

Mechanistic-based Ductility Prediction for Complex Mg Castings

X SUN (PI)

PACIFIC NORTHWEST NATIONAL LABORATORY
RICHLAND, WA, USA

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► Timeline

- Start: Oct. 2010
- End: Sep. 2014
- 65% 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

- ▶ 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

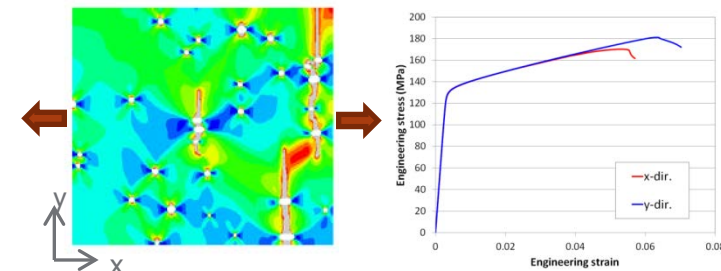
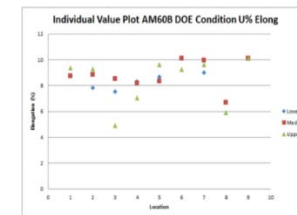
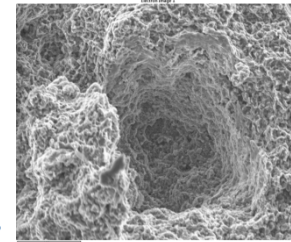
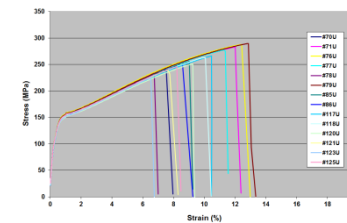
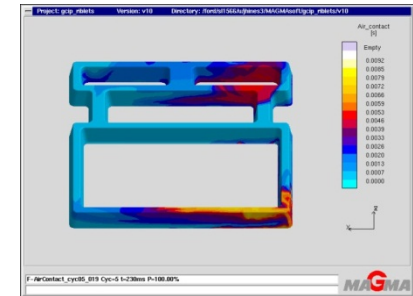
- ▶ A validated simulation tool (quality map approach) for estimating the spatial variation of ductility and the influence of casting process variables (completed)
- ▶ Modeling and experimental methods in quantifying location-dependent intrinsic and extrinsic ductility limiting factors for complex Mg castings (on-going; due 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

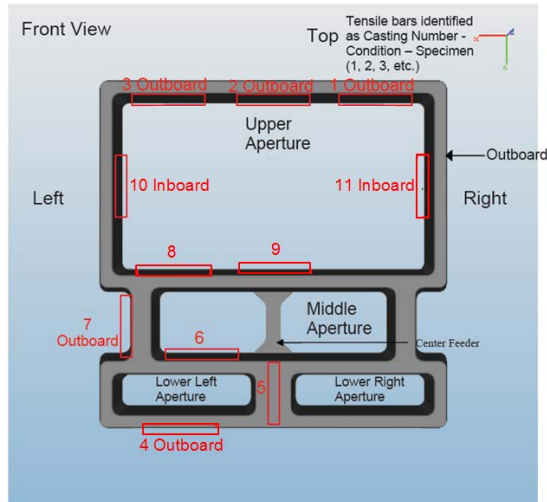


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Battelle Since 1965

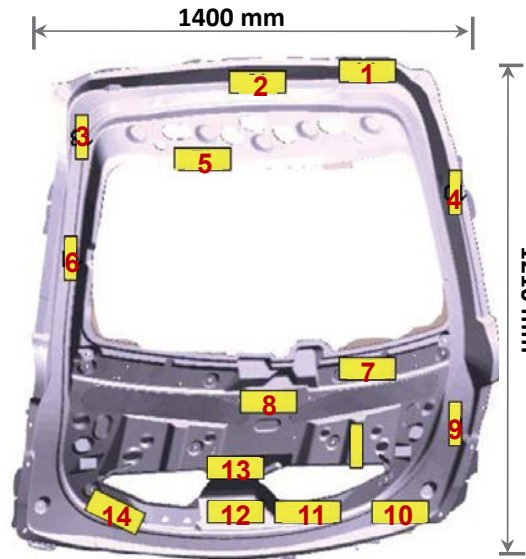


Ford - Quality Mapping Validation

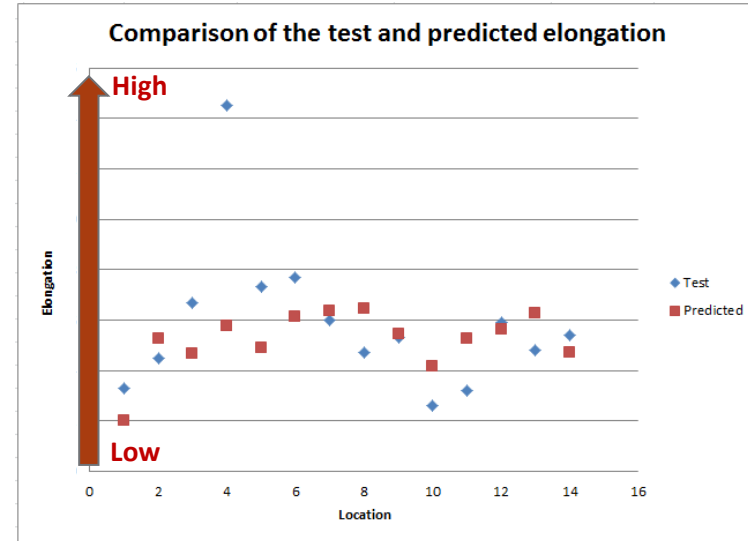
Processing parameter setting with GCIP



Geometry and locations of excised sample bars on GCIP casting



Geometry and locations of excised sample bars on Ford MKT liftgate



Comparison of the test and predicted elongation of Ford MKT liftgate

$$\text{Strain} = 20.5 - 18.96 * ST_{\text{norm}}^{0.19934} - 1.8144 * FL_{\text{norm}}^{0.91472} - 5.8475 * AE_{\text{norm}}^4 - 7.0759 * AC_{\text{norm}}^{0.92389} + 27.613 * Temp_{\text{norm}}^4$$

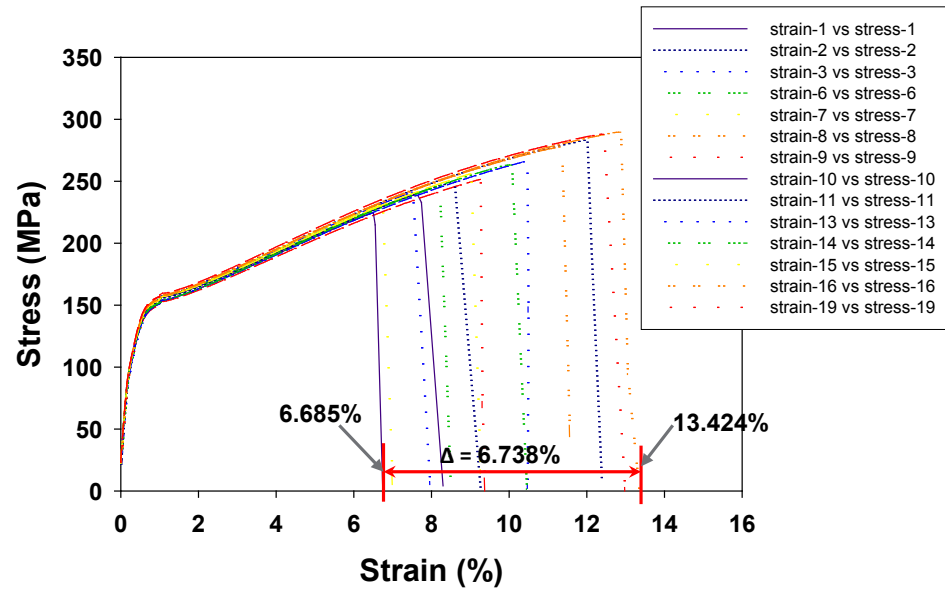
The criteria functions were normalized as follows:

$ST_{\text{norm}} = \text{Liq to Sol}/4$; $AE_{\text{norm}} = AE/35$; $FL_{\text{norm}} = FL/2000$; $AC_{\text{norm}} = AC/0.02$; $Temp_{\text{norm}} = (T_{100\%} - 620)/620$

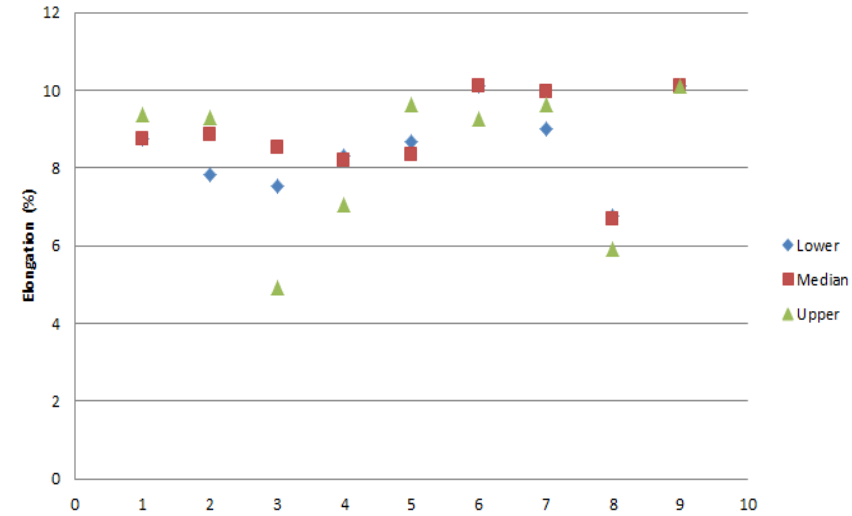
❖ **The test and predicted ductility match well.**

Ford - Predicted Ductility Statistical Variation (GCIP)

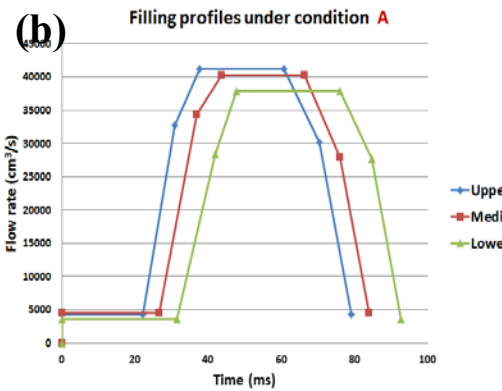
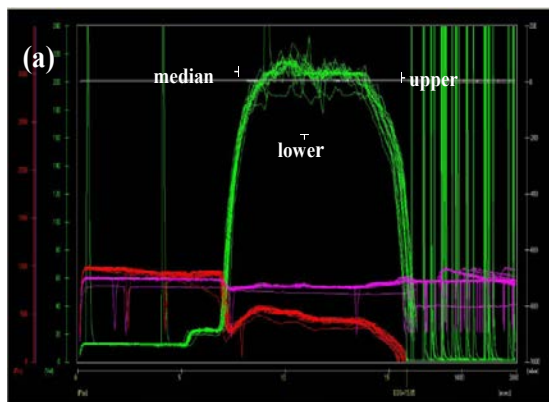
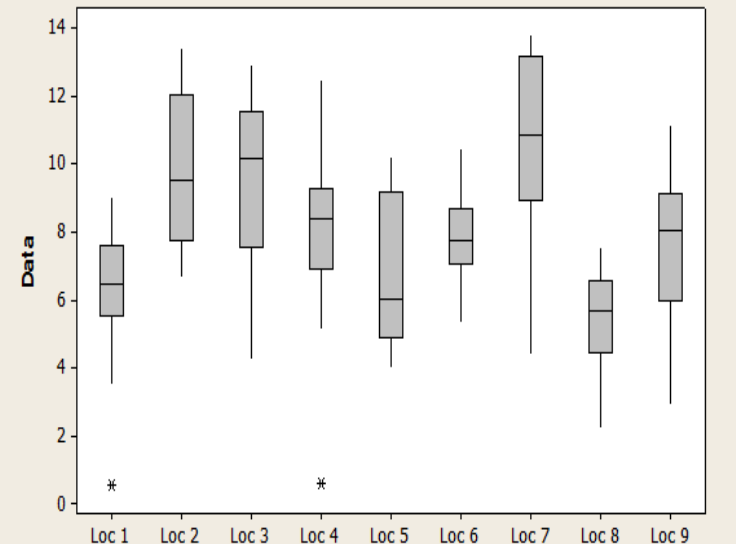
Condition U Location 2



Individual Value Plot AM60B DOE Condition U% Elong

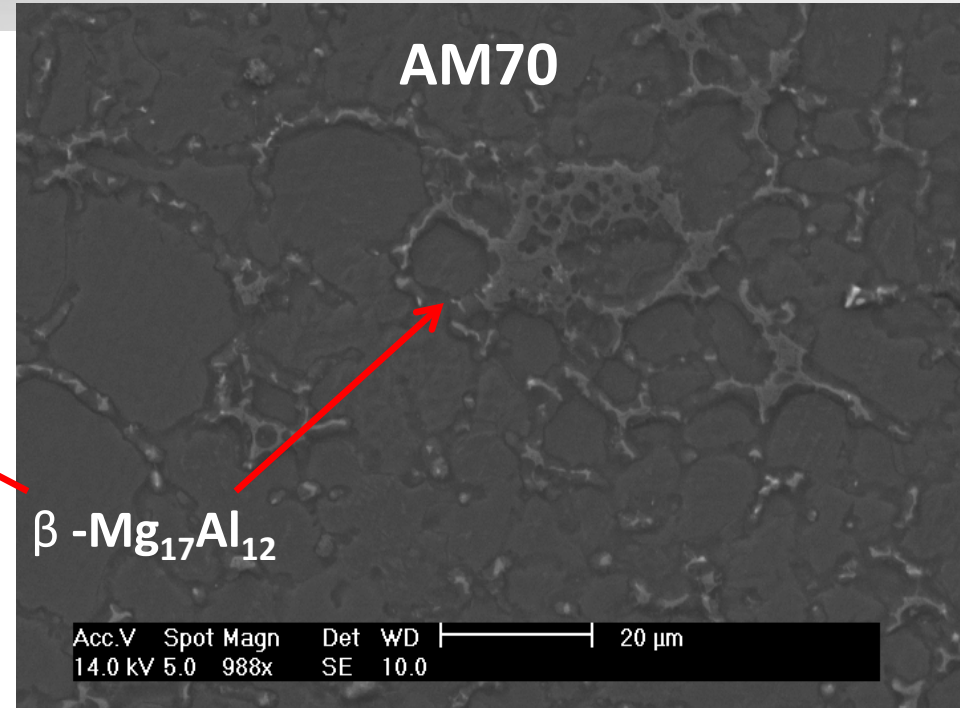
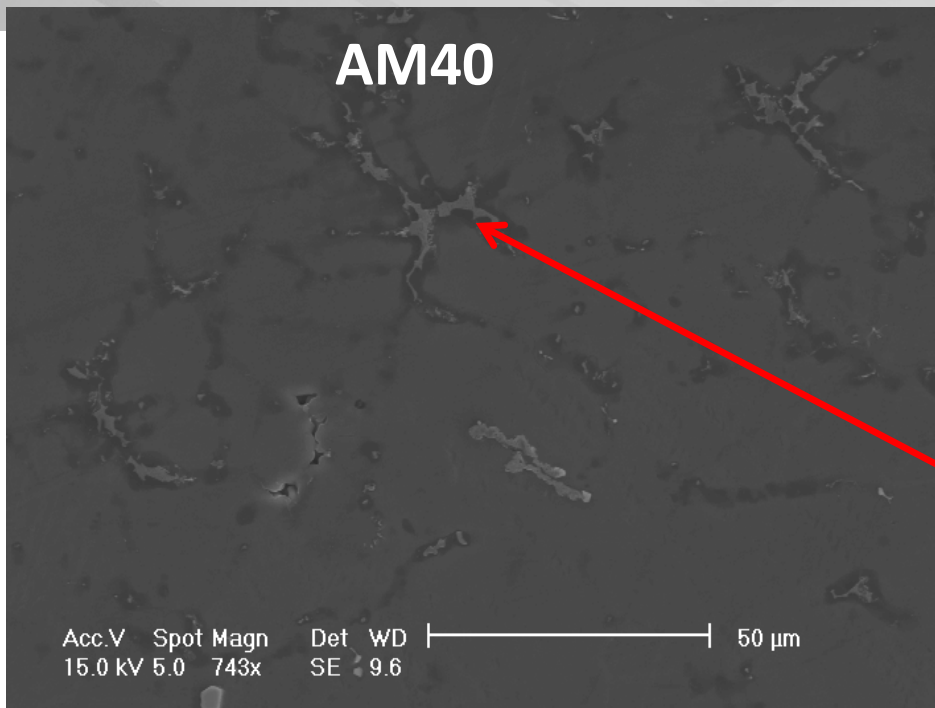


Boxplot of % Elongation Condition U



Filling profile of A condition (a) shot-trace for the set of castings
(b) filling profile used in MAGMASoft simulation

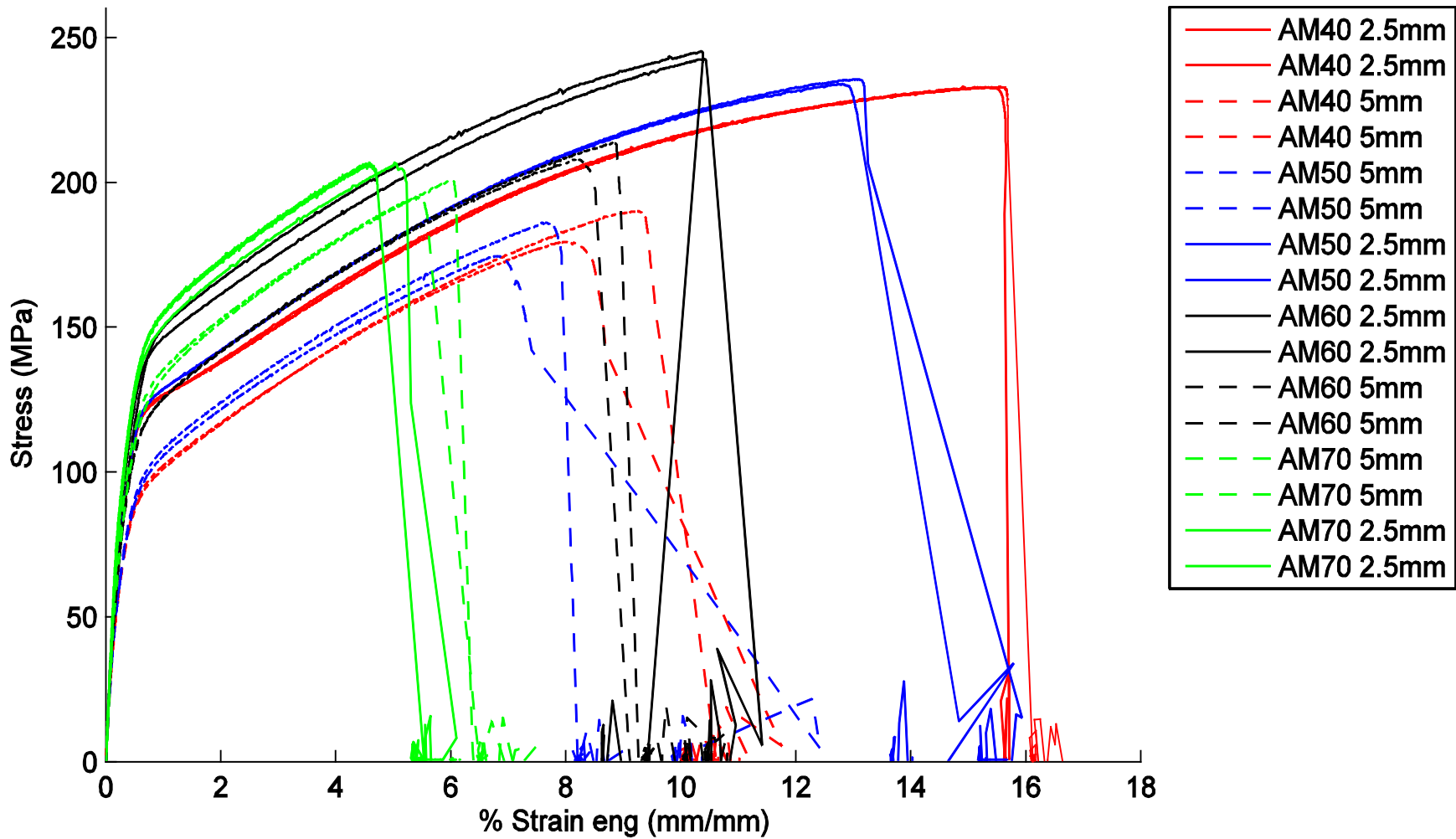
UM + Ford - Increasing Alloy Aluminum Content Changes Grain Boundary Phase Characteristics



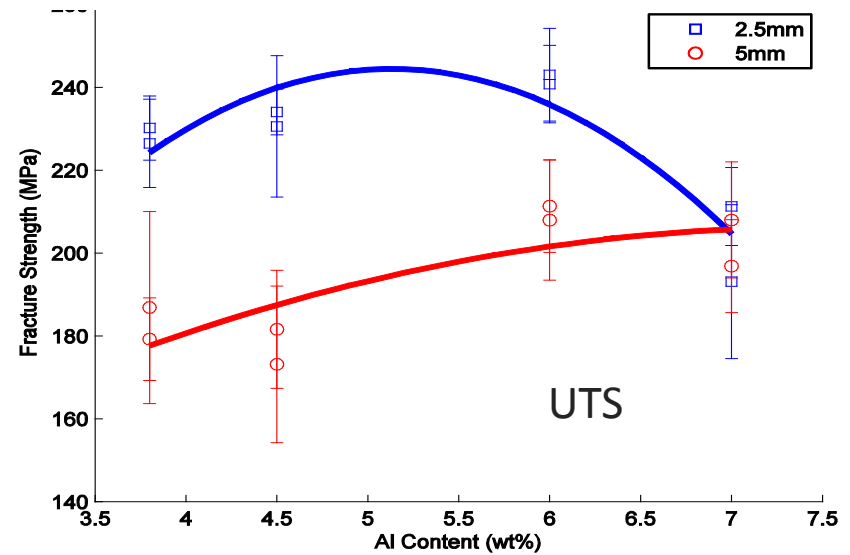
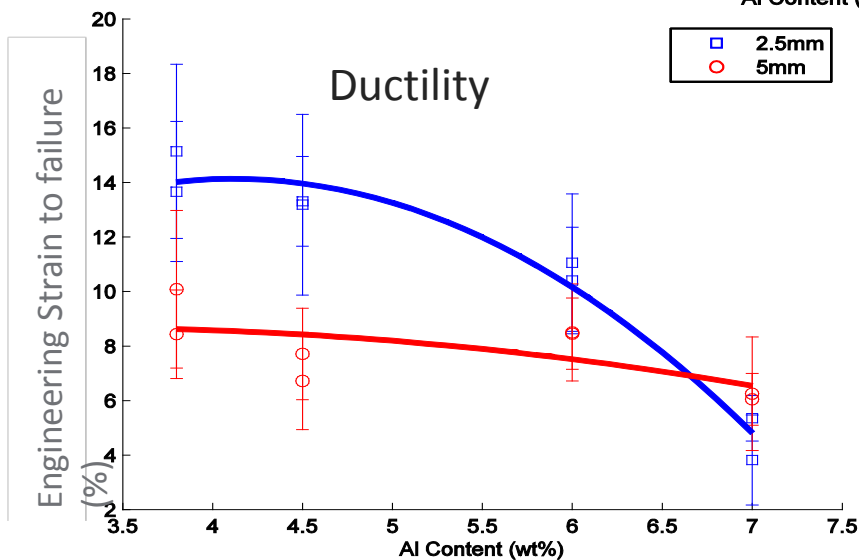
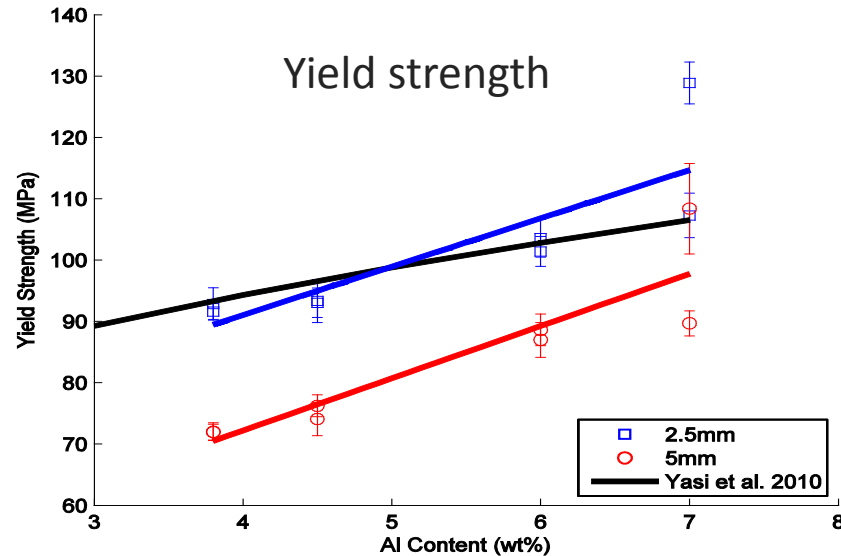
- ▶ 2.5mm and 5mm thick plates were super vacuum die cast (SVDC) with 3.8, 4.5, 6, and 7 (weight%) aluminum contents
- ▶ Secondary electron and optical images show that with increasing Al content, the β phase goes from disconnected particles along grain boundaries to an interconnected network

UM + Ford - Representative Tensile Curves Showing the Influence of Al Content and Sample Thickness

Representative Tensile Samples



UM + Ford – Influence of Aluminum Content and Sample Thickness on Tensile Properties



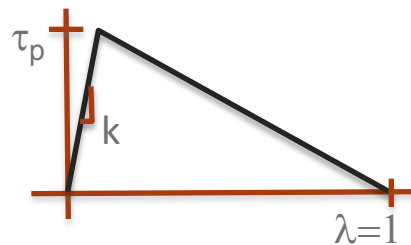
PNNL -- Finite Element-based Intrinsic Strength and Ductility Modeling

► Developed tools for generating synthetic sample

- Generate microstructure representation
- Include β phase along grain boundaries

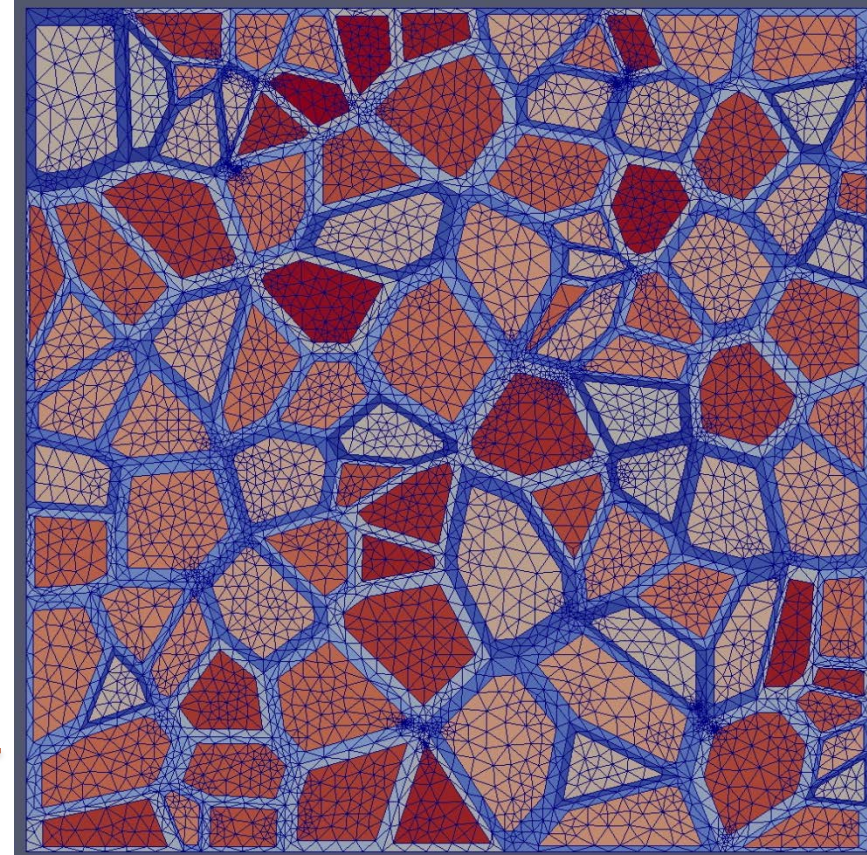
► Finite Element Analysis

- Automatic meshing generation
- 2.5D
- FEAWD
- Various material models
 - Grains: von Mises plasticity
 - β : LEI
 - Grain boundaries: cohesive zone



► Simulation cases

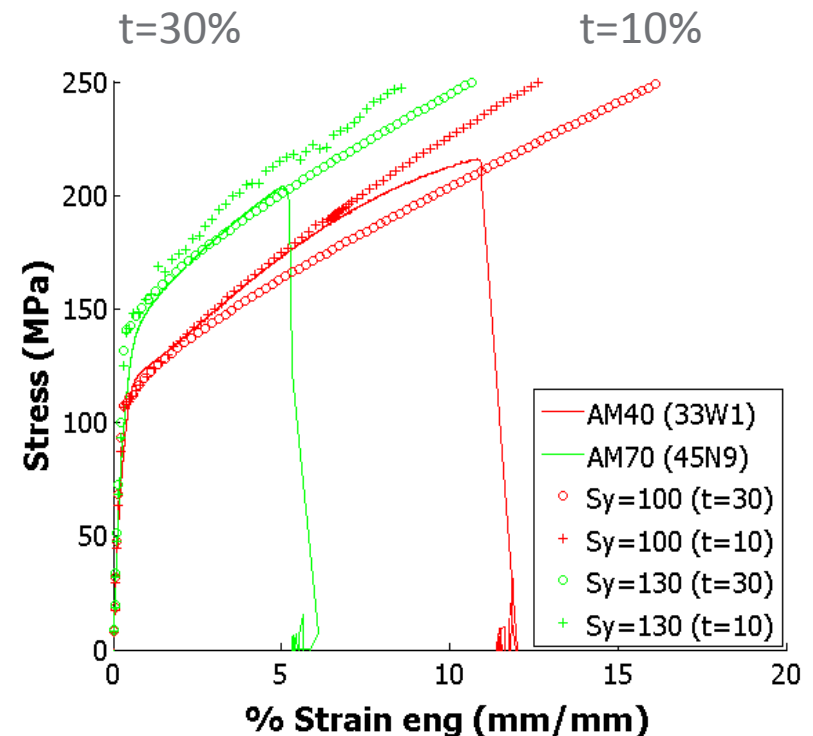
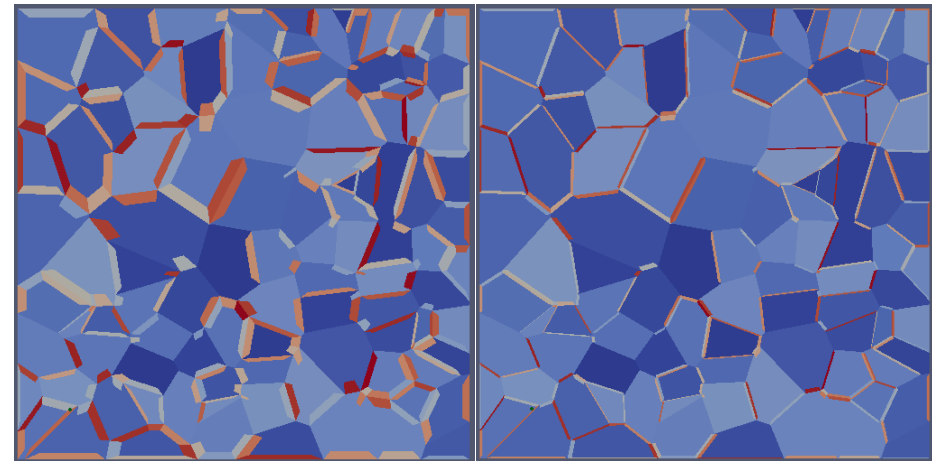
- Fully connected β phase
- Partially connect β phase
- β phase geometry
- Damage inclusion through cohesive grain boundaries



150 μm
100 grains

PNNL -- Predicted Intrinsic Stress vs. Strain Curves

- ▶ Initial analyses conducted to determine impact of geometry features
 - Including fully connected β network increased hardening
 - Partially connected β , increase hardening but not as much
 - Same volume fraction of β with increasing size, continued to decrease hardening
- ▶ Introduced failure through cohesive grain boundaries
 - Modified hardening behavior
 - Elongation dependent on input material parameters
- ▶ Comparison of simulation and experimental results
 - $E=38\text{GPa} \pm 5\%$
 - $\text{Sigma_yld} = 130 \text{ MPa} \pm 5\%$ for AM70
 - $\text{Sigma_yld} = 100 \text{ MPa} \pm 5\%$ for AM40
 - β Volume fraction = $21\%^3$ for AM70
 - β Volume fraction = 10% for AM40
 - β parameters ($\text{Mg}_{17}\text{Al}_{12}$) – selected from first-principle calculations^{1,2}
 - $E = 77.7 \text{ GPa}$

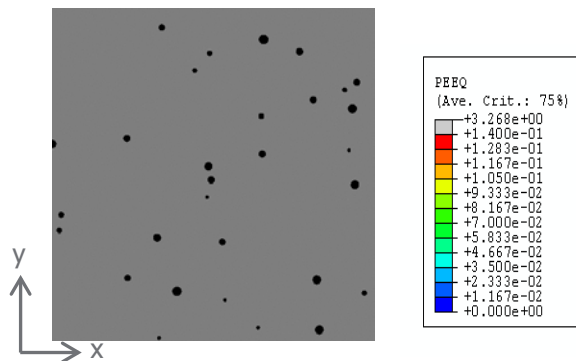
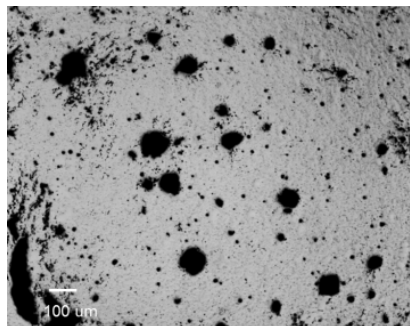


¹ Zhang, et. al., *Acta Materialia*, v58(11), 2010, pg. 4012-4018

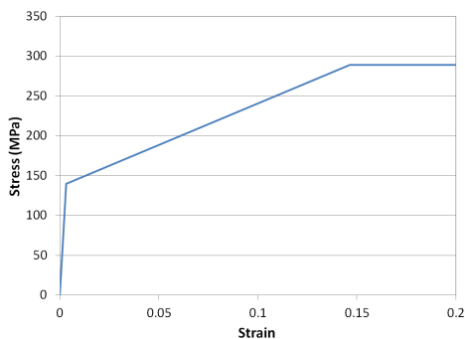
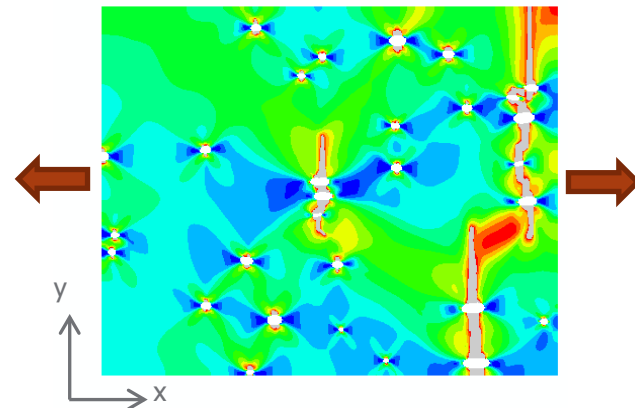
² Wang, et. al., *Calphad*, v35(4), 2011, pg. 562-573

³ Sachdeva, et. al., *Metal Mat Trans B*, v41B, 2010, pg. 1375-1383

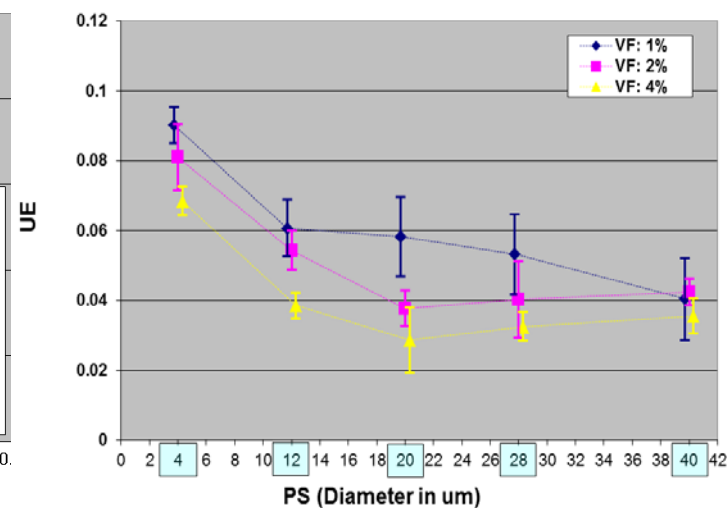
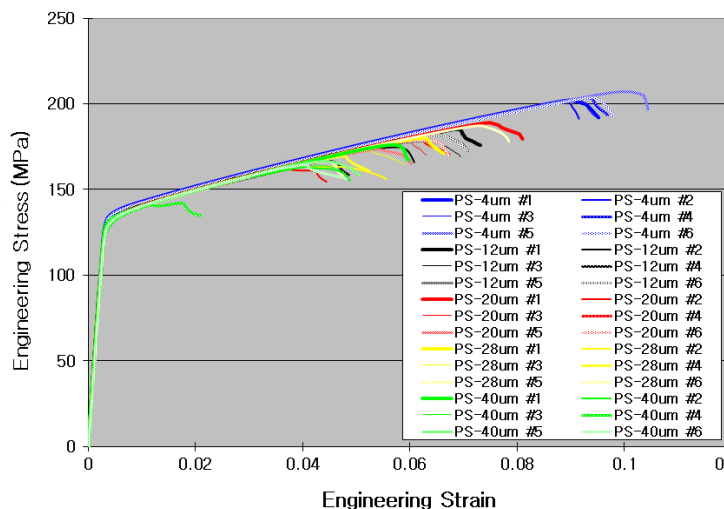
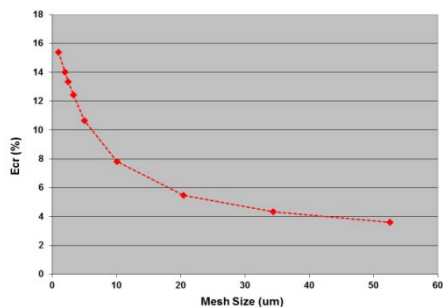
PNNL -- Finite Element-based Ductility Prediction Technique for Mg Castings



VF: 1%
PS: avg 20um (10~30um)

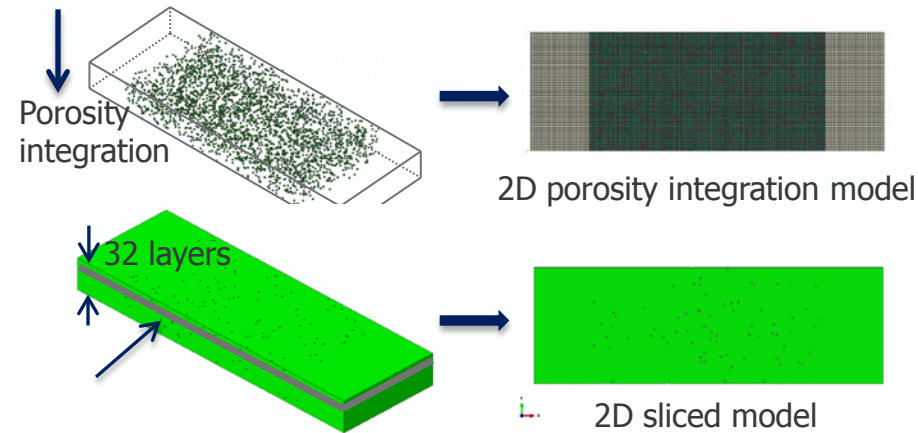


Size dependence of E_{cr}

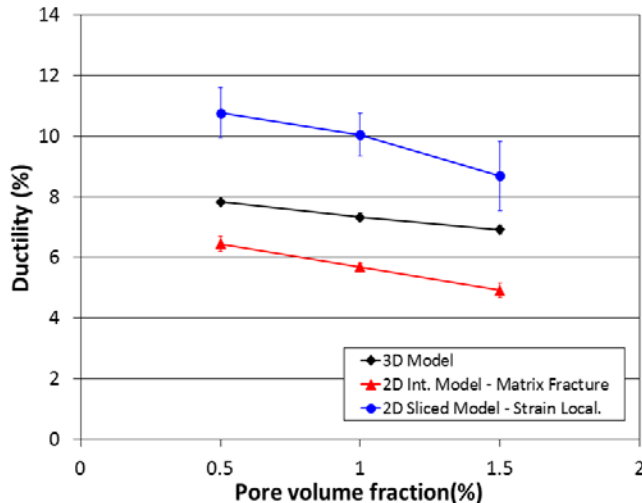


Predicted effects of pore size
and volume fraction

PNNL –2D Model Verification with 3D Results & Effects of Skin Thickness on Ductility

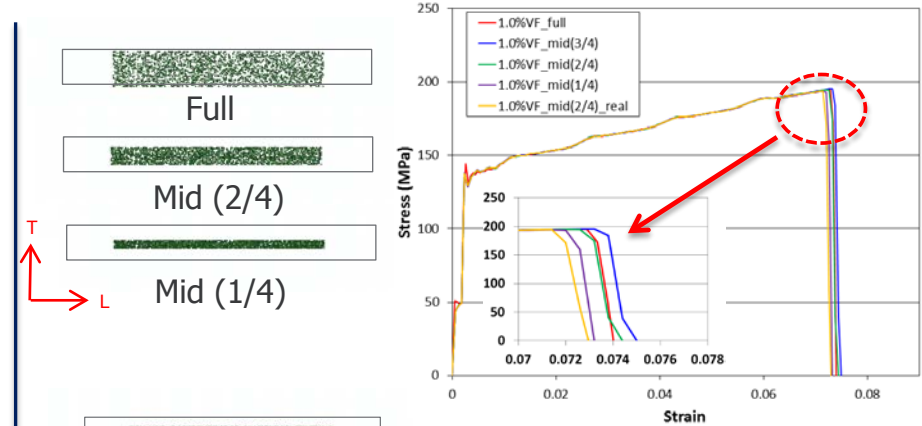


Cutting out 1 layer



Effect of pore volume fraction on ductility

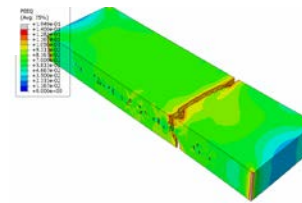
- Some results of 2D modeling show similar trends to those of 3D modeling.
- Possible correlation may exist between 2D/3D modeling results.



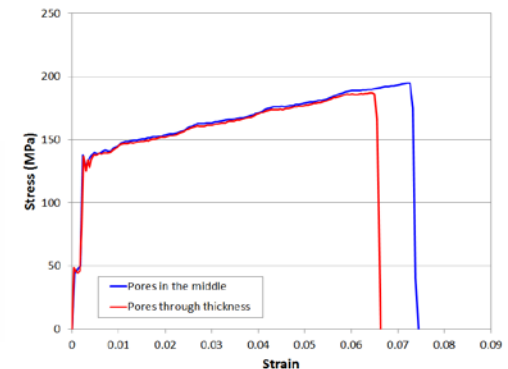
Effect of skin thickness

Pores in the middle

Pores through thickness



Predicted failure mode



Skin effect

- For the same overall pore volume fraction, the skin thickness effects on the ductility seem to be negligible.
- For the same local pore volume fraction in the mid region, skin region helps for better ductility.

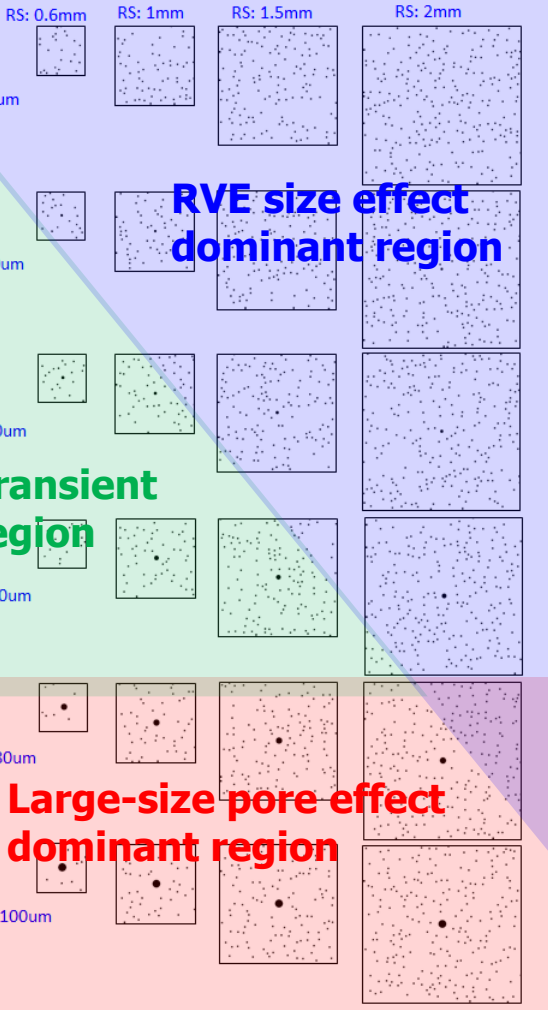


Modeling of Extrinsic Factors on Ductility

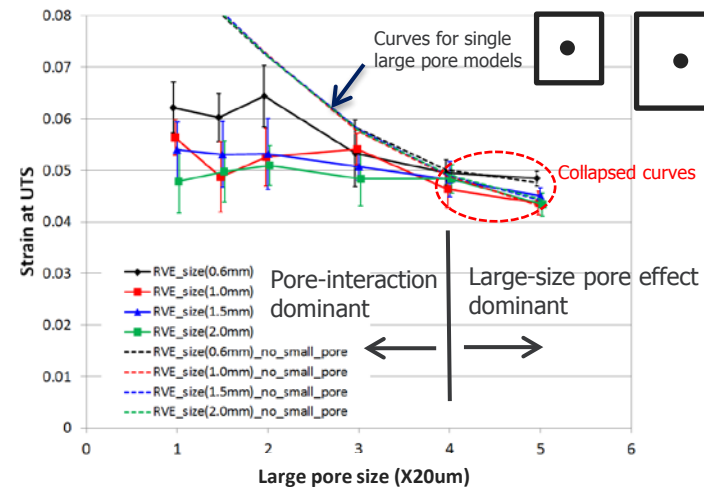
– Effects of Large-Size Pore and Virtual Sample Size

Mesh size (MS): 2um
Pore size (PS): 20um
Volume fraction (VF): 2%
Critical Strain: 14%

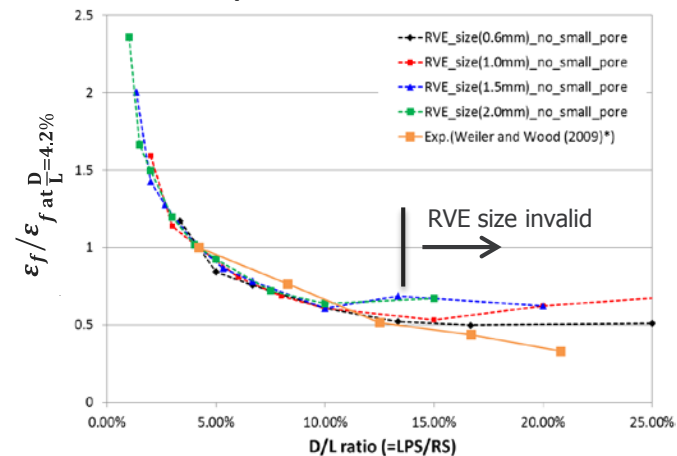
Virtual sample size (RS) increases



Large pore size (LPS) increases



Ductility for different RS and LPS



Comparison with Exp. Results.

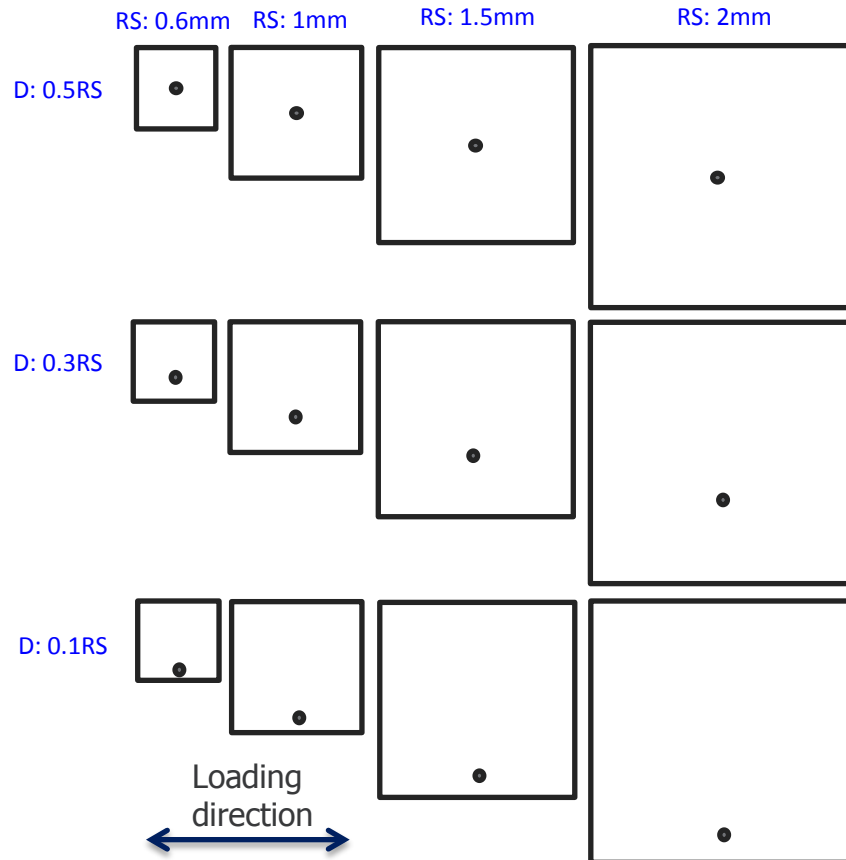
- ▶ Pore-interaction dominant region and large-size pore effect dominant region may exist.
- ▶ Valid sample size needs to be used depending on the largest pore size.

2D plane stress models with different RS and LPS

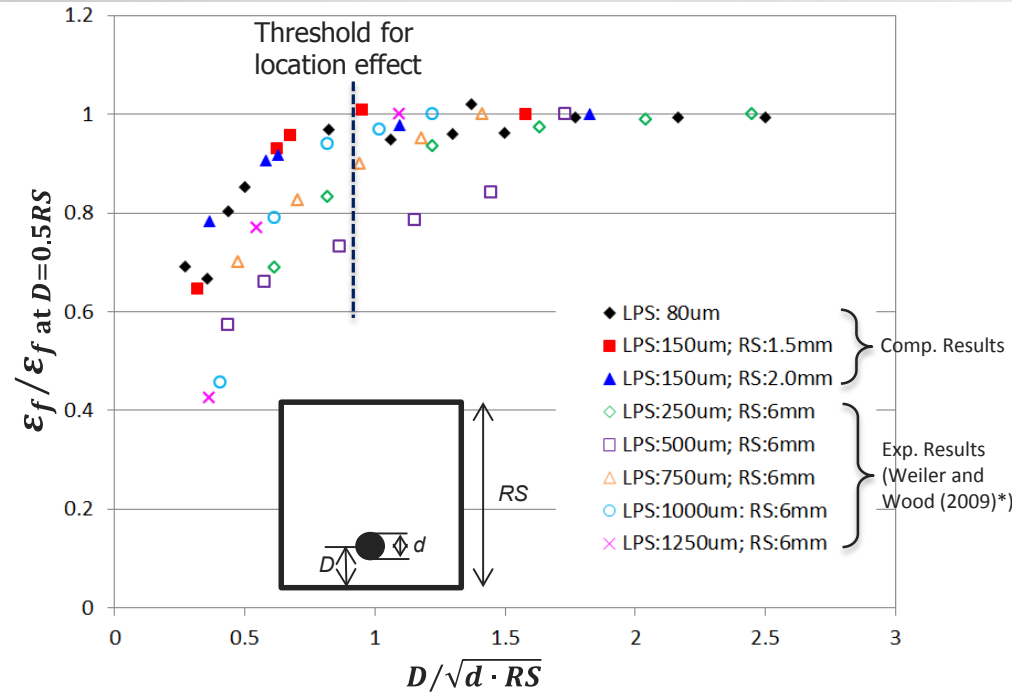
Modeling of Extrinsic Factors on Ductility

– Effects of Large-Size Pore Location

- ▶ Large-size pore (80um) is chosen within its effect dominant region.
- ▶ Small size pores are not considered.



2D plane stress models considered with different RS and pore location



Combined effects of large pore size, virtual sample size and distance from the edge on ductility

- ▶ Threshold region near the sample edge exists, in which large pores start to have significant effects on the ductility.
- ▶ In general, predicted trends based on simple 2D models agree well with those of the experimental results.

Summary

- ▶ Validated quality mapping approach with Ford MKT liftgate.
- ▶ Extended quality mapping approach to examine statistical variation of ductility.
- ▶ 2.5mm and 5mm thick plates were super vacuum die cast (SVDC) with 3.8, 4.5, 6, and 7 (weight%) aluminum contents.
- ▶ Established effects of plate thickness and aluminum contents on yield strength, ductility and UTS.
- ▶ Developed finite element based intrinsic strength and ductility prediction capability with FEAWD and cohesive zone elements.
- ▶ Predicted intrinsic stress vs. strain curves for different Al content with first-principle-based β phase properties.
- ▶ Synthetic microstructure-based 2D/3D finite element analyses have been conducted to examine the effects of skin thickness and the correlations between 2D/3D modeling results.
- ▶ Quantified the effects of large-size pore and its location on ductility together with the virtual sample size effects

- ▶ Ford, Mag-Tec Casting Corporation, CANMET Materials Technology Laboratory (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.
 - Developing empirical weak-link based ductility model
 - Collaborated on characterization of microstructure and defect feature
 - Collaborated on development of Mg casting quality map

Proposed Future Work

- ▶ Evaluate approaches for incorporating ductility and yield strength variability into the quality map approach (Ford)
- ▶ Produce as cast samples to support quality map development (Ford)
- ▶ Setting up in-situ SEM capability to examine crack growth under 3-point bend loading for alloys with different aluminum contents (Ford+UM)
- ▶ Complete fractographic analysis for empirical micromechanical model (UM)
- ▶ Use quantitative fractography and microstructural analysis to establish relationships between properties, microstructure and alloying/processing variables (UM+PNNL)
- ▶ Establish a weak link model to account for the above relationships (UM)
- ▶ Develop plate bulge testing method to simulate structural response of die cast Mg (UM)
- ▶ Predict intrinsic ductility for Mg with different aluminum content by examining the interactions of eutectic β phase and grain boundary decohesion (PNNL)
- ▶ Link bulk intrinsic properties into extrinsic ductility prediction framework (PNNL)
- ▶ Perform microstructure-based 2D/3D finite element analysis with consideration of different pore size, variable pore size distribution and large size pores (PNNL)