Computational design and development of a new, lightweight cast alloy for advanced cylinder heads in high-efficiency, light-duty engines

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General Motors

6/10/2015

Project ID # PM061

Overview

Timeline

Project start date 02/2013

Project end date 09/2017

Percent complete 50%

Budget

- Total project funding
  - DOE share $3,498,650
  - Contractor share $1,646,423
- Funding **received** in FY14
  - $456,103
- Funding for FY15
  - $557,500

Barriers

Engine Durability

- Current materials limit engine efficiency by limiting peak cylinder temperatures and pressures
- Insufficient tensile and fatigue properties beyond 150 C

Material Cost

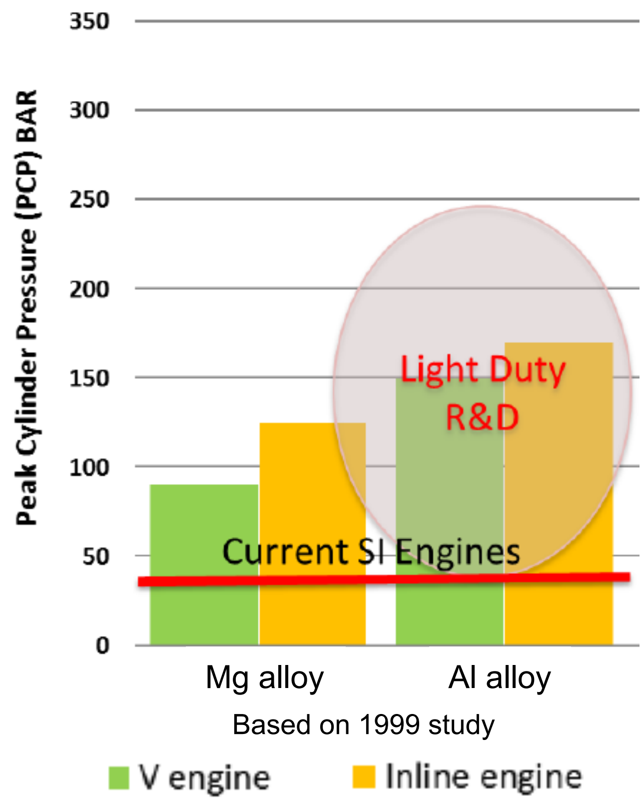
Partners

- Questek Innovations LLC
- Northwestern University
- American Foundry Society
- Dr. Fred Major
- Camaneo Associates
- MIT
- **Project lead** General Motors

Relevance- Project Objectives

DOE FOA 648-3a Material Property Targets

Property	Baseline	DOE Target
Tensile Strength (ksi/MPa)	33/227	40/276
Yield Strength (ksi/MPa)	24/165	30/207
Elongation (%)	3.5	3.5
Shear Strength (ksi/MPa)	26/179	30/207
Endurance Limit (ksi/MPa)	8.5/59	11/76
Fluidity (Spiral test)	Excellent	Excellent
Hot Tearing Resistance	Excellent	Excellent
Tensile Strength (ksi/MPa)	7.5/52 @250 C	9.5/65 @300 C
Yield Strength (ksi/MPa)	5.0/34 @250 C	6.5/45 @300 C



To meet energy efficiency targets, peak engine pressures and temperatures will greatly exceed current material properties and therefore material needs to be improved

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Relevance - Project Objectives 2014-2015

VTO Lightweight materials

Increase understanding of Materials through modelling and computation

Material Property Improvement (strength, stiffness, and ductility)

Improving manufacturing of materials (cost, production rate, or yield)

GM lightweight cast alloy project

Thermodynamic and mobility database development of three alloy concept structures

Investigation of 18 elements for new concept discoveries using electronic structure methods (DFT)

Precipitate growth and strength models calibrated and validated using LEAP and TEM imaging, isothermal and isochronal hardness testing

Room and high temperature tensile property measurements made on a 10 new and baseline alloys and multiple heat treatment schedules.

Approach/Strategy

Using expert knowledge, thermodynamic and DFT models develop alloy concepts with potential for meeting high temperature properties and cost constraints.

Milestone: Concept Generation Complete

Select alloy concepts based on prediction of potentially viable structures.

Milestone: Alloy Model Selection Complete

Button castings for observation of precipitate structures, isothermal and isochronal hardness studies. Plate castings for room and high temperature mechanical property measurements.

Milestone: Sub-scale Castings Complete

Generate data to support kinetic precipitate growth and material strength models

Milestone: Sub-scale Data Development Complete

Validation of sub-scale concepts through microstructural observation and mechanical testing.

Milestone: Sub-scale Concepts and Models Validated Complete

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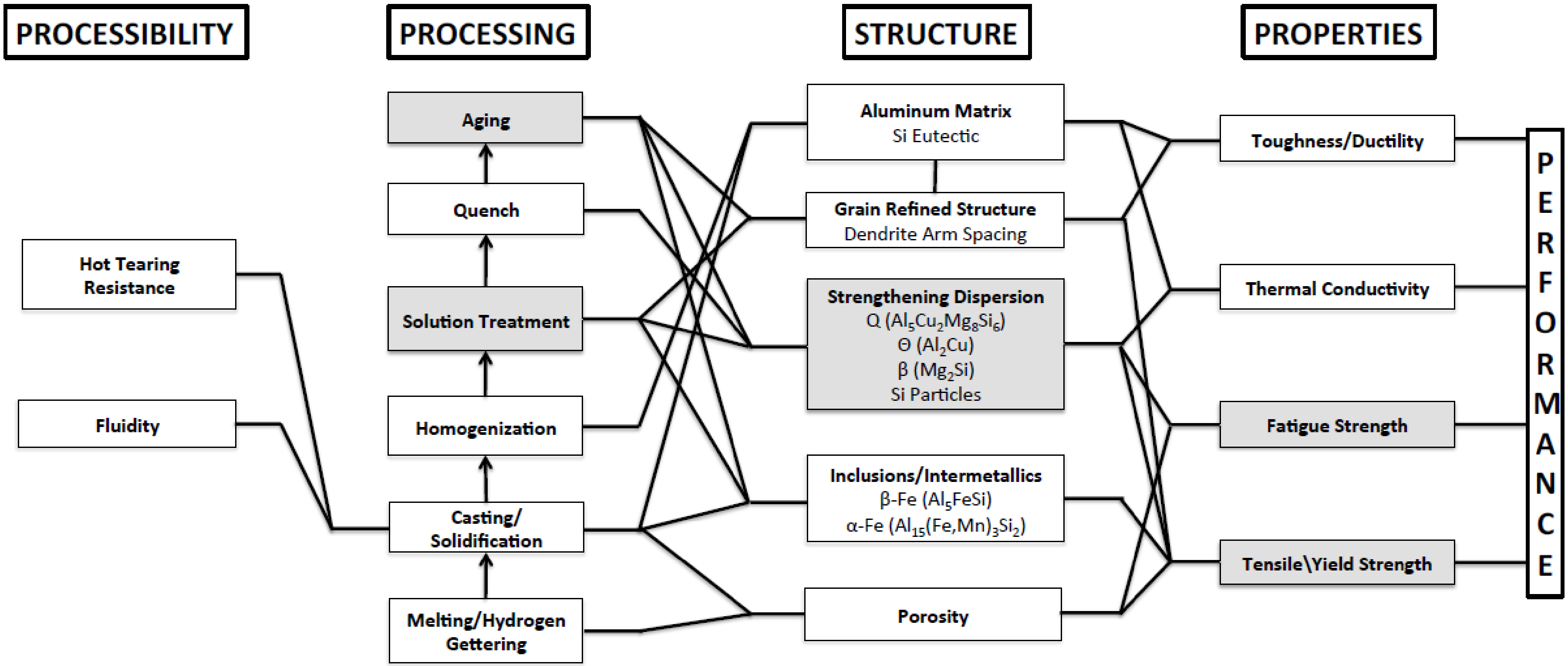
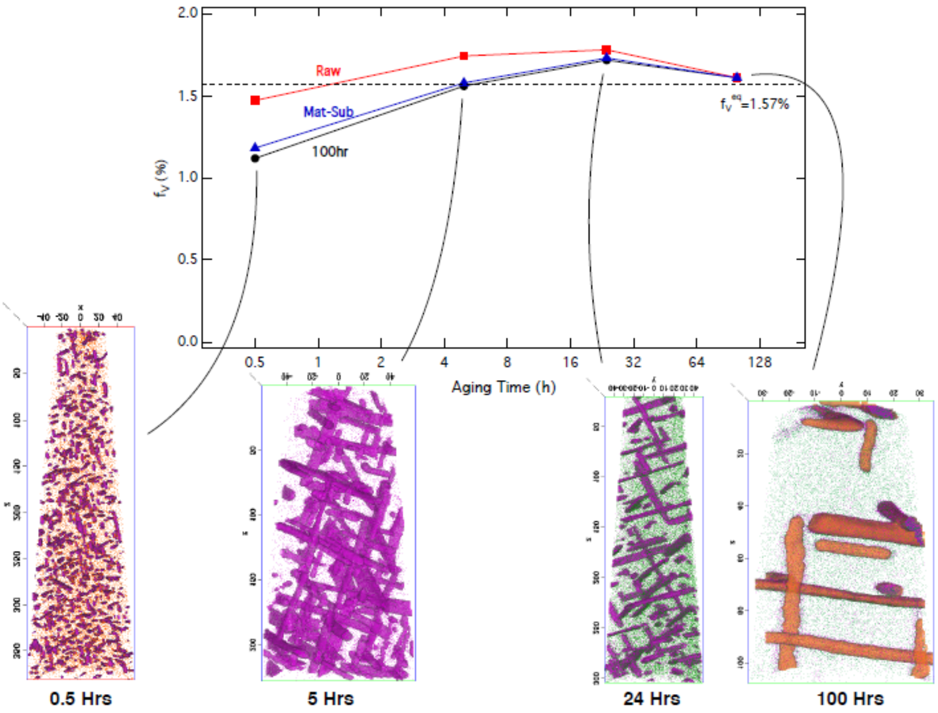
Approach/Strategy

System design chart illustrating links among processing/structure/properties relationships



A system design chart was established to identify integrated computational materials engineering (ICME) links to be used in materials design efforts

Approach/Strategy



LEAP images showing precipitate phase evolution (volume fraction/size) versus aging time

Characterization efforts include local electrode atom probe (LEAP), TEM, etc.

Data obtained from experimental results is used to refine computational models and thermodynamic and mobility databases

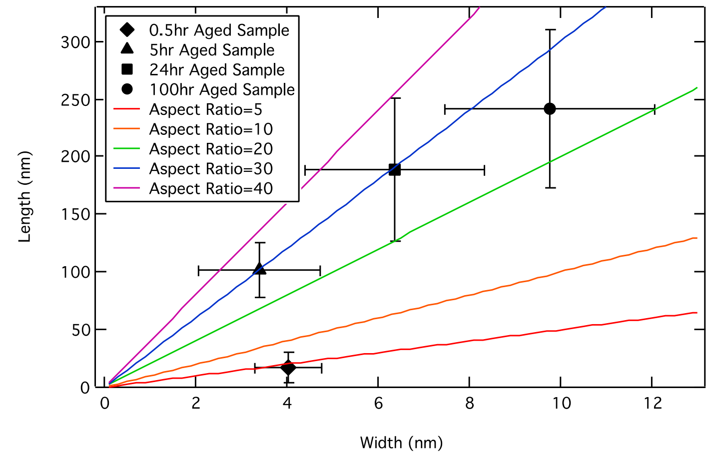
Milestones

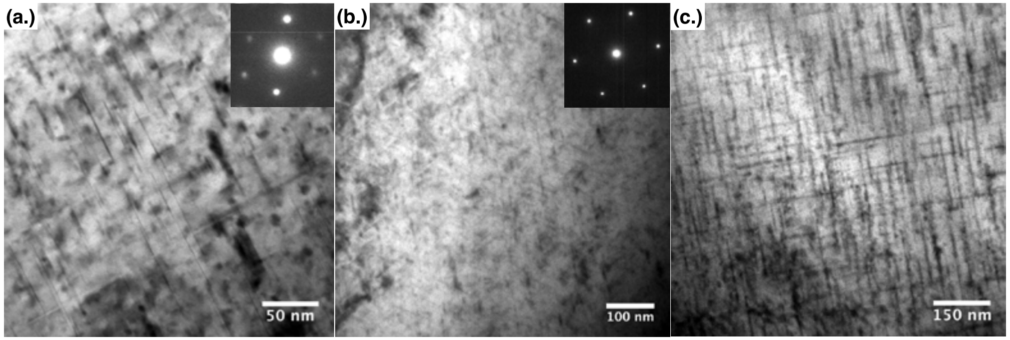
Milestone	Date planned	Status
1. Alloy Requirements Matrix	01/14	Complete 03/14
2. Alloy Concepts Generated	01/14	Complete 03/14
3. Alloy Models Selected for Castings	03/14	Complete 04/14
4. Produce Sub-scale Castings	04/14	Complete 05/14
5. Data Development of Sub-scale Castings	07/14	Complete 10/14
6. Validation of Sub-scale Concepts and Models	10/14	New date 04/15
Go/No-Go Validation of models adequate to continue	10/14	New date 04/15
7. First Generation Alloy Designs	01/15	New date 06/15
8. Lab-scale Castings of First Generation Designs	04/15	New date 09/15
9. Alloy Characterizations and Validation	07/15	New date 12/15
Go/No-Go Demonstrate property improvement	07/15	New date 12/15

New date reflects 6 month extension applied to budget period 2

Technical Accomplishments
Strengthening Particle Evolution

- Precipitate growth and shape changes determined by transmission electron microscopy (TEM) and local electrode atom probe (LEAP)
- *In-situ* TEM planned for calibration of precipitate growth models for ICME tool expansion
- ***Calibrated precipitate growth models enable the design of aluminum with optimal strength***





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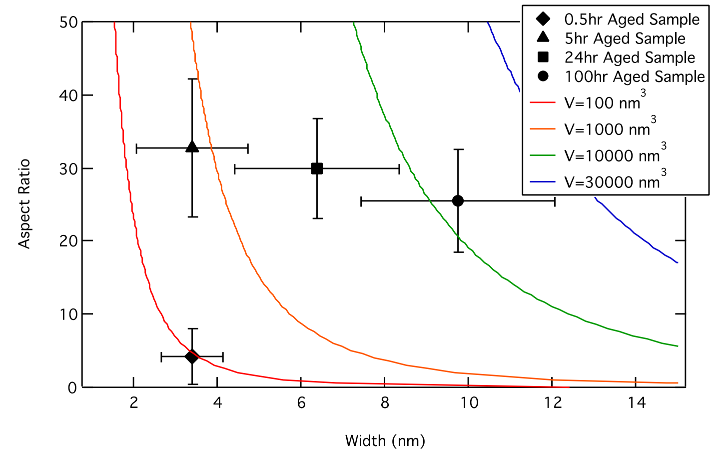
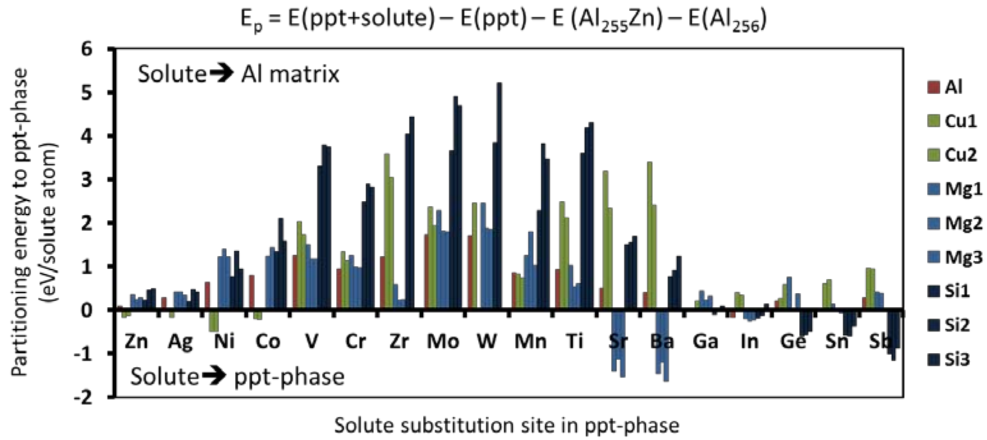
TEM images in various orientations performed to the shape of strengthening precipitates in Concept 1



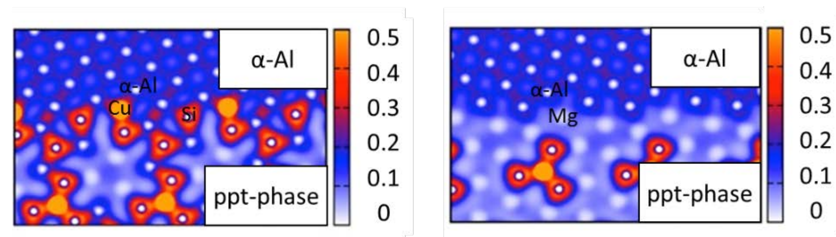
The evolution of the precipitate length, width, and aspect ratio versus aging time of Concept 1

Technical Accomplishments
DFT Determination of Solute Segregation

- DFT (density functional theory) calculations for solutes in aluminum to slow precipitate coarsening
  - Elements identified with potential to segregate to precipitate
- Interfacial energy calculations performed to calibrate precipitation models
  - Charge density plots show which elements increase chemical bonding on interface
  - Calculations show ordering of preferable interface
- ***DFT results used to find elemental additions to enhance properties of cast aluminum***



Precipitate segregation energies for various elements

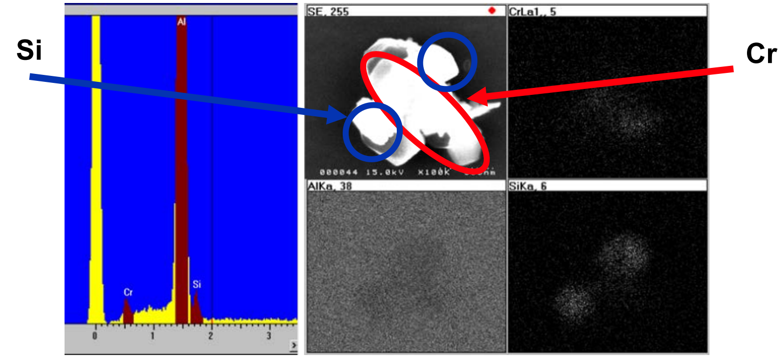


1st nearest atom to interface	2nd nearest atom to interface	3rd nearest atom to interface	Interfacial energy (J/m^2)
Si	Mg	Mg	≈ 0.72
Cu	Mg	Si	0.66
Cu	Si	Al	0.52

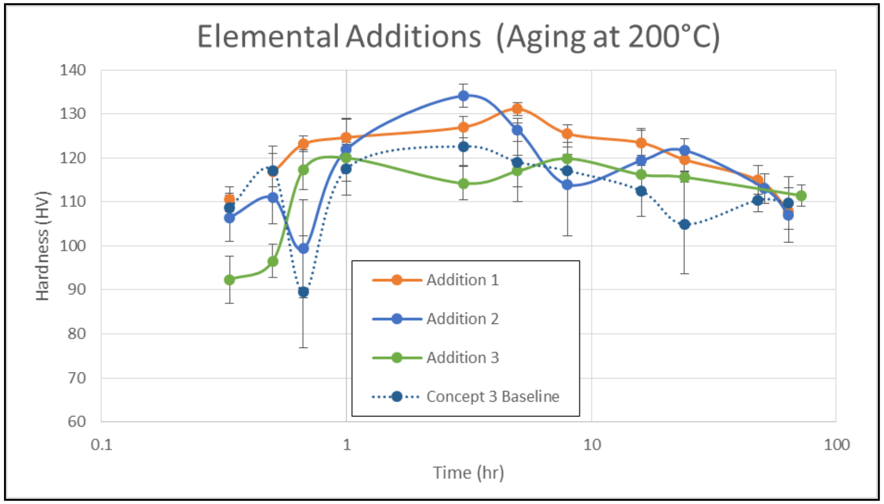
DFT Interfacial energy calculations and charge density plots

Technical Accomplishments
Evaluation of Concept Alloys

- HTDFT concepts found to have undissolved elemental additions
  - No aging peak found
  - Increased solution treatment used for elemental additions in response to finding of undissolved particles
- Elemental additions to concept 3 showed slower coarsening of precipitate phase—higher hardness at longer aging times
  - Elevated hardness seen at long aging times (> 10 hrs.) for all additions
  - Additions will be evaluated in casting versions of alloys
- ***Concepts identified with ICME methods shown to have superior properties in sub-scale castings***



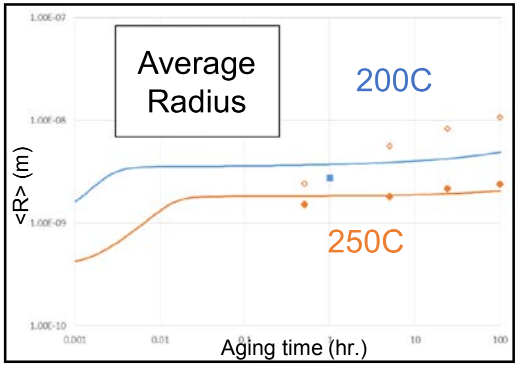
Un-dissolved Cr and Si particles in HTDFT concept

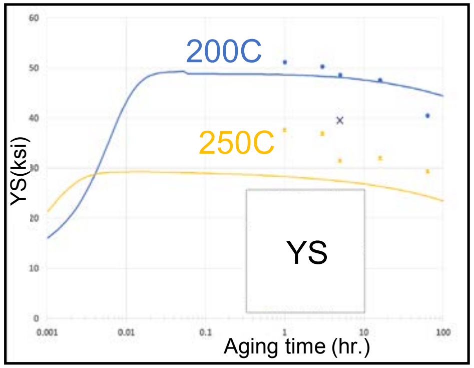


Hardness versus 200°C aging for elemental additions to Concept 3 buttons

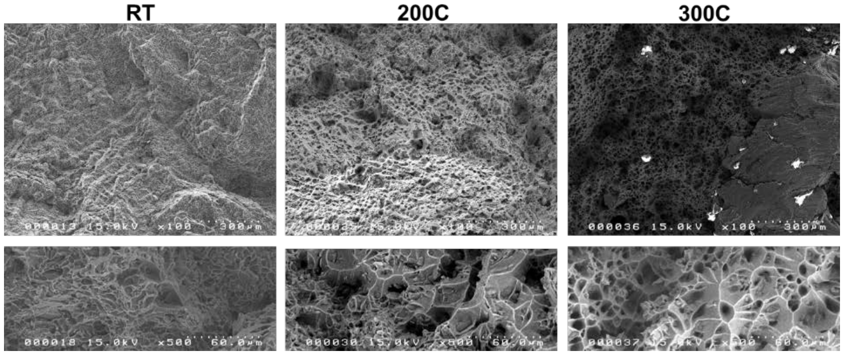
Technical Accomplishments
Strength Model Development

- Initial strength models developed for precipitation strengthening
  - Precipitation models (*PrecipiCalc®*) show precipitation size evolution
- Fracture surface analyzed with SEM/EDS: initiation sites found
- ***Strength model development will enable parametric design of alloys with maximized strength***

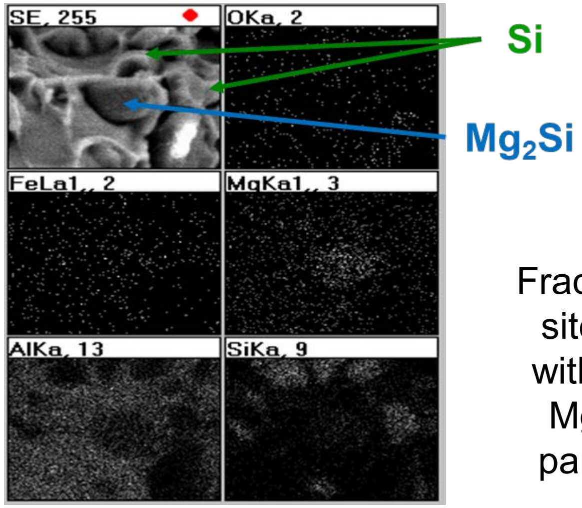




Precipitation radii growth (left) and alloy yield strength prediction (lines) versus experiment (points) at 200 and 250°C

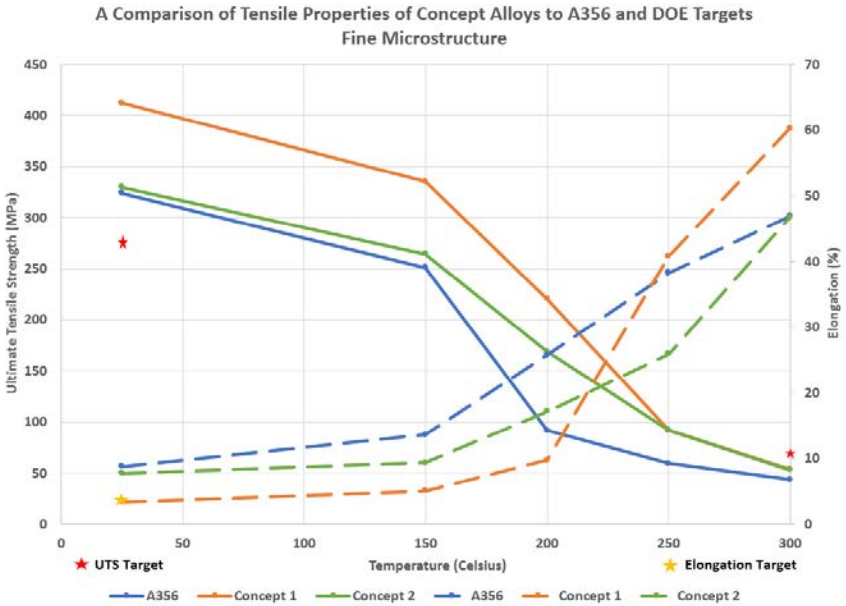


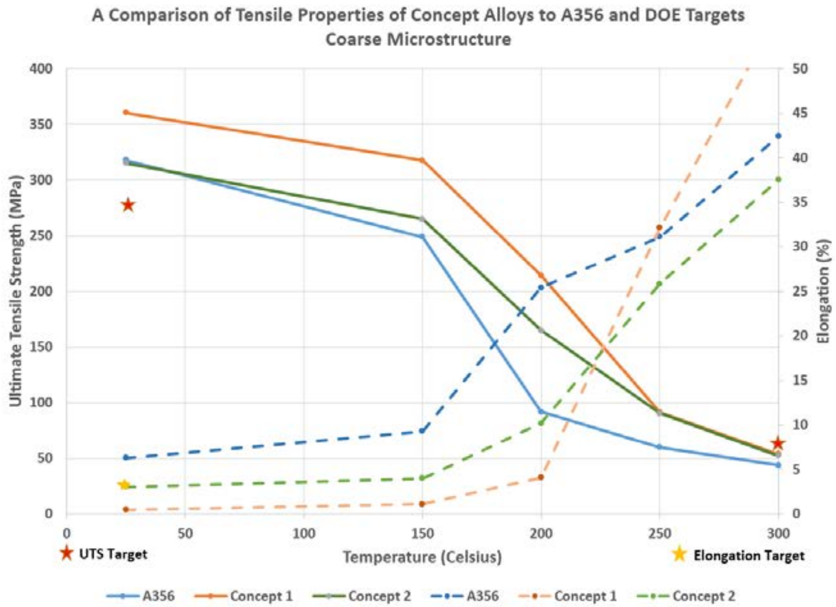
SEM of fracture surfaces versus conditioning temperature for Concept 1 alloy



Fracture initiation sites identified with SEM/EDS: Mg2Si and Si particles found

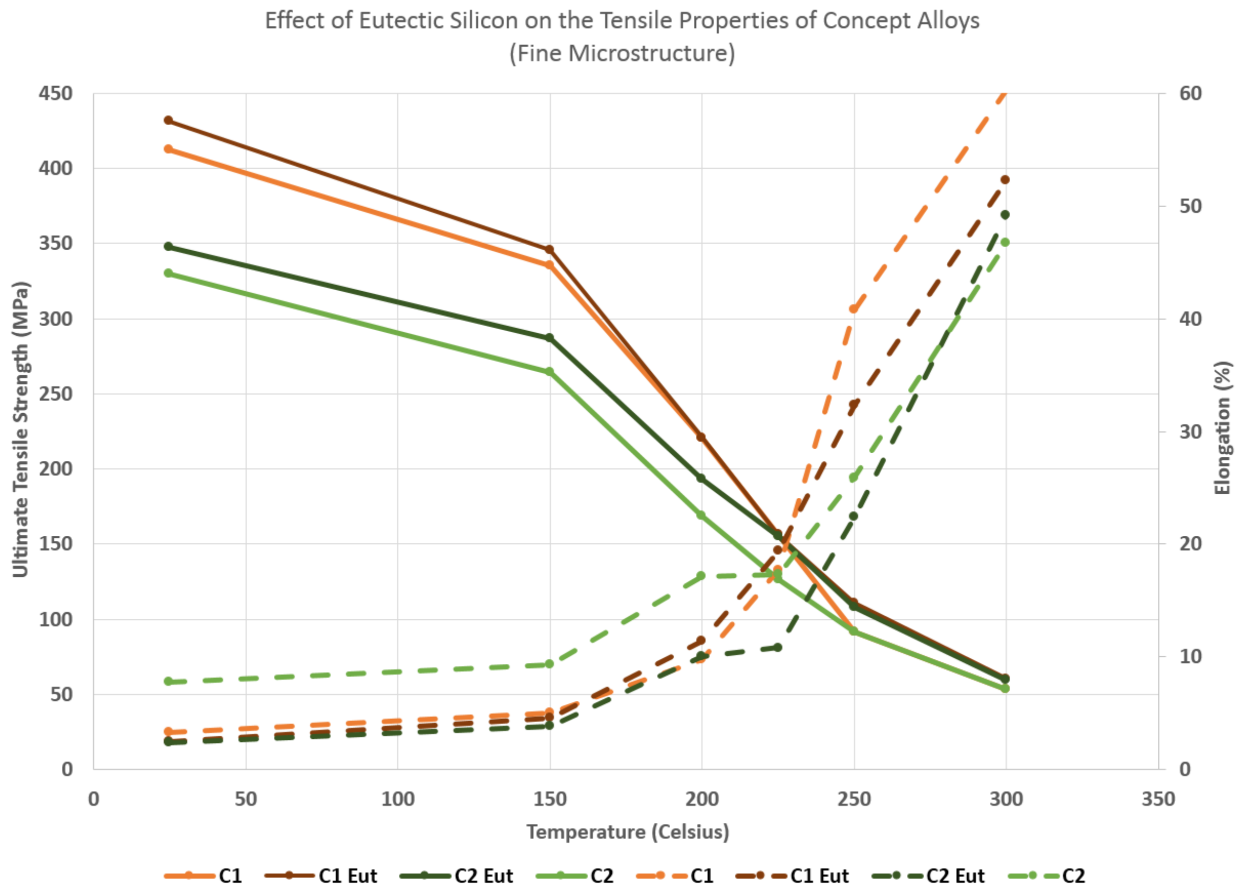
Technical Accomplishments
Tensile Properties of Initial Alloys





Concept alloys have mechanical properties above baseline A356 but increased strength is needed at 300 C. Maintaining room temperature ductility is necessary to achieve fatigue targets.

Technical Accomplishments
Alloy Parameterization



Silicon provides added strength at all temperatures but causes loss in ductility.

Responses to Reviewers Comments

Reviewer comment: Project team was missing a major aluminum company to make alloy.

Response: General Motors purchases aluminum from multiple suppliers for its casting operations depending on price and availability and does not want to be tied to a single supplier. GM has included a consultant previously employed by an aluminum manufacturer to gain knowledge from the aluminum producers.

Reviewer comment: The reviewer noted that adding a national laboratory partner would help strengthen the project team.

Response: General Motors and project partners Northwestern University and Questek LLC have sufficient computational, experimental expertise and equipment to develop an aluminum alloy.

Responses to Reviewers Comments

Reviewer commented that the project defines needs but does not yield the answers through the development of a new alloy.

Reviewer explained that the evaluation of the current alloys and analysis of the needs was good but the progress or pathway to a new alloy is lacking.

Reviewer Can you explain the link with the introduction of alternative chemical species to further enhance high-temperature stability, ductility, fatigue properties, and castability with the enhanced models.

Response: It is critical to properly define the needs for any new alloy development. Although strengthening mechanisms and factors affecting castability are well known in the literature for aluminum alloys, it is important to incorporate these in the strength, fatigue, and castability models. A high temperature resistant alloy will be developed using the advanced ICME tools that have already incorporated well-known strengthening models and capability in predicting castability and multi-scale defects and microstructures.

Collaboration and Coordination

General Motors – Principle Investigator

- Project administration, casting simulation, casting experiments, mechanical properties, microstructural evaluation

QuesTek Innovations LLC – Industrial sub-partner

- Industrial Sub-partner
- ICME calculations – thermodynamics, kinetics, DFT alloy generation, alloy concept generation, parametric and final alloy designs, heat treatment process recommendations

Northwestern University – University sub-partner

- DFT alloy generation, Phase Field modelling of microstructure, experimental validation - Optical, SEM,TEM, LEAP

Fred Major, Tom Prucha (AFS),– Industrial sub-partners

- Technical advisors

Camanoe Associates – Industrial sub-partner

- Process Based Cost Modelling

MIT – University sub-partner

- Recyclability Analysis

Remaining Challenges and Barriers

All new and baseline alloys still show a precipitous drop in material strength beyond 150 C. Unable to achieve DOE 300 C strength targets of 65 MPa and a 100 MPa GM strength target at 250 C have also not been met.

Alloy concepts with the best high temperature strength or slowest decline in strength with elevation of temperature show inadequate ductility at room temperature. Room temperature ductility is critical to low cycle fatigue resistance.

Maintaining costs within targets eliminates the use of scandium, silver, etc., well known additions to achieving high temperature strength in aluminum.

Future Work

2015

Parametric designs of alloys.

- Optimize castability, strength, and ductility
- Refine strength models, update thermodynamic/mobility databases
- Milestone 7 Completion of First Generation Alloy Design (06/15)
- Milestone 8 Lab scale casting of new alloys (09/15)
    - Buttons and plates
- Milestone 9 Alloy Characterization and Designs Validated (12/15)
    - Microstructural determinations, castability evaluation, property measurements

2016

Develop Final Embodiment of New Alloy

- Milestone 10 Final Computational Design (06/16)
- Milestone 11 Lab scale Casting of Final Alloy (09/16)
    - Plates for tensile properties, fatigue analysis
- Milestone 12 Component Scale Castings (12/16)

Summary

Developed and selected several key alloy concepts using ICME methods
Through button casting, microstructural analysis, isochronal and isothermal heat treatment studies populated important databases for further alloy development and validated key concepts and strength models
Through end-chill plate casting and tensile testing created first set of castable alloys stretching to target properties.

Property	DOE Target	Fine SDAS	Coarse SDAS
Tensile Strength @ 25C	276 MPa	330 MPa	315 MPa
Yield Strength @ 25 C	207 MPa	273 MPa	277 MPa
Elongation @ 25C	3.5%	7.8 %	3.07 %
Tensile Strength @ 300 C	65.5 MPa	53.1 MPa	52.4 MPa
Yield Strength @ 300 C	45.0 MPa	41.0 MPa	41.3MPa