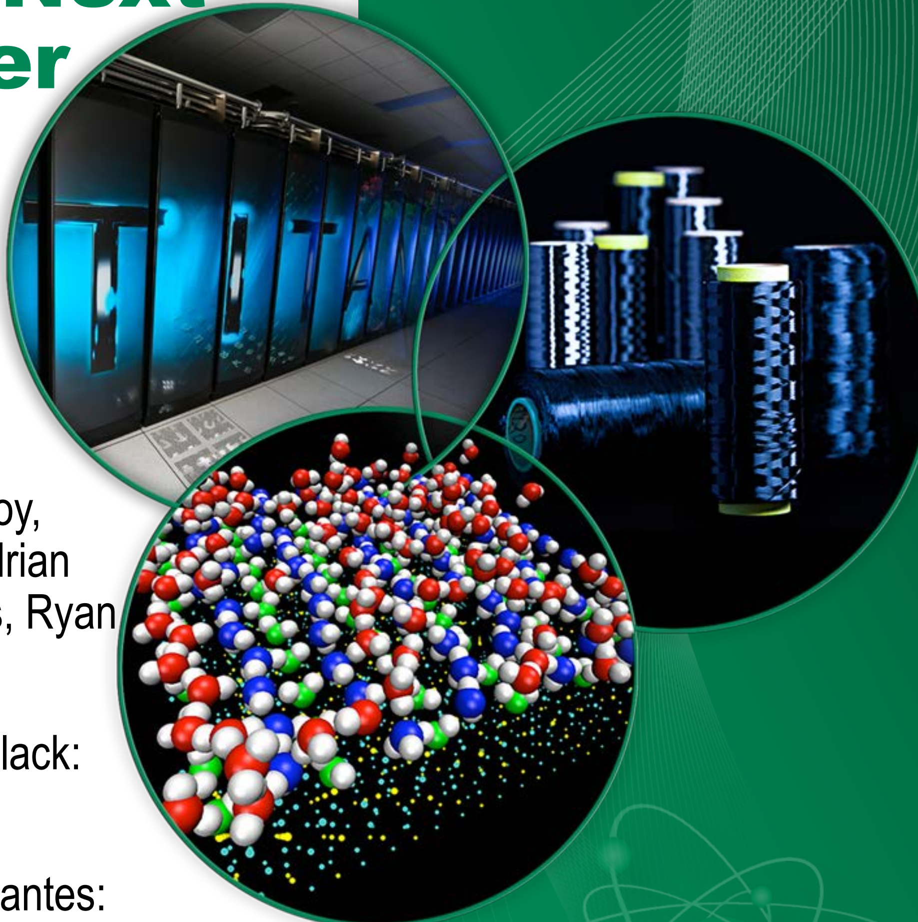
Project ID: PM062

High Performance Cast Aluminum Alloys for Next Generation Passenger Vehicle Engines



2015 DOE Vehicle Technologies Annual Merit Review and Peer Evaluation Meeting
June 9, 2016

Amit Shyam (Principal Investigator), Shibayan Roy, Larry Allard, Yukinori Yamamoto, Dongwon Shin, Adrian Sabau, Phil Maziasz, Wally Porter, Thomas Watkins, Ryan Cooper, Patrick Shower and Allen Haynes: *ORNL*

Lin Zhang, Chris Glaspie, Seyed Mirmiran, Gregg Black: *Fiat Chrysler Automobiles (FCA US LLC)*

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

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

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Overview

Timeline

- Start: November 2012
- *CRADA* Executed: Nov 2013
- End: November 2017
- 63% Complete

Budget

- Total project funding.
  - DOE-$3500 K
  - Cost share ~$2000 K
- FY15 DOE Funding - $1000 K
- FY16 DOE Funding - $700 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.

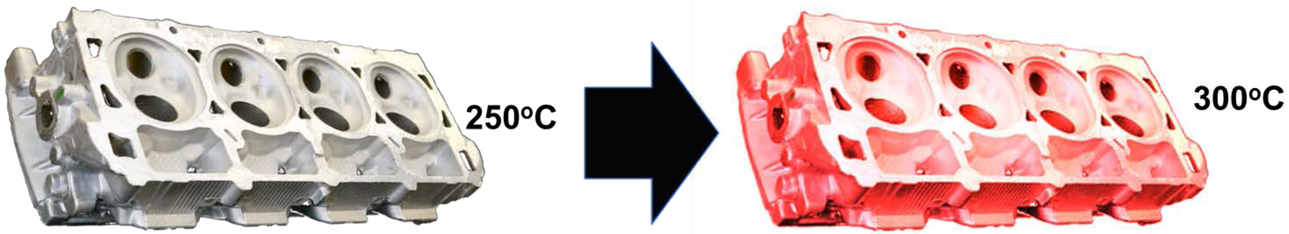
Partners

- 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*

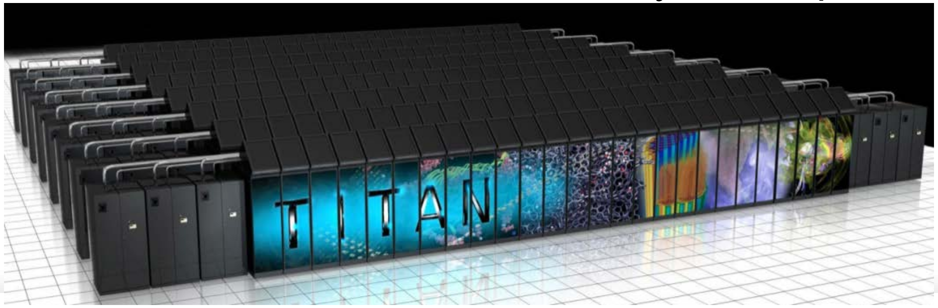
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

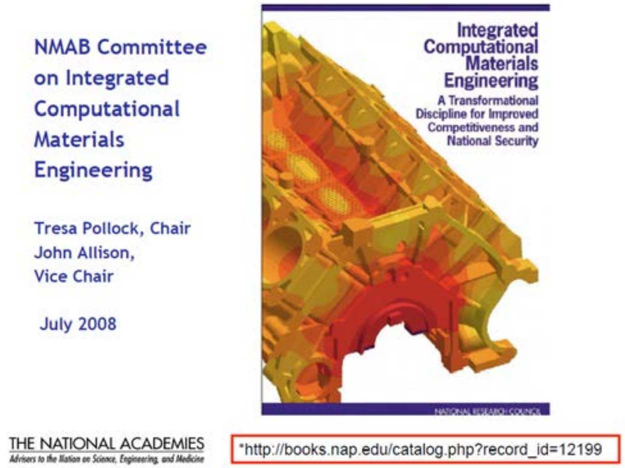
Relevance

- 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.



  - 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.



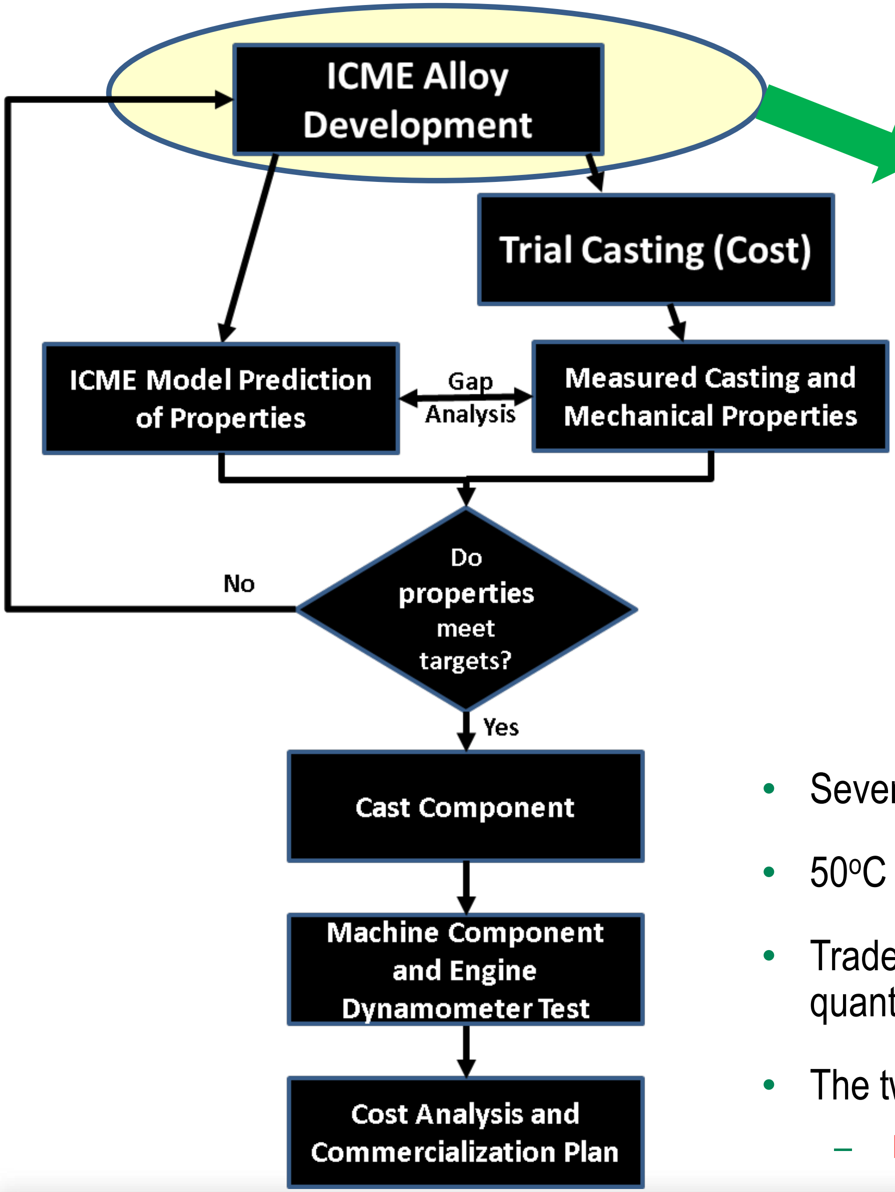


Project Milestones

- 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 (completed)
- Milestone 3: Finish identification of new alloy composition(s) with improved properties.
  - Planned Date: 11/30/16 (on track)
- 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

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Approach/Strategy

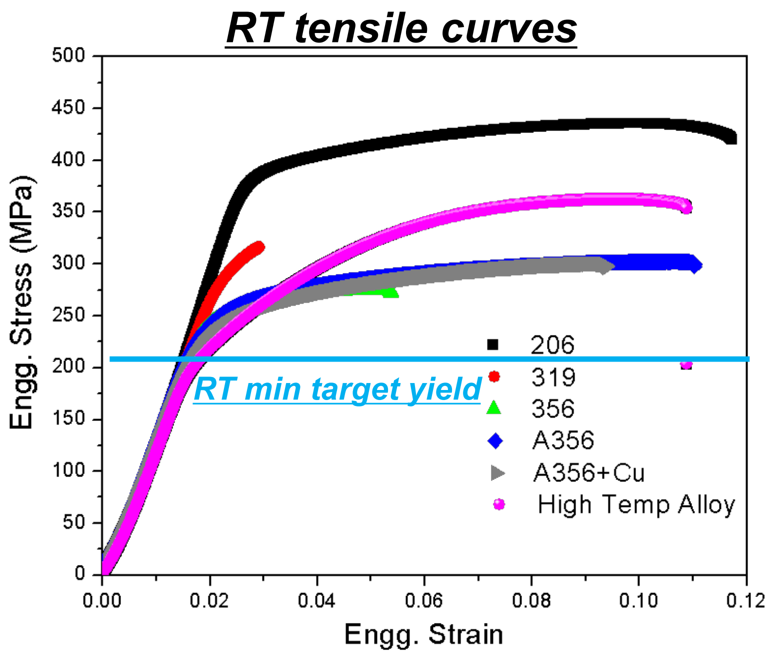


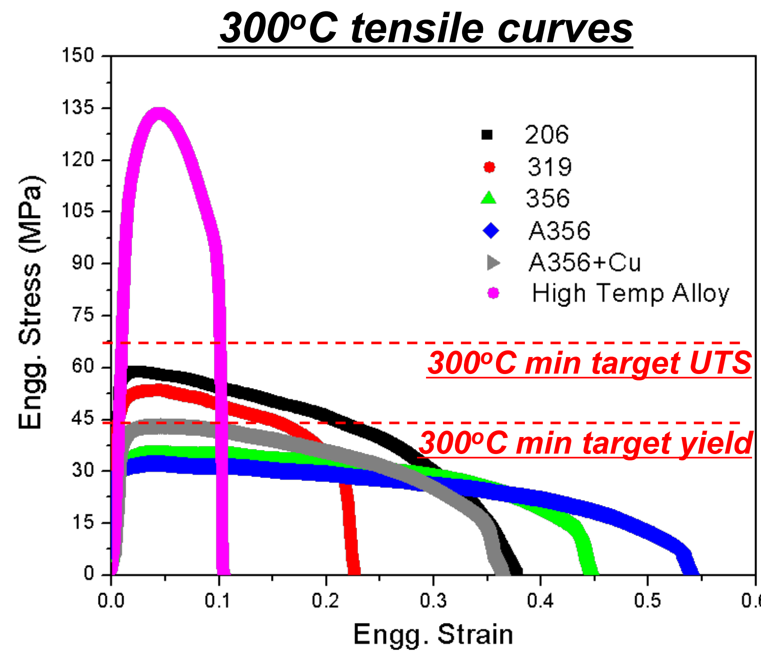
Property	Cast Al Baseline	Cast Alloy Targets	Key Properties
Tensile Strength @ RT	33 ksi	40 ksi	Key
Yield Strength @ RT	24 ksi	30 ksi	Key
Density	2.7 g/cc	< 6.4 g/cc	
Elongation	3.5%	3.5%	
Shear Strength	26 ksi	30 ksi	
Endurance Limit	8.5 ksi	11 ksi	
Fluidity (Spiral test)	Excellent	Excellent	Key
Hot Tearing Resistance	Excellent	Excellent	Key
High Temp Performance	@ 250°C	@ 300°C	
Tensile Strength @ HT	7.5 ksi @ 250°C	9.5 ksi @ 250°C	Key
Yield Strength @ HT	5 ksi @ 250°C	6.5 ksi @ 250°C	Key
Elongation in 2"	20% @ 250°C	<20% @ 250°C	
Cost	$ x/lb	$ 1.1x/lb	Key

- Several properties need to be satisfied simultaneously
- 50°C increase in temperature was a very challenging target
- Tradeoffs need to be performed. These tradeoffs can be performed quantitatively with the ICME approach.
- The two key technical targets are related to:
  - Elevated temperature mechanical properties
  - Castability and hot tear resistance

Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Technical Accomplishments

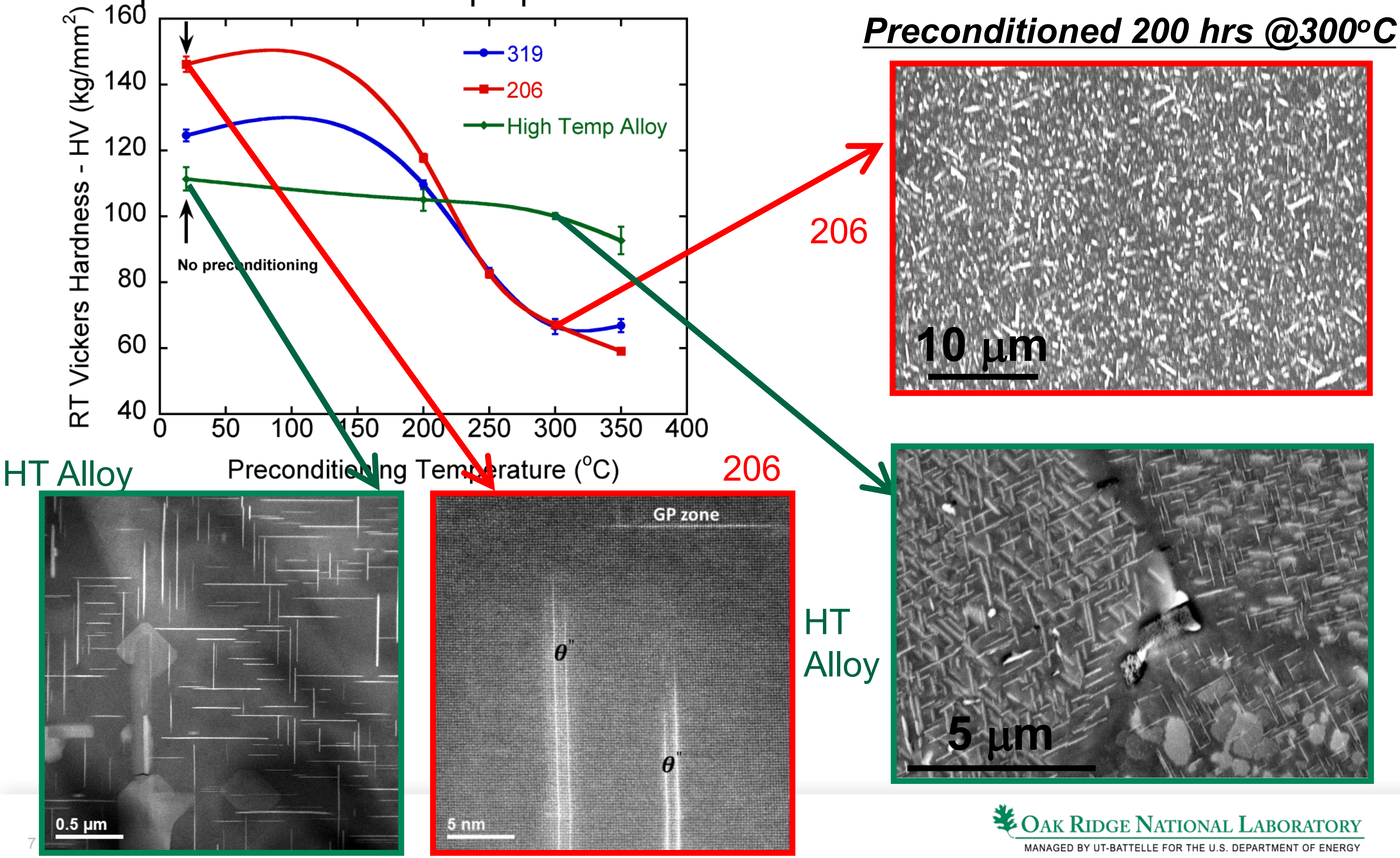




- Cylinder head materials supplied by Nemak
  - 319-T7; 356-T6; A356-T6; A356+0.5Cu-T6; 206-T6; 1 High Temp Alloy
  - All materials have grain size/secondary dendrite arm spacing (SDAS) of ~ 30 μm
- **High temperature alloy exceeds 300°C technical target by >2X**
- Alloy is in Al-Cu family and has exceptionally stable microstructure after sustained elevated temperature exposure
- Patent Application filed

Technical accomplishments

- *<u>High temperature microstructural stability is key</u>* to improved elevated temperature mechanical properties

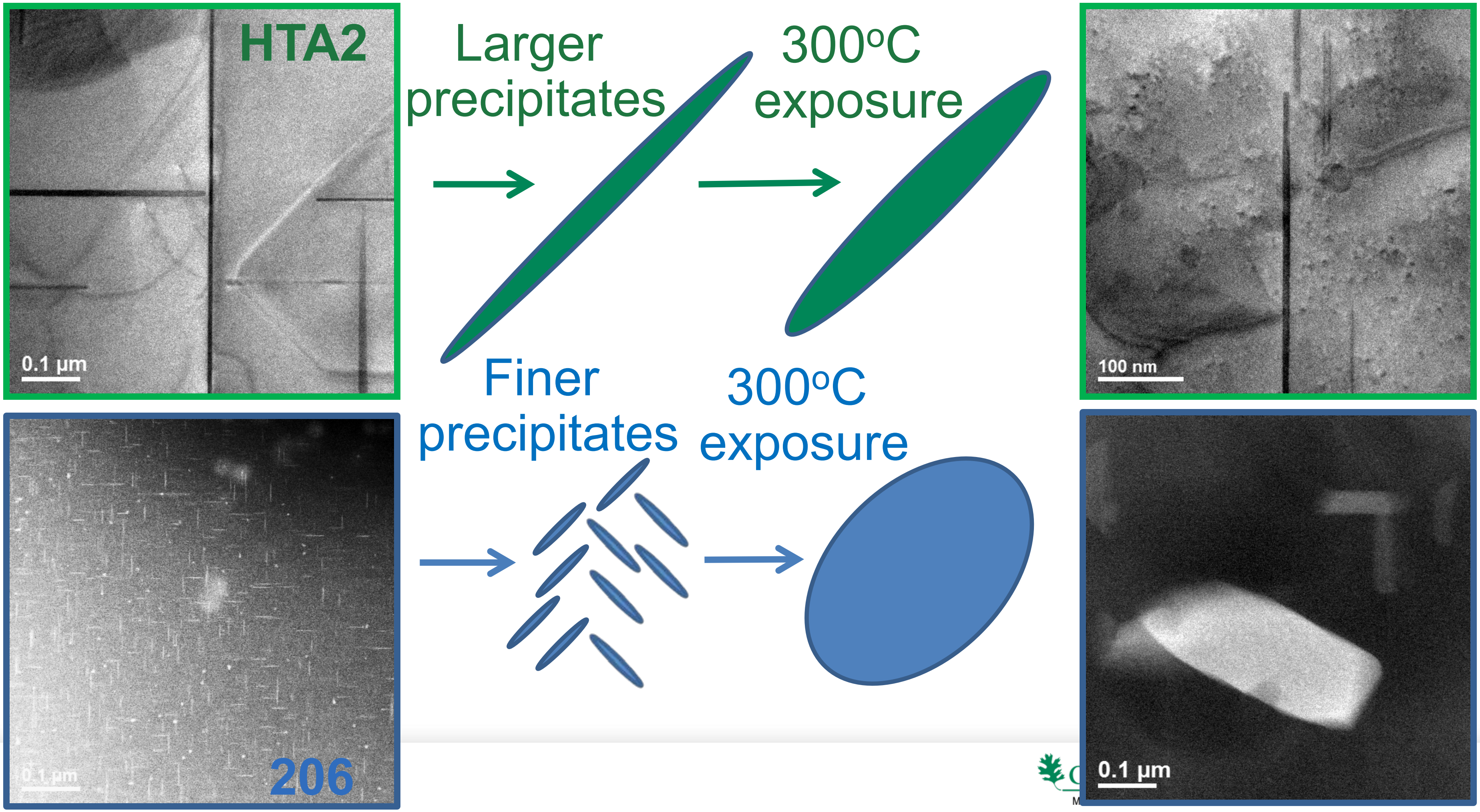


Technical Accomplishments

Higher temperature capable alloys have ***stable*** precipitates at elevated temperature

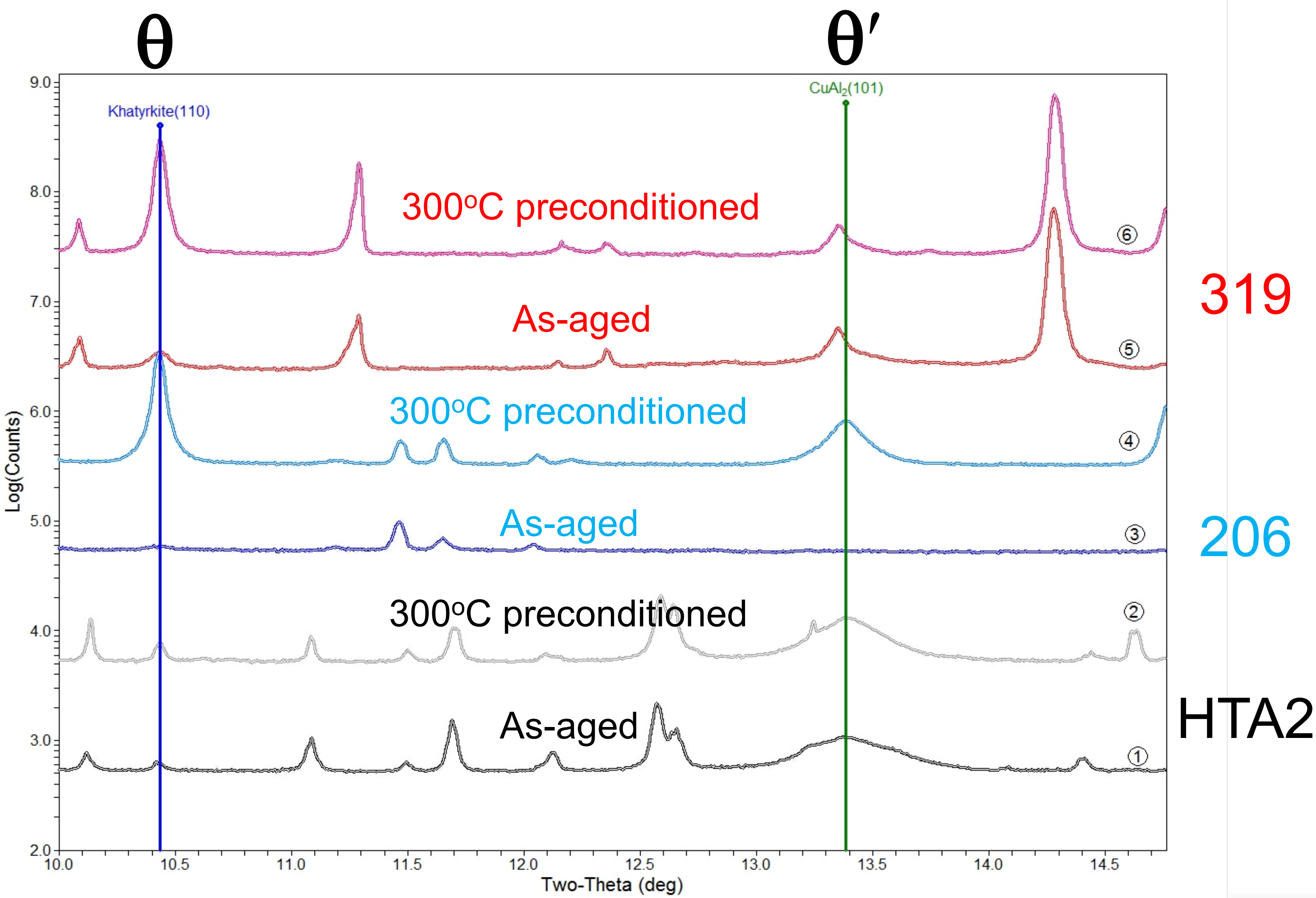
High aspect ratio/crystallographic precipitates are good for strength!

Need to preserve aspect ratio after high temperature exposure



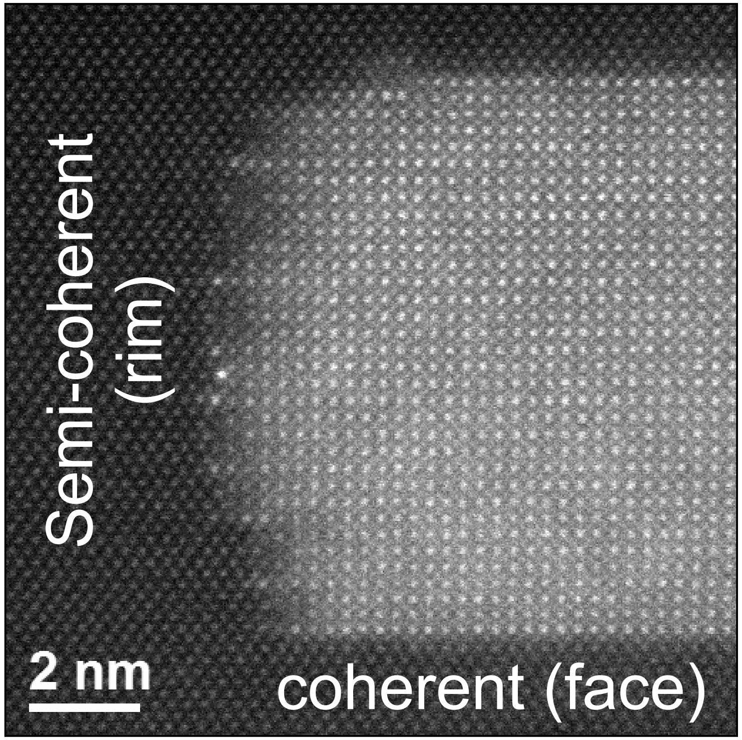
Technical Accomplishments

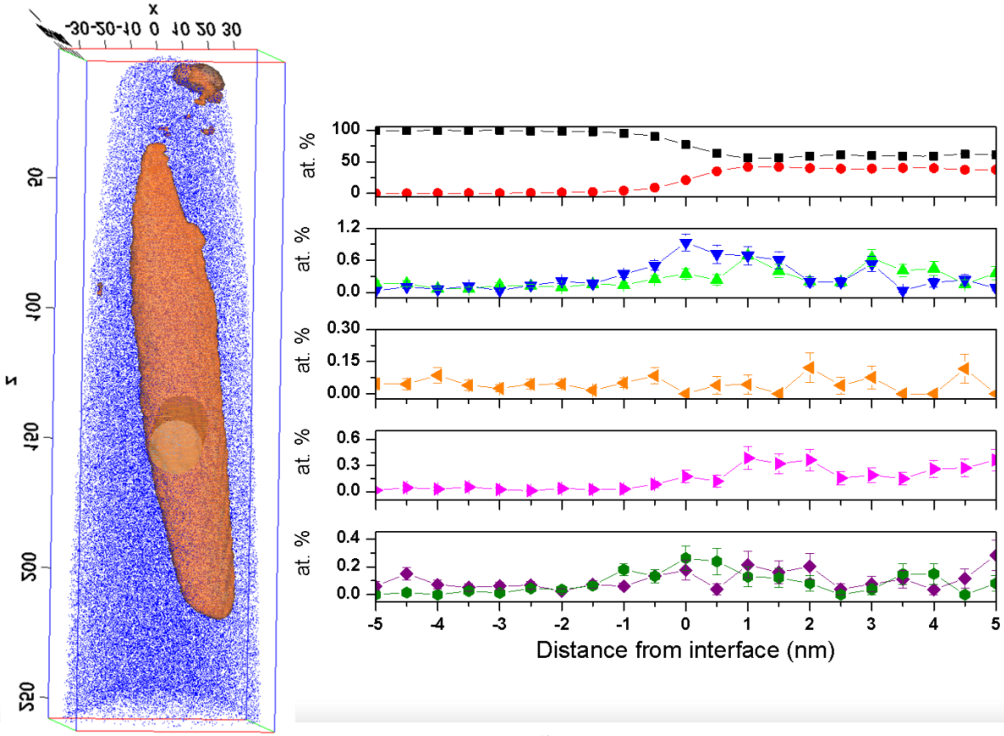
Synchrotron Diffraction (NSLS – BNL) confirms phase (and shape) stability in high temperature alloys – need intensity and resolution of synchrotron X-ray



Technical Accomplishments

- Interfaces are key. Two types of interfaces in θ' (Al_2Cu)
- Semi-coherent interfaces have higher mobility due to higher energy
- TEM and Atom probe tomography (APT performed at CNMS-ORNL) indicate high Z elemental combination can stabilize semi-coherent interface

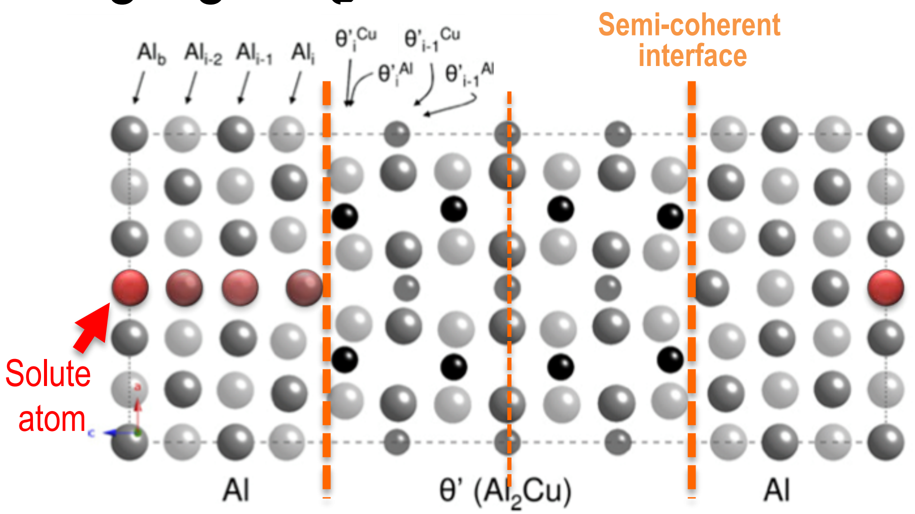


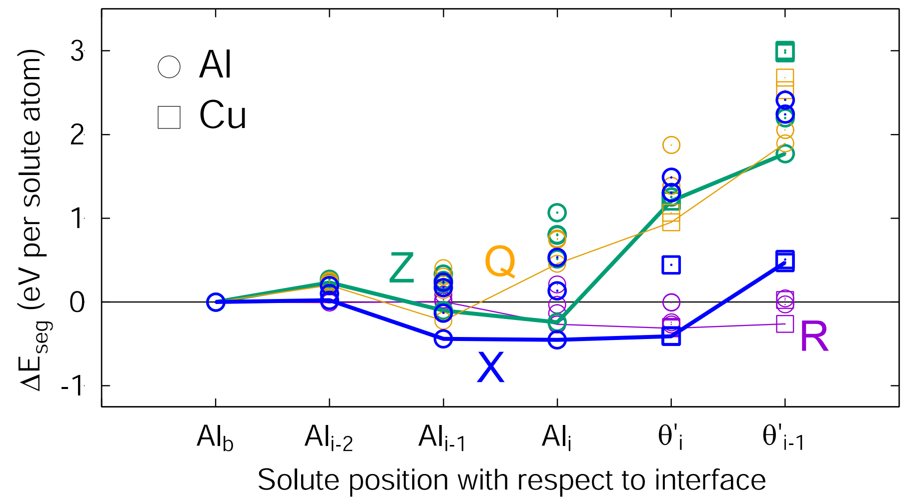


Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

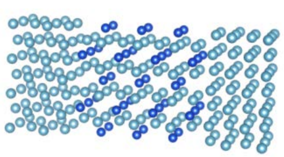
Technical Accomplishments

- Computational capability has been developed to predict other elemental combinations that lead to microstructural stability by segregating to the interfaces





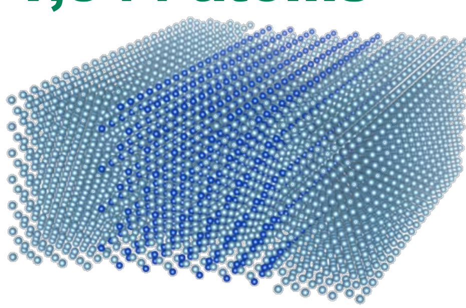
168 atoms

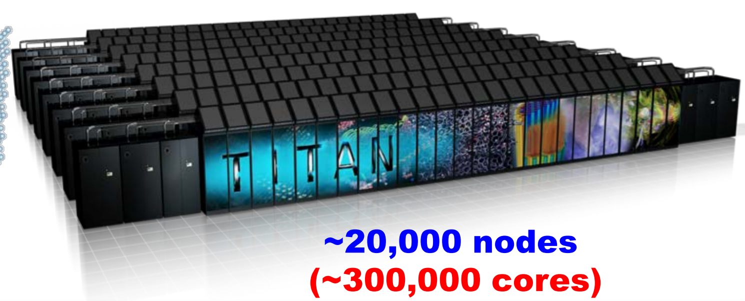


32 cores × 48 hours
~ 1,500 CPU hours per supercell
(hundreds of serial calculations)

~30 nodes
(~400 cores)

1,544 atoms





~20,000 nodes
(~300,000 cores)

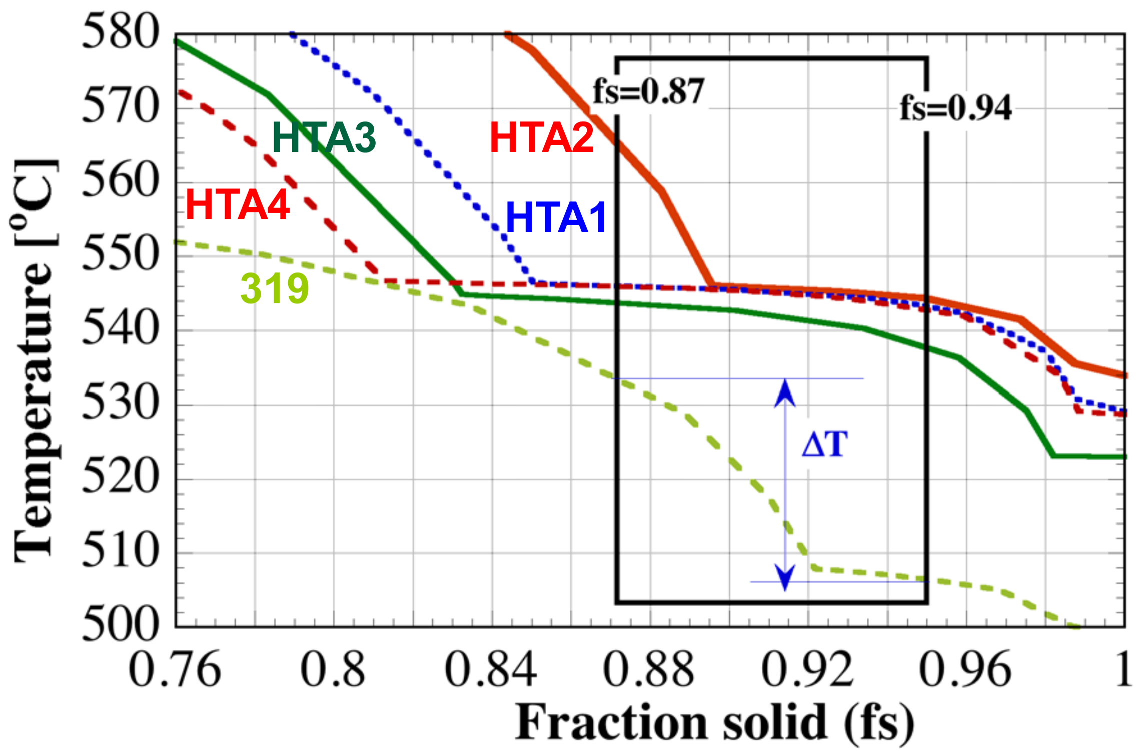
Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Technical Accomplishments

- Tensile properties of developed alloys exceed 300^{o}C targets by >2X. High temperature goals exceeded by a significant margin and alloys have stable microstructures up to 350^{o}C have been developed.
- Key lesson – **Certain elements** provide high temperature stability by segregating to the semi-coherent interface; avoid **certain other elements**
- Currently, we have cast several (~30) alloy compositions with the above alloying concept and filed a US Patent Application (for 350^{o}C stable alloys)
- **We know the elemental hierarchy that exists in terms of providing high temperature stability**

Technical Accomplishments

- Hot tear model of Kou* *et al*. implemented for baseline and HT alloys

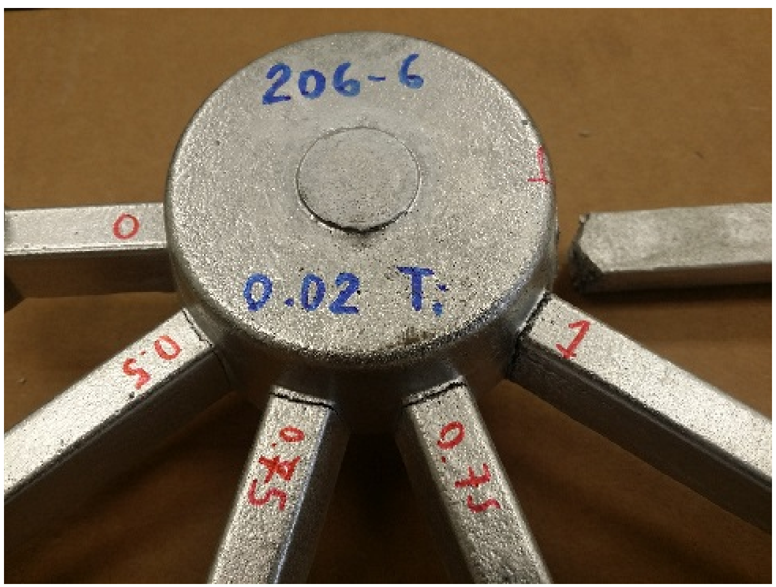


- Hot tearing propensity increases with slope $\dfrac{\Delta T}{\Delta\left(\sqrt{f_s}\right)}$ (evaluated between f_s=0.87 and 0.94)
- HTA1, 2, 3, 4, 5 and 6 are high temperature alloys
- Model does not account for processing induced changes in hot tearing

*Kou, Acta Materialia 88 (2015) 366–374

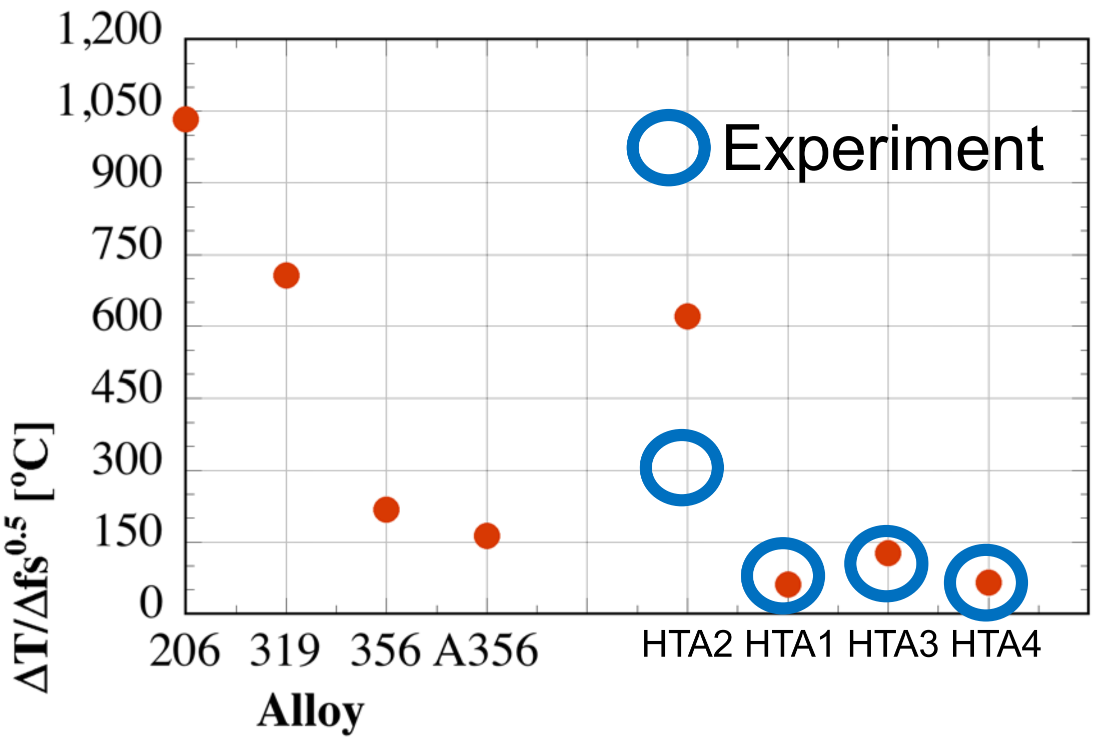
Technical Accomplishments

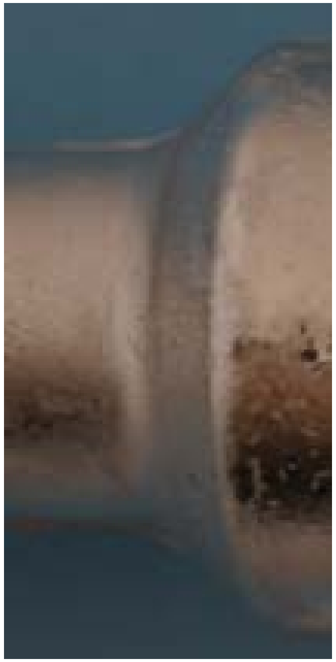
- High temperature alloys have excellent hot tear resistance (comparable or better than 319). Also tests performed at WPI. > 400 castings at WPI + Nemak for hot tear evaluation
- Lower value (in table) is better
- Hot tear cracking issue is manageable



Alloy	Average Hot crack value
HTA1	**2.05**
HTA2	3.55
HTA5	3.45
HTA6	3.85
319 Alloy	2.45
319 Alloy	2.5

Technical Accomplishments
Note: Hot tear tests performed at WPI





No hot tear crack

Hot tearing propensity increases with slope $\frac{\Delta T}{\Delta\left(\sqrt{f_s}\right)}$
(evaluated at f_s=0.87 and 0.94)

- Three of above four High Temp Alloys have excellent hot tear resistance

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Collaboration and co-ordination

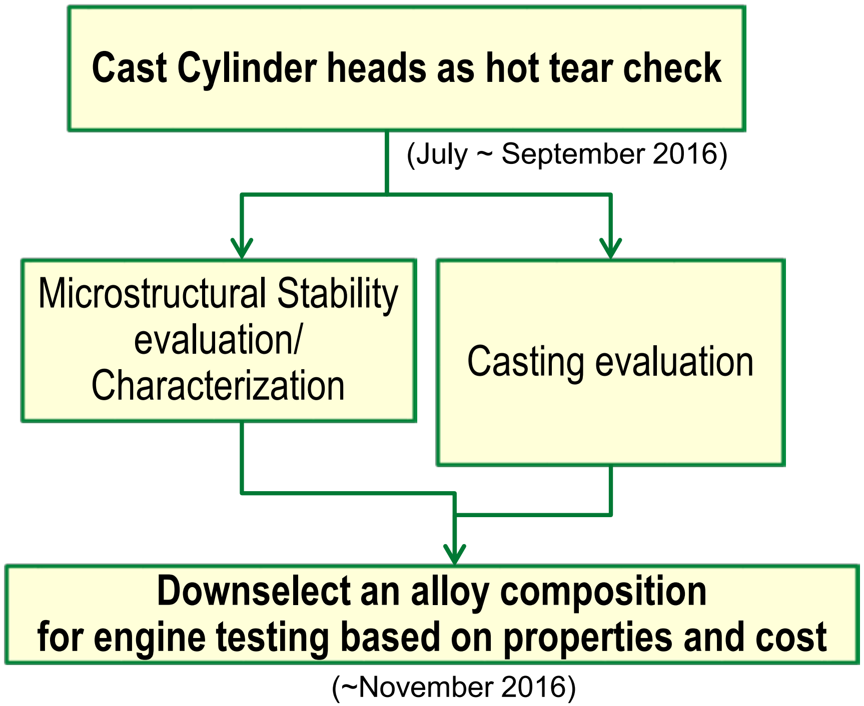
- Monthly conference calls and biannual face-to-face all hands meeting
- *CRADA* partners with significant cost share
  - FCA US LLC - OEM automotive manufacturer
    - FCA (Chrysler) provides technical guidance to the overall effort and leads tasks such as LCF/machinability evaluation
    - Guides casting effort. Provides the larger scale casting to ORNL
  - Nemak S. A. – Cylinder head supplier to FCA
    - Guides casting 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
- Other partners
  - Granta MI – Data management partner
  - ESI North America, Flow Science, Magma Foundry Technologies – casting simulation software
  - Minco Inc – casting supplies
- Subcontractors
  - WPI – Hot tear evaluation
  - Element – Specimen preparation and some materials testing

Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Remaining challenges and barriers

- The technical targets have been achieved in several alloys. Optimizing the alloys for technical and cost targets is the major remaining challenge.
- Cylinder heads can perform differently compared to laboratory scale castings. There are unknowns such as thermal conductivity, corrosion resistance, machinability, residual stress in castings that need to be characterized before the alloys can be commercialized.
- Several gaps exist in ICME models; for example for microstructural evolution. These are barriers for further improvement of the alloy family.

Future work



- Further property evaluation and characterization of the down-selected alloys (mechanical properties such as thermomechanical fatigue)
- Estimation/measurement of properties such as corrosion resistance, residual stress (neutrons) and thermal conductivity
- ICME approach for development of new alloy compositions
- FY16 and FY17 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
  - Cost Analysis and Commercialization Plan

Responses to Previous Year Reviewers' Comments

- The reviewer saw the obvious goal as producing an alloy with higher capabilities, but was unclear as to how the ICME tools are being incorporated into subsequent heats. The characterization work the reviewer found impressive, but asked how it was being leveraged. Likewise, the reviewer queried whether there is specific distribution of theta phase, for instance, that is expected to prove more stable through nucleation strategies such as heat treatments or composition changes. How the microstructural evolution is being modeled, the reviewer continued. Based on what has been learned in the project, the reviewer believed that redefining the goals using microstructural terms rather than final properties would be very interesting.
  - **Response:** This is a fair criticism based on what was presented at last year's AMR. We did not present the results from new alloys based on IP concerns. The leveraging of characterization work should be obvious from this year's presentation. Microstructural evolution modeling is a big gap in this area. Final goals redefined through microstructural terms is an interesting idea. We have, for example, determined that if we can make Al_2Cu precipitates with an aspect ratio of >13 at 300^oC, the strength targets will be met.
- Reiterating that strength of Al alloys is derived from precipitation hardening and that the major barrier to high-temperature stability is coarsening of precipitates, the reviewer underlined the necessity of identifying precipitates which are stable at high temperatures (i.e., approximately 300^oC) if the strength is to remain stable.
  - **Response:** We agree with the reviewer. We believe that exactly this strategy was followed to develop the new higher temperature capable alloys.
- To this reviewer, it seemed that the industrial partners were largely slated for consultation rather than hands-on contributions. Castings, the reviewer noted, are still being produced using lab-based conditions, although Nemak is supplying master alloys. Thus the reviewer assumed that complementary analyses show casting results from ORNL heats are similar to industrial castings.
  - **Response:** There is close collaboration between CRADA partners for alloy development. Complementary analysis has been performed as needed. The industry partners bring in a lot of experience in processing, application and chemistry changes. Our patent application has been submitted jointly as well.

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:**
  - New higher temperature alloys developed that meet all technical criteria for the funding opportunity
  - Tensile properties exceed 300°C targets by >2X. High temperature goals exceeded and alloys have stable microstructures up to 350°C
  - Hot tear resistance of new alloys is excellent
  - High temperature microstructural stability is key characteristic (US patent application submitted)
- **Collaborations:** FCA, Nemak and smaller software cost-share partners
- **Future Work:**
  - Cast cylinder heads; characterization of properties of new alloys; test new alloys on engine platform
  - ICME Gap Analysis; cost model for cylinder heads