Mechanistic-based Ductility Prediction for Complex Mg Castings

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2014 DOE VEHICLE TECHNOLOGY PROGRAM REVIEW
JUNE 16-20, 2014

Project ID#: LM057

Overview

- Timeline
  - Start: Oct. 2010
  - End: Sep. 2014
  - 80% Complete
- Budget
  - DOE - $1,800K
    - FY11 - $600k
    - FY12 - $600k
    - FY13 - $500k
    - FY14 - $100k
  - Industries (in-kind) - $900K
    - Industry - $300k/YR FY11-13
- Barriers
  - Limited ductility of Mg castings hindering its wider applications as vehicle components
  - High ductility variations
  - Lack of capability of conventional computational software/models in predicting ductility of Mg castings, resulting from various types of defects
- Partners
  - Ford Motor Company
  - University of Michigan
  - Mag-Tec Casting Corporation
  - CANMET Materials Technology Laboratory

Project Objectives

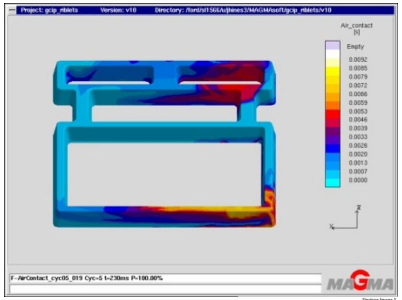
- Background and motivation
  - Conventional computational technique (i.e., homogenization, continuum damage mechanics, crystal plasticity) and some phenomenological approaches have no or very limited ductility predictive capability for Mg castings
- Objectives: To provide a modeling framework that can be used in future Mg alloy design and casting process optimization by
  - Developing an empirical casting process simulation tool that can *estimate the variation in ductility* and be used by the casting industry in the near future
  - Developing a *mechanistic-based predictive capability* on key factors controlling Mg ductility that can be coupled with future advances in casting process simulation and will lead to further casting process optimization and alloy design

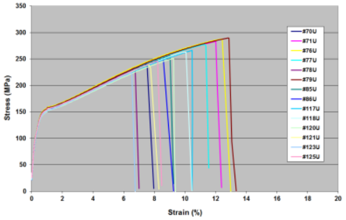
Deliverables

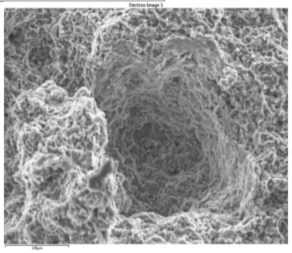
- A validated simulation tool (quality map approach) for estimating the spatial variation of ductility and the influence of casting process variables (completed)
- Modeling and experimental methods in quantifying location-dependent intrinsic and extrinsic ductility limiting factors for complex Mg castings (completed 9/30/2013)
- Experimentally validated predictive models for stress versus strain curves, including ductility, for Mg castings considering both intrinsic and extrinsic ductility limiting factors (on-going; due 9/30/2014)

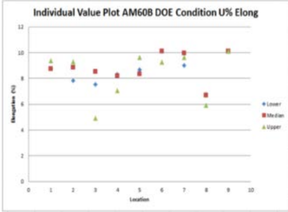
Technical Approaches

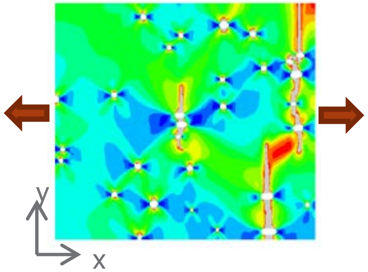
- Cast a number of AM50/AM60 castings of complex geometries under a variety of conditions (i.e., melt temperature, shot speed, die temperature, gating geometry) – *Ford, MagTec Ind., CANMET Mat. Tech. Lab.*
- Perform alloying and casting process simulation to predict spatial variations in casting defects and other microstructural features under different conditions – *Ford*
- Characterize microstructure and defect features at various locations of the castings and perform tensile tests with samples machined from various locations – *U. of Michigan, Ford*
- Develop a quality-mapping capability for estimating/controlling ductility of Mg castings based on tensile test results and various casting parameters – *U. of Michigan, Ford*
- Develop a mechanistic-based ductility prediction capability with separate consideration of intrinsic factors and extrinsic factors - *PNNL*

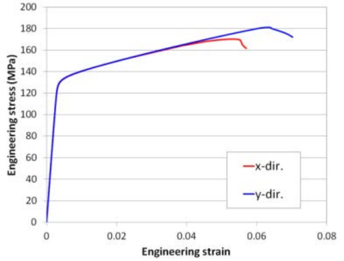




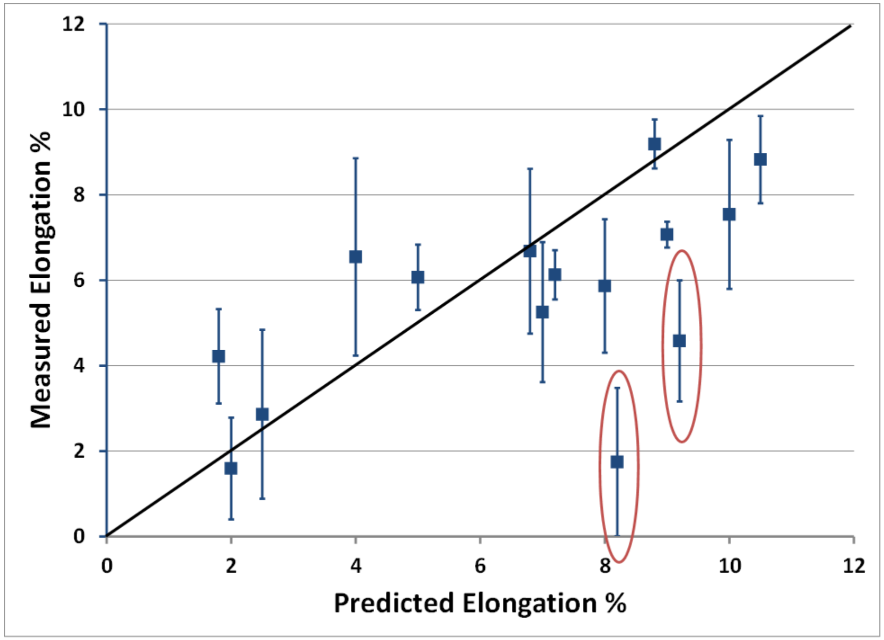


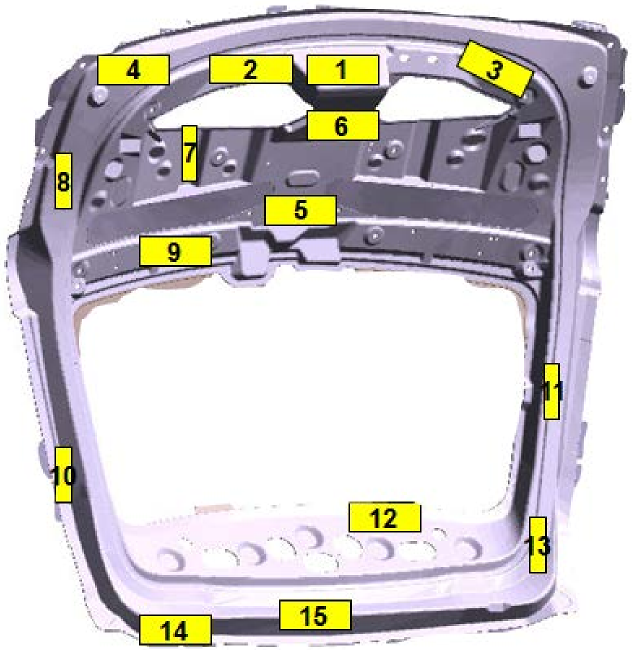






Previous Ford Accomplishment



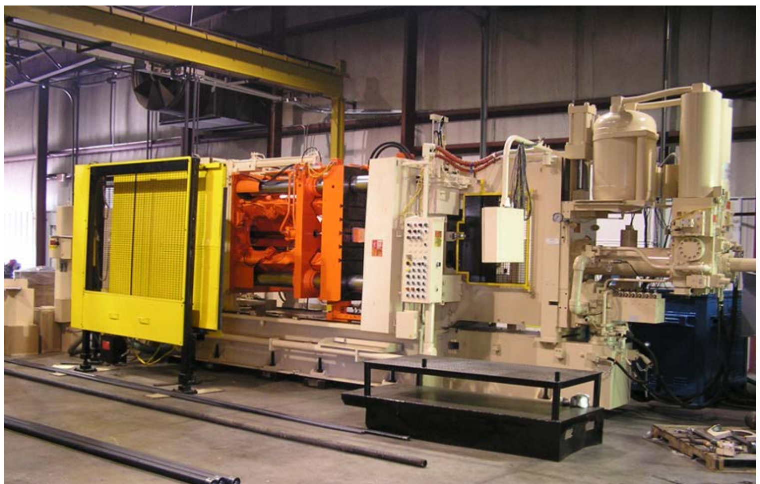


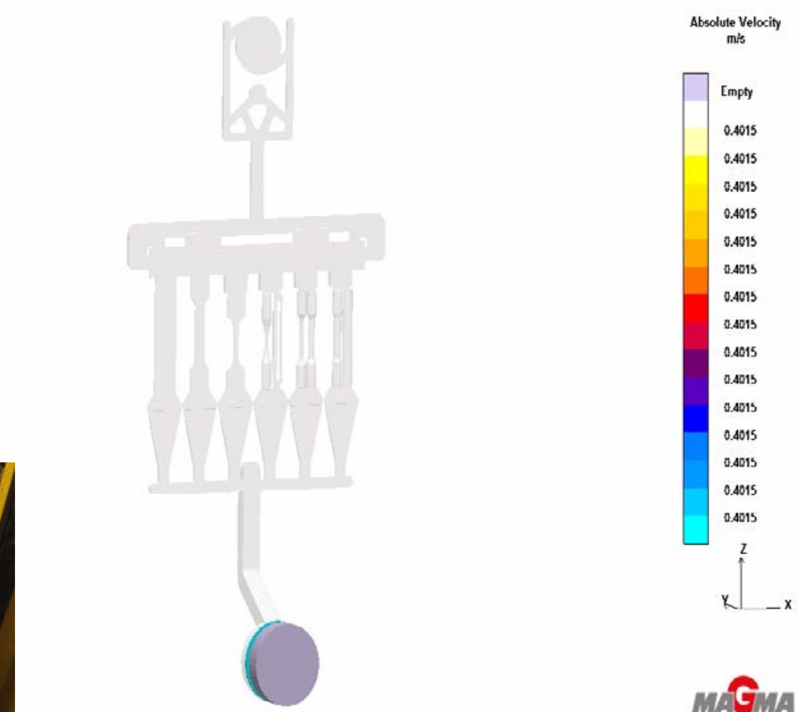
Sample locations

- Measured elongation with error versus predicted elongation. Agreement was acceptable except for 2 locations (circled)
- Need further understanding of statistical variation of elongation

FY14 Accomplishments - Ford

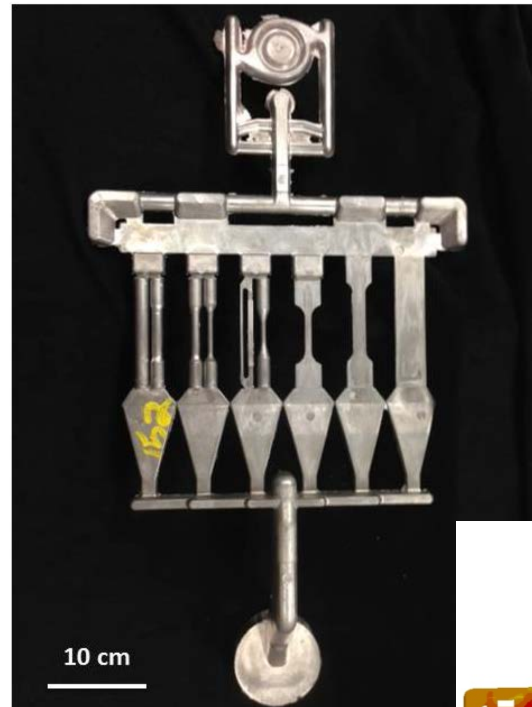
- Designed and manufactured new die cast insert to produce tensile and bend specimens

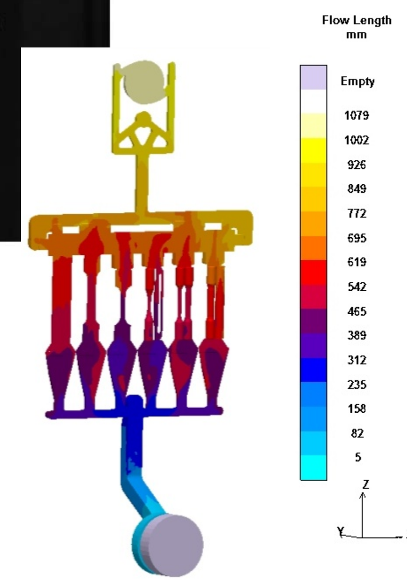




FY14 Accomplishments - Ford

- Test specimens to be used for determination of:
  - Statistical variability from machined versus as-cast samples
  - Skin effects

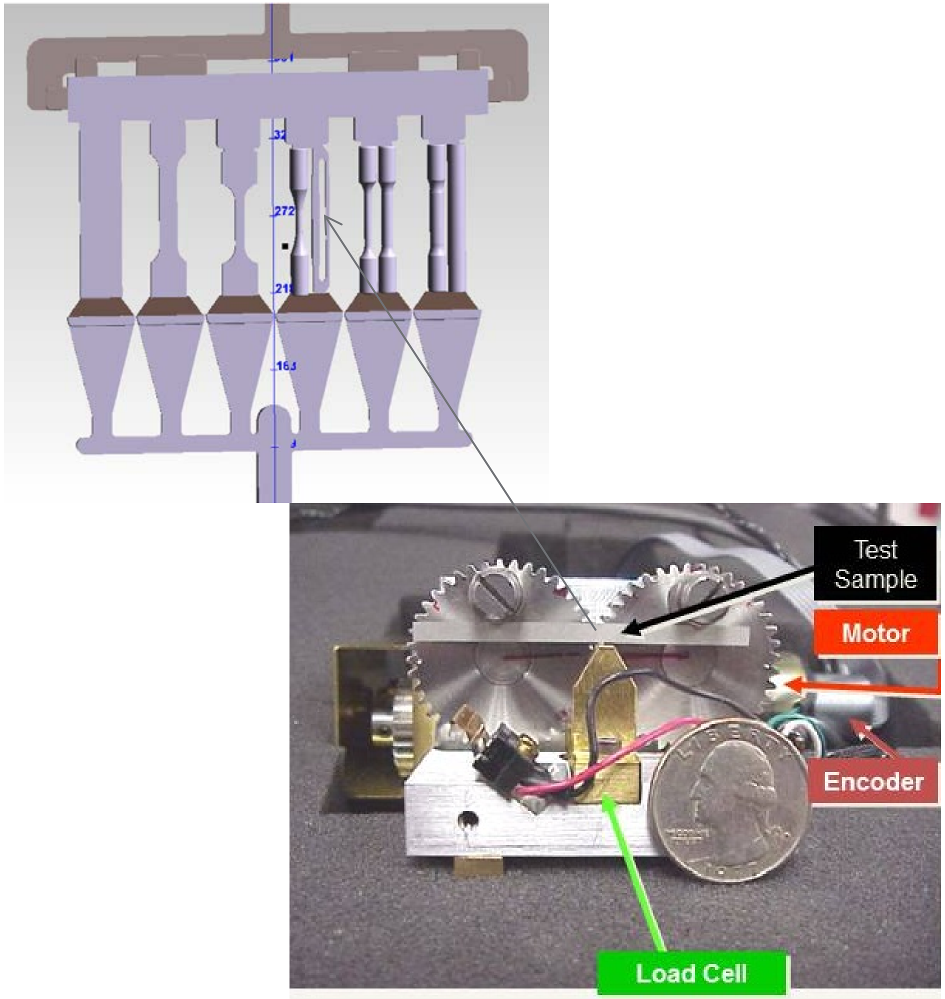




MAGMA

FY14 Accomplishments - Ford

- Retro-fit existing SEM to accommodate “in-situ” bending of Mg alloy samples
- Crack Propagation in samples with different aluminum content will be investigated to determine influence of:
  - β phase
  - α phase
  - Porosity
  - skin

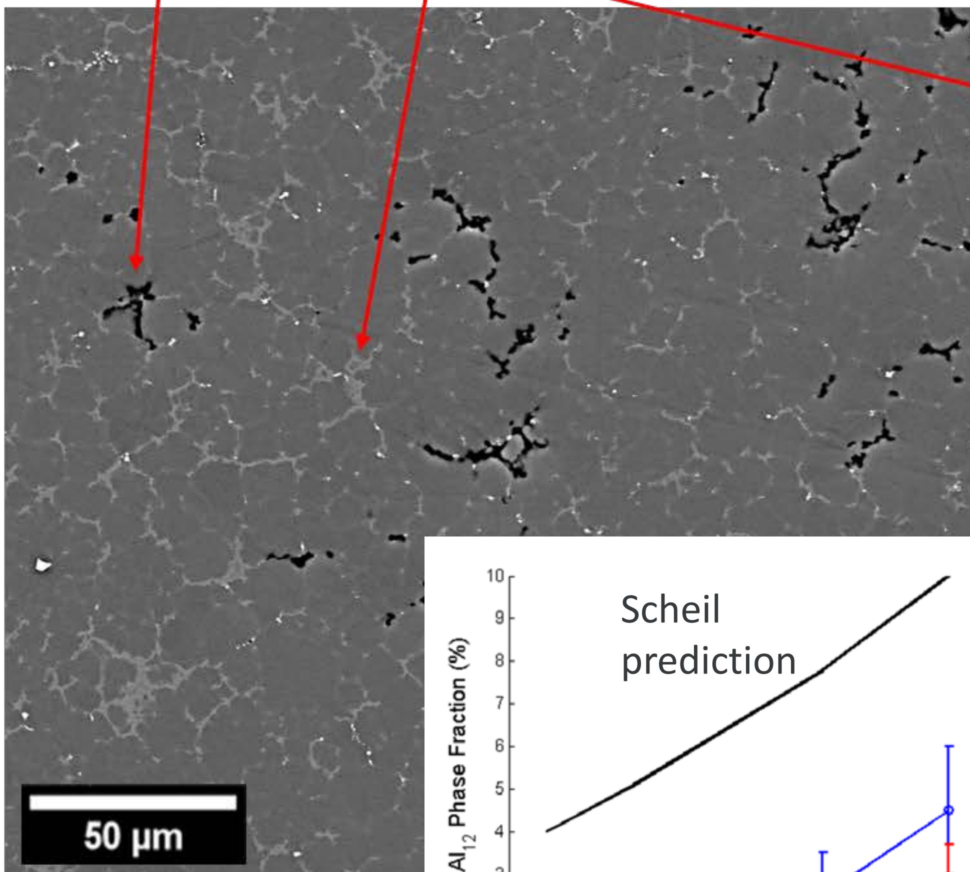


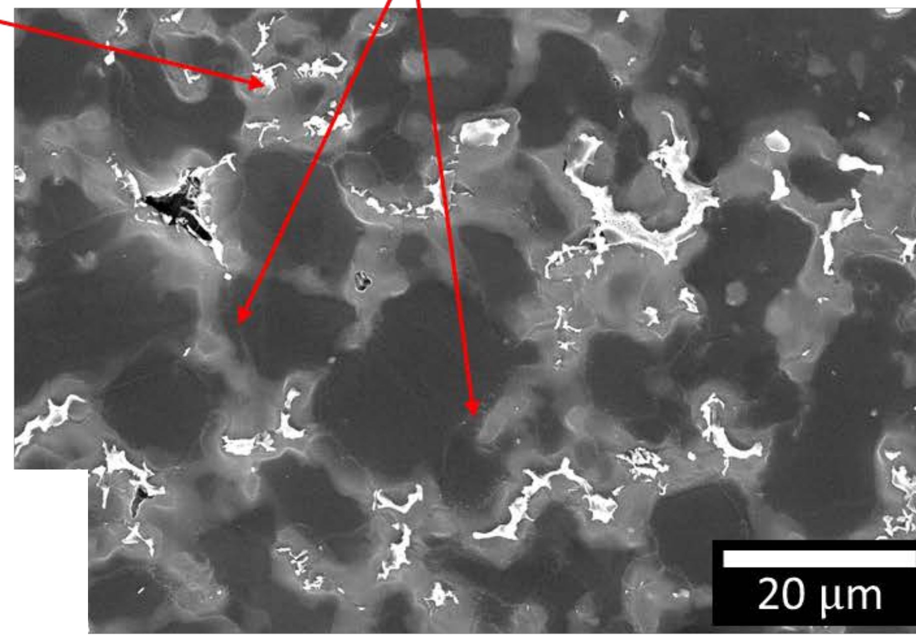
UM + Ford – Cast and Characterize Shrinkage Porosity and β-$Mg_{17}Al_{12}$ in SVDC AM Series

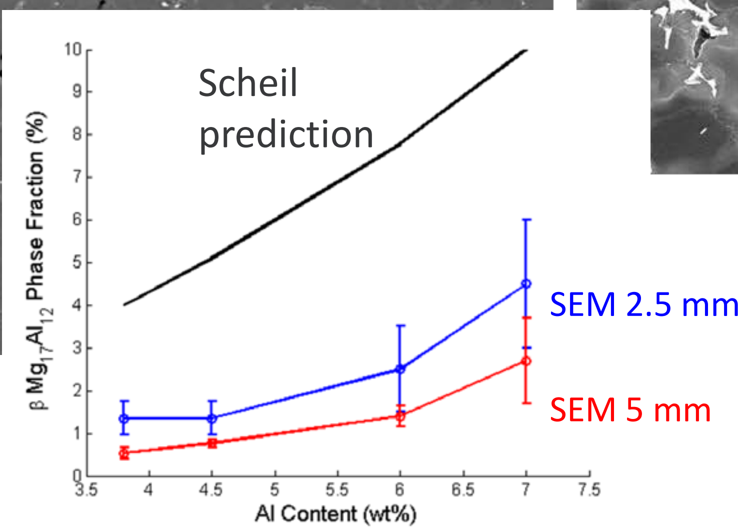
Shrinkage porosity

β-$Mg_{17}Al_{12}$

Grain boundaries



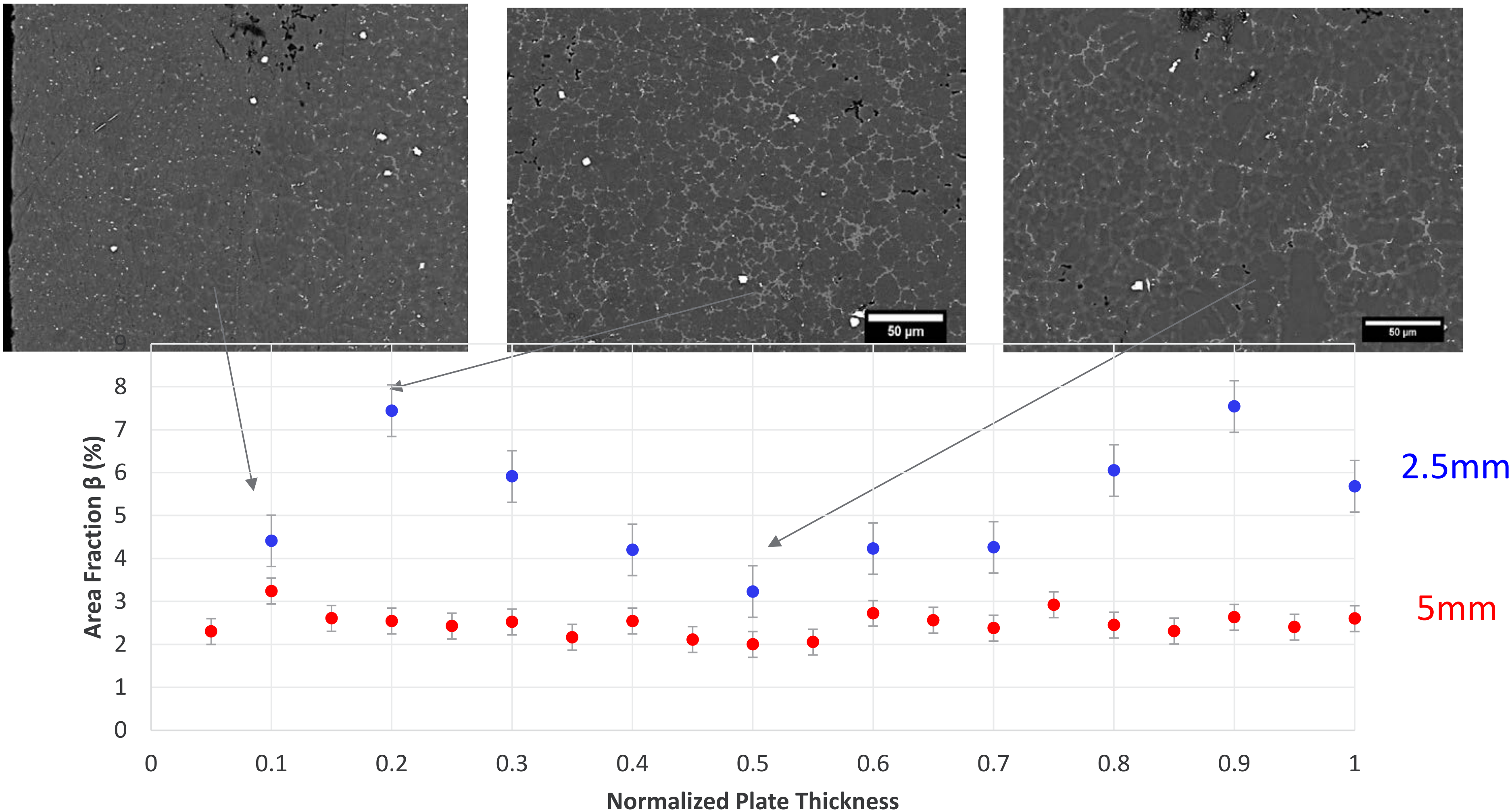




Average β area fraction increases as Al content is increased and as thickness is decreased. It is much lower than that predicted from “Scheil” solidification calculations

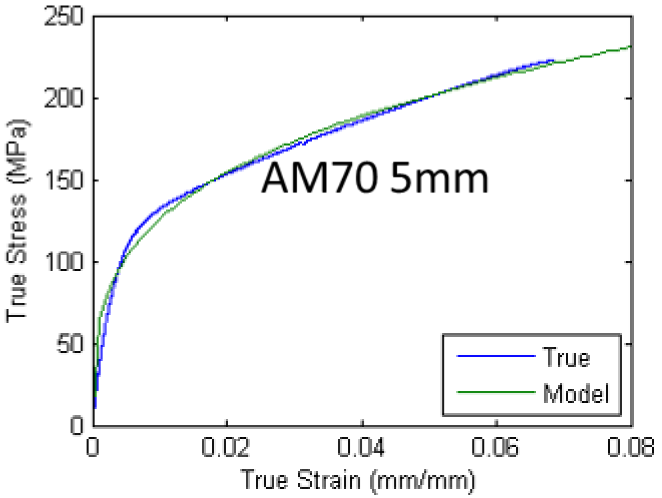
UM -- Developed quantitative methods for characterizing β-phase volume fraction and morphology

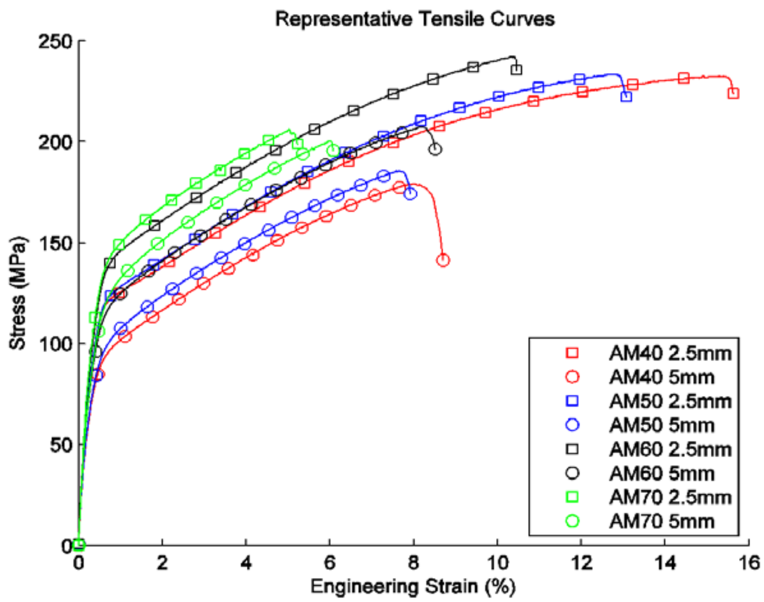
- Morphology changes from "isolated" at plate surface to "interconnected" in center of SVDC cast plates
- β phase formation varies strongly through thickness of the plates and depends on plate thickness



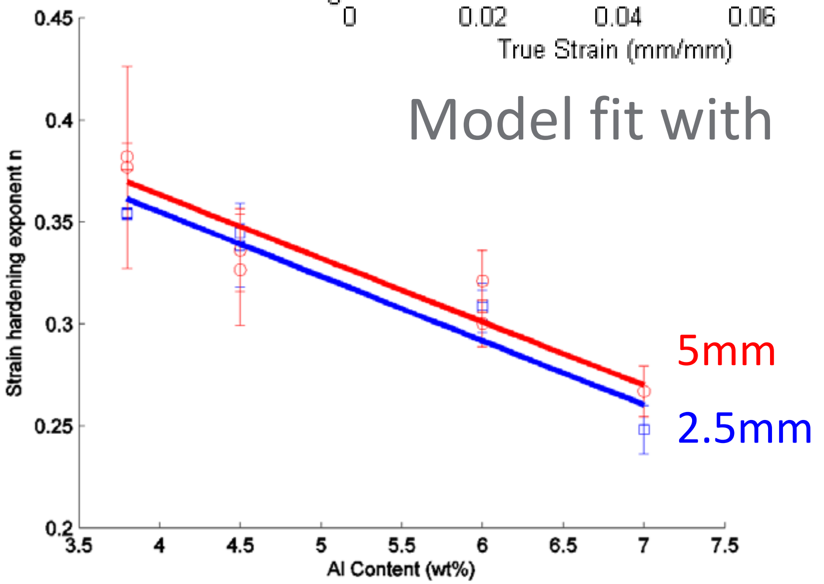
UM - Tested over 140 Tensile Samples from 16 SVDC Plates Produced by Ford

- Established major, statistically significant reference database quantifying the influence of composition and plate thickness on tensile behavior
- Quantified influence of Al composition and plate thickness on strain hardening exponent decreases



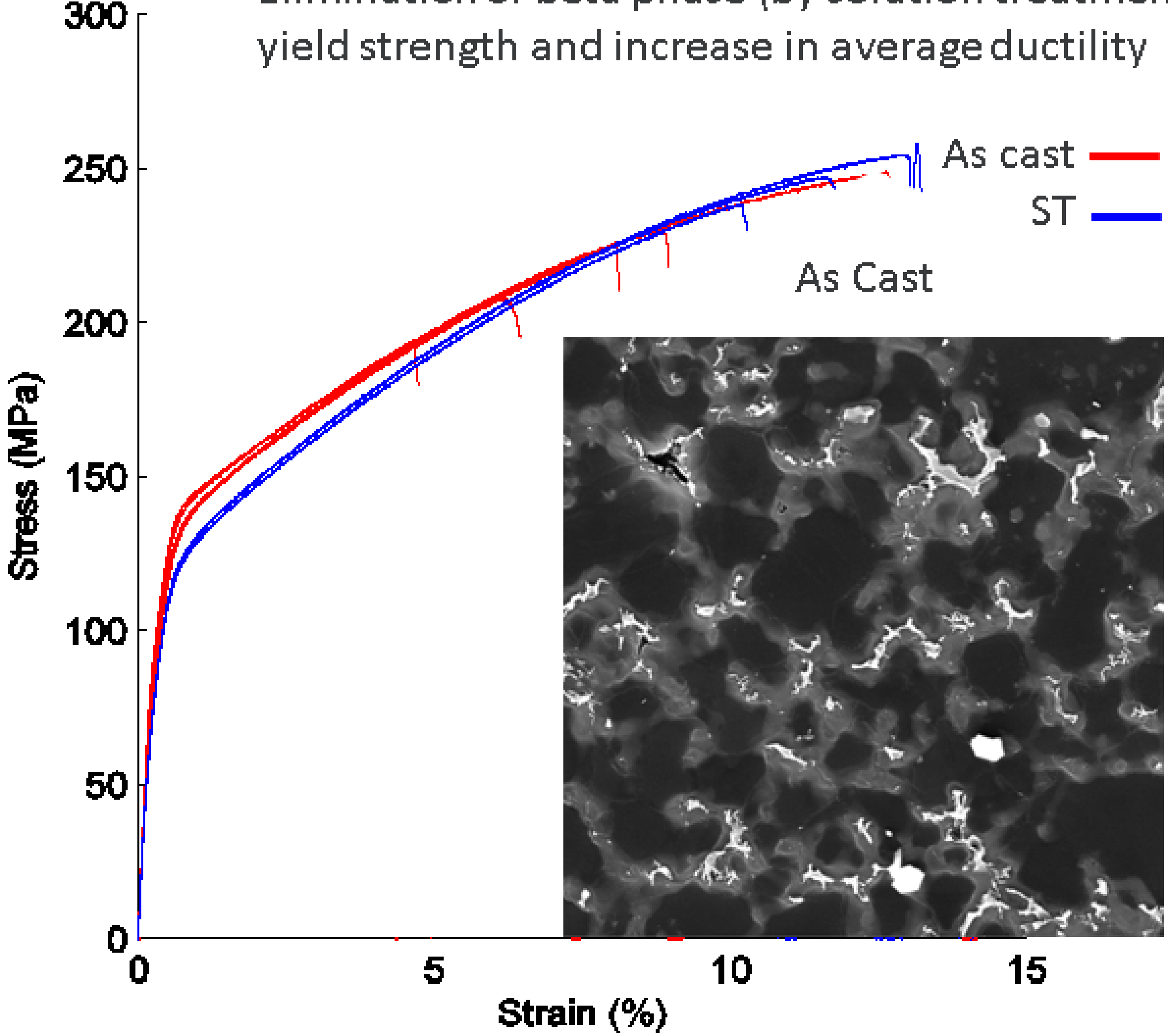


Model fit with



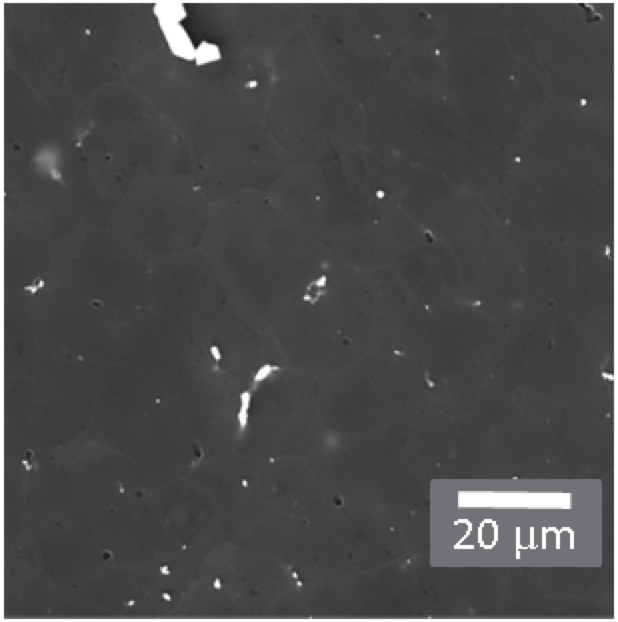
UM -- Completed initial solution treatment and planned for hot isostatic pressing experiments
- Quantify the influence of β and shrinkage

- Elimination of beta phase (by solution treatment) leads to decrease in yield strength and increase in average ductility



As Cast

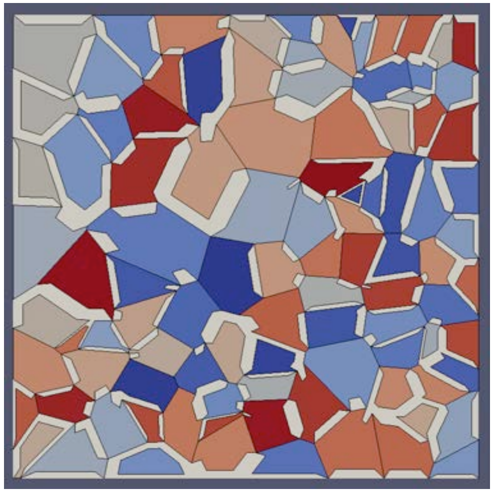
Solution Treated



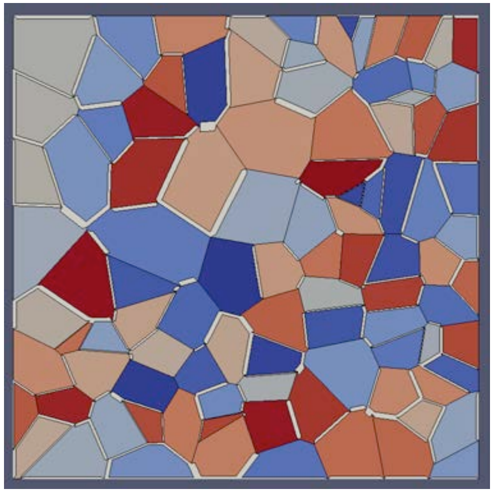
PNNL – Validated Intrinsic Model Considering Various β Volume Fraction and Morphology

- α phase properties extracted from nanoindentation[1,2]
- β phase properties calculated from first-principles[3]
- Synthetic geometries generated to represent UM/Ford observations

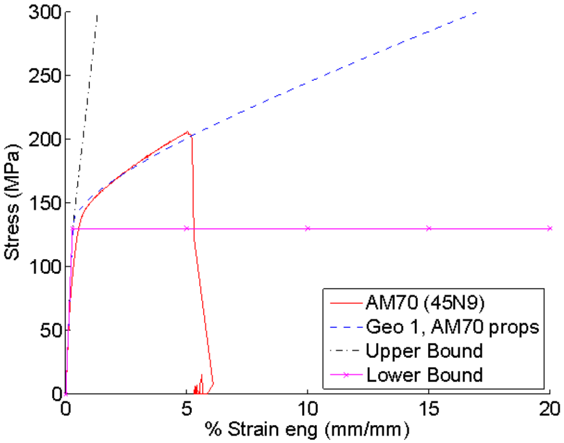
- AM70
  - E = 38 GPa 5%
  - σ_y = 130 MPa 5%
  - h' = 0.1 MPa 10%
  - ν = 0.35
- AM40
  - E = 35 GPa 5%
  - σ_y = 120 MPa 5%
  - h' = 0.1 MPa 10%
  - ν = 0.35
- β
  - AM70: 21% VF (*t*=10%)
  - AM40: 8% VF (*t*=5%)
  - E = 77.7 GPa
  - ν = 0.35

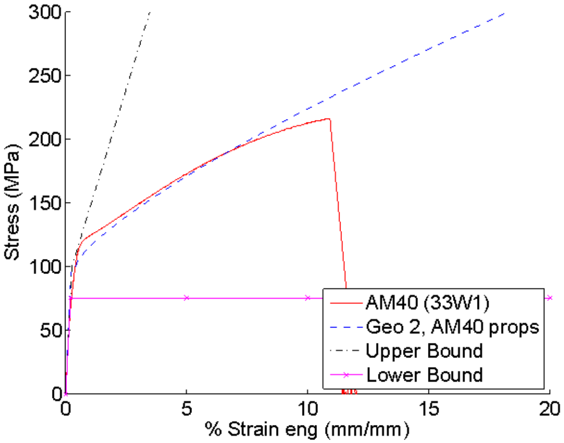


AM70



AM40

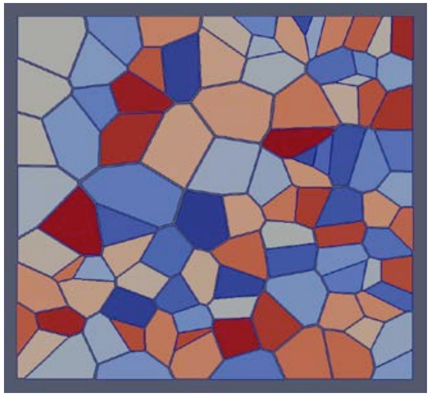




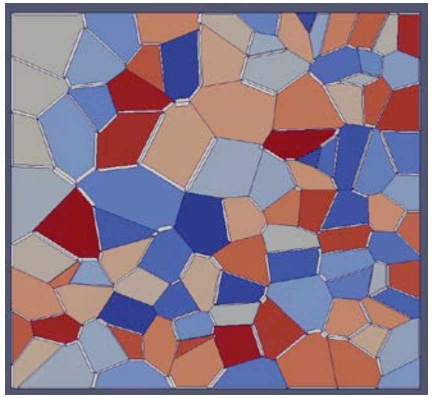
[1] Han et al., Materials Science and Engineering A, 473 (2008) 16-27
[2] Shan, Gokhale, Materials Science and Engineering A, 361 (2003) 267-274
[3] J. Wang, et al., Calphad, 35 (2011) 562-573

PNNL -- Effects of β Phase Morphology

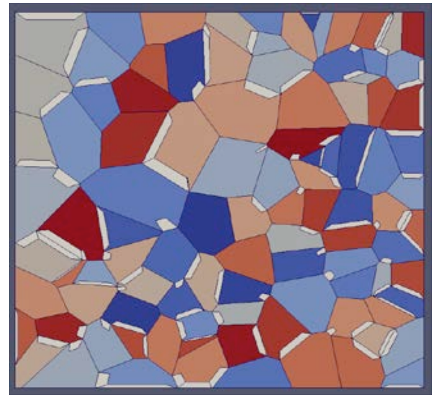
Using AM40 Properties



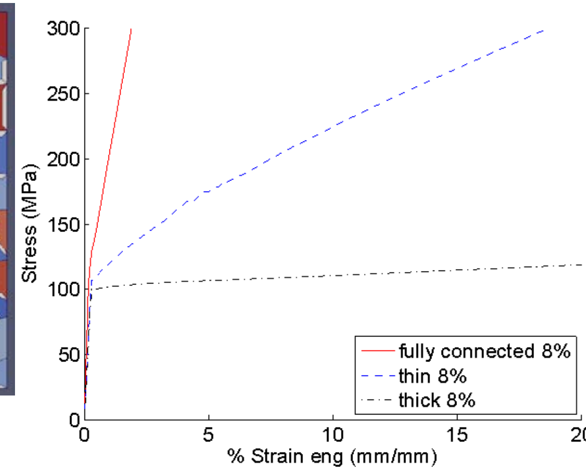
8% β, *t*=4%



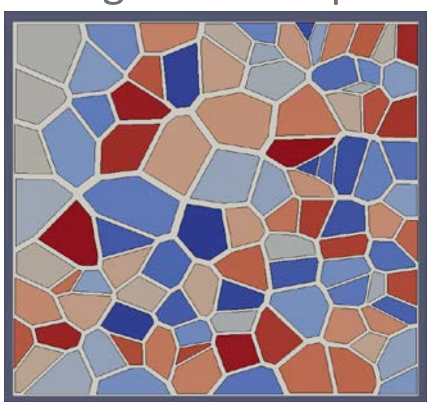
8% β, *t*=10%



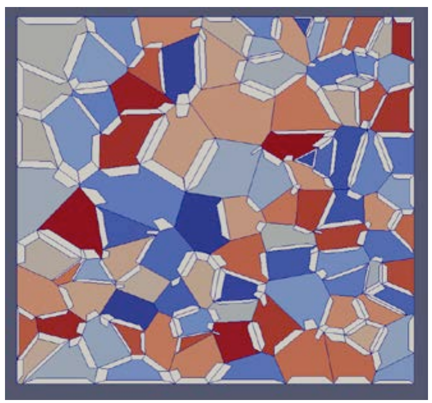
8% β, *t*=30%



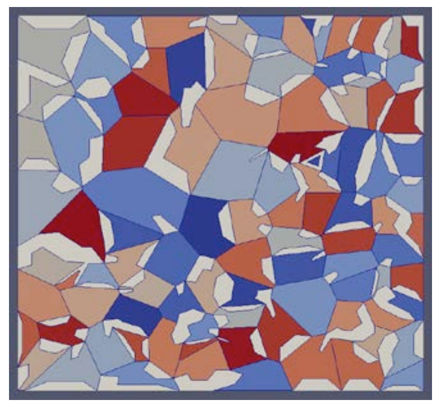
Using AM70 Properties



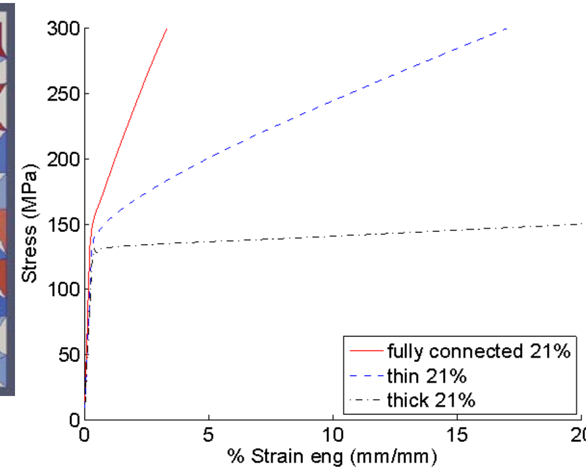
21% β, *t*=11%



21% β, *t*=30%



21% β, *t*=50%



Barker, et al., in press *Comp. Mat. Sci.*, 2014.

PNNL -- Incorporating Intrinsic Microstructure-based Results into Extrinsic Models to Consider Pores

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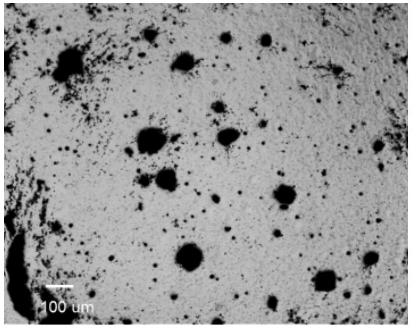
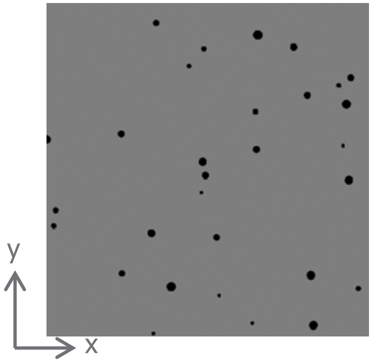
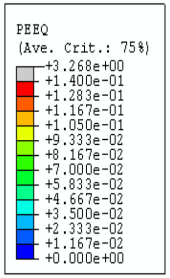
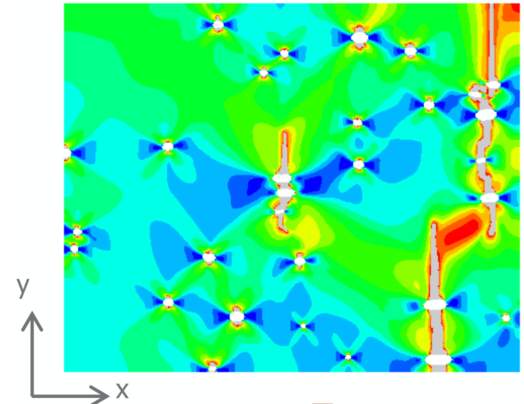
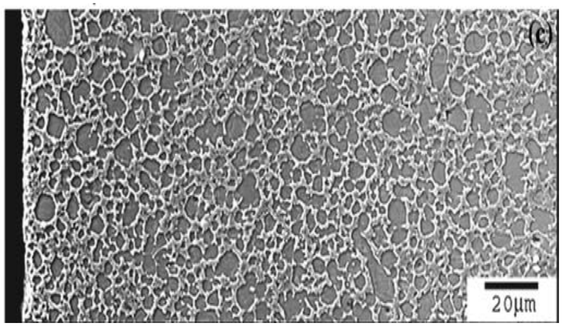


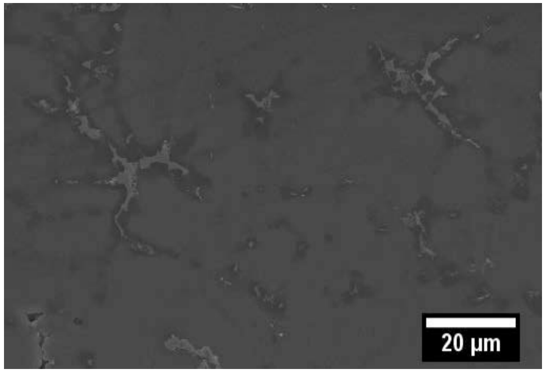


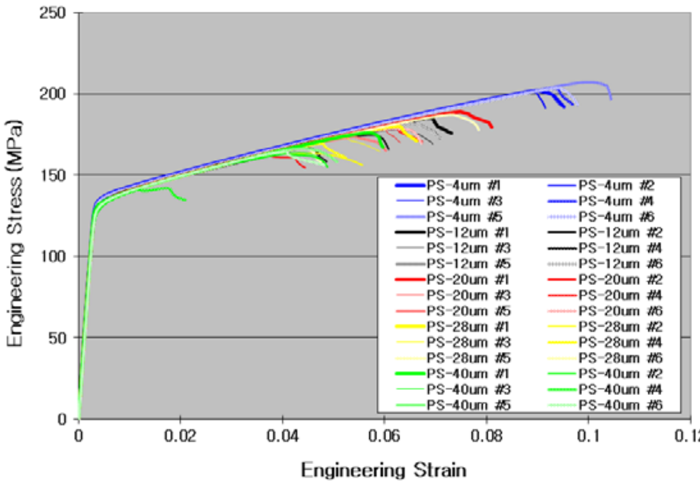




VF: 1%
PS: avg 20μm (10~30μm)



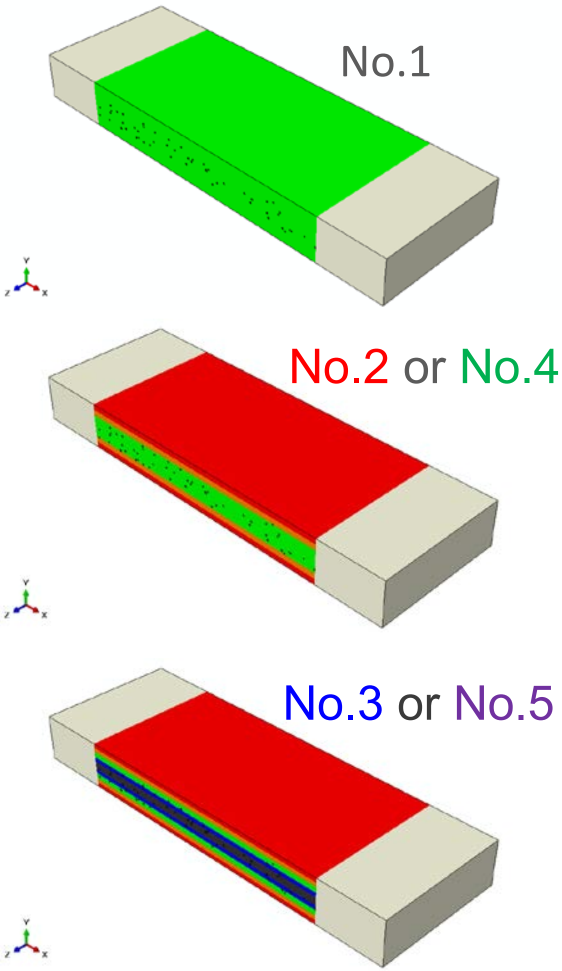




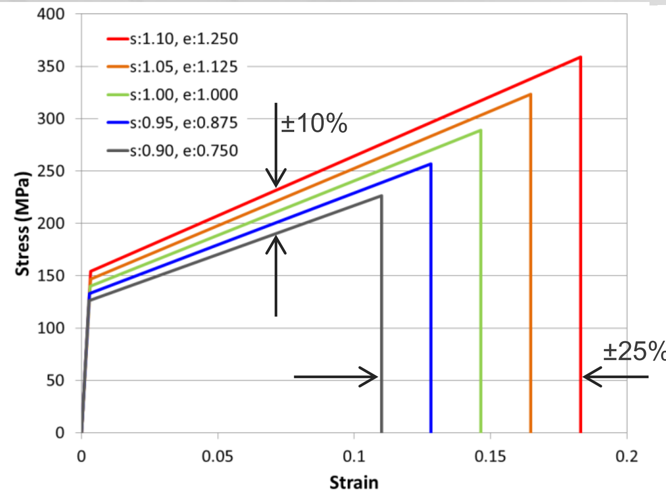
Sun, et al., *Mat. Sci. Eng. A*, 2013.

AM50 sample; Chadha, et al., *Metal Mat Trans A*, 2007

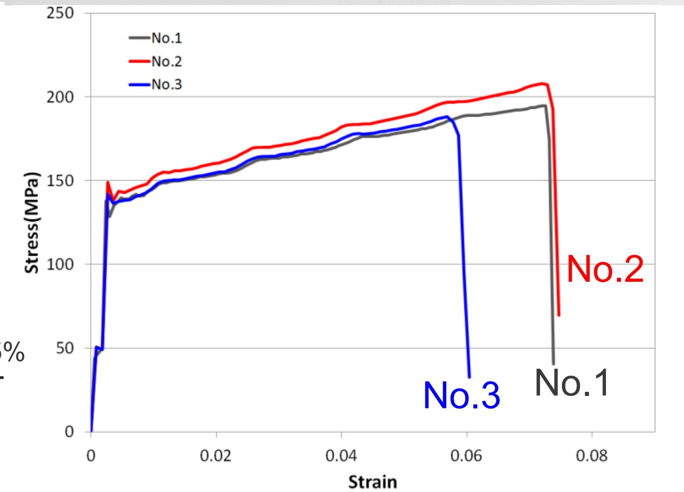
PNNL (Extrinsic Modeling) – Effects of Intrinsic Properties on Ductility



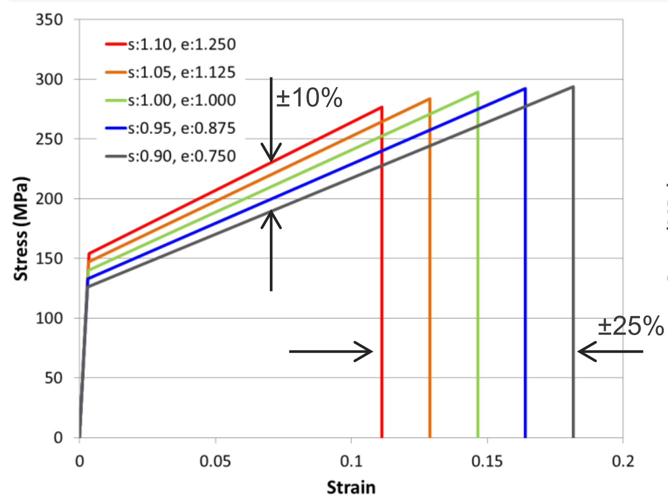
3D models with different properties for different layers



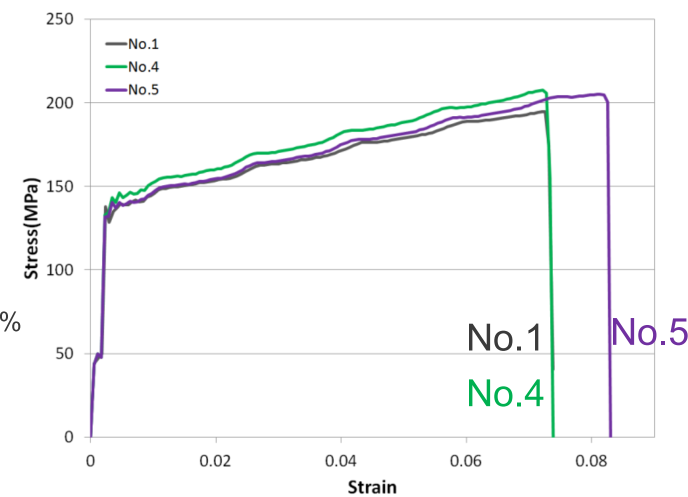
Input s-e curves for model #1,2,3



Resulted s-e curves



Input s-e curves for model #1,4,5



Resulted s-e curves

- The intrinsic property in the high-porosity core region has dominant effects on the ductility.
- The intrinsic property in the core may be used for 2D simulation.

PNNL (Extrinsic Factor Modeling) – Predicting Ductility based on Actual Microstructures with 2D/3D Correlation

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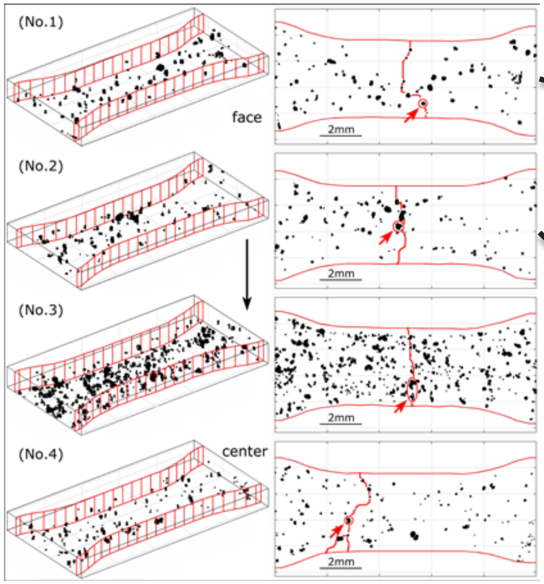
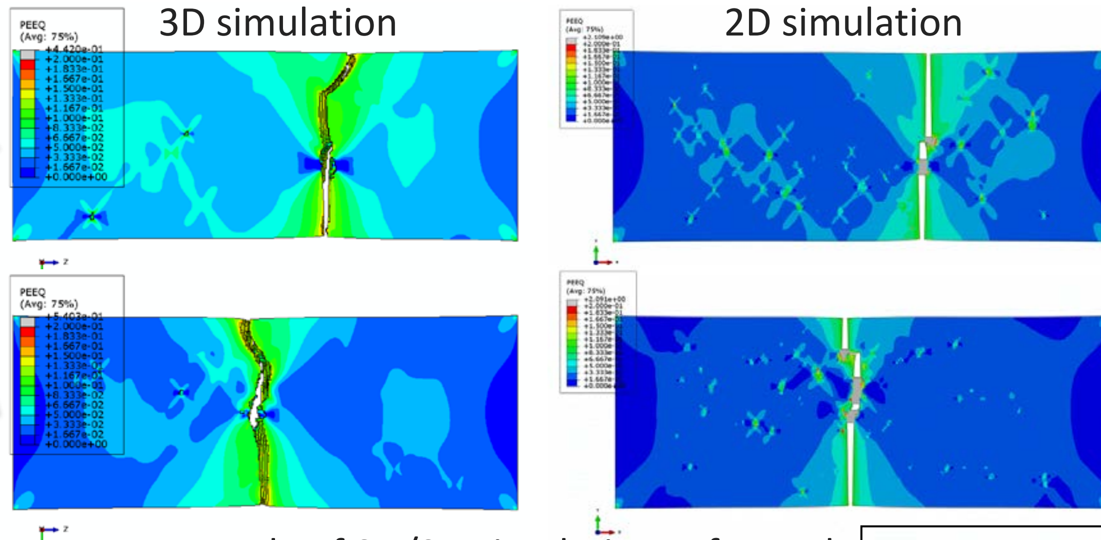


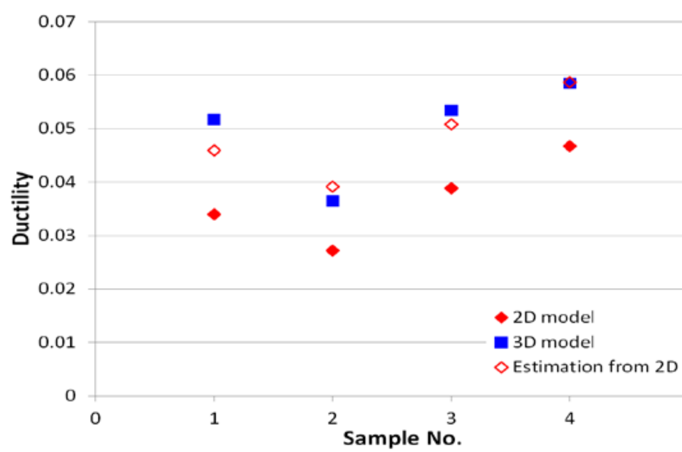
Actual pore distributions *



Example of 3D/2D simulations of actual microstructure-based models

Element size :~25um
$\varepsilon_{cr,tension}$: 20%
Flatness : ~0.6

	Ductility(%)			Error (%) (3D-Est.2D)/3D
	2D model	3D model	Estimation from 2D	
No. 1	3.40	5.18	4.60	11.16
No. 2	2.72	3.64	3.92	-7.55
No. 3	3.88	5.35	5.08	4.89
No. 4	4.67	5.85	5.88	-0.46



Comparison of 2D/3D ductility

*Song, Xiong, Li, Allison (2009) J. Alloys and Compounds, 477, pp.863-869.

Address Previous Year Reviewers' Comments

- Approach
  - Reviewer 2: This reviewer pointed out that a mechanistic model would be a dramatic improvement; the reviewer was unclear how the necessary input parameters will be determined. The reviewer stated that overall the project draws heavily from experimentation, but the reviewer did not see how the modeling work will be fed back to affect the experimental work.

  Response: The experimental work at different scales are designed to provide modeling parameters and serve as model validations. The initial modeling results on effects of b phase morphology and pore distribution have also guided the experimental design of solution treatment and HIP.

  - Reviewer 3: This reviewer opined that the work at Pacific Northwest National Laboratory (PNNL) always seems to be brute-force modeling of a particular system from which no generalizable insights can be drawn.

  Response: The objective of this project is to develop a mechanism-based modeling framework that can be used to predict cast Mg ductility. We start with some specific AM alloys due to data availability and the general methodology should apply to other Mg systems.

- Collaboration
  - Reviewer 2: This reviewer observed that other participants do not seem as deeply involved as personnel at PNNL.
  - Reviewer 3: This reviewer stated that not many details were provided other than Ford cast the parts, and Michigan modeled this.

  Response: This is a PNNL-led project with active Ford and UM contribution as shown in the project structure and overall progress report. Ford has made significant contribution with the quality mapping for ductility and all microstructural and sample level characterizations are carried out by UM.

- Future Work
  - Reviewer 2: This reviewer pointed out that the remaining goals seem very broad and appear to be a large challenge to complete.

  Response: We agree. We are currently on carryover from FY13 funding.

Collaborations

- Ford, Mag-Tec Casting Corporation (Industry)
  - Provided/operated high pressure casting and super vacuum die cast equipment
  - Characterized coupon level stress versus strain curves for different conditions and locations
  - Produced casting samples with varying aluminum content and performed casting process simulations
  - Collaborated on characterization of microstructure and defect features at various locations on castings
  - Developed and validated Mg casting quality map with statistical variation
- University of Michigan (Academic)
  - Established effects of plate thickness and aluminum contents on yield strength, ductility and UTS.
  - Developed characterization techniques to quantify b volume fraction and morphology across sample thickness and for different aluminum contents
  - Examined effects of solution treatment and hot isostatic pressing on hardening parameters and ductility
- CANMET Materials Technology Laboratory
  - Performed phase field simulation on pore and dendrite interactions

Summary

- Relevance
  - Limited ductility and high ductility variations hinder the wider applications of Mg casting in vehicle structures for lightweighting
- Approach
  - Develop a quality-mapping capability for estimating/controlling ductility of Mg castings based on tensile test results and various casting parameters
  - Develop a mechanistic-based ductility prediction capability with separate consideration of intrinsic factors and extrinsic factors
- Technical Accomplishments
  - Validated quality mapping approach in predicting ductility and ductility variations
  - Designed and manufactured new die cast insert for tensile and bending samples for in-situ SEM observation on α and β deformation mechanisms
  - Quantified β-phase volume fraction and morphology for various aluminum content and casting plate thickness
  - Validated intrinsic model considering various β volume fraction and morphology
  - Predicted ductility based on actual pore structure produced by 3-D x-ray tomography
- Collaborations
  - Ford, Mag Tech, U Mich
- Future work

Proposed Future Work

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- Setting up in-situ SEM capability to examine crack growth under 3-point bend loading for alloys with different aluminum contents (Ford+UM)
- Use quantitative fractography and microstructural analysis to establish relationships between properties, microstructure and alloying/processing variables (UM+PNNL)
- Perform nano-indentation tests to evaluate grain boundary cohesive strength (PNNL/UM)
- Predict intrinsic ductility for Mg with different aluminum content by considering eutectic β phase and grain boundary decohesion (PNNL)
- Final deliverable – Validate prediction framework by comparing measured ductility with predicted ductility from x-ray tomography (PNNL)