

High Performance Cast Aluminum Alloys for Next Generation Passenger Vehicle Engines

2015 DOE Vehicle Technologies
Annual Merit Review and Peer
Evaluation Meeting
June 10, 2015

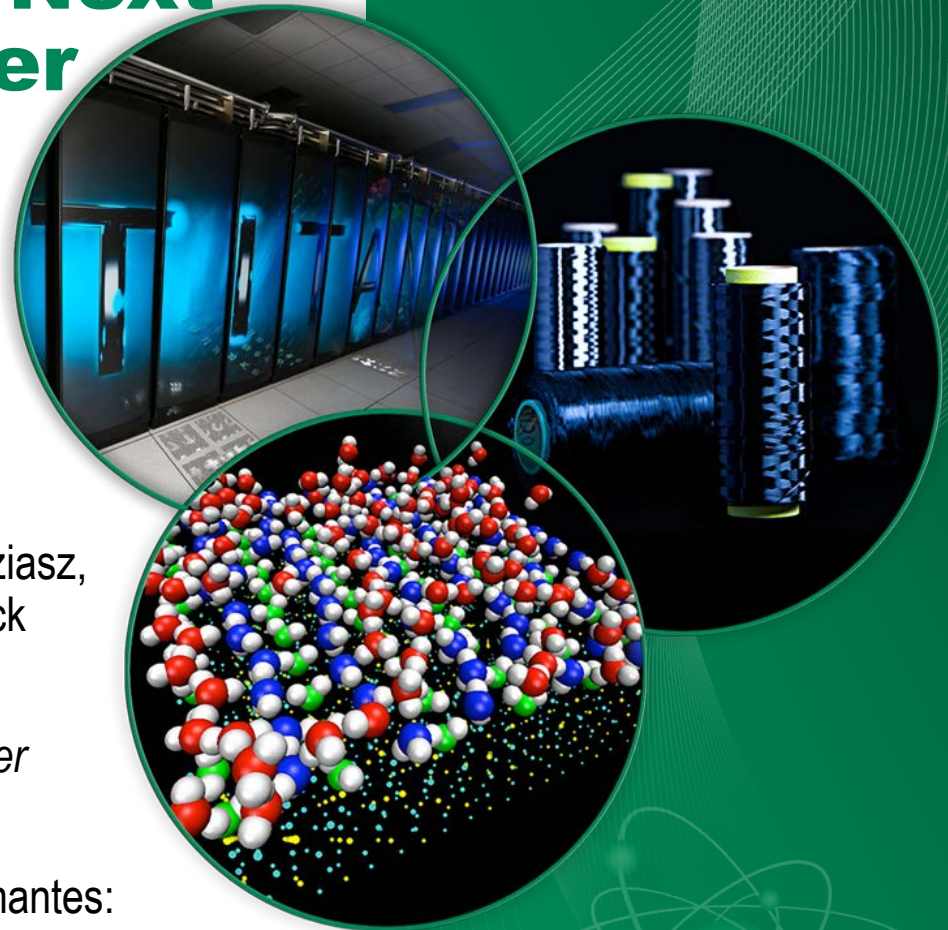
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Lin Zhang, Chris Glaspie, Gregg Black: *Fiat Chrysler Automobiles (FCA)*

Andres Rodriguez, Alejandro Gonzalez, Jose Talamantes: *Nemak S.A.*

Sponsored by
**U.S. Department of Energy, Energy Efficiency and
Renewable Energy, Vehicle Technologies Office**

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Overview

Timeline

- Start: November 2012
- CRADA Executed: Nov 2013
- End: November 2017
- 38% Complete

Budget

- Total project funding.
 - DOE-\$3500 K
 - Cost share ~\$2000 K
- FY14 DOE Funding - \$1100 K
- FY15 DOE Funding - \$1000 K

Barriers

- Absence of **economical** lightweight materials with improved castability, high temperature strength and fatigue performance.
- A major barrier to the development of new alloys is the time-intensive trial and error approach applied to these complex systems. **Integrated computational materials engineering** (ICME) approach to accelerate the development and deployment of new cast aluminum alloys.

Partners

- CRADA Partners: Fiat Chrysler Automobiles (FCA), ORNL, Nemak Inc.
- Collaborators: Granta MI, ESI North America, Flow Science, Magma Foundry Technologies, Minco Inc.
- Project lead – ORNL

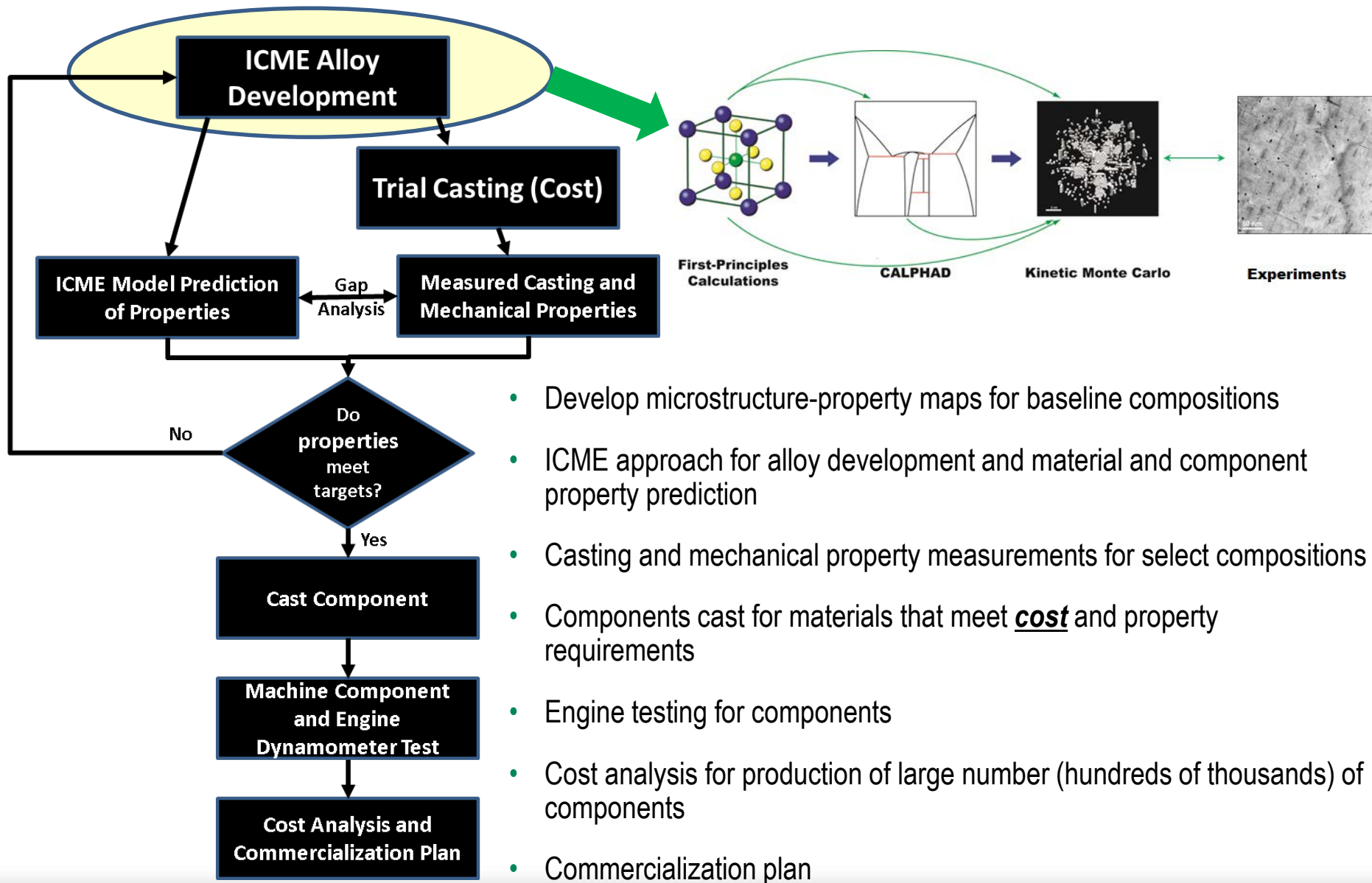
Relevance

- Opportunity to develop and commercialize the next generation of materials for higher efficiency light duty engines (with higher peak cylinder pressure and temperature) where Aluminum alloy use is limited due to these materials rapidly losing strength at temperatures $> 200^{\circ}\text{C}$.
- Objectives
 - Develop high performance cast aluminum alloys that have following characteristics
 - improved castability, high temperature strength and fatigue performance.
 - engine cylinder heads fabricated with new alloy will have $> 25\%$ strength improvement (at 300°C compared to baseline properties at 250°C) and will cost $< 10\%$ more than heads manufactured by 319 or 356.
 - will enable an increase in maximum component operating temperature by $\sim 50^{\circ}\text{C}$.
 - Evaluate the adequacy of existing ICME models and codes for the prediction of properties and development of cast aluminum alloys
 - A gap analysis report for existing ICME codes for cast aluminum alloy development.

Project Milestones

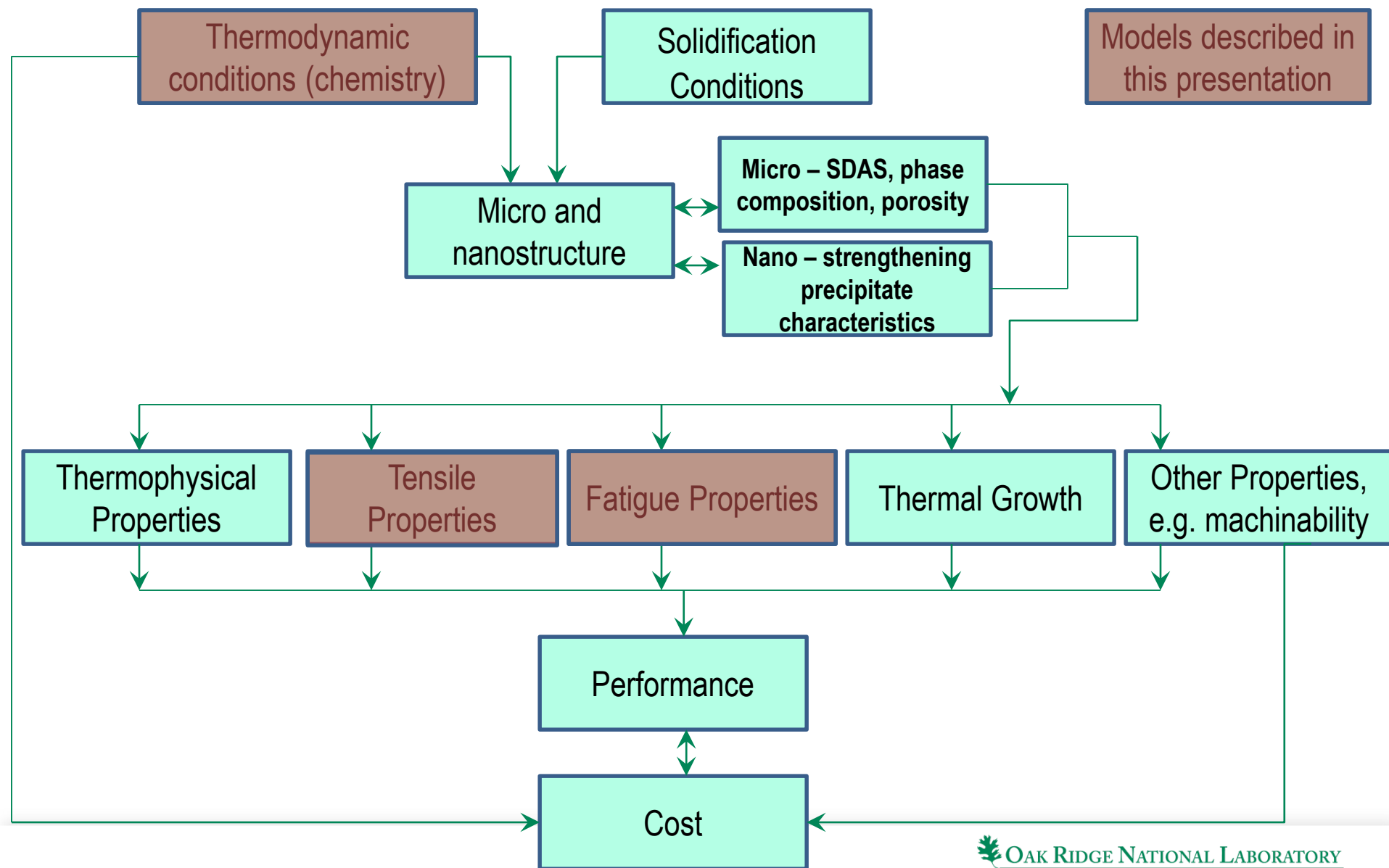
- Milestone 1: Selection of the cast aluminum alloy family for further development to refine alloy development path.
 - Planned Date: 11/30/14 (**completed**)
- Milestone 2: Finish implementation of ICME models that could be iterated to accelerate the alloy development.
 - Planned Date: 11/30/15 (on track)
- Milestone 3: Finish identification of new alloy composition(s) with improved properties.
 - Planned Date: 11/30/16
- Milestone 4: Complete cost model for component fabrication with new alloy.
 - Planned Date: 7/31/17
- Milestone 5: Finish commercialization plan for the new alloy.
 - Planned Date: 11/30/17

Approach



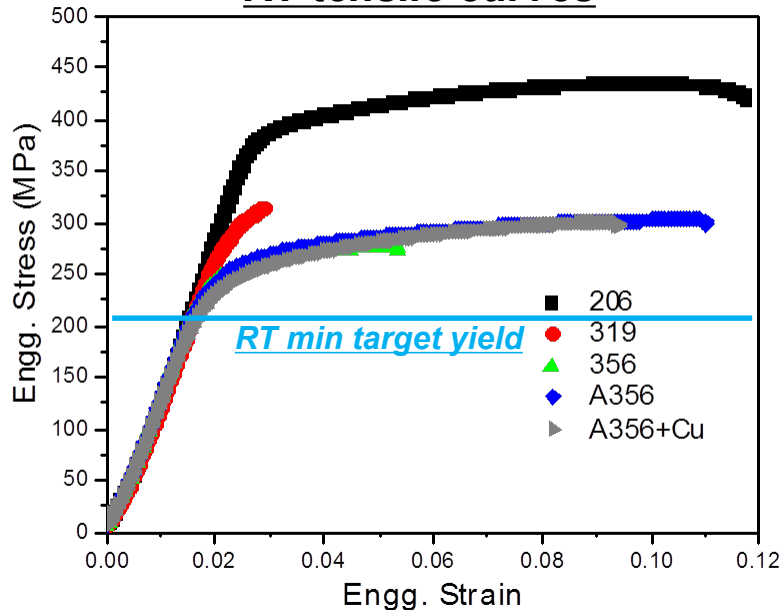
- Develop microstructure-property maps for baseline compositions
- ICME approach for alloy development and material and component property prediction
- Casting and mechanical property measurements for select compositions
- Components cast for materials that meet **cost** and property requirements
- Engine testing for components
- Cost analysis for production of large number (hundreds of thousands) of components
- Commercialization plan

Approach – Computational models for cast aluminum alloy development

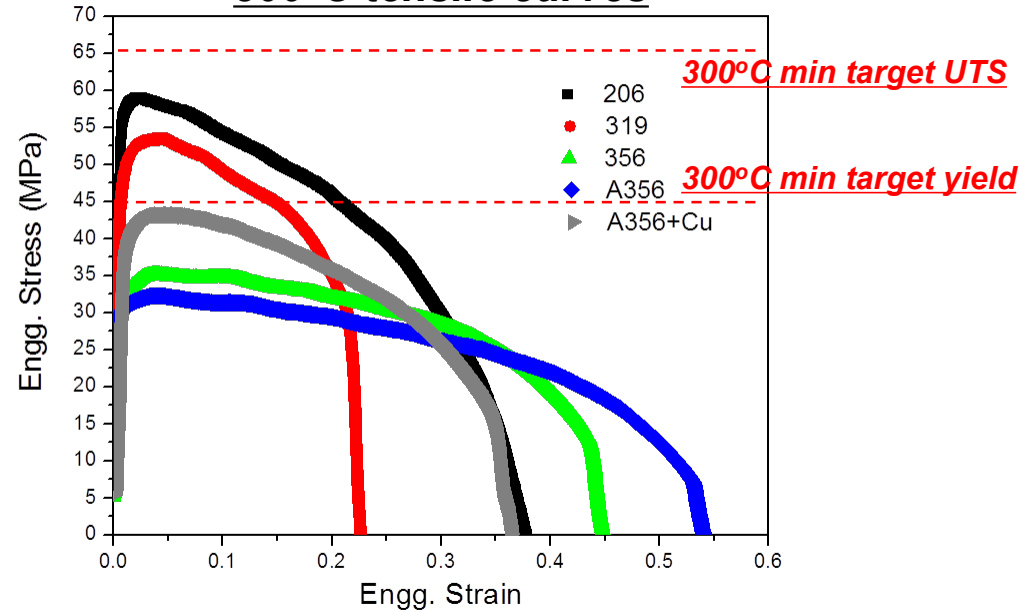


Targets and Technical Accomplishments

RT tensile curves



300°C tensile curves

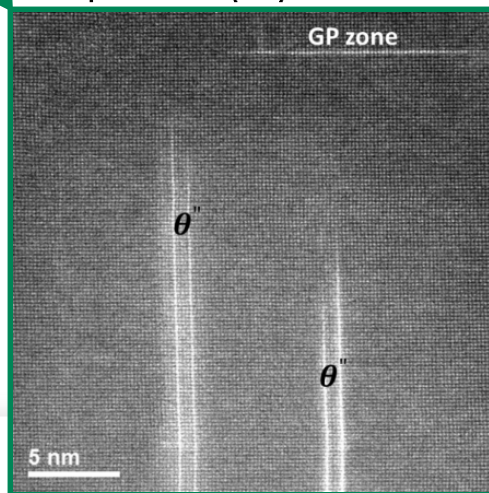
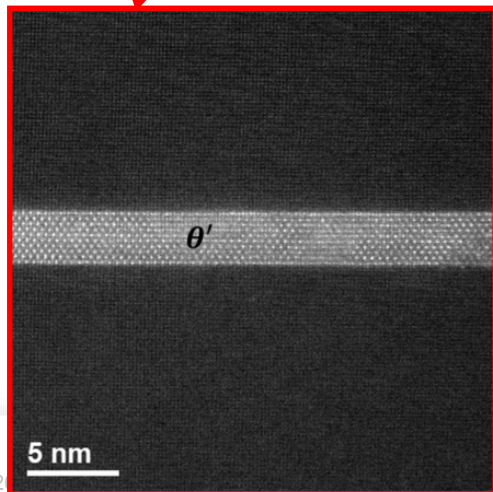
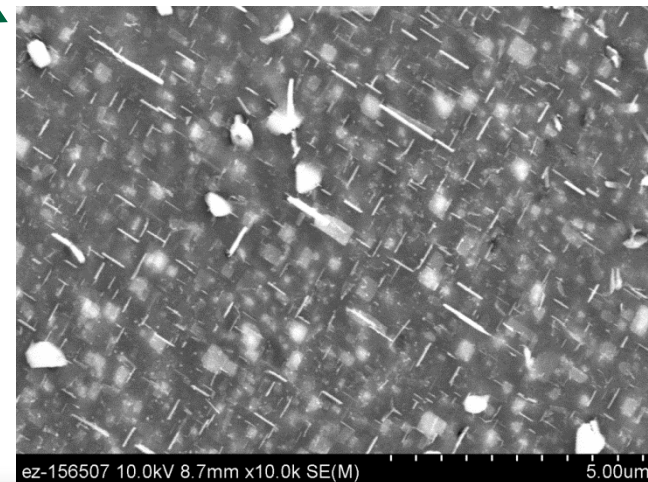
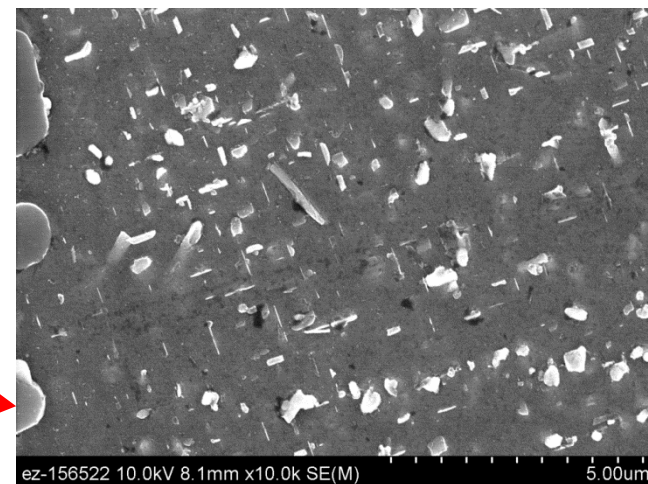
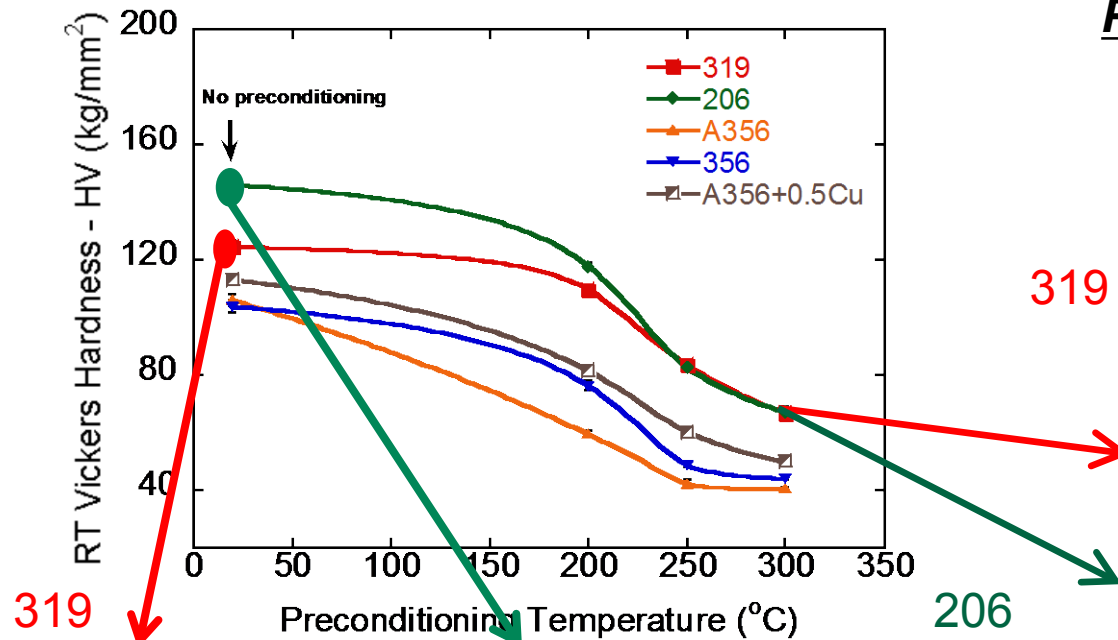


- Baseline materials supplied by Nemak
 - 319-T7; 356-T6; A356-T6; A356+0.5Cu-T6; 206-T6; two high performance baseline alloys
 - All materials have grain size/secondary dendrite arm spacing (SDAS) of ~ 30 μm
- Characterization (for cylinder head application) of baseline materials
 - Microstructure characterization
 - Mechanical properties; high temperature tests on preconditioned specimens
 - Thermal properties (thermal expansion, heat capacity, thermal diffusivity, thermal conductivity)

Technical accomplishments

- High temperature microstructural stability is key to improved elevated temperature mechanical properties (flat response is desired in graph below)

Preconditioned 200 hrs @300°C



Technical accomplishments

Effect of ageing on 206 alloy

GP I

2 nm

5 hrs

16 hrs

2 nm

GP II or θ''

2 nm

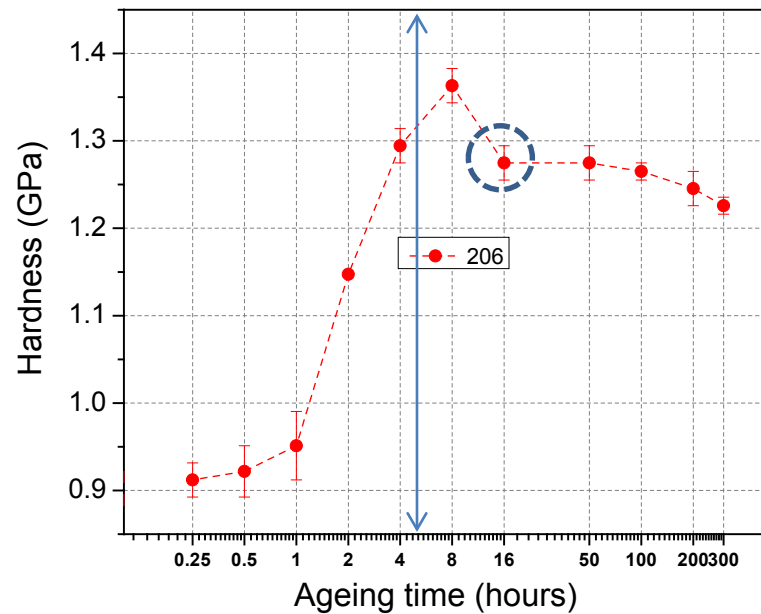
θ'

Q Phase

2 nm

Q Phase

2 nm

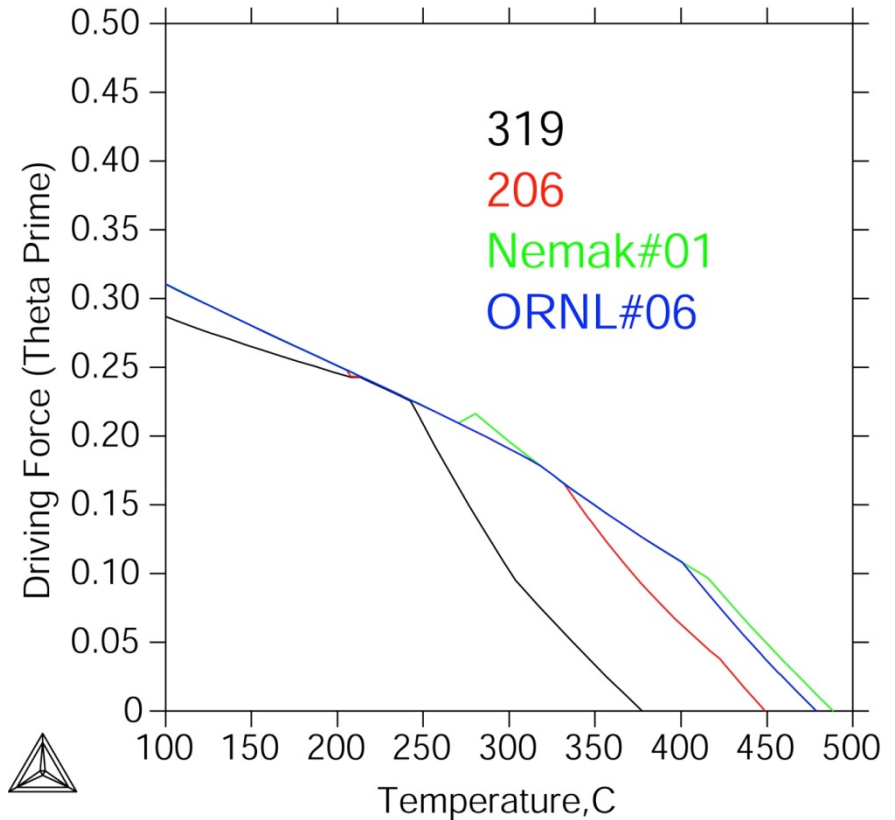
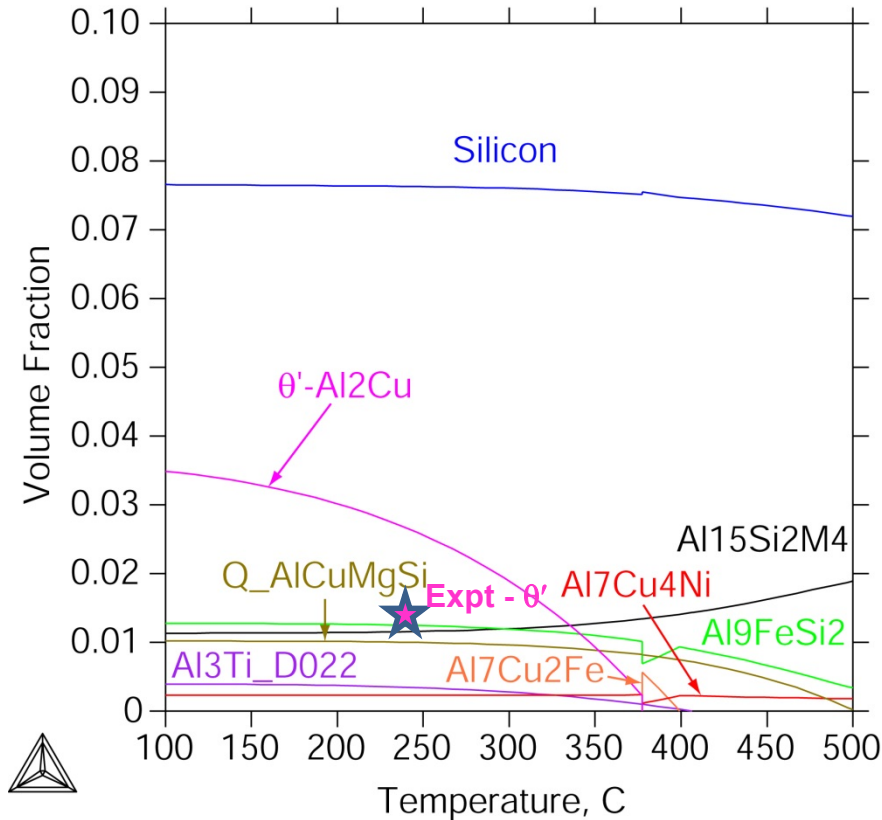


Ageing temperature – 190°C

2 nm

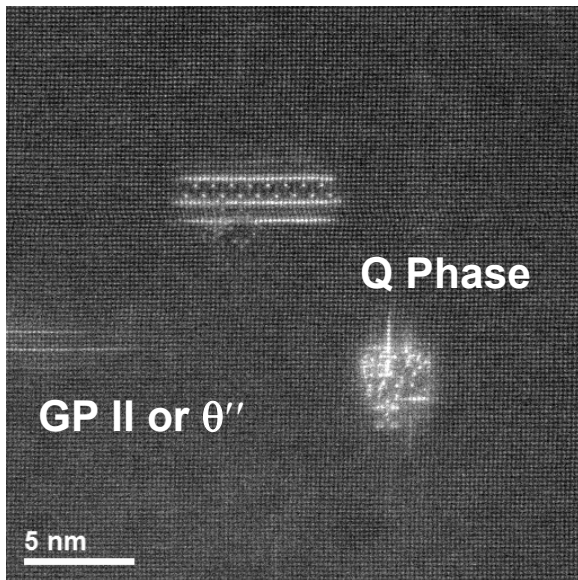
Technical accomplishments - Predicted Phases for 319 Al

319: Al-8.29Si-3.17Cu-0.34Mg-0.31Zn-0.68Fe-0.03Ni-0.39Mn-0.17Ti



Computational thermodynamic modeling (CALPHAD) approach has been used to predict thermodynamic stabilities including meta-stable phases with the TCAL3 database from Thermo-Calc™

Technical accomplishments – Density Functional Theory (DFT) Calculations for Al alloys with high temperature stability



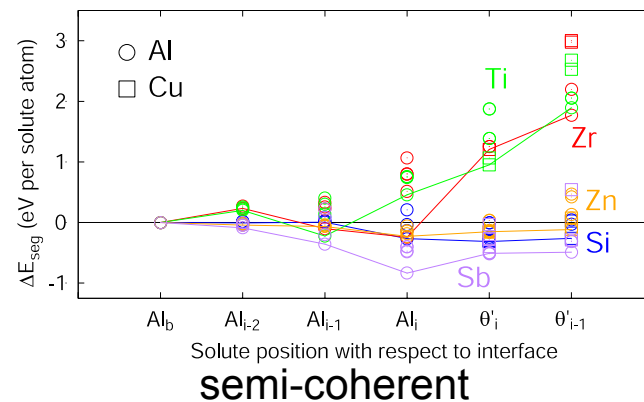
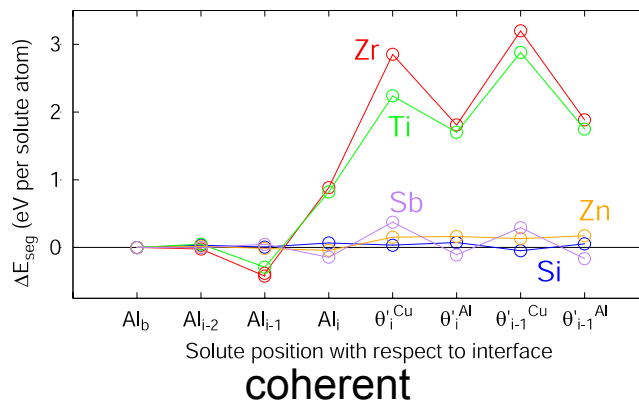
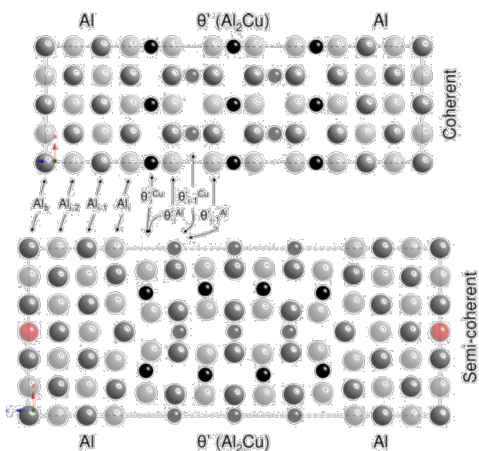
Solute clustering and vacancy interaction in Al alloys



Nucleation and early growth is important for determining precipitate morphology

Interaction between solute clusters and vacancies have been calculated from first-principles to correlate the nucleation and growth of precipitates at the early stage of diffusion kinetics.

Solute segregation at the θ' /Al interface



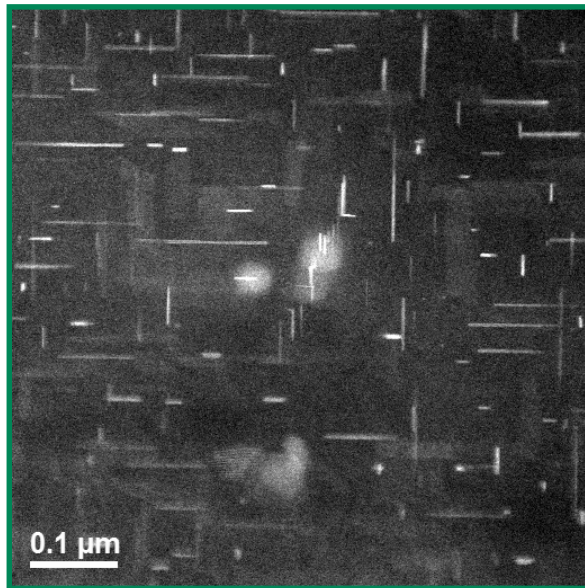
Some elements strongly segregate at the semi-coherent interfaces between matrix Al and θ' -Al₂Cu and determine the high temperature stability of the precipitate

A. Biswas et al., Acta Mater., 59 (2011) 6187–6204

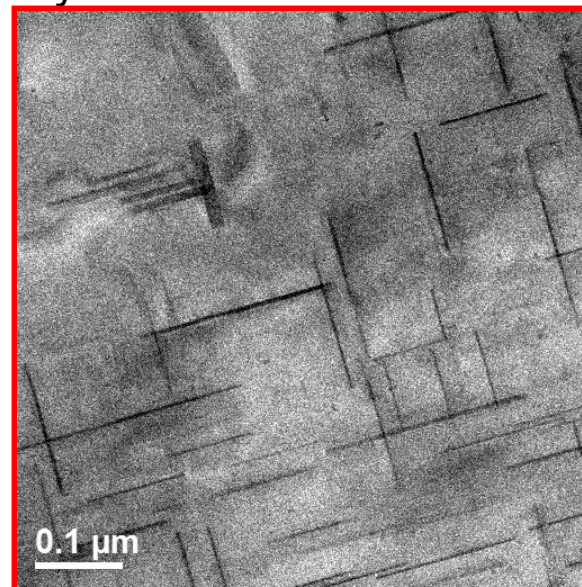
Technical Accomplishments – Strength model

- Motivation for strength modeling: Design the microstructure to achieve the desired level of mechanical response from the material system

206 - DF



319 - BF

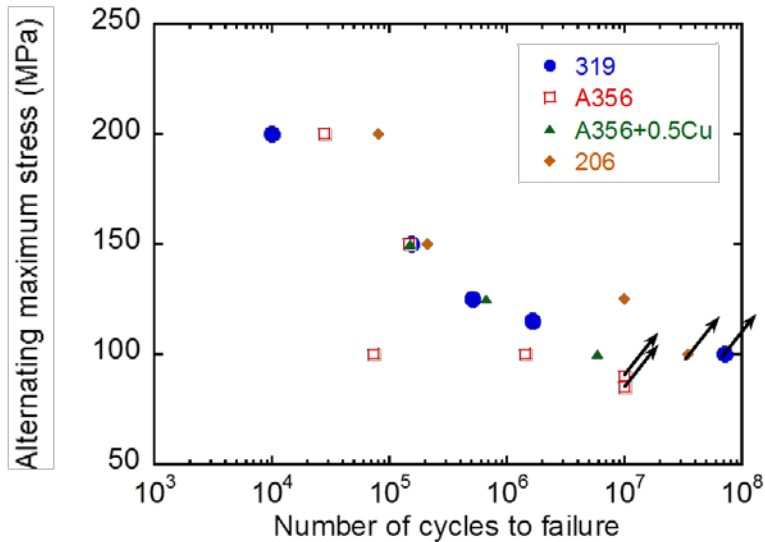


- Yield strength (σ_y) is the sum of (a) intrinsic strength of the material system (σ_i), (b) strength due to precipitates (σ_{ppt}), and (c) strength due to solid-solution (σ_{ss}): $\sigma_y = \sigma_i + \sigma_{ppt} + \sigma_{ss}$

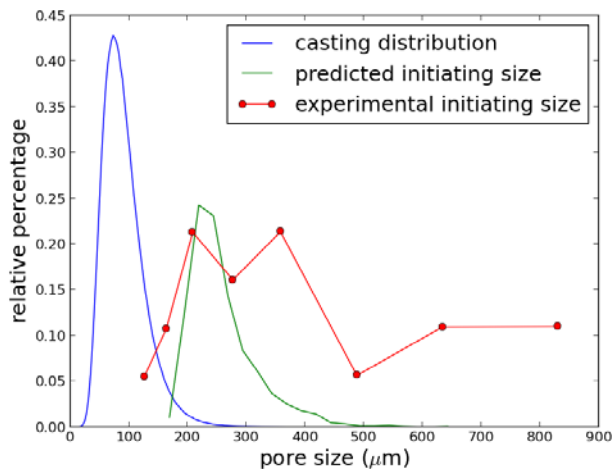
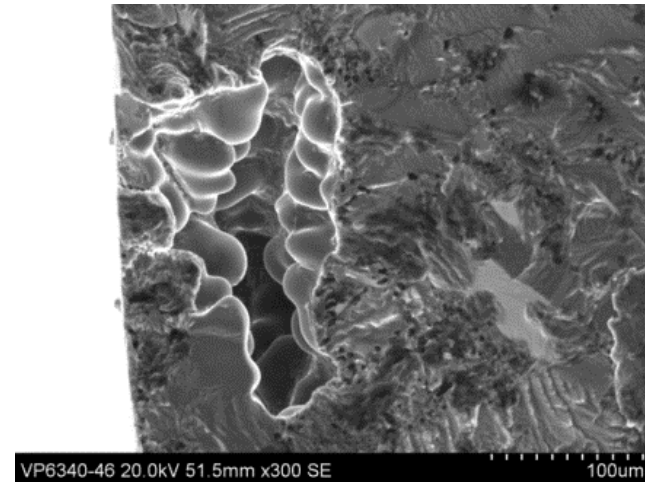
Alloy	Ppt. dia. (nm), d_t	Ppt. thickness (nm), t_t	Number density, (N_v) (nm^{-2})	$\Delta\tau$ (MPa)	$\Delta\sigma = M\Delta\tau$ (MPa)	σ_{ss} (MPa)	σ_i (MPa)	σ_{Cal} (MPa)	$\sigma_{Expt.}$ (MPa)
319-T7	124.9	2.8	3.6×10^{-7}	43.1	131.7	15.7	104.5	245.2	279.8
206-T6	40.5	1.8	54.1×10^{-7}	70.3	215.1	2.4	132.6	350.1	380

Refs: A.J. Ardel *Met. Trans.* 16A (1985) 2131-2165; S.C. Weakly-Bollin et.al. *Metal. Mater. Trans. A* 35A (2004) 2407 – 2417; J. da Costa Teixeira et. *Al. Acta Mater.* 56 (2008) 6109–6122; J.F. Nie and B.C. Muddle, *J. Phase Equil.* 19 (1998) 543-551; A.W. Zhu and E.A. Starke Jr., *Acta Mater.* 47 (1999) 3263–3269

Technical Accomplishments - Fatigue limit model



A356-T6 fatigue fracture surface



We ran 1900 fatigue simulations for 319 type alloy!
General model developed

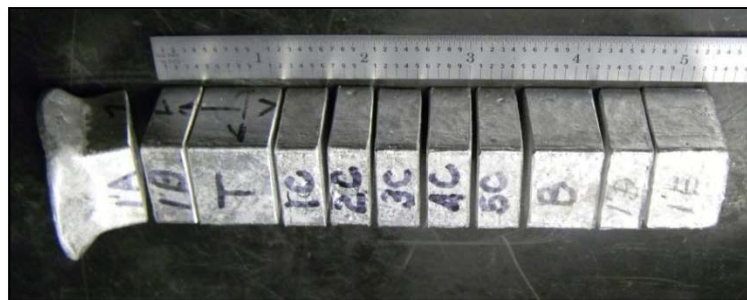
Simulation results summary

	Mean Fatigue strength (MPa)	Standard deviation (MPa)
experiment	85	8.5
prediction	83	8.9

Technical Accomplishments – New Alloys

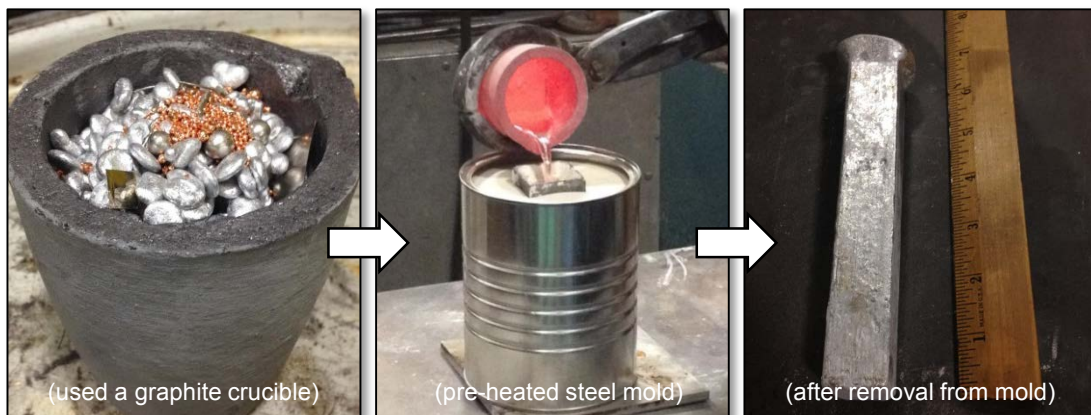
- ❑ Minor alloying effects on high-temp. properties, thermal stability, castability, and cost effectiveness are to be evaluated for 25 compositions developed;

- Lab-scale heats have been cast by using pre-heated steel mold
- Nemak, provided master alloys (total ~90kg) to ORNL



Sectioned heat

Typical melt process of lab-scale heat



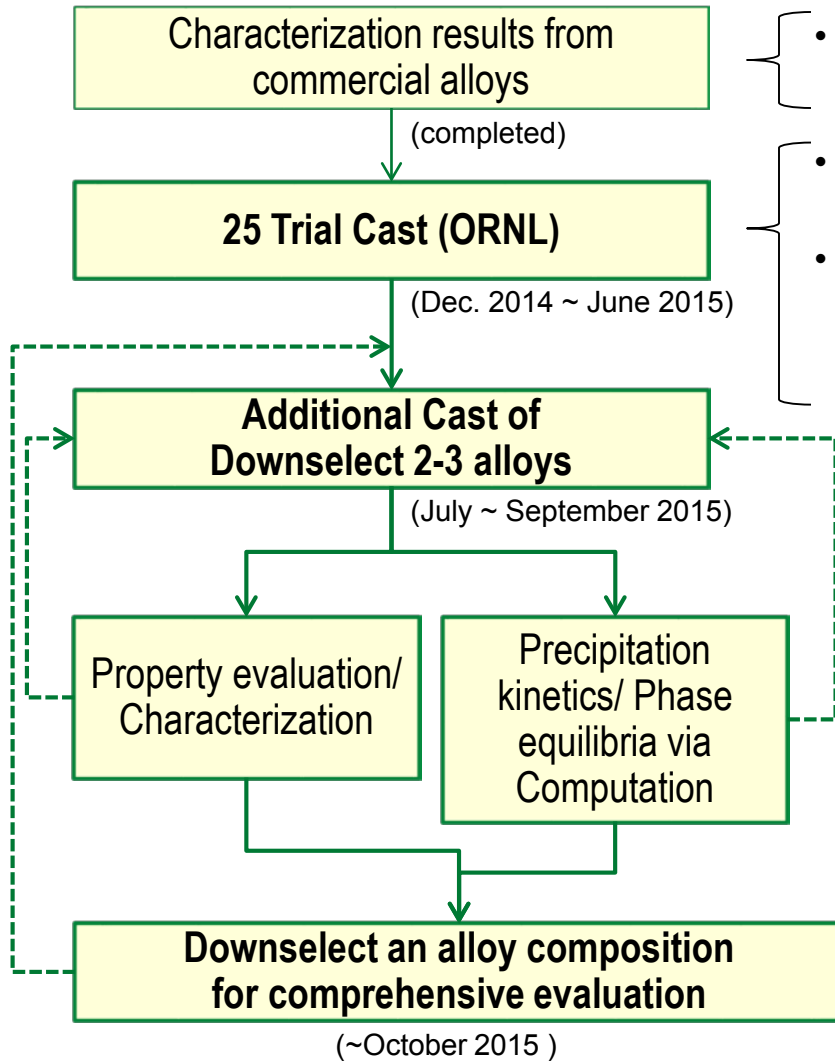
Master ingots from Nemak



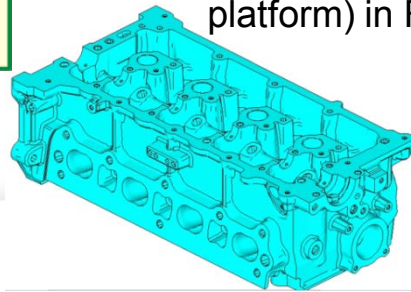
Collaboration

- Monthly conference calls and biannual face-to-face all hands meeting
- *CRADA* partners with significant cost share
 - Chrysler - OEM automotive manufacturer
 - FCA (Chrysler) provides technical guidance to the overall effort and leads tasks such as LCF/machinability evaluation
 - Powertrain Laboratories Engine, Transmission, & Component Testing lead
 - Nemak S. A. – Cylinder head supplier to Chrysler
 - Guides casting and alloy development effort. Provides the larger scale casting to ORNL
 - Product prototyping development at these centers utilizes the latest software and technologies to simulate processes and determine optimal product configurations
 - The Semi-Permanent Molding (SPM) technologies for cylinder heads include Gravity, Direct Pouring, Low Pressure, and Rotacast.
- Other cost share partners
 - Granta MI – Data management partner
 - ESI North America, Flow Science, Magma Foundry Technologies – casting simulation softwares
 - Minco Inc – casting supplies

Future work



- Some baseline alloys perform better but also cost more
- Remove key elements (or add to) baseline alloys based on ICME approach
- Evaluate the RT hardness after aging and pre-conditioning at 200~300° C (no HT testing/ microstructure characterization) to downselect the alloy composition
- Further property evaluation and characterization of the down-selected alloys
- ICME approach for development of new alloy compositions
- FY16 Future work
 - Identify the new composition of aluminum alloy
 - Larger heats on new composition and optimization of heat treatment
 - Publish gap analysis report
 - Prepare for large scale evaluation (on engine platform) in FY17



Responses to Previous Year Reviewers' Comments

- Reviewer comments on approach and collaboration were generally complementary
- One reviewer stated that the problem is that the alloys being evaluated are all existing and do not have the required properties. Another reviewer noted that hopefully the researchers can tell in the 2015 review how the link was made between the investigation of the baseline materials and the enhanced materials, or the new alloys.
 - Some higher performance baseline alloys have adequate properties but are more expensive. The higher performance baseline alloys are being used as basis for alloy development.
- The reviewer said hopefully the researchers can explain in next year's review why the secondary dendrite arm spacing (SDAS) of approximately 30 μm is such an important factor for the selection of these base materials.
 - This is because 30 μm is the SDAS size produced by gravity die casting in the combustion chamber region of cylinder heads and this region is most susceptible to cracking.
- The reviewer said that adding an academic institution would strengthen the team even more.
 - This is not possible due to the CRADA terms.
- The reviewer added that any ultra-high-performing alloys that do not meet the cost parameters for this project should be identified and possibly assessed for other applications where cost is less of a concern.
 - Great suggestion. We are already thinking in terms of other applications such as water cooled turbocharger housings and pistons for the more expensive alloys.
- The reviewer reported that the team needed to look into newer alloy systems rather than existing alloys. The reviewer said that the new elements may be needed to be added to the existing alloys to improve high-temperature strength. The reviewer added that if the team was aware of this fact it is not evident from the presentation.
 - Agree with the reviewer. The new alloys are made on the basis of lessons learned from baseline alloys along with some plausible high temperature strengthening mechanisms
- Reviewers commented that DOE objectives of petroleum displacement were met and that resources available were adequate

Summary

- **Relevance:** New alloys that can enable the development and implementation of higher efficiency passenger car engines
- **Approach/Strategy:** ICME approach used to accelerate the development of cast aluminum alloys. Partner with major players in this area.
- **Accomplishments:**
 - Baseline aluminum alloys characterized
 - ICME models implemented for alloy development and relevant property prediction
 - High temperature microstructural stability is key characteristic for a 300°C capable cast aluminum alloy
 - Existing alloys along with ICME models provided pathway for the development of 25 new alloy compositions
- **Collaborations:** Chrysler, Nemak and smaller software cost-share partners
- **Future Work:**
 - Alloy chemistry refinement; casting and screening of trial alloys; characterization of new alloys
 - Casting of components and engine testing; cost model for cylinder heads