material AZ31-O

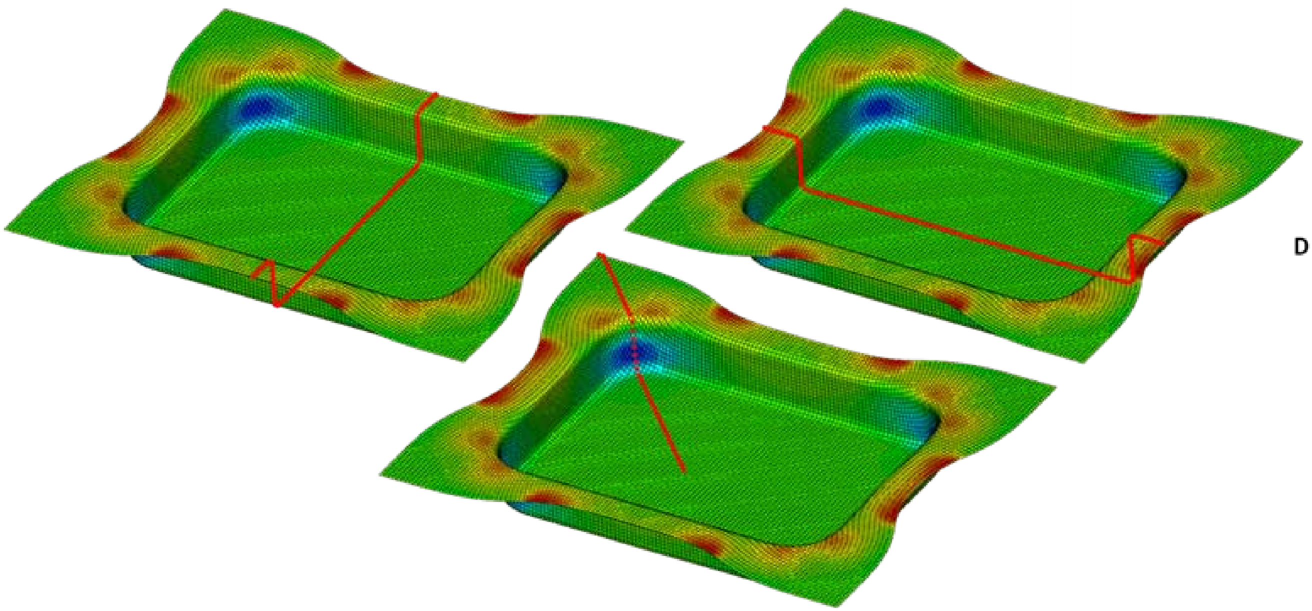
Draw Dimensions d_1, d_2 and d_3 used for comparing numerical and experimental pan forming results

$d_1 = (AC-A'C')+(BD-B'D')$

$d_2 = HH'+FF'$

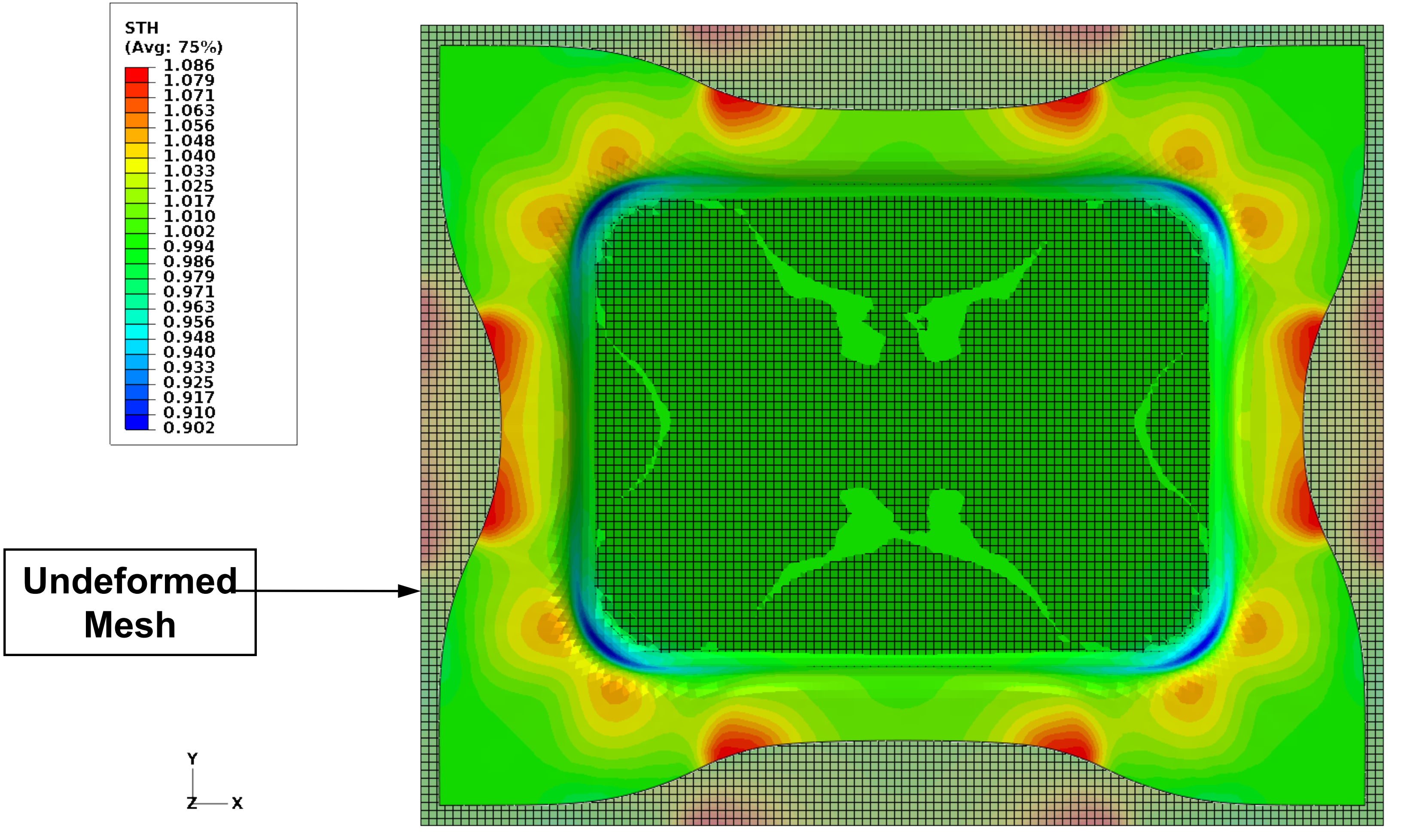
$d_3 = = EE'+GG'$



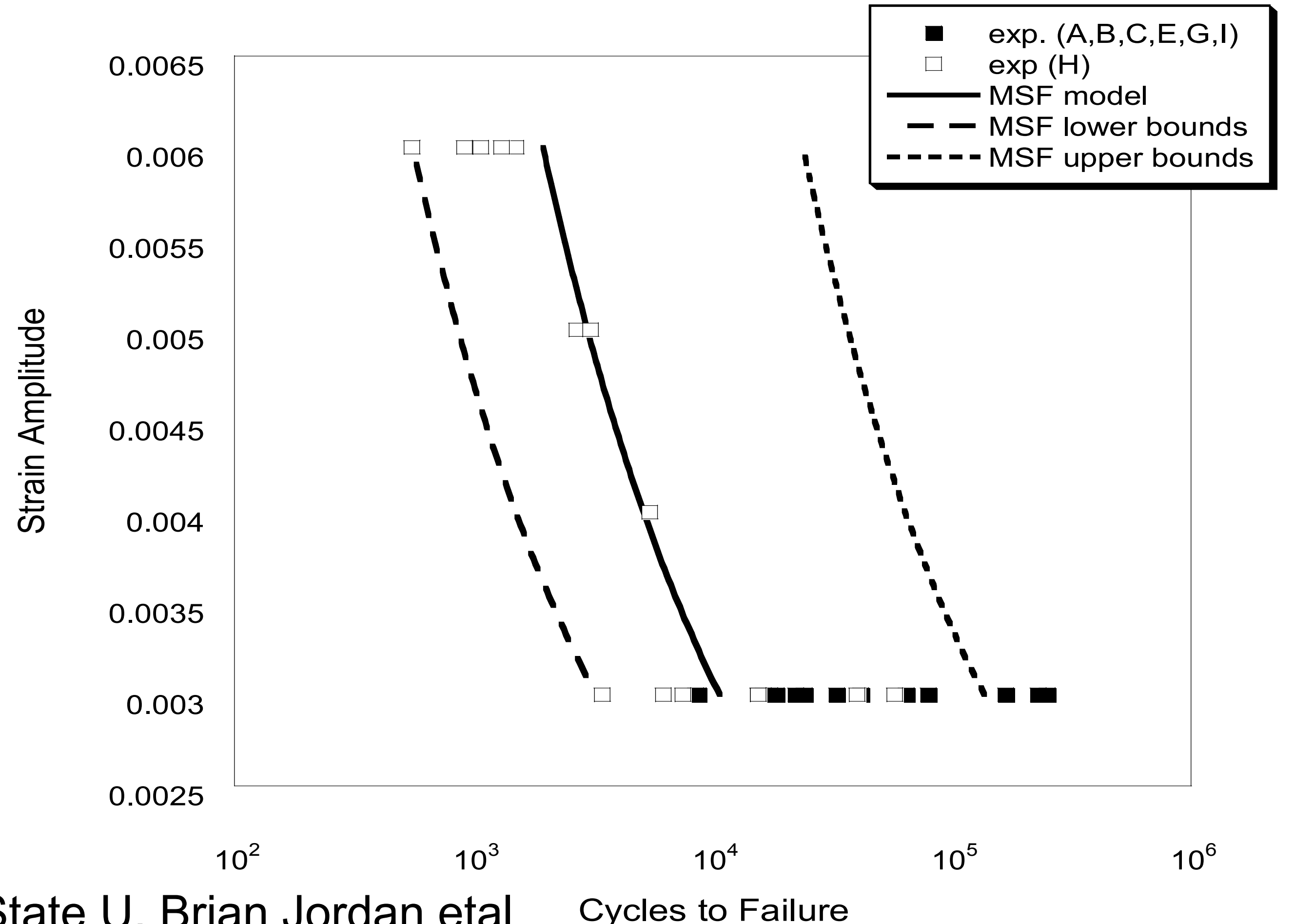


Different nodal paths for outputting thickness profiles.

Pan Forming Simulations – Shell and 3D Elements
Thickness Distribution

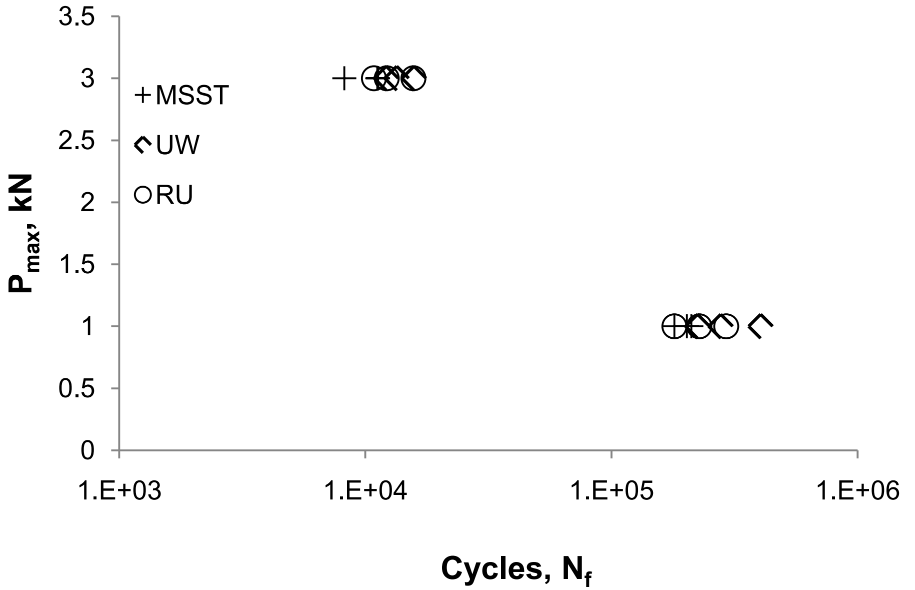


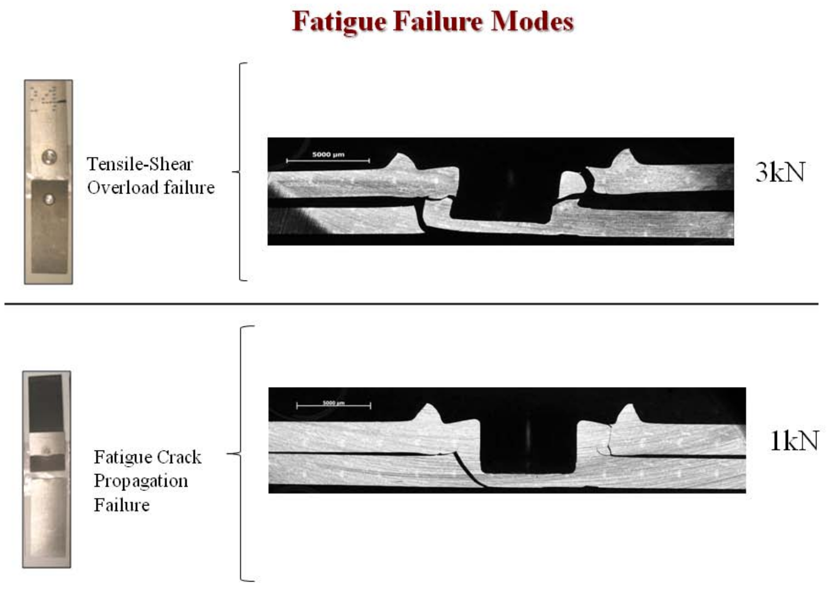
Multi-stage Fatigue Model Prediction compared with experimental results for extruded AM30



Mississippi State U, Brian Jordan etal

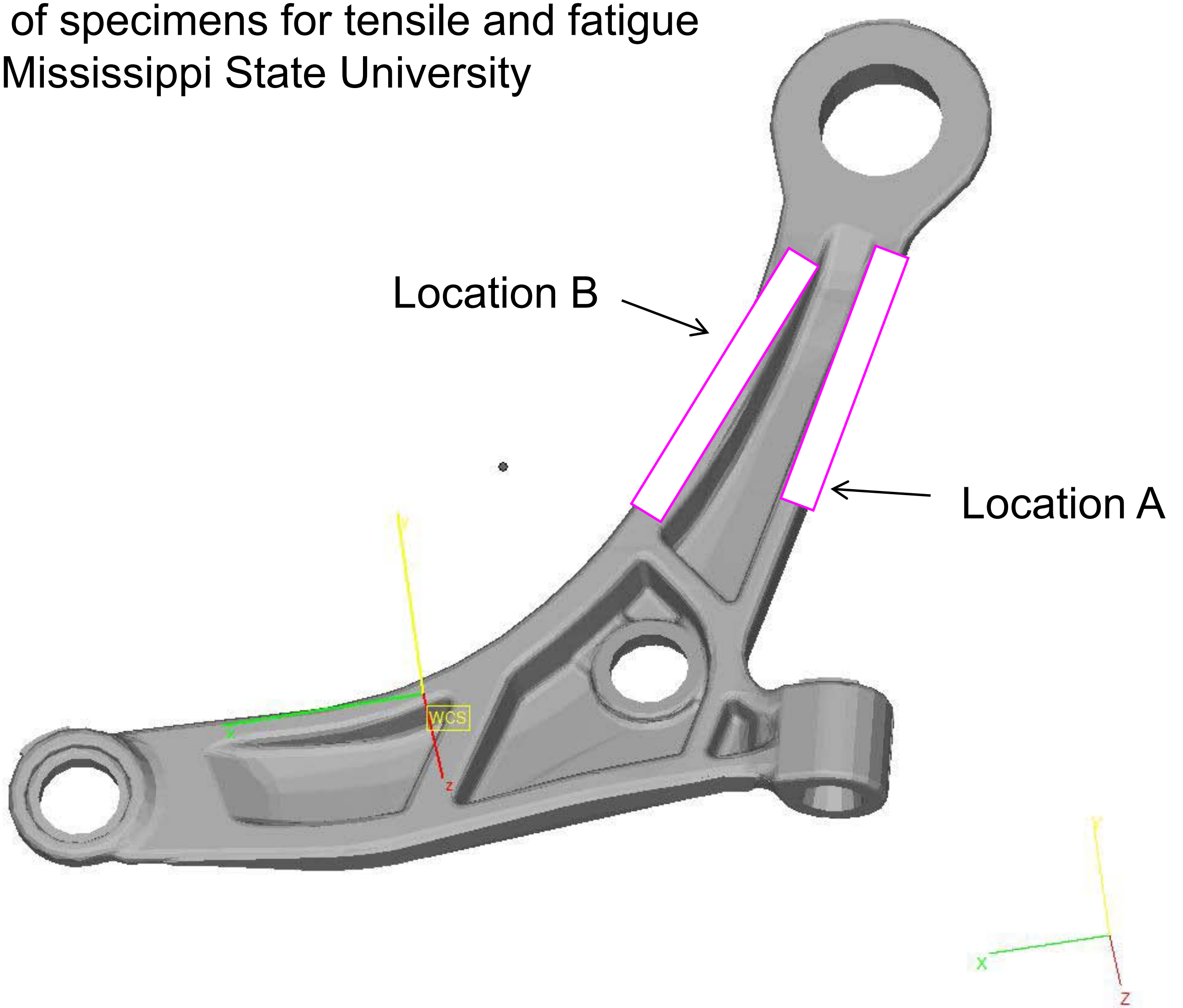
Fatigue Round-Robin: FSSW



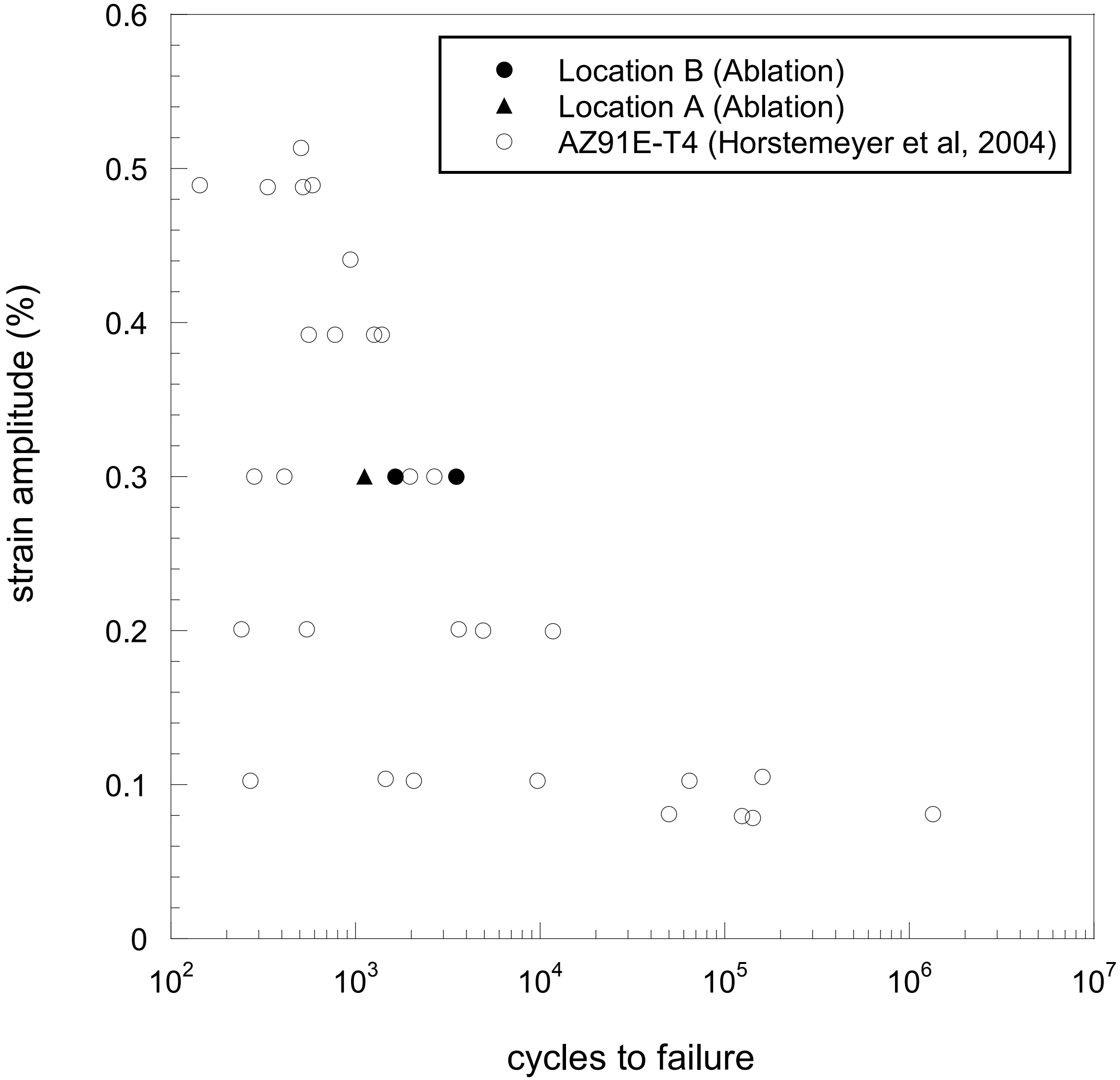


HIMAC

Locations of specimens for tensile and fatigue testing at Mississippi State University



HIMAC: Ablation vs Literature Data

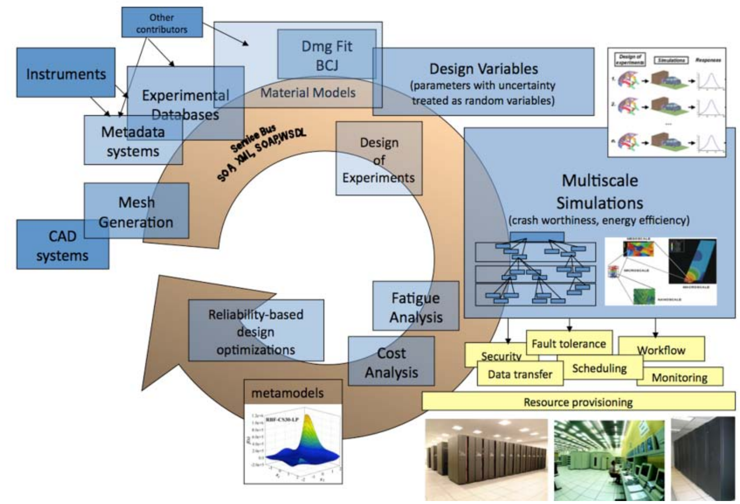


Fatigue results of Ablation castings compares well with Horstemeyer et al. data (AZ91E-T4)

Cyberinfrastructure for ICME

Goal: The objective is to develop a cyberinfrastructure to exploit the recent transformative research in material science involving multiscale physics-based predictive modeling, multiscale experiments, and design.

The development of the cyberinfrastructure will leverage tools, technologies, and software developed by other large-scale scientific cyberinfrastructure projects and will be augmented by original research in Computer Science and Software Engineering towards the creation of large, distributed, autonomic and cooperative software systems supporting virtual organizations.



SWOT Analysis:

Strengths: Experienced and recognized team of developers; unique and dominant position in MFERD/ICME community; in house expertise in both Material Science and Computer Science

Weaknesses: Insufficient number of researchers/staff to realize goals of ICME and autonomic computing; insufficient collaboration with external partners

Opportunities: Rising interest of material science communities expressing the need for the CI and refining the requirements; autonomic computing is critical for the practical use of multiscale simulations; platform for the dissemination of knowledge to peer researchers and industrial partners

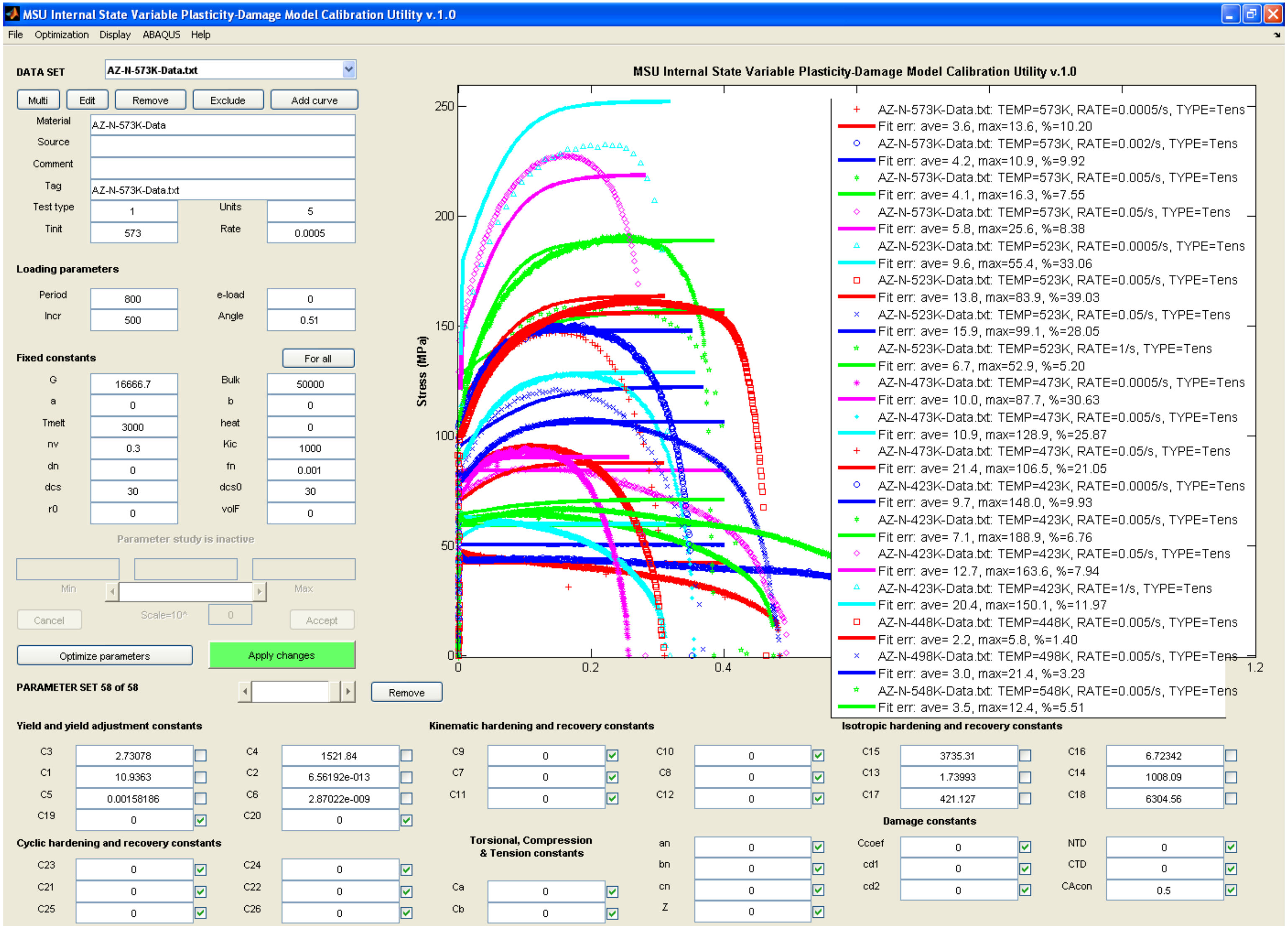
Threats: Rapidly changing technologies, competition from other cyberinfrastructure groups (e.g., Nano-Hub); possible conflict between base research and maintenance including user support.

MSU Personnel:
Tomasz Haupt (CAVS)
Florina Ciorba (CAVS)
Igor Zhuk (CAVS)
Bhargavi Parihar (CAVS)
Gregory Henley (CAVS)

Corporate Partners:
Ford Motor Co.
General Motors
Chrysler

MsSt Version I Material Fitting

AZ31-N Material Fitting using DMGfit.v1.0



Relevancy to 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

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., $MgZn_2$ 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 (MsSt)
  - 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 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.*

Key Actions and Deliverables

• Develop 10-year plans on composite/polymer with ORNL teams (Dave Warren, …)

• Refine 10-year plans on Mg and Steel with DOE teams (Will Joost)

• Participate in ICME and MFERD (Phase II, Design, Joining, …teams)

• Courting Korean companies (Hyundai – auto and steel, KiTech, Posco, several universities)

• HIMAV: Complete microstructure and fatigue data of four casting processes in June, 2010, to assist the selection of Mg cast process.

• Natural fiber: SMC panel will be delivered to ACC for review in yr. 2010.

• Multiscale Material models: Mg DMG 1.0 for sheet forming delivered to GM in May, 2010.

10 Year Plan for Magnesium Alloys

Predictive tools, new alloy design, and new Mg fabrication/product company (PDT) at MS

Magnesium (Mg) : Cast, Extrusion, Sheet, Joining

Outcomes

- ❑Verified / validated Internal State Variable material model including anisotropy, damage, twining, recrystallization, grain growth, precipitates.
- ❑Verified / validated multistage fatigue model
- ❑Material Database for Mg alloys from cast, extrusion, sheet processes.
- ❑ Lab/pilot and component/industry levels validation of modeling tools

Cyberinfrastructure

Experiments

Coupon Level. Structure-property relations for cast, extrusion and sheet specimens under diff strain rates / temperatures:
- Characterize stress response for damage, recrystallization, grain growth, twining, texture, anisotropy and precipitates.
- Tests: uniaxial/biaxial tension, plane strain compression, torsion, loading paths / directions changes, yield probing.
- Microstructure analysis at different length scales: OIM, SEM/EBSD, TEM, Xray-CT.

Fatigue. Low/high cycle fatigue, small & long crack growth, spectrum analysis, effects of mean stress, temperature, and frequency.

Heat Treatment:. Solution treatment, aging, precipitation, eutectic phases, intermetallics

Lab-Scale / Pilot Scale Level. Processing-structure-property relations using in-house fixtures for casting, extrusion (direct / indirect) and sheet (stamping / hemming).

Component / Industry Scale Level. Characterize property-performance relations through component testing (extruded tube / sheet pan crushing) and industrial collaboration testing (extrusion and multistage sheet forming processes)

Modeling / Simulation

Internal State Variable (ISV) material model incorporating texture-induced anisotropy, damage, twinning, recrystallization, grain growth and precipitate hardening.

Multistage Fatigue (MSF) model.

Precipitation and aging modeling. Include precipitate hardening into ISV model

Robust Finite Element models and Uncertainty-Based Optimization Techniques for extrusion/ sheet forming processes and lab / pilot scale and component / industry levels applications.

Year 2 | Year 4 | Year 6 | Year 8 | Year 10

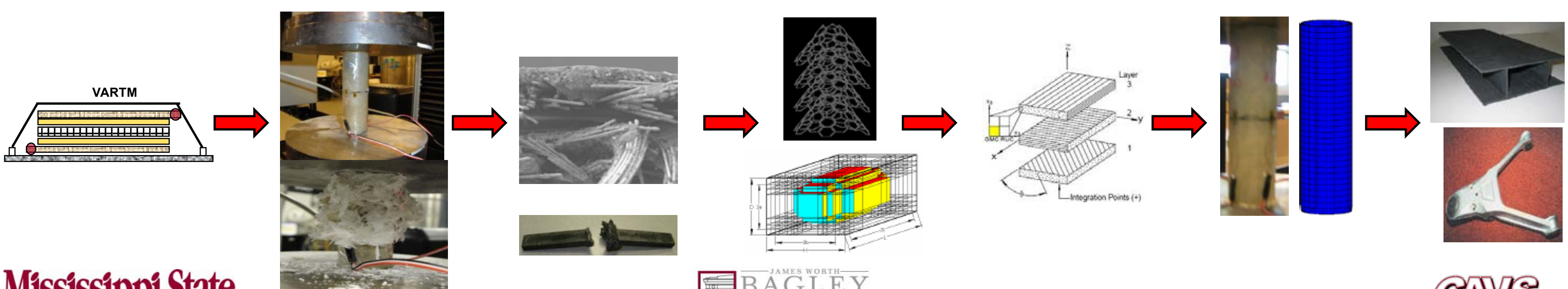
Mississippi State UNIVERSITY

CAVS

Back up slides

NanoComposite: Tactical Timeline

Year	2008				2009				2010				2011			
Quarter	Q 1	Q 2	Q 3	Q 4	Q 1	Q 2	Q 3	Q 4	Q 1	Q 2	Q 3	Q 4	Q 1	Q 2	Q 3	Q 4
Task 9. Structural Nanocomposite Design																
9.1. Investigate effect of configuration /processing parameters on optimal nanocomposite properties																
9.2. Investigate effect of configuration /processing parameters on optimal nanoreinforced continuous fiber composite properties																
9.3. Quantify the structure-property relations experimentally																
9.4. Study material failure modes under different loading conditions																
9.5. Develop multiscale materials modeling methodology for nanocomposites																
9.6. Develop a proof of concept experiment																
9.7. Incorporate experimental data and models into cyberinfrastructure.																



Task 12: K-12 Education

K-12 Education

Researchers: R. Cuicchi, P. Cuicchi

Goal:

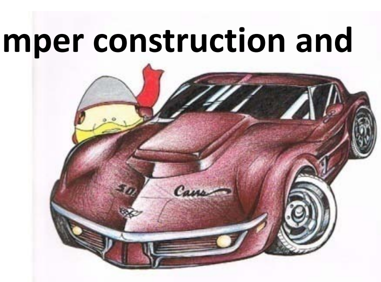
- Development of a K-PhD program (Mission Eggcellence) that communicates the importance of crashworthiness and safety issues in design and construction of vehicles
- Utilization of a "Car Crash Curriculum" to educate K-12 teachers and students through teacher workshops and student competitions

Scope of Work:

- Create a grade appropriate curriculum with experiments and problems associated with the Physics of car crashes for grades K-2, 3-5, 6-8, 9-12.
- Develop a Teacher Workshop and supply equipment for grades K-12 teachers for training in use of the grade appropriate curriculum in the regular classroom.
- Design a competition for grades K-2, 3-5, 6-8, 9-12 incorporating bumper design for passenger safety.
- Design a competition for grades K-2, 3-5, 6-8, 9-12 incorporating car design for passenger safety.

Approach:

Address the needs of the children of the State of MS in the areas of mathematics and physics through the applications of physics through real world applications in the areas of automotive bumper construction and automotive design to ensure passenger safety in car crashes



Mississippi State UNIVERSITY

SAE will adopt these Kits for its community outreach nationwide

CAVS

Phase II Cost Share Committed (yrs 3 and 4)

- USAMP* $120,000 $120,000 $360,000
- SAC $98,800 $100,000
- POSCO $93,000 $93,600
- AlphaStar* $172,000 $172,000
- Mimics $16,680
- Dassault System $13,885
- ESI $**130,500**
- Lousisiana Pacific $150,000
- M&S Co $144,000
- MSC $59,400
- Manufacturing Service and Development, Inc., $15,000
- CAVS $100K
- Total Phase II >= $1M

SRCLID Partners (Blue Designates Potential Partners)

ISV w Uncertainty
Tower Automotive
AMPS Technology
USAMP
Ford Motor Co.
General Motor Co.
ABAQUS
Wade Services, Inc.
Mitsubishi
USX
Norsk Hydro
Gibbs
American Iron and Steel Institute
Alcoa

Fatigue
Front-end Mg Project (GM, Dick Osborne/Don Penrod)
nCode
Alcoa

Cyberinfrastructure
Ford Motor Co.
General Motor Co.
USAMP

Nano-Composite
Alpha Star
USAMP
Southern Clay Products

Natural Fiber
Kengro Co
Louisiana Pacific
Wood Forest, MsSt
ME Dept, MsSt

Design Optimization
Vanderplaats Research and Development, Inc
MSC Software
Wade Services, Inc.
Front-end Mg Project (GM, Ford, DCC)
Mitsubishi Motors
Simufact-America
F-Tech

Materials Design
Wade Services, Inc.
POSCO
SAC
M & S
AISI
Auto Steel Partnership

LENS
NASA
NSF
Army-TARDEC
Optomex

Bio-Inspired
Mimics

Education
Vista Engineering
Mississippi Children Museum
Nissan Foundation

DOE Partners: HIMAC, MFERD, ORNL, PNNL Teams

Budget History for DOE SRCLID Program

Aug. 2006 – Aug.

$2 M

Aug. 2007 – Aug. 2008

$2 M

$4 M, Phase I

Aug. 2008 – Aug. | **Aug. 2009 – Aug. 2010**

$3 M | **$1 M**

$4 M, Phase II

Aug. 2009 – Aug. 2011

$2 M | **$2 M**

$4 M, Phase III

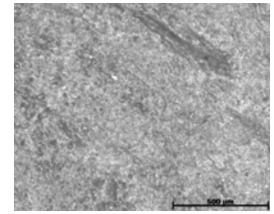
Mg Corrosion Quad Chart

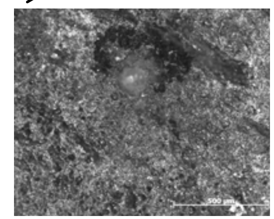
Goal

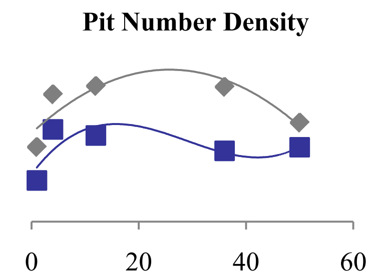
Develop a multiscale internal state variable model relating structure-property effects from bulk hydrogen and corrosion effects on magnesium alloys

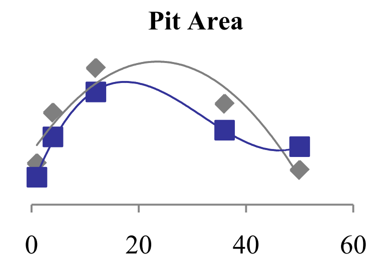
Team Members

M.F. Horstemeyer (PI), **S. Groh** (MD/DD), **H. Martin** (corrosion tests)**, K. Solanki** (continuum ISV model)**, D.J. Bammann** (continuum ISV model).









Sub-Tasks

4.1: Determine effects of bulk hydrogen on Mg from molecular dynamics.

4.2: Determine hydrogen effects on mobilities from molecular dynamics for dislocation dynamics codes.

4.3: Include hydrogen induced mobilities into dislocation dynamics codes for Mg alloy design.

4.4: Develop and Implement new damage laws into crystal plasticity with consideration of hydrogen.

4.5: Explore the development of Internal State Variable laws incorporating hydrogen effects from lower length scale results.

4.6: Perform experiments to validate the results: perform corrosion spray tests and measure pitting responses.

Approach

➢Perform multi-scale modeling to quantify mechanisms for corrosion and bulk hydrogen effects on magnesium alloys

➢Perform experiments with various environmental conditions to quantify corrosion mechanisms and effects

➢Use data collected from experiments to calibrate an Internal State Variable Model

Corrosion Annual Deliverables

- 2009
  - Modeling:
    - Development of Mg and Mg-H MEAM potential
    - Influence of H on dislocation from basil slip system
  - Experimental:
    - Completion of as-cast AE44 and polished AE44 data collection and data analysis
    - Determination of most corrosive cyclical test cycle
- 2010
  - Modeling:
    - Influence of H on dislocation from prismatic slip system
  - Experimental:
    - Completion of AZ61, AM60, AZ31, and AZ91 data collection and data analysis
- 2011
  - Modeling:
    - Effect of H on the mechanical response by DDD
  - Experimental:
    - Completion of Corrosion and Creep of AZ61 and AM60

Task 5: High Strain Rate Impact Fracture Modeling

Researchers: Phil Gullett, Mark Horstemeyer, Don Ward, Neil Williams, Matthew Priddy, Will Whittington

Goal:
- Establish a relationship between damage evolution and stress state under high strain rate loading for lightweight materials
- Implement relationship in microstructure-property model
- Evaluate numerical procedures for modeling of monotonic fracture.

Approach:
- Perform Split Hopkinson bar experiments in compression, tension and torsion at strain rates of (10^3 to 10^4/sec).
- Develop interrupted testing procedures for high strain rate tests.
- Establish quantitative analytical relationships for high strain rate damage evolution and incorporate into the microstructure-property model.
- Validate these tools, for robustness, by a critical set of experiments representing fracture mechanisms occurring in engineering applications.
- Implement microstructure-property model in a fracture simulation code

Sub-Tasks

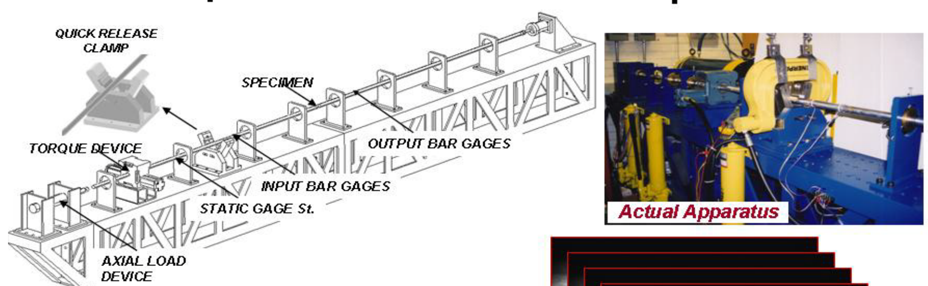
Experimentation

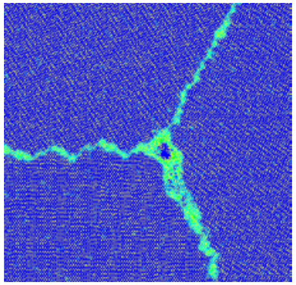
5.1 – Split Hopkinson Bar – Tension/ compression/ torsion
5.2 – Coupon/Component Scale Tests
5.3 – Metallurgical characterization – Pretest NDE

Modeling

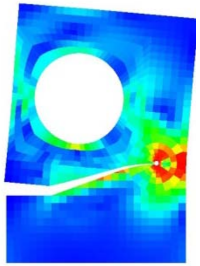
5.4 – Microscopic Damage Processes – Polycrystalline molecular dynamics simulation, Microscopic damage evolution, Hierarchical model development, ISV model development.
5.5 – Meso and Continuum Damage Modeling
5.6 – Computation Method Development – Plastic localization, Fracture simulation techniques

Hopkinson Bar Setup

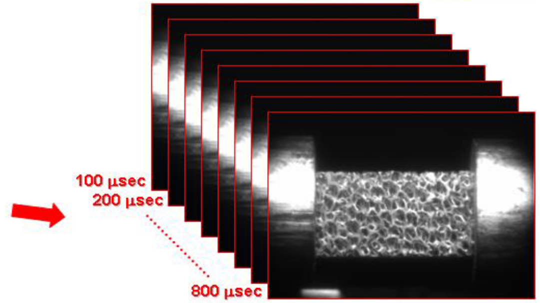




Nanoscale



Macroscale Fracture



Experimentation