2020 DOE Vehicle Technologies Office Annual Merit Review Presentation

Properties of Cast Al-Cu-Mn-Zr (ACMZ) alloys*

** Task 1B under the Powertrain Materials Core Program (PMCP)*

Amit Shyam (PI)

Other contributors: J. Allen Haynes, Dongwon Shin, Sumit Bahl, Xiaohua Hu, Jiaohao Cheng, Jiheon Jun, C. Shane Hawkins, Dana McClurg

Oak Ridge National Laboratory

Bharat Gwalani and Arun Devaraj – *Pacific Northwest National Laboratory*

Lianghua Xiong and Dileep Singh – *Argonne National Laboratory*

June 4, 2020

Project ID # mat188

Program Overview: VTO Powertrain Materials Core Program

Timeline/Budget

- Lab Call Award: July 2018
- Budget: $30M/5 years
- Program Start: Oct 2018
- Program End: Sept 2023
- 30% Complete

Barriers

- Increasing engine power densities & higher efficiency engines; resulting in increasingly extreme materials demands (increased pressure and/or temperature)
- Affordability of advanced engine materials & components
- Accelerating development time of advanced materials
- Scaling new materials technologies to commercialization

FY20 Program Research Thrusts	FY20 Budget	Participating Labs
1. Cost Effective LW High Temp Engine Alloys	**$1.05M**	**ORNL**
2. Cost Effective Higher Temp Engine Alloys	$1.525M	ORNL, PNNL
3. Additive Manufacturing of Powertrain Alloys	$1.075M	ORNL
4A. Advanced Characterization	$1.025M	ORNL, PNNL, ANL
4B. Advanced Computation	$0.60M	ORNL
5. Exploratory Research: Emerging Technologies	$0.75M	ORNL, PNNL, ANL

Partners

- Program Lead Lab
  - Oak Ridge National Lab (ORNL)
- Program Partner Labs
  - Pacific Northwest National Lab (PNNL)
  - Argonne National Lab (ANL)

Program structure includes three alloy development thrusts (1-3), a foundational support thrust (4), and a thrust for one-year exploratory projects (5).

Project Overview: Task1B: Properties of Cast Al-Cu-Mn-Zr (ACMZ) alloys

Timeline/Budget

- Project start: Oct 2018
- Project end: Sep 2021
- Percent complete: 30%
- **1B Budget**
  - **FY19: $425k**
  - **FY20: $325K**

Barriers

- Microstructural levers for alloy design are not well understood.
- Scaling new alloy technologies to commercialization.
- Critical property targets are not well-understood for components
- Development time. Project leverages an *Integrated computational materials engineering* (ICME) framework to reduce the early & mid-stage development time of new LW alloys by 50%.

Thrust 1: Tasks/Subtasks	Lab	TRL	PI(s)	FY19	FY20
Task 1A. New Al Alloys with Improved High Temperature Performance					
• 1A1. Fundamental studies of complex precipitation pathways	ORNL	Low	Shin	$350k	$350k
• 1A2. New higher performance Al alloys (>400C)	ORNL	Low	Shyam	$400k	$375k
Task 1B. New AlCuMnZr alloy variants with tailored performance					
• **1B1. Intermediate temperature variants of cast ACMZ alloys**	**ORNL**	**Mid**	**Shyam**	**$300k**	**$225k**
• **1B2. Commercial collaborations for ACMZ alloys**	**ORNL**	**Mid**	**Shyam**	**$125k**	**$100k**
			Subtotals	**$1,175k**	**$1,050k**

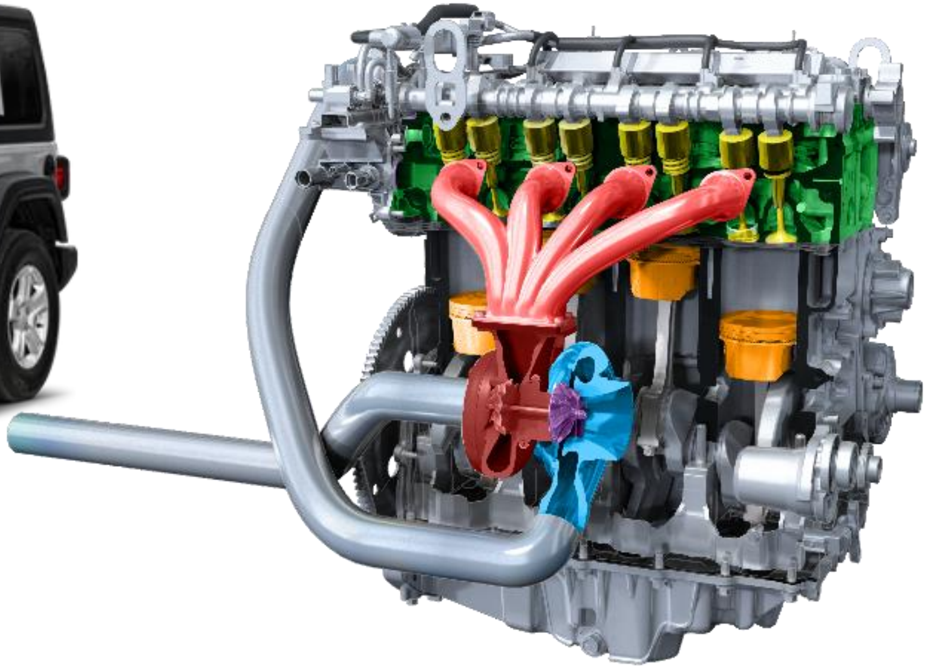
Partners

- Subtask 1B Lead
  - Oak Ridge National Lab (ORNL)
- Subtask 1B Partners
  - Thrust 4A
    - Argonne National Lab (ANL)
    - Pacific Northwest National Lab (PNNL)
  - General Motors (CRADA in Progress)

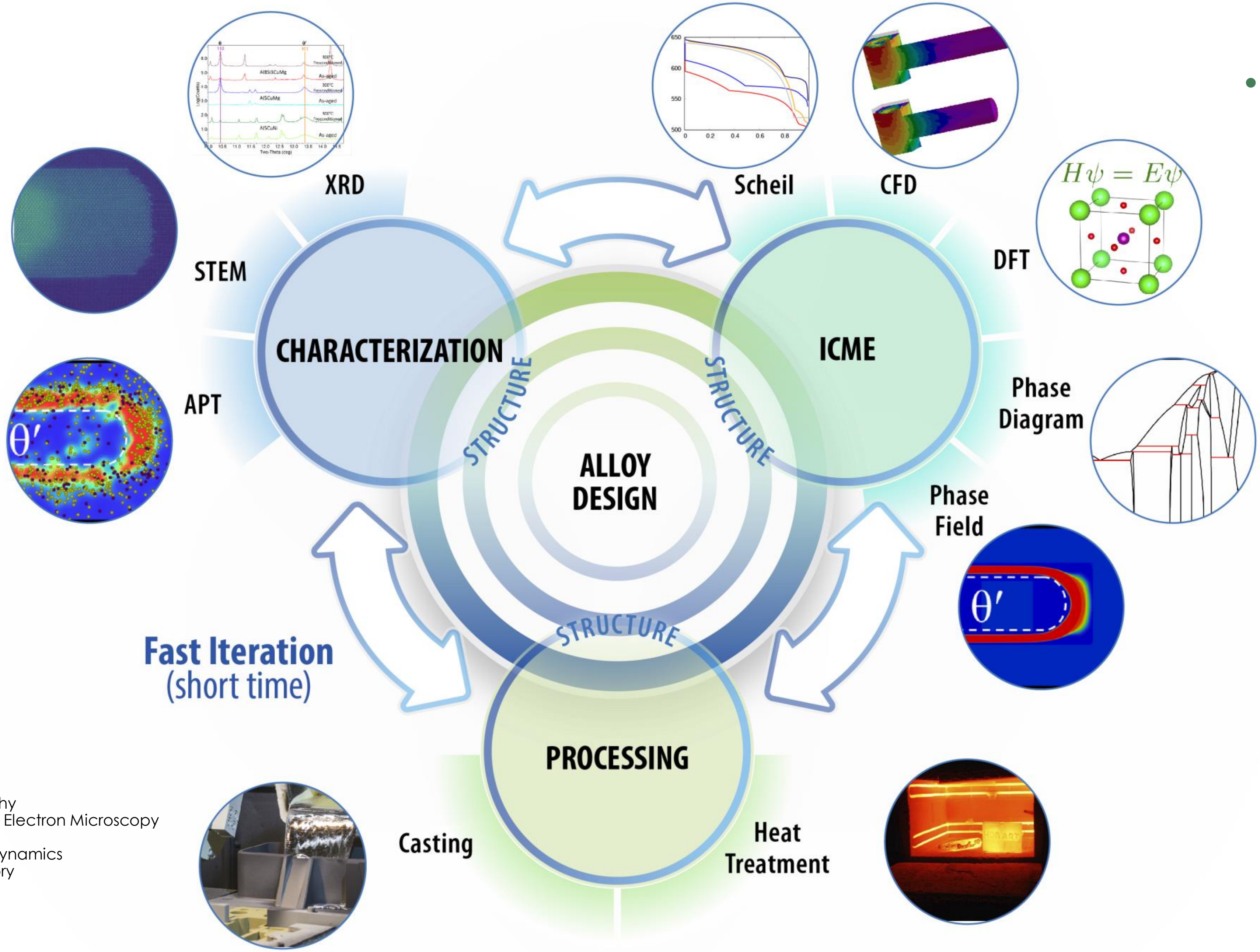
Relevance

Problem: Most higher-efficiency ICE designs result in higher cylinder pressures & gas temperatures. This creates more severe conditions for engine materials - presently operating at their limits.

Opportunity: Lightweight alloys with **improved strength & microstructural stability** at higher temperatures are necessary to enable higher efficiency engines.



Introduction to Lightweight Alloy Design for Powertrains



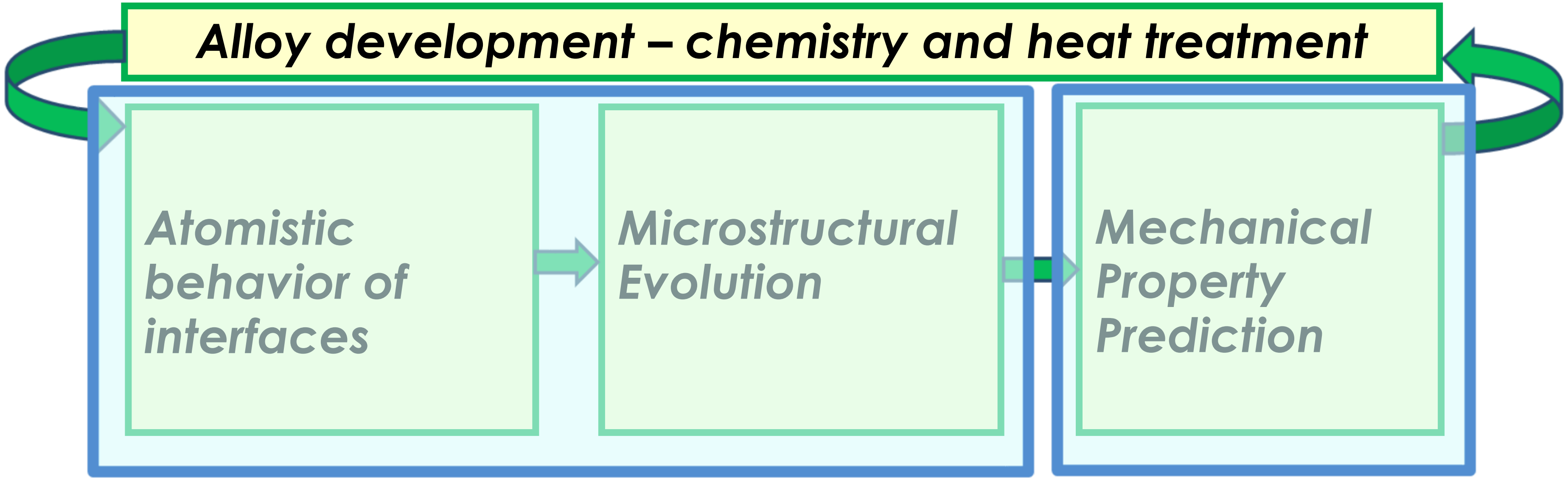
- Develop, ***using Integrated Computational Materials Engineering (ICME)***, higher temperature lightweight engine materials with improved strength and thermal stability, leading to further increases in power densities of engines.

APT – Atom probe tomography
STEM – Scanning Transmission Electron Microscopy
XRD – X-ray Diffraction
CFD – Computational Fluid Dynamics
DFT – Density Functional Theory

Thrust Structure

Thrust 1: Cost Effective Lightweight High Temperature Engine Alloys

Thrust 3: Tasks/Subtasks	Lab	TRL	PI(s)
Task 1A. New Al Alloys with Improved High Temperature Performance			
• 1A1. Fundamental studies of complex precipitation pathways	ORNL	Low	Shin
• 1A2. New higher performance Al alloys (>400C)	ORNL	Low	Shyam
Task 1B. New AlCuMnZr alloy variants with tailored performance			
• **1B1. Intermediate temperature variants of cast ACMZ alloys**	**ORNL**	**Mid**	**Shyam**
• **1B2. Commercial collaborations for ACMZ alloys**	**ORNL**	**Mid**	**Haynes, Shyam**



Subtasks 1A1 and 1A2

Subtask 1B
-Focus of this talk

OAK RIDGE National Laboratory

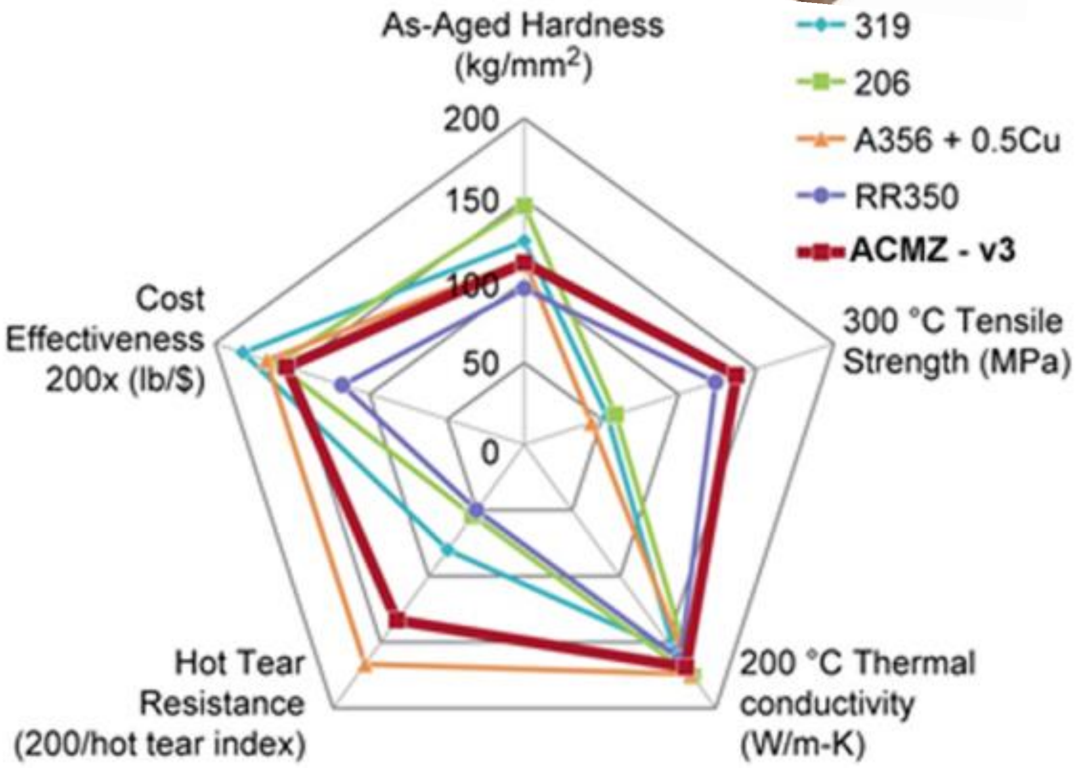
Milestones for Task 1B

Milestone Name/Description	Criteria	Planned End Date	Status
Submit manuscript on ductility prediction in ACMZ alloys	Statement in Quarterly report	End of **Q1**, FY20	**Complete** Manuscript published
Finish LCF testing on three temperatures (150, 200, 250°C) on ACMZ and baseline alloys	Statement in Quarterly report	End of **Q2**, FY20	**Complete**
Submit CRADA documents on ACMZ alloys with OEM	Statement in Quarterly report	End of **Q3**, FY20	**Complete**
Submit invention disclosure on high copper aluminum alloy with improved ductility	Statement in Quarterly report	End of **Q4**, FY20	**Complete** Patent filed

High Temperature Cast AlCuMnZr (ACMZ) alloys

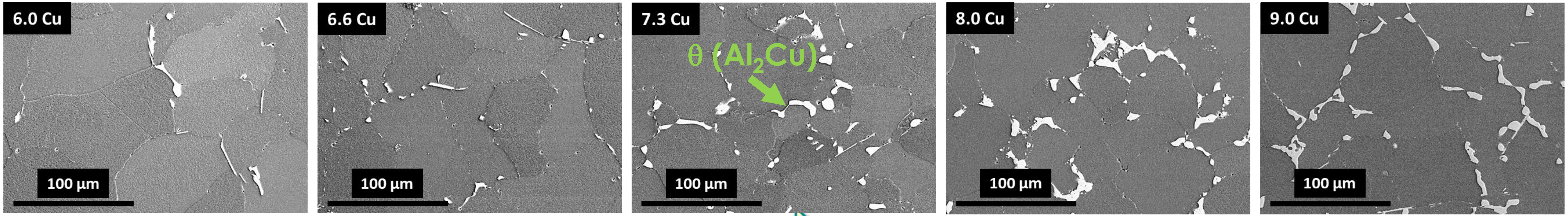
- VTO FOA award led to 4 year CRADA with industry & ICME played a key role
- Goal of FOA: Affordable, cast alloys for next generation cylinder heads with improved power density
- Requires **improvement in ductility and low cycle fatigue resistance** at low-intermediate temperature (<150°C)

First generation ACMZ won a 2017 R&D 100 Award



OAK RIDGE National Laboratory

ACMZ microstructure as a function of alloy Cu content

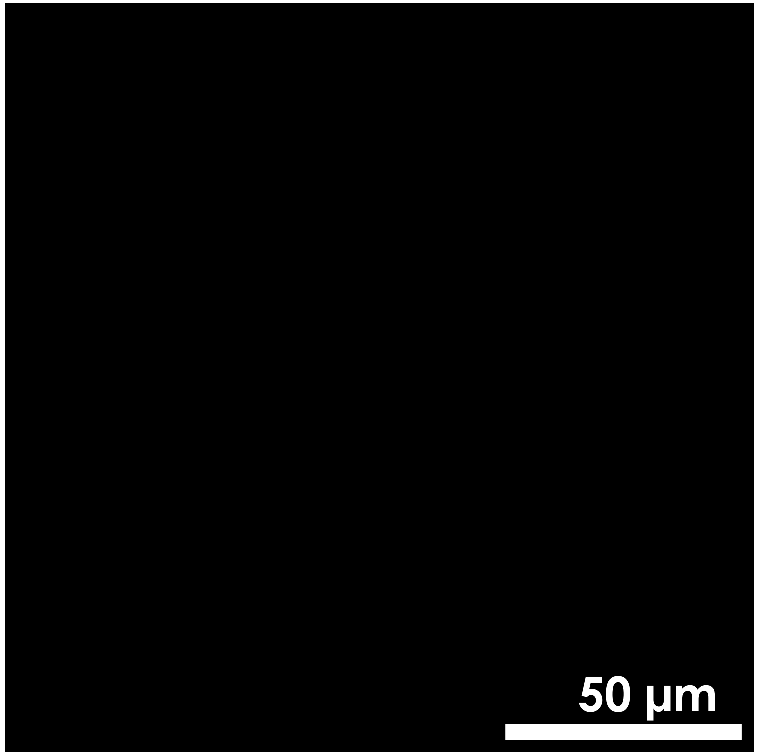


Increase in Cu content

Increase in grain boundary particle area

Improved castability/hot tear resistance

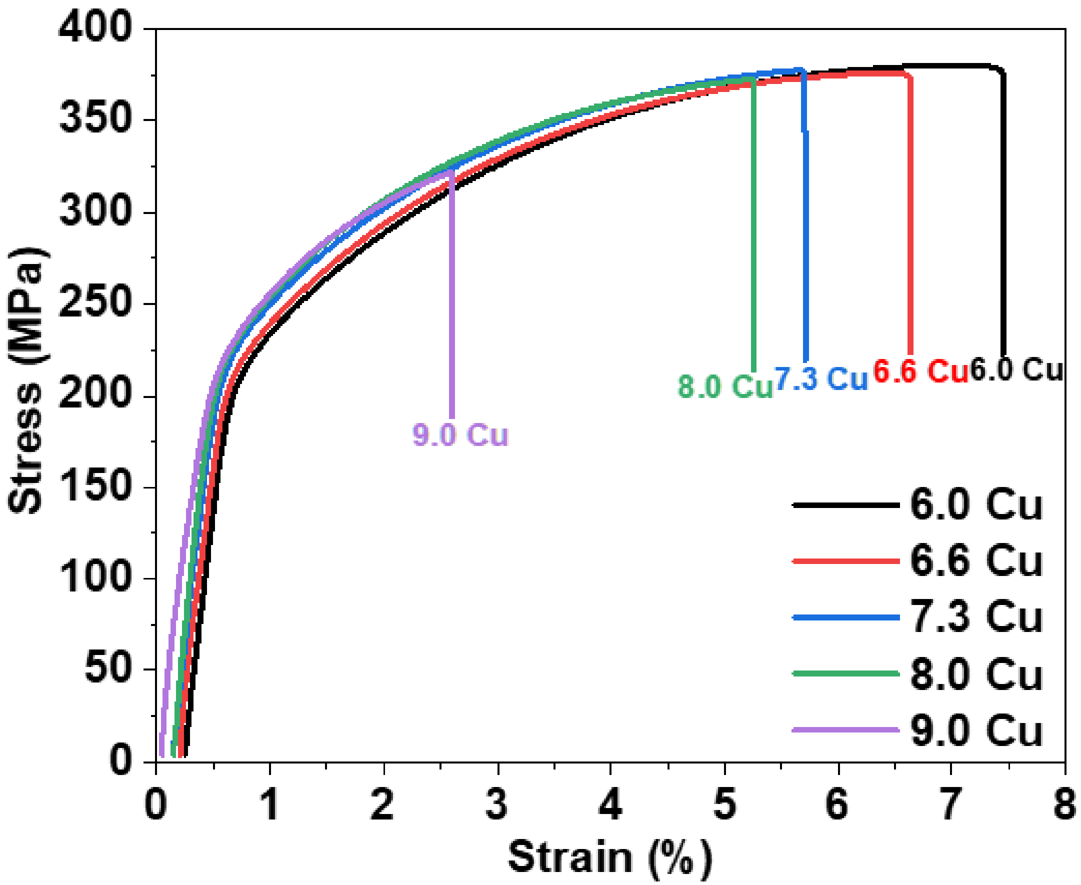
- Size and volume fraction of grain boundary θ particles increases with Cu content
- Intragranular microstructure (θ') invariant with Cu content

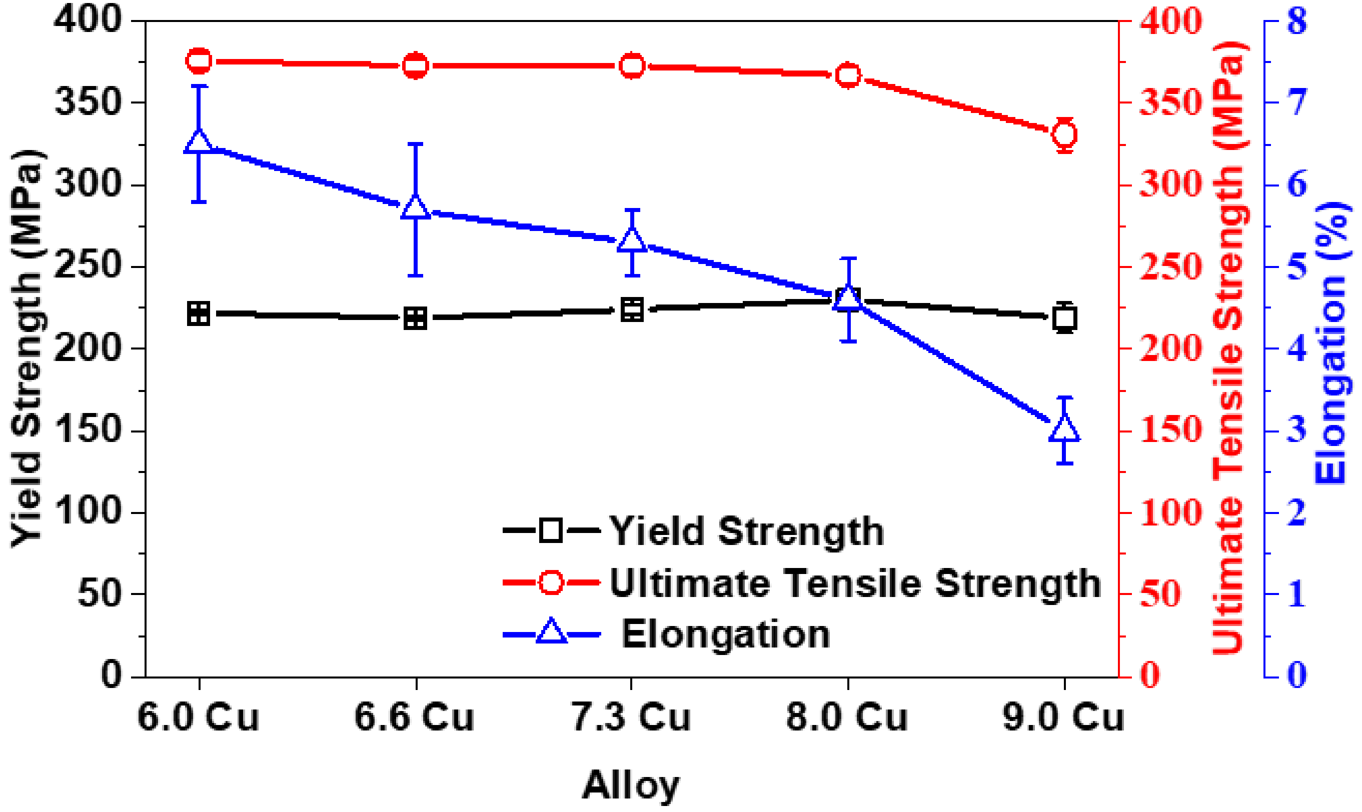


X-ray tomography video of interconnected grain boundary particles (for 9 wt% Cu)

Bahl et al. Mater. Sci. Eng. A, 772, (2020), 138801

Ductility decreases monotonically with Cu content

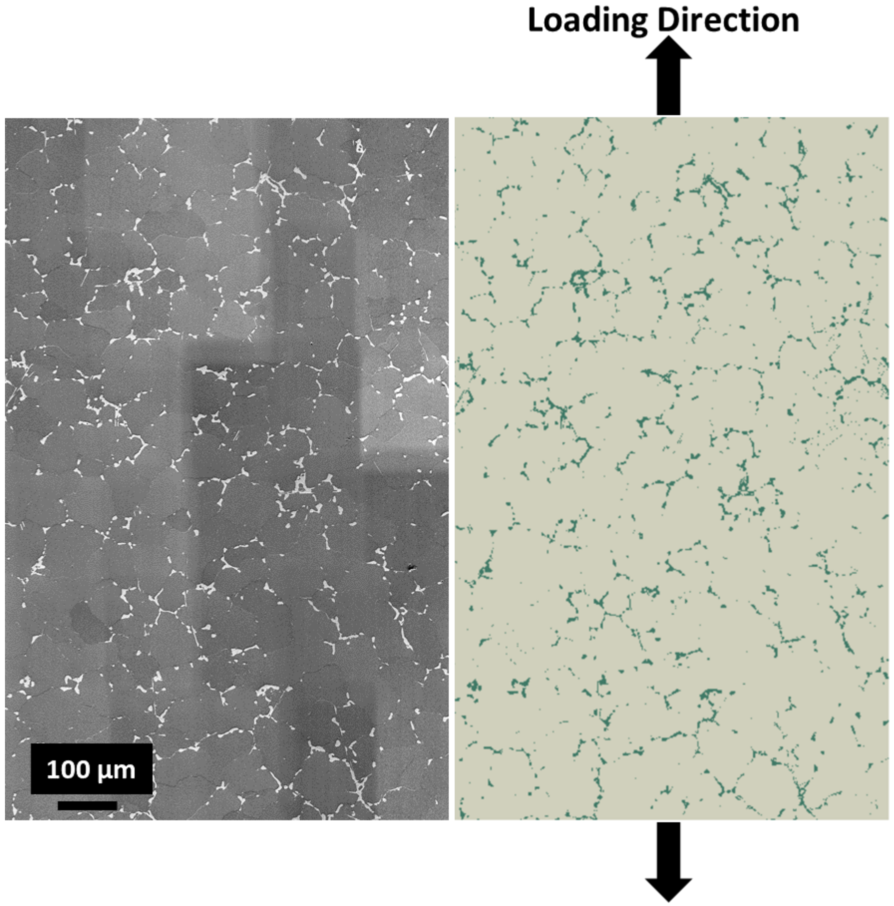


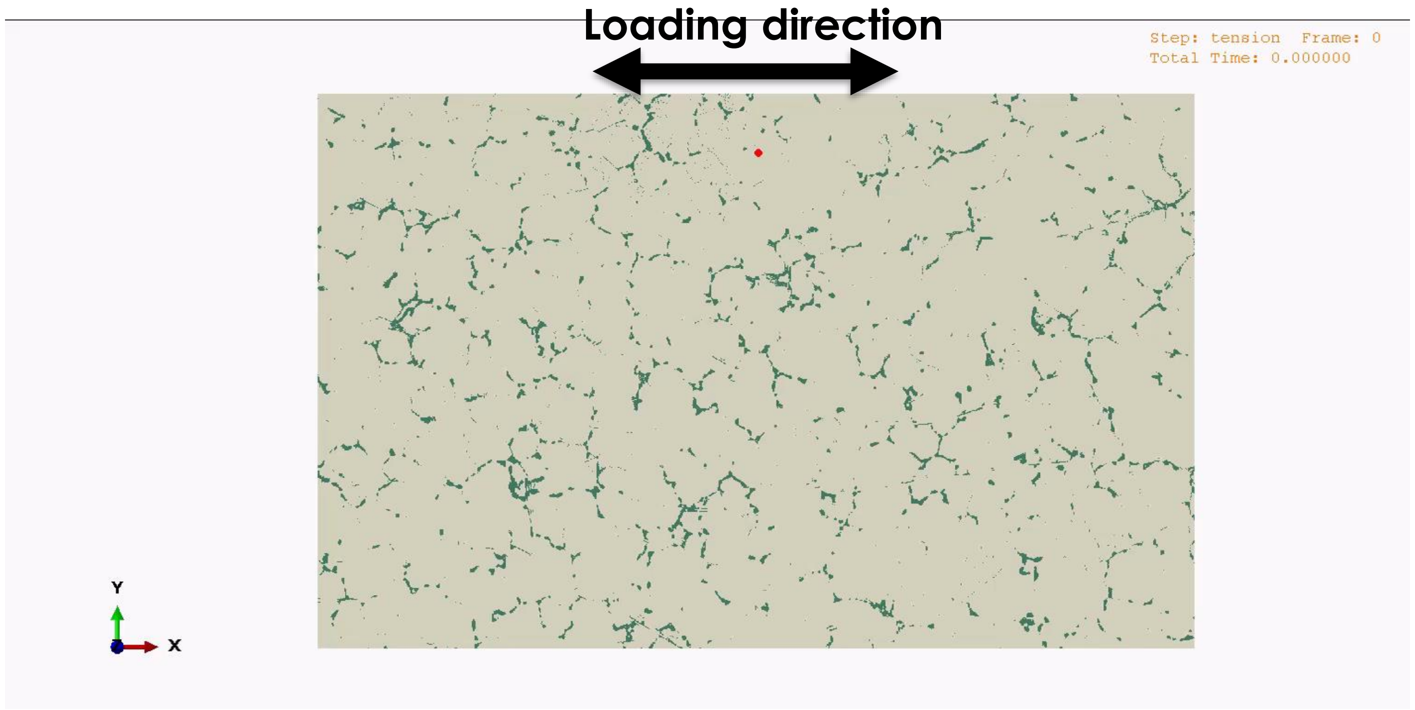


- Ductility decreases from 6.5 % (6.0 Cu) to 3.0 % (9.0 Cu)
- Yield strength and strain hardening behavior unaffected

OAK RIDGE National Laboratory

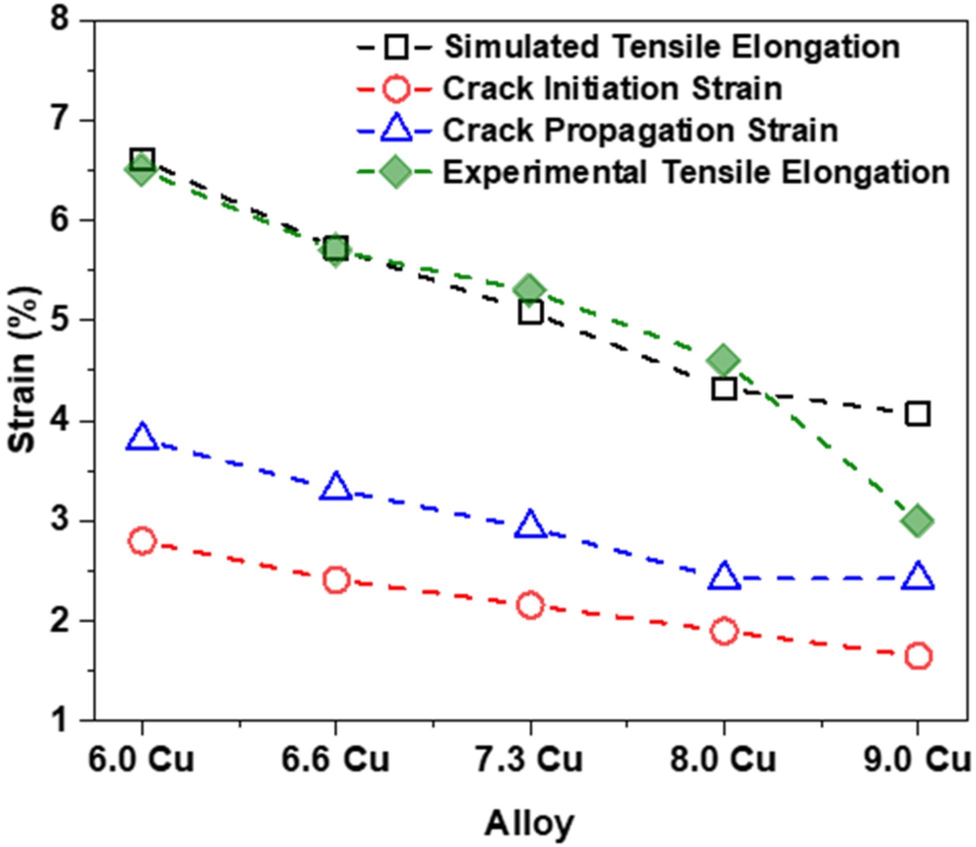
Progression of cracking shown by finite element modeling of tensile elongation during monotonic loading

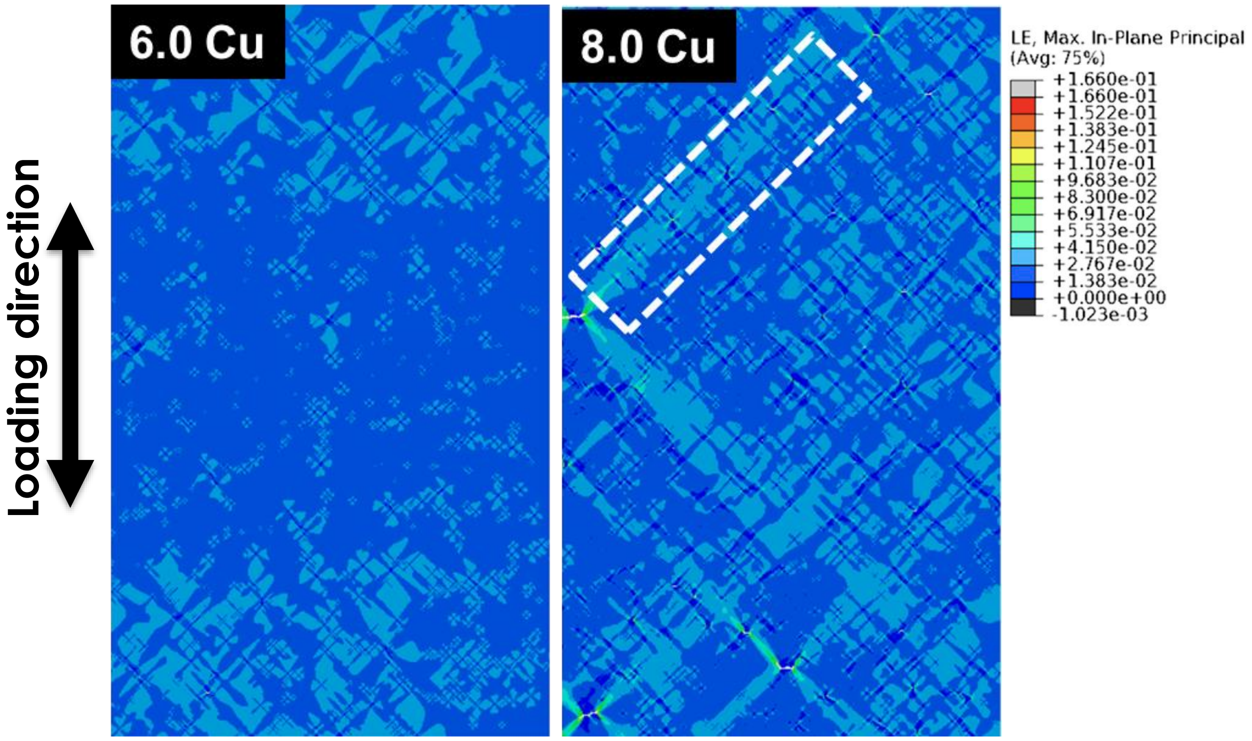




- Grain boundary particles modeled as purely elastic
- Matrix (Al + θ') modeled as elasto-plastic

Good match between modeled and experimentally measured elongations

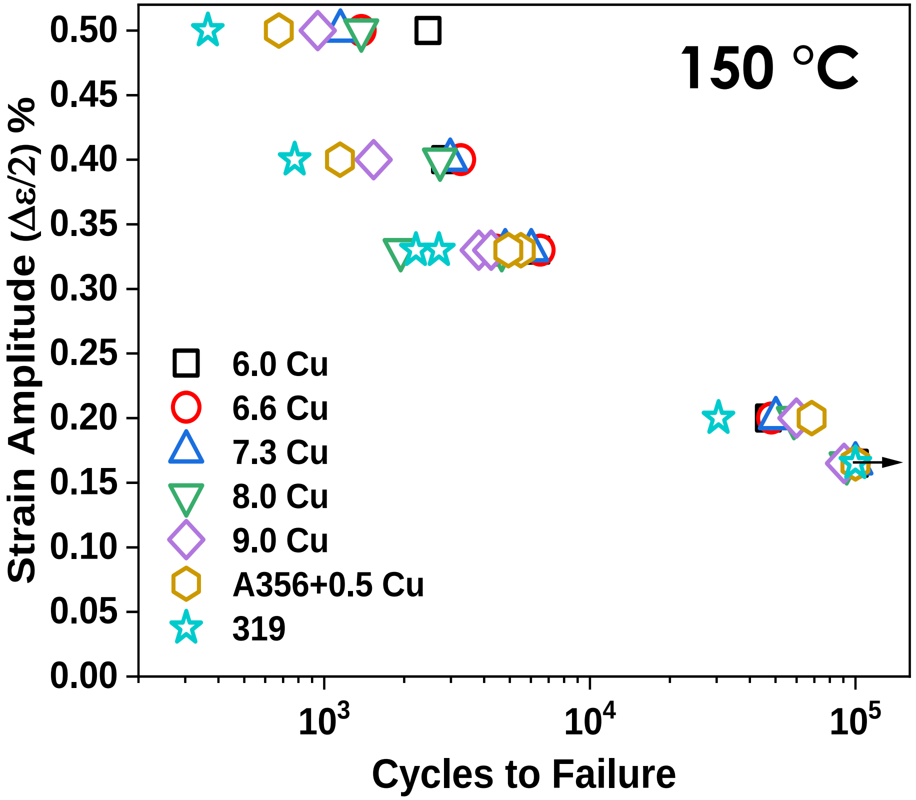


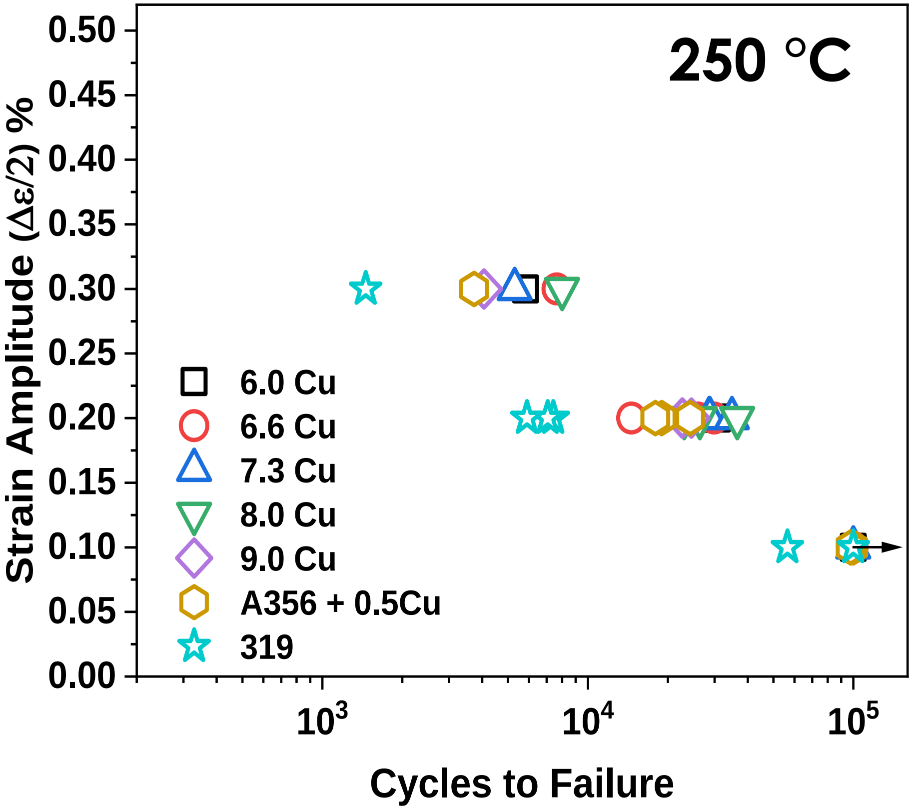


Simulated maximum in-plane principal strain map at 3% strain. White dotted line is a macro shear zone.

- Total elongation = crack initiation + crack propagation strain
- Both initiation and propagation easier at higher Cu content
  - More θ volume fraction and larger average size leads to earlier cracking

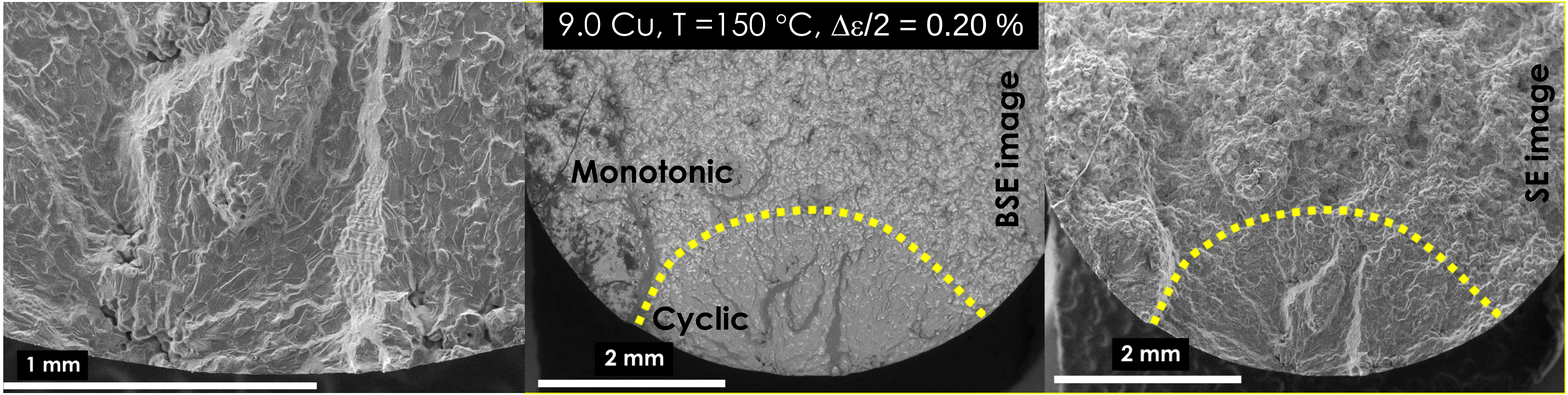
Low cycle fatigue life independent of Cu content



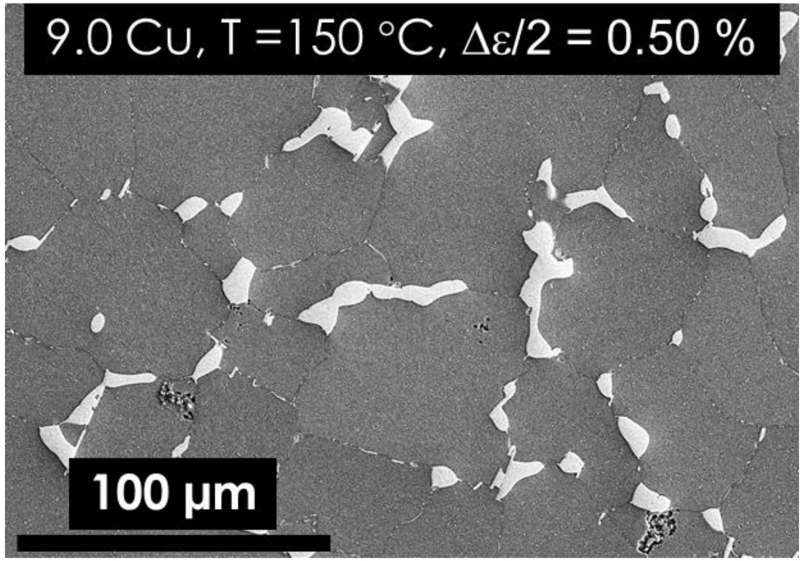


- Fatigue life of ACMZ alloys comparable to A356+0.5Cu and better than 319.
- A356+0.5Cu and 319 are commercial cast cylinder head alloys

Fatigue crack initiation occurs at near-surface porosity

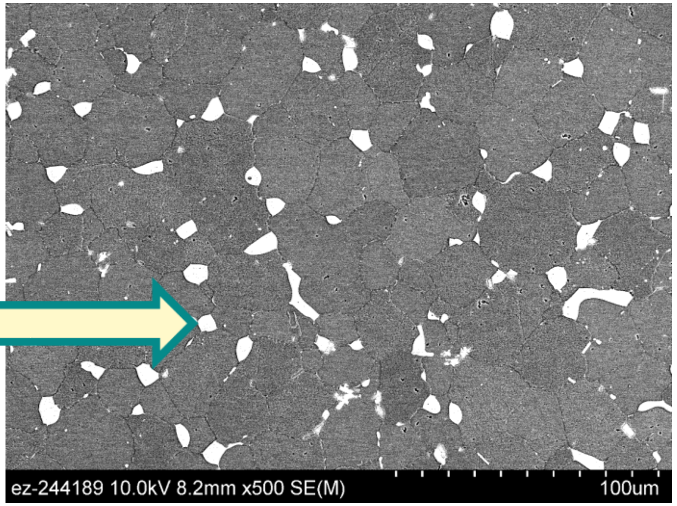


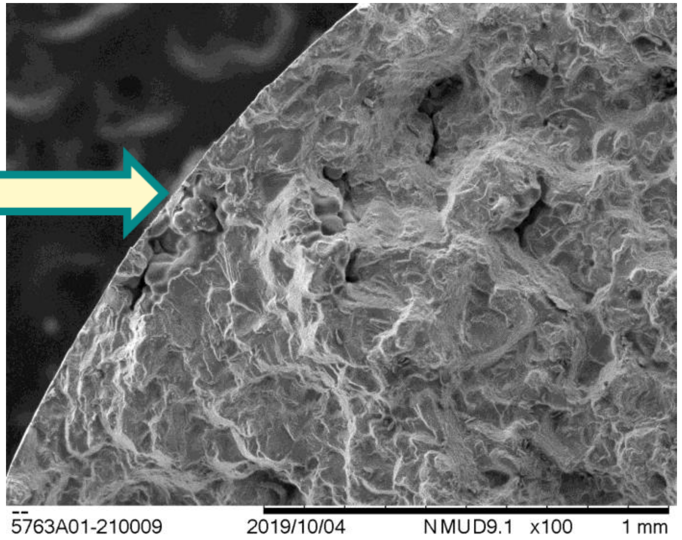
- Grain boundary particles are **<u>not</u>** the sites for fatigue crack initiation
- Grain boundary particles do not play a major role in fatigue crack propagation



Outcome of Research: Focus on grain boundary particles and near surface porosity

- Key lever for ductility improvement: ***Shape of grain boundary particles***
- Control particle formation through alloy chemistry – patent filed
- Key lever for LCF improvement: ***Near surface porosity***
- Control near surface porosity through processing modifications





ACMZ 150C LCF Series

Responses to Previous years Reviewer’s comments

- General remarks about project were positive
- *“It would be interesting to see the creep/fatigue behavior of the material due to the high temperatures that we are discussing (more than 400C). ”*
  - *Response:* Extensive creep (backup slide) and fatigue tests were performed this FY. Higher temperatures in out year.
- *“It would be nice to reach out to a primary Al ingot supplier to determine the cost of the material.” “It will be interesting to see if CRADA's form in near future”*

  \- *Response*: Good suggestion on ingot supplier. A new CRADA involving ACMZ alloys is currently being negotiated with an industry partner.
- *“It would be interesting to determine the series of phases that transforms before the θ' phase.”* One reviewer asked if sufficient focus is being applied to corrosion.

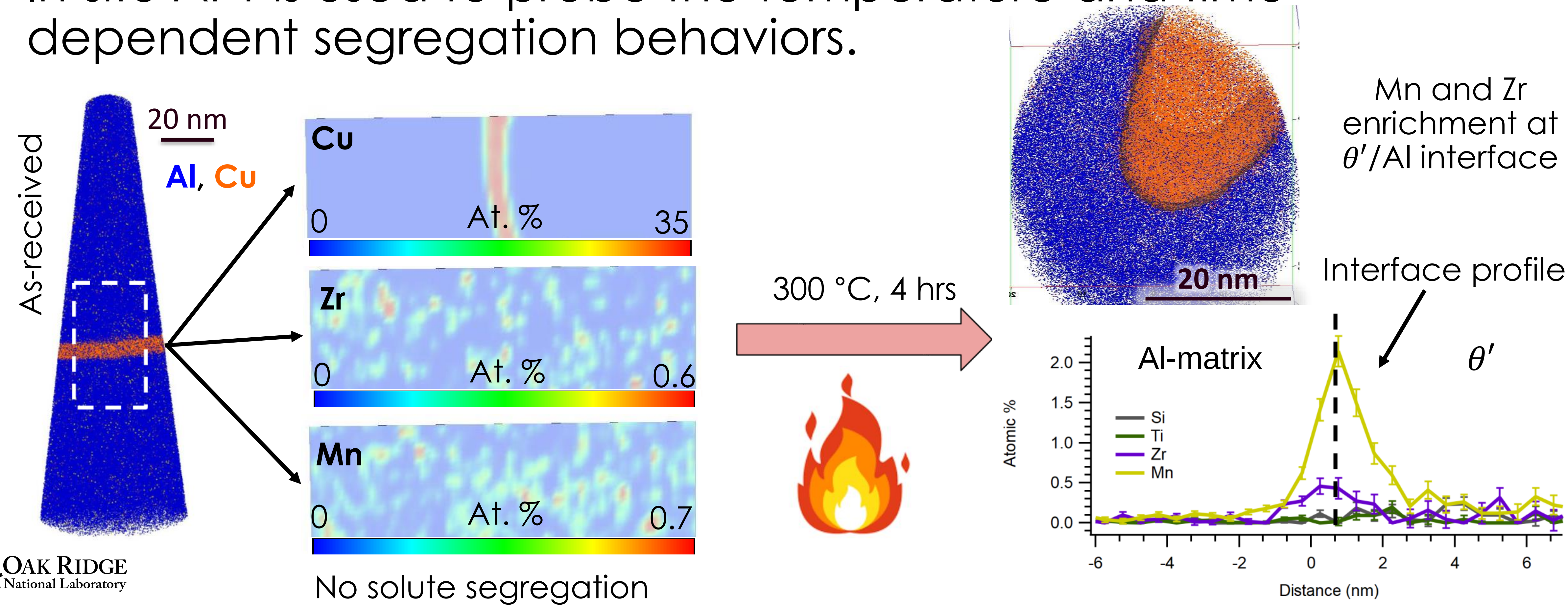
  \- *Response*: Various phase transformations have been studied in the past and are being investigated still. There is ongoing work on alloy corrosion.

Collaboration and Coordination

- **Program Lead**
  - Oak Ridge National Laboratory (ORNL)
    - Spallation Neutron Source (SNS)
    - Center for Nanophase Materials Sciences (CNMS)
- **Program Partners**
  - Thrust 4A - Pacific Northwest National Laboratory (PNNL)
    - *In-situ* atom probe
  - Thrust 4A - Argonne National Laboratory (ANL)
    - *In-situ* synchrotron diffraction and phase identification
- **Other Partners**
  - General Motors (GM) – CRADA in progress
  - Northwestern University – Creep testing
  - Colorado School of Mines - Neutron diffraction

Collaboration Example: In-situ Atom Probe Tomography (APT) – with Arun Devaraj and team at PNNL

- Solute segregation at θ' precipitate interfaces is important for high temperature θ' stability (the strengthening phase)
- In-situ APT is used to probe the temperature and time dependent segregation behaviors.



OAK RIDGE National Laboratory

Remaining Challenges and Barriers

- Further improve fatigue performance of ACMZ alloys at intermediate temperatures vs A356+0.5Cu to fully reap the strength & stability advantages of ACMZ at >250°C
- Critical property targets for specific new engine components are not well-understood in many instances - resulting in lack of clarity in alloy design guidance
- Several gaps exist in ICME models; Examples are models for microstructure evolution or fatigue life prediction.
- Commercialization barriers
  - Engine components can perform differently compared to lab scale castings.
  - OEMs require a full materials card before they consider going into the design phase of a component
  - OEMs are needed to transition technology to their applications

Proposed Future Research

- Fundamental efforts will include
  - New alloy systems investigated based on their thermal stability e.g. Al-Ni (i.e., subtask scientific focus is broader than ACMZ alloys)
  - Thermal conductivity-microstructure relationships
  - Continue to establish the microstructure and mechanical property relationships of interest

- Applied efforts will include
  - Work on commercialization of ACMZ alloys for engine applications
  - Application of advanced processing techniques on ACMZ type compositions
  - Continue corrosion studies
  - Generate property datasets of interest for ‘tailored’ ACMZ alloys

Any proposed future work is subject to change based on funding levels

Summary

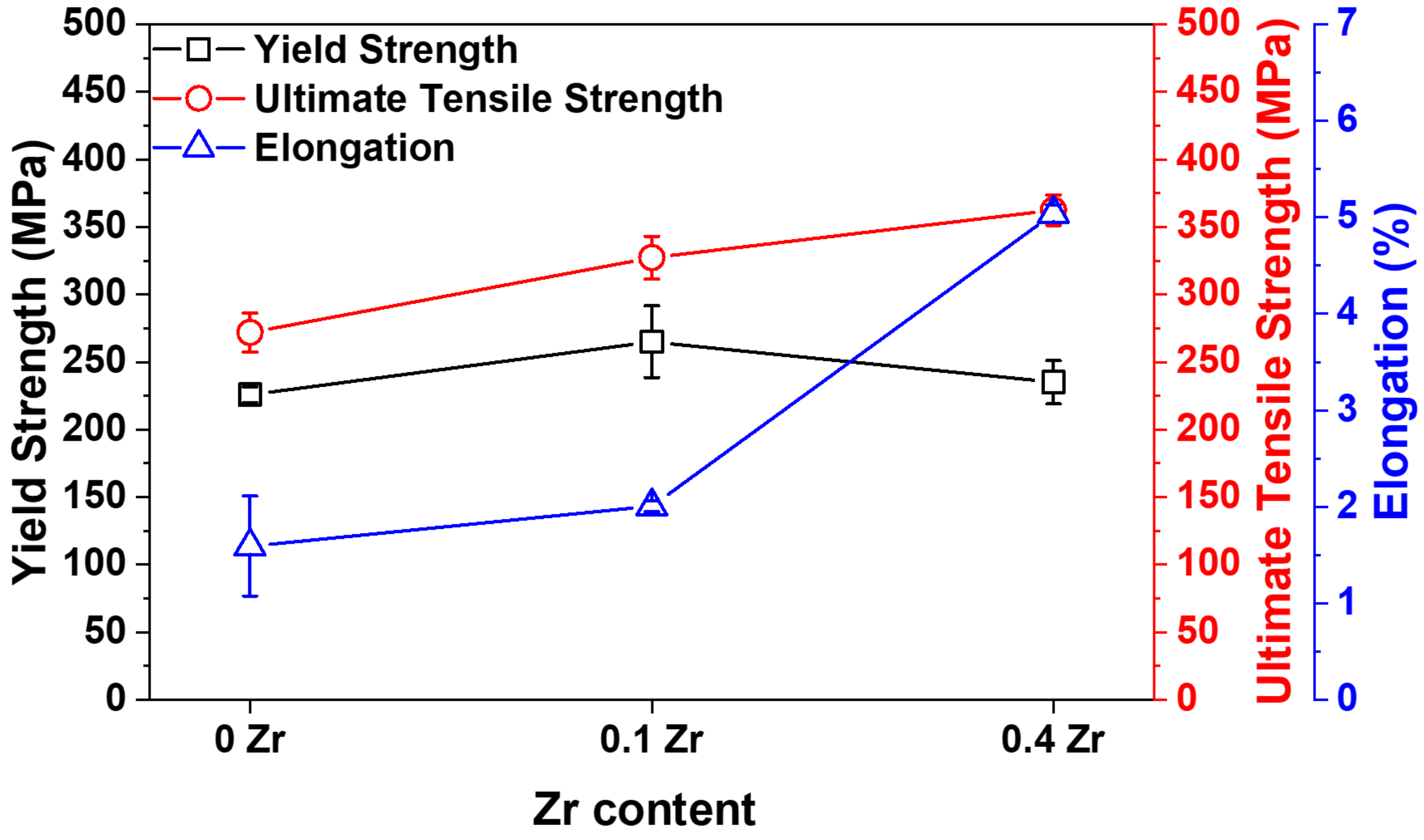
- **Relevance:** Develop, using ICME, more robust engine materials that can withstand higher temperatures and combustion pressures, leading to further increases in power densities of engines.
- **Approach:** ICME approach used to accelerate the development of cast aluminum alloys.
- **Collaborations:** PNNL and ANL (three national labs are actively participating). Working on one CRADA negotiation and looking for additional CRADA opportunities.
- **Technical Accomplishments:**
  - **Identified required microstructural improvements in ACMZ alloys to increase their durability under powertrain component service conditions**
  - **Crack initiation sites in a series of ACMZ alloys were different in monotonic and cyclic loading. Alloy compositions and processing techniques were pursued to improve the performance of the ACMZ alloys for engine applications**
  - **Advanced characterization techniques applied to further understand mechanical behavi**or
- **Future Work:**
  - **New alloy system(s) will be explored**
  - **Microstructure-thermal property relationships.**
  - **Generate property datasets for tailored ACMZ alloy compositions**

Any proposed future work is subject to change based on funding levels

Backup Slides

Key outcome: Microstructural features that control ductility and LCF are different

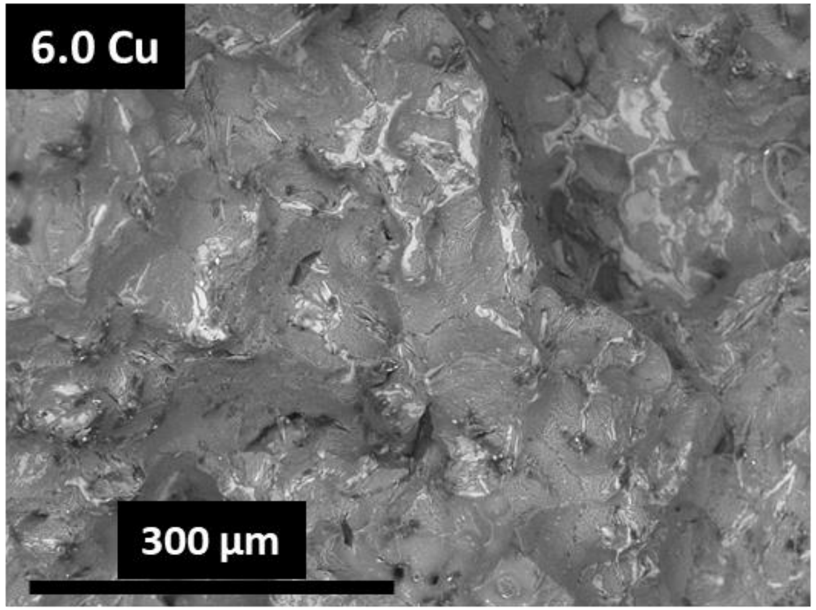
Increasing Zr content in cast alloys improves their ductility by modifying grain boundary precipitates

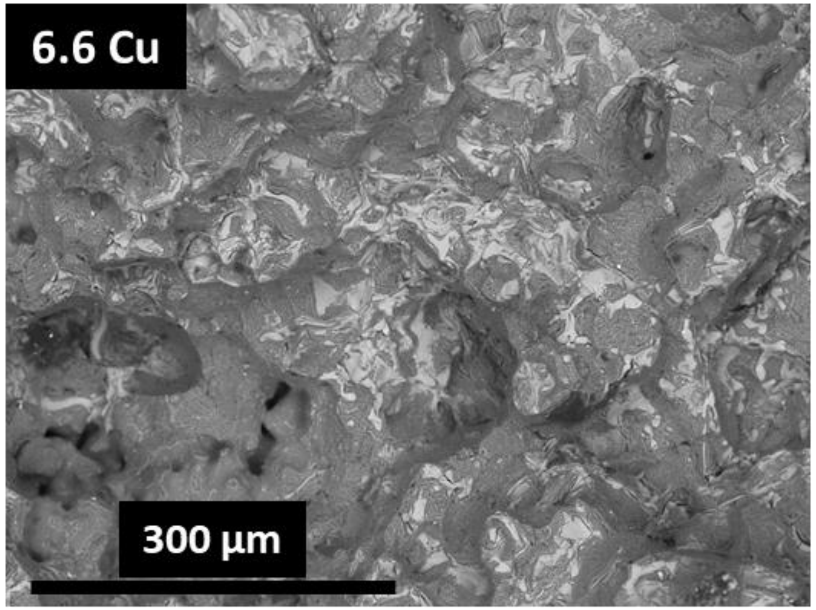


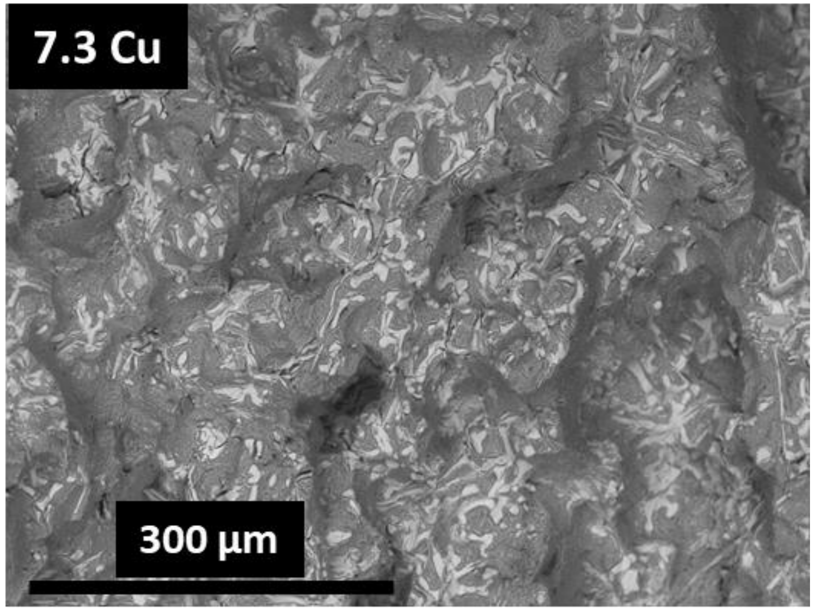
* Patent application is filed (Cu content is 7.3-8.0 wt%)

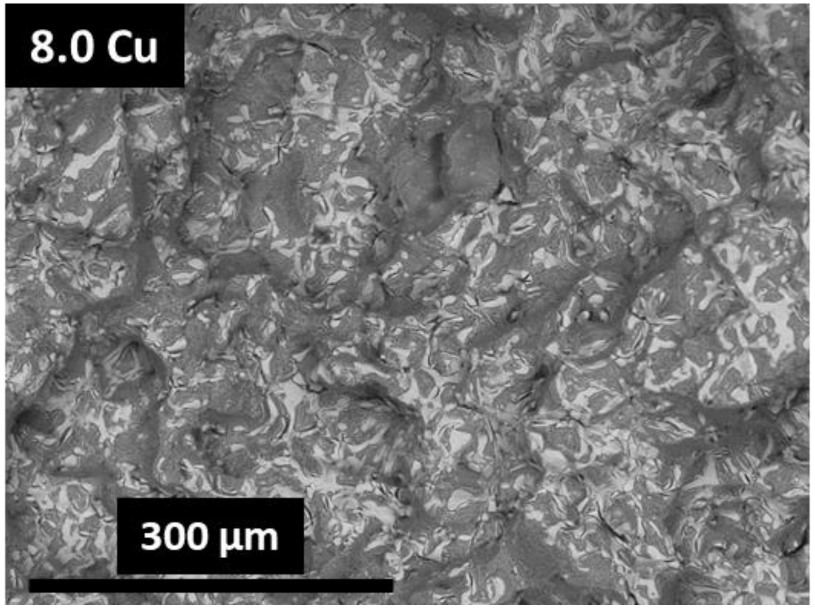
Technical Back Up

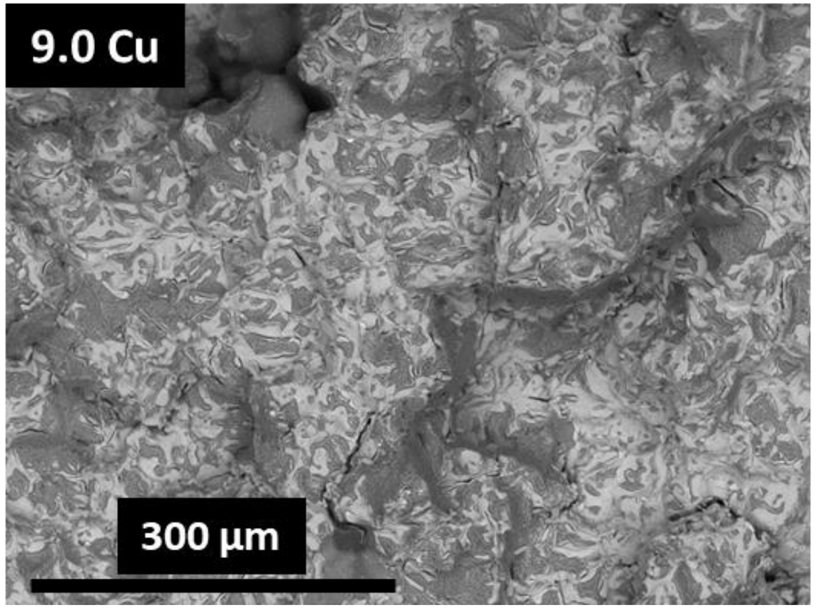
Fracture surface preferentially occupied by particles





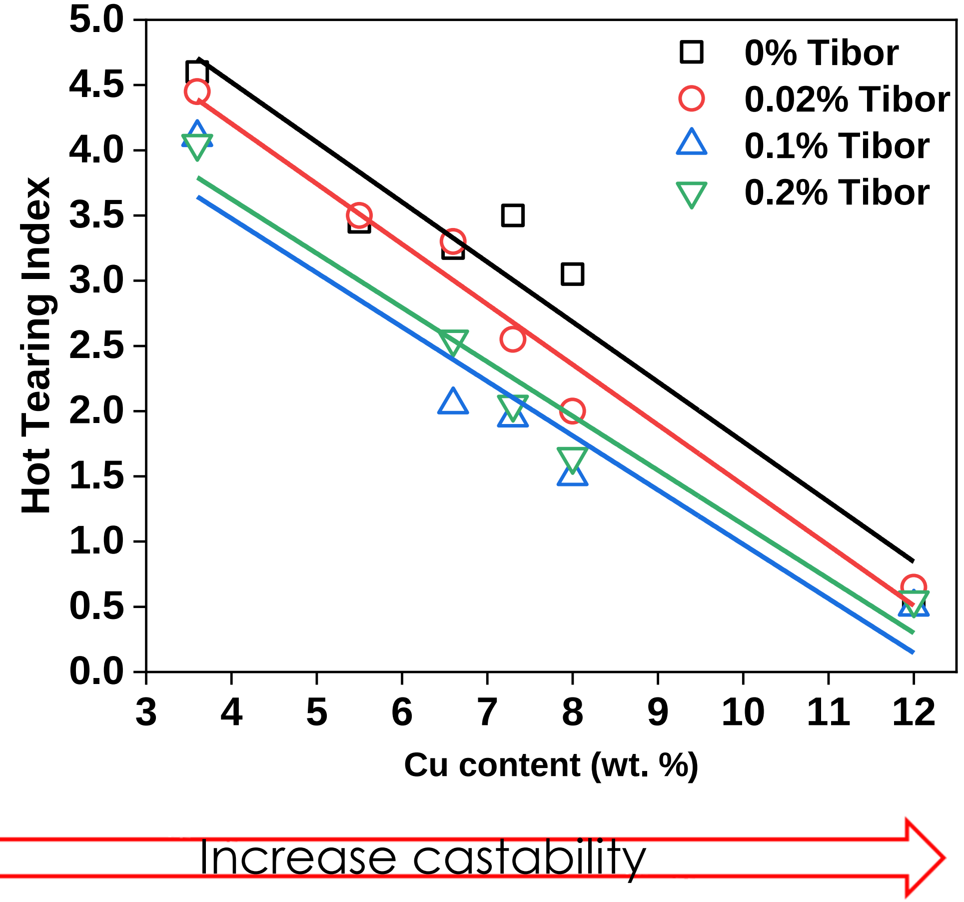






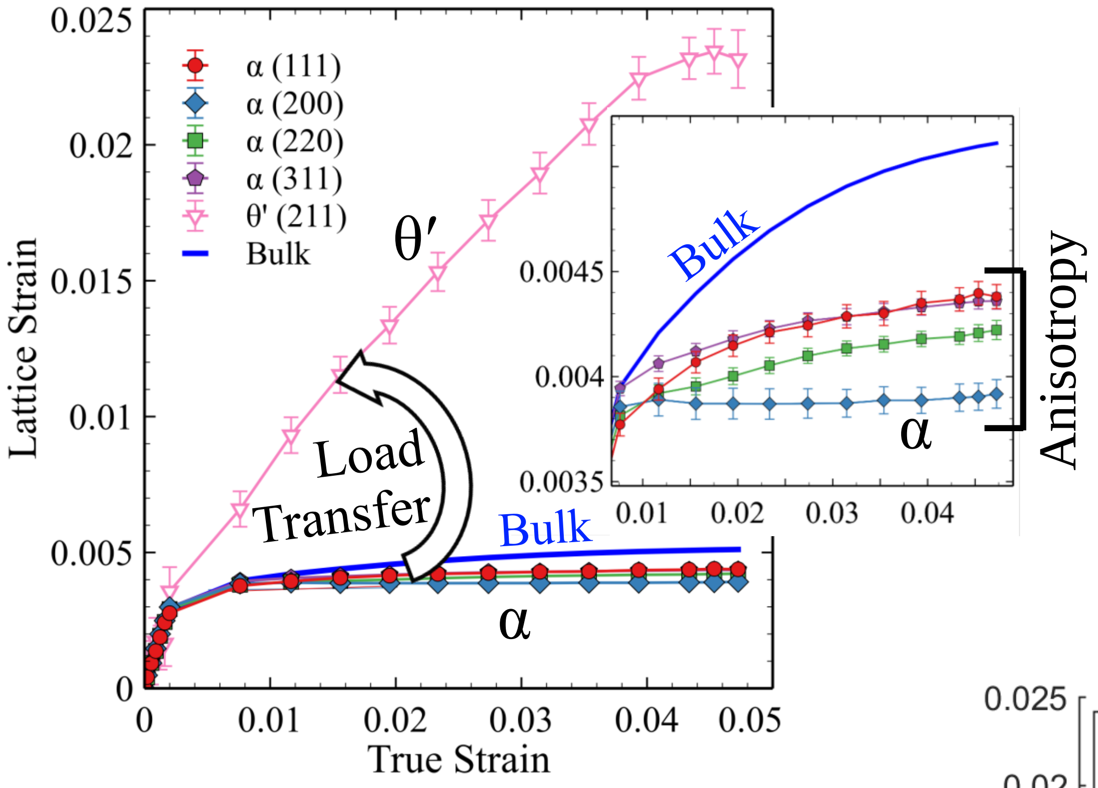
Targets: Improvement in mechanical properties of high Cu ACMZ alloys will help enable higher efficiency engines

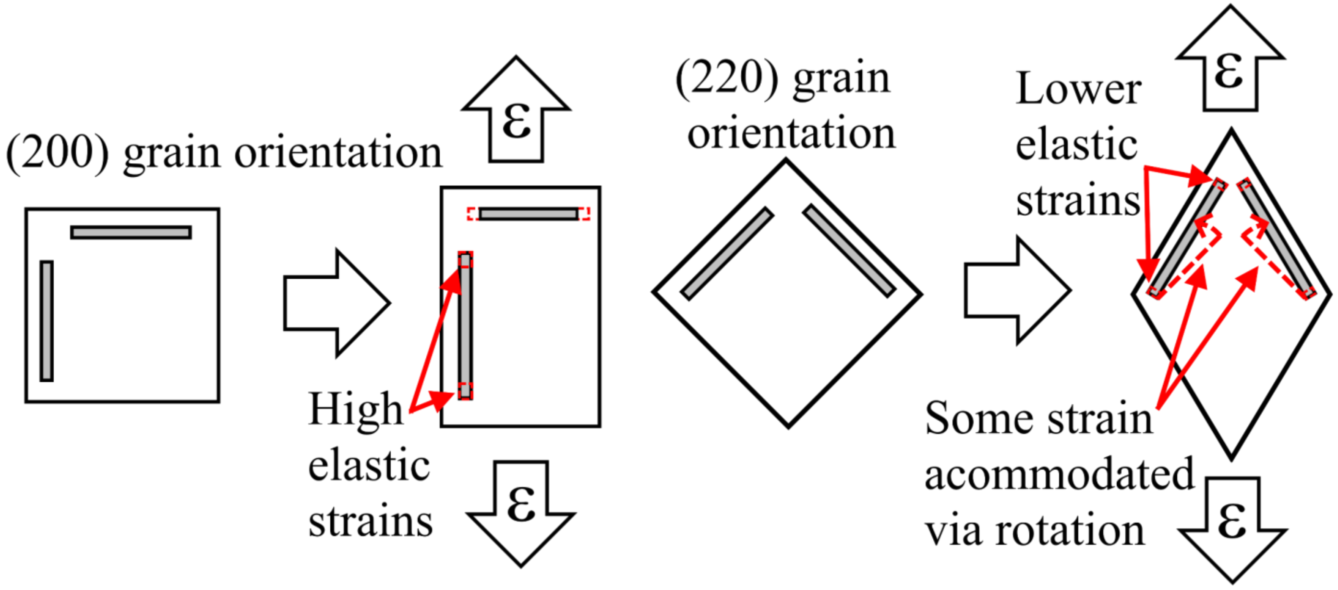
- Room temperature ductility of 5-6% in high Cu (>7% Cu) ACMZ alloy
- Low cycle fatigue life superior to A356+0.5 Cu and 319 baseline alloys at all temperatures
- Higher Cu necessary for better hot tearing resistance

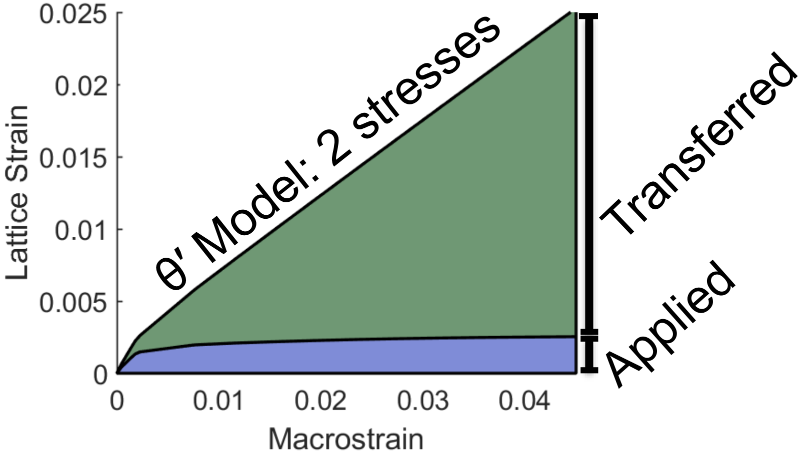


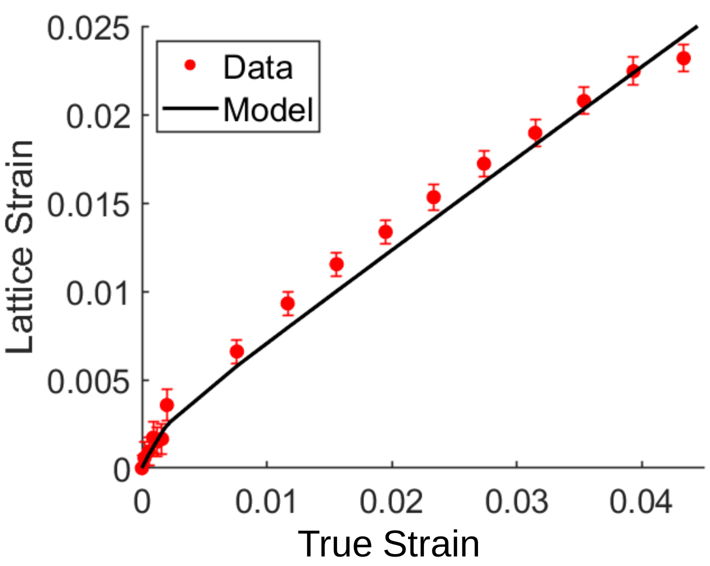
Technical Back Up

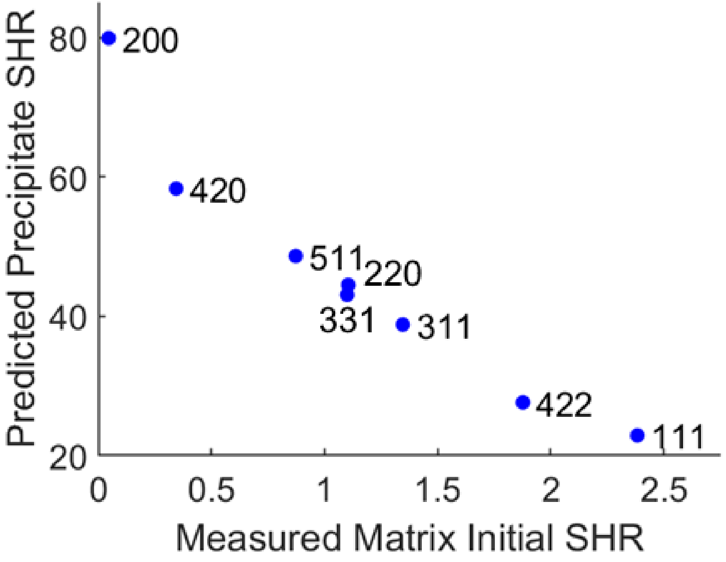
Anisotropic Strain Hardening in Alloys with θ′ Precipitates



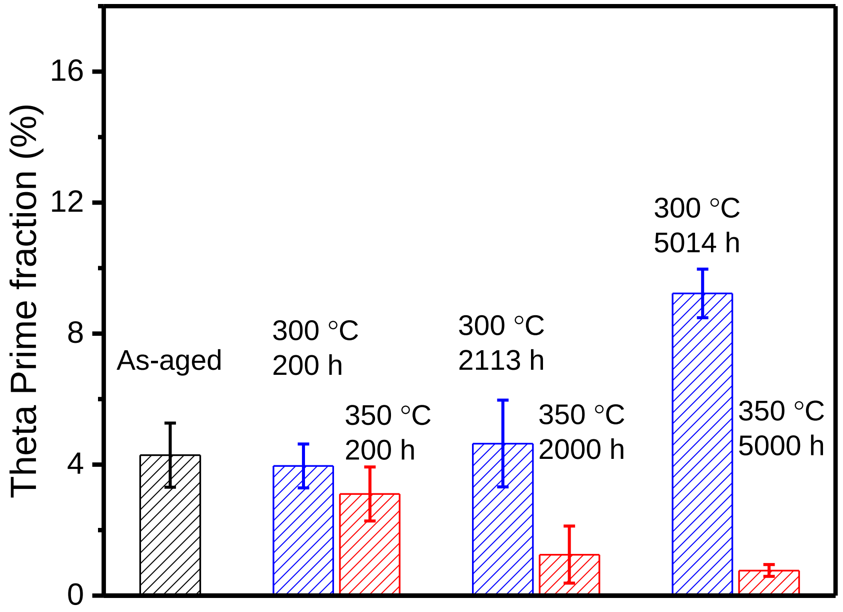


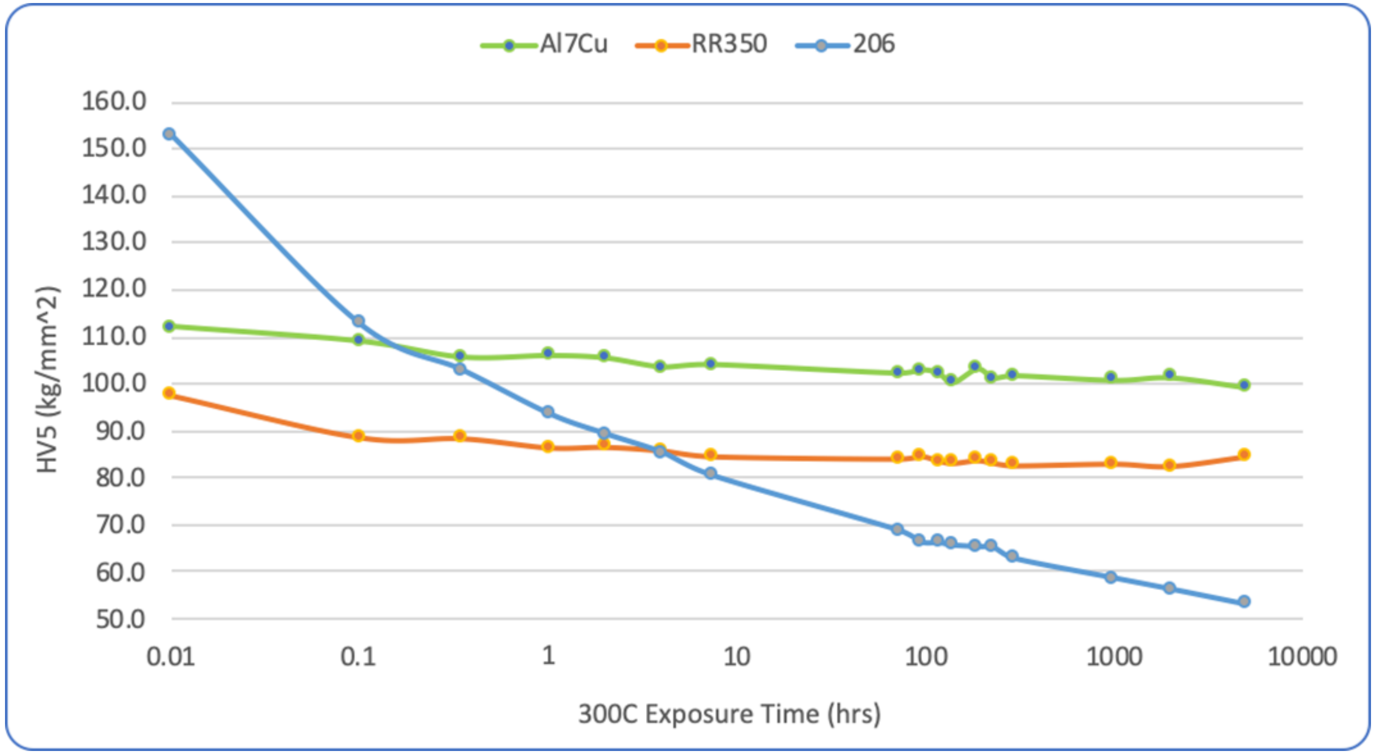






$\theta' - \theta$ volume fraction evolution in ACMZ alloy measured with synchrotron diffraction at Advanced Photon Source





- Fraction of θ' phase increases at 300°C with increasing annealing time in ACMZ alloy (with 6.6 wt% Cu), but decreases at 350°C with increasing annealing time.

OAK RIDGE National Laboratory