Light Metals Core Program - Thrust 4 - Characterization, Modeling and Lifecycle

Project ID# mat235

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June 24th 2021

Overview

Timeline

- Project start date: 1st Oct 2020
- Project end date: Sept 30th 2023
- Percent Complete: 5%

Budget

- FY21: $1.15 million
- Advanced characterization & modeling:
  - PNNL: $250K
  - ORNL: $300K
  - ANL: $200K
- Residual stress: PNNL $250K
- Material lifecycle: ANL $150K

Barriers and Technical Targets

- Need to effectively characterize and measure mechanical properties of Al & Mg alloys with intentionally heterogeneous microstructure
- Need for linked atomic/meso/macro-scale predictive models for magnesium/Aluminum, capable of predicting material structure, properties, residual stresses and corrosion behavior based on alloy composition, processing, and fabrication techniques.
- Effective recycling approaches are needed for Mg and Al alloys
- Integration across three labs to accelerate light weight materials R&D

Partners

- Program lead lab: Pacific Northwest National Laboratory (PNNL)
- Program partners
  - Oak Ridge National Laboratory (ORNL)
  - Argonne National Laboratory (ANL)

Relevance

- **Objectives:**
- Bring together advanced microstructural characterization, local mechanical testing and predictive modeling to help establish processing-microstructure-property/performance relationships
- Characterize, predict and optimize residual stresses introduced by the local processing approaches used to achieve intentionally heterogenous microstructure
- Study recyclability of intentionally heterogenous Al and Mg alloys
- Thrust 4, projects selected through internal proposal and review

Thrust 1: Localized property enhancements for sheet Al applications

Thrust 2: Localized property enhancements for cast structural Al applications

Thrust 3: Localized property enhancements for cast Mg applications

Thrust 4:
- Advanced Characterization & Modeling
- Residual Stresses
- Material Lifecycle

Approach: Matrix of unique tools and scientific expertise across PNNL, ORNL & ANL

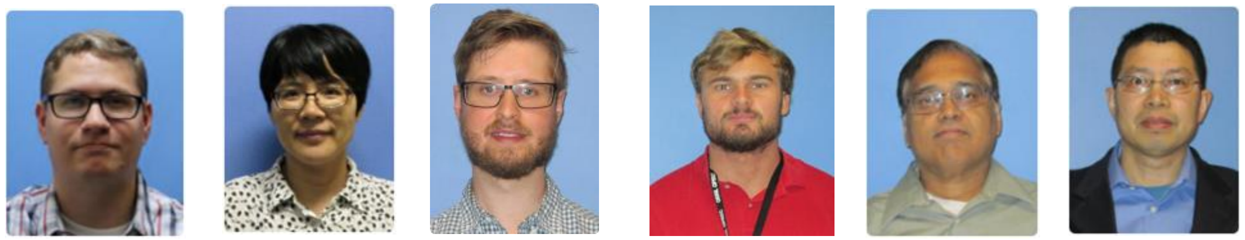
Electron Microscopy, Atom Probe, Nanomechanical Testing

Synchrotron X-rays: Diffraction, Small Angle X-Ray Scattering (SAXS), X-Ray Computed Tomography (XCT)

Material Lifecycle

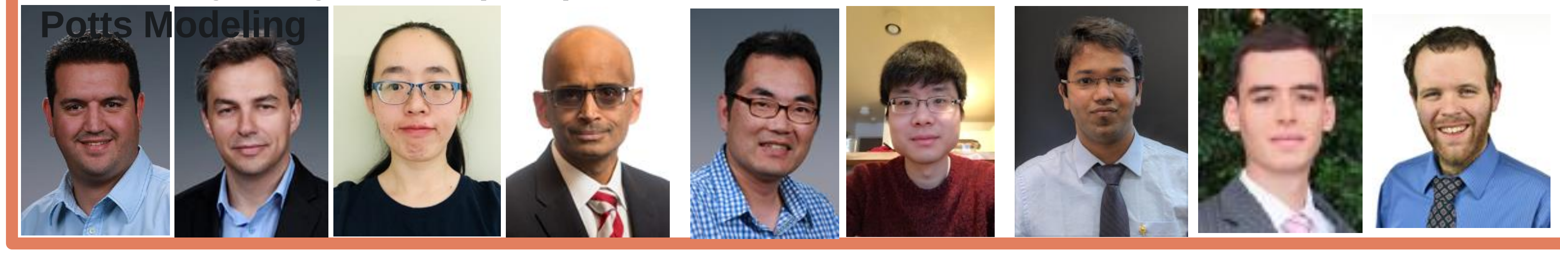
Electron Microscopy, Atom probe, X-rays, XCT, Neutron Diffraction

Computation: Solidification, thermodynamic, process, micro-macro finite element modeling (FEM) for bendability



Residual stress Characterization, Prediction, Optimization

Computational Modeling: High performance computing (HPC), Density Functional Theory (DFT), Molecular Dynamics (MD), Smooth Particle Hydrodynamics (SPH), FEM Potts Modeling



Approach: Advanced Characterization & Computation

- Issued FY21 Call 1 for support thrust advanced characterization and computation on Feb 5th 2021
- Selected 5 highest impact proposals for funding in this call after rigorous internal reviews and projects started on 30th March 2021

Support Thrust: Advanced Characterization and Computation	Relevant Thrust & Project	Lab ownership
Advanced characterization of microstructure-mechanical property relationship in friction stir processed 7085-T78	1C	PNNL & ANL
High performance computing for Density Functional Theory (DFT) studies of cast magnesium local corrosion mitigation	3A	PNNL
In situ beamline experiments at Advanced Photon Source (APS) to study dendrite-ultrasound interactions	2B	PNNL & ANL
Multi-resolution macro-micro Finite Element Modeling (FEM) to study local microstructures' impact on bendability of Al sheets	1C	ORNL
Coupled thermodynamic & process modeling to understand factors affecting the printability and heat treatment response for additive manufacturing (AM) of aluminum alloys onto dissimilar cast or stamped parts	1B & 2C	ORNL

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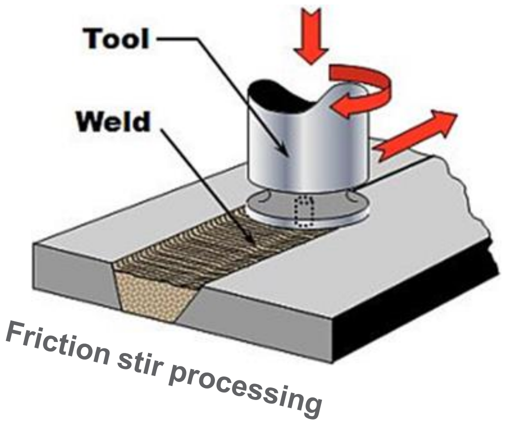
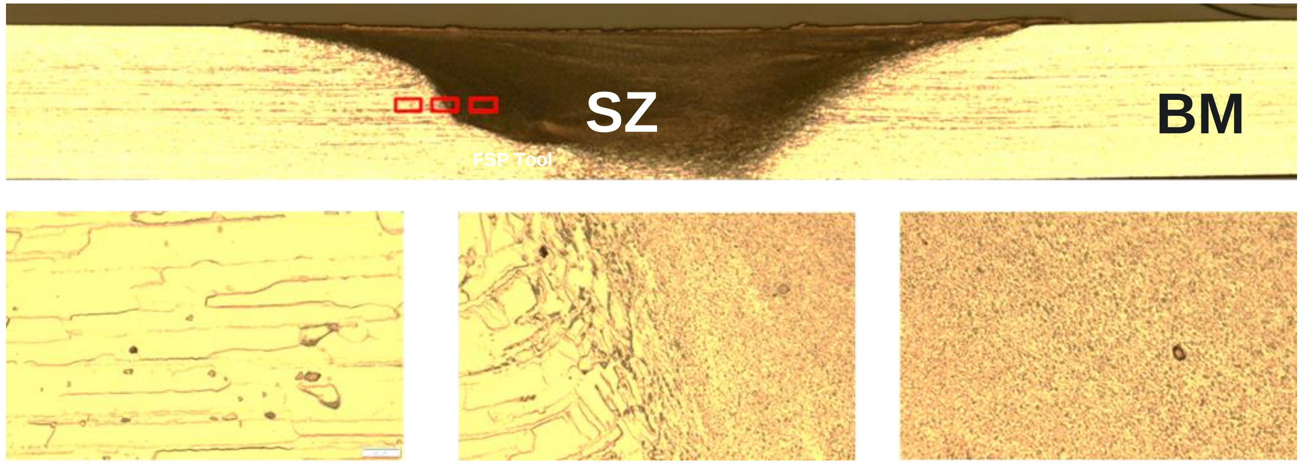
Technical Accomplishments and Progress: High Speed Friction Stir Processing of 7085-T78

1C
Piyush Upadhyay (PI)
Mert Efe
Hrishikesh Das
Tim Roosendaal

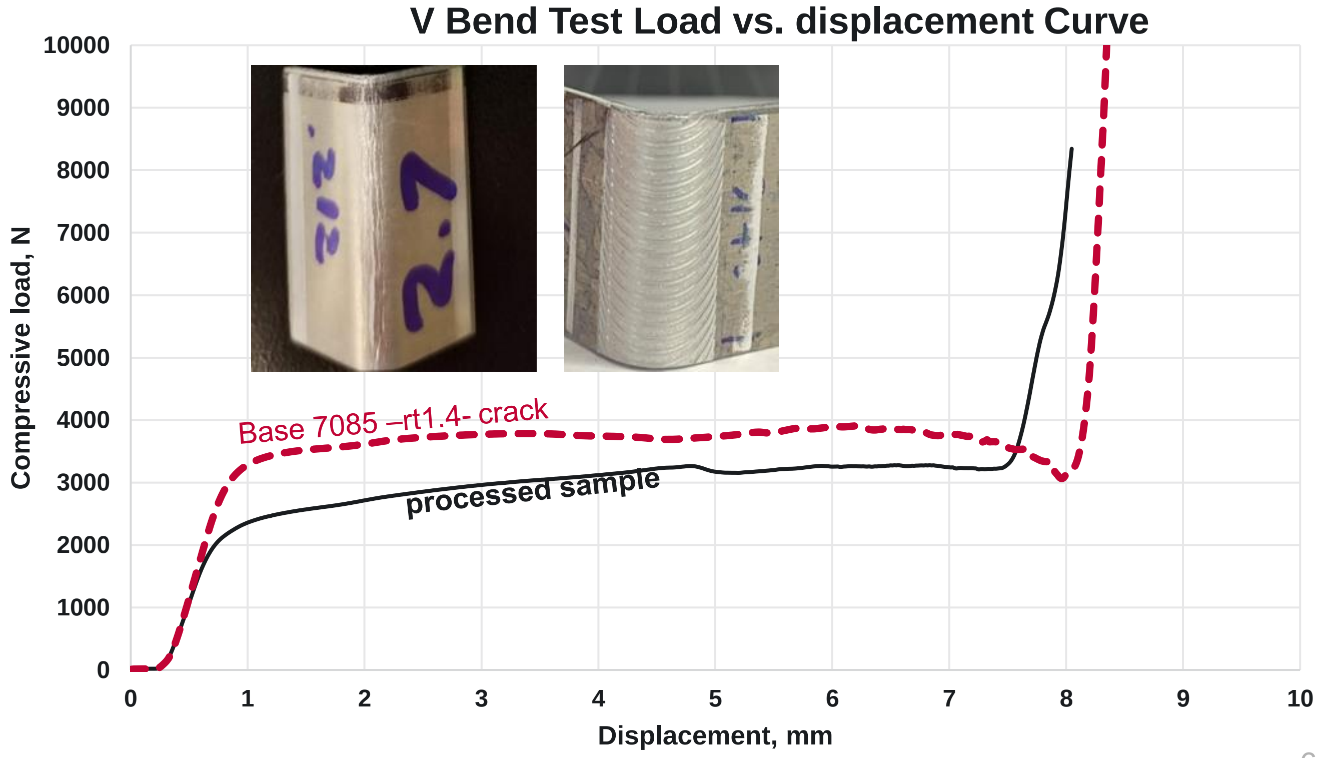




- Friction stir processed (FSP) stir zone (SZ) has low hardness and contains very fine dynamically recrystallized grains and shear textures
- Successful samples show reduced load to yield point in bend tests.

<u>Thrust 4 focus</u>

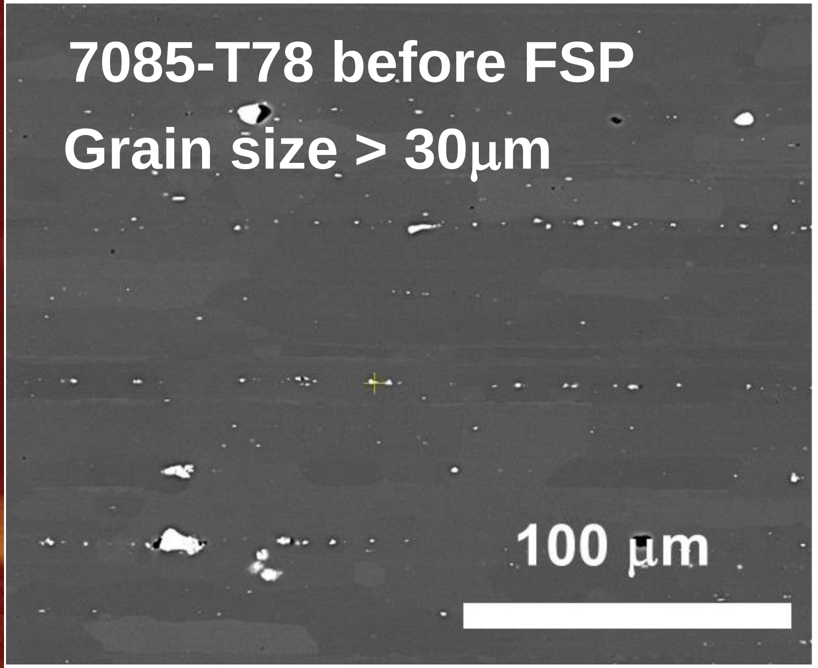
- ➢ Advanced microstructural characterization of nanoscale precipitates in base alloy and stir zone using PNNL aberration corrected Transmission Electron Microscope (TEM) and Atom Probe Tomography (APT) to correlate to bend test results and FSP conditions
- ➢ In situ nanomechanical testing of friction stir processed microstructure and correlate with bend test performance

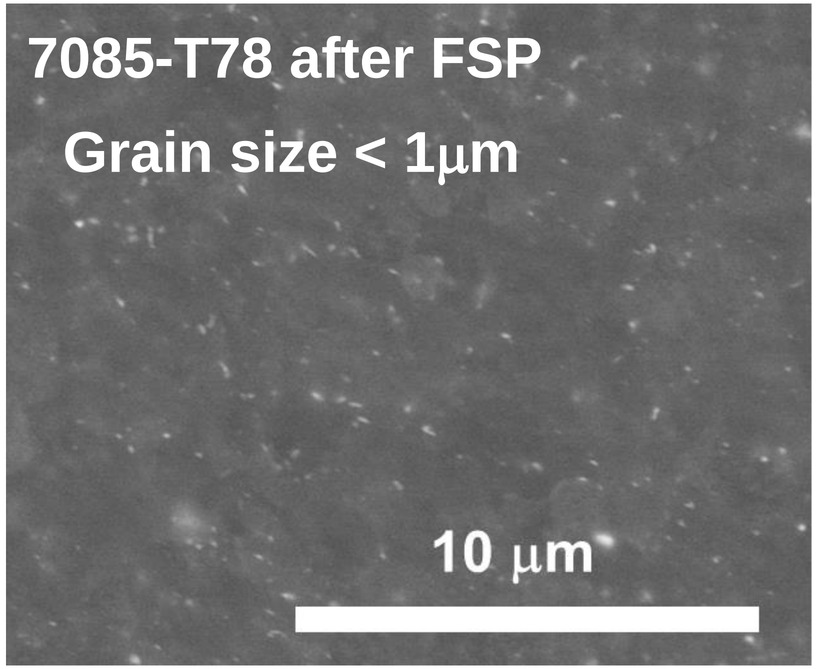


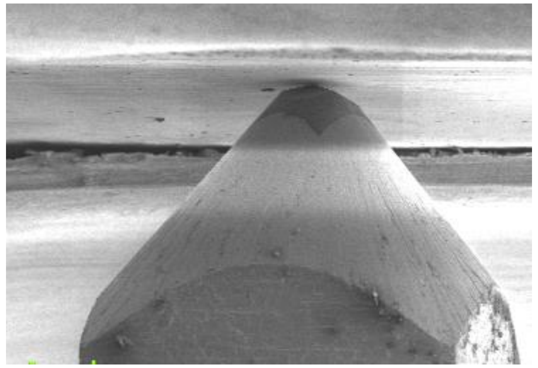
Advanced characterization of influence of FSP on Al 7085

Arun Devaraj (PI)
Christian Roach
Matt Olszta
Tanvi Ajantiwalay

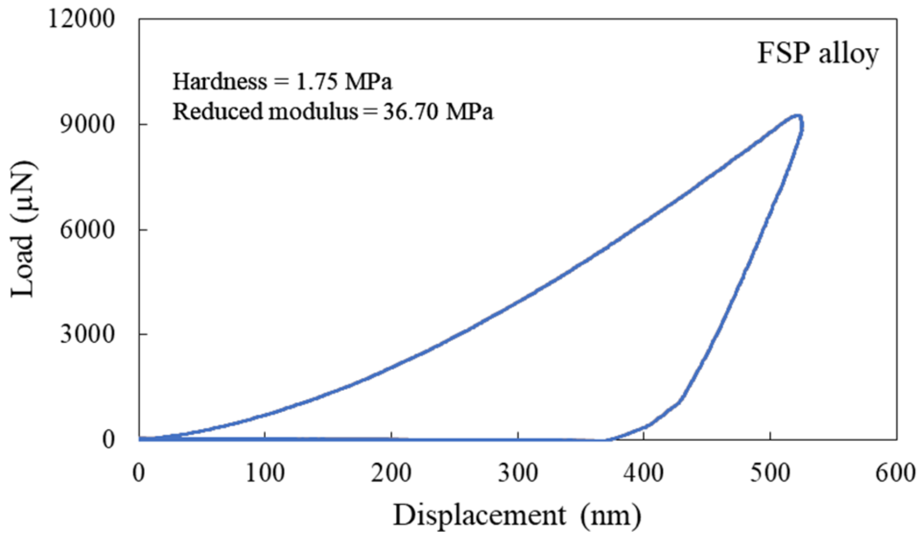
Dileep Singh (PI)
Jonova Thomas







Local Stress-strain curve in FSP SZ vs base alloy 7085 extracted using in situ nanoindentation



- Beamline proposal for High-energy X-ray diffraction at APS submitted
- TEM and APT analysis under progress to identify the structure and composition of precipitates in the stir zone

High performance computing for DFT studies of cast magnesium local corrosion mitigation

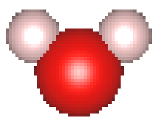
3A2
Peter Sushko (PI)
Qin Pan
Vineet Joshi

- **Objective:** Using Density Functional Theory (DFT) to understand energetics for adsorption of water molecules on the ideal and compositionally modified Mg surfaces: configurations and binding energies of adsorbed H_2O estimated

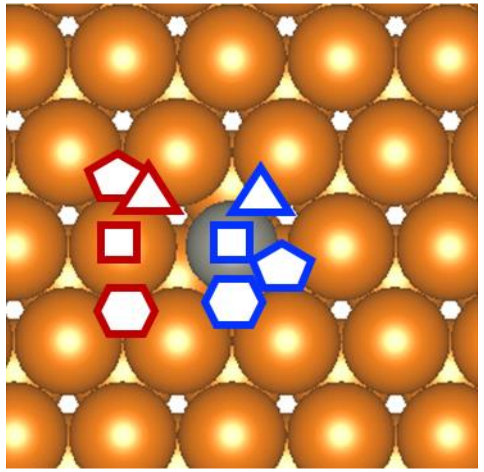
- DFT can show influence of alloying element (Zn) on Mg surfaces on water binding energies

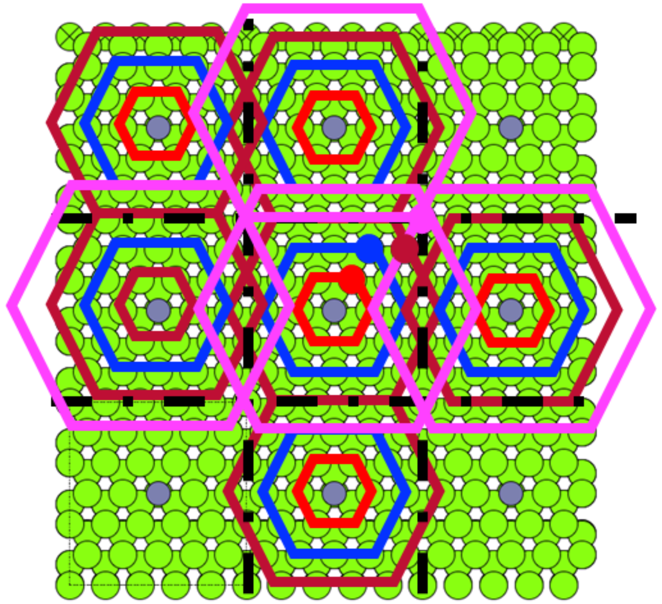
- Effort ongoing to translate scientific understanding to corrosion resistance enhancement by modifying detrimental MgO/Mg(OH2) native surface film.

Mg (0001) surface; lateral cell



Water molecule





Change in H_2O adsorption as a function of distance from Zn dopant on Mg

top	Top – near Zn
bridge	Bridge – near Zn
hollow - fcc	hollow – fcc – near Zn
hollow - hcp	hollow – hcp – near Zn

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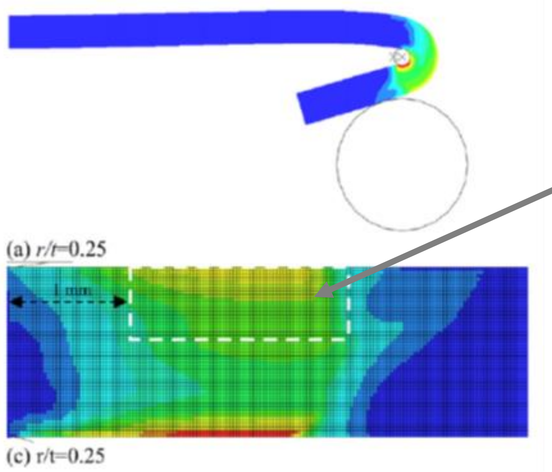
Macro-Micro finite element modeling scheme to study local microstructure influences on bendability

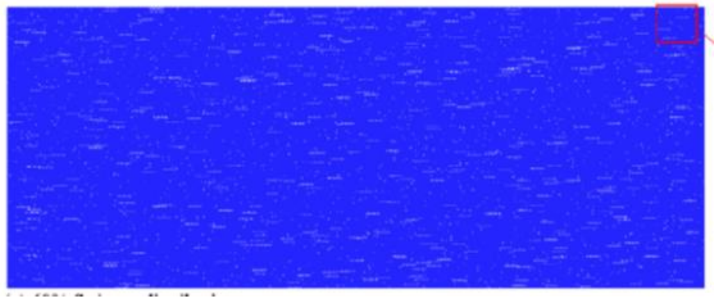
1B/2C

Ying Yang
Alex Plotkowski
Govindarajan Muralidharan
Xiaohua Hu (PI)

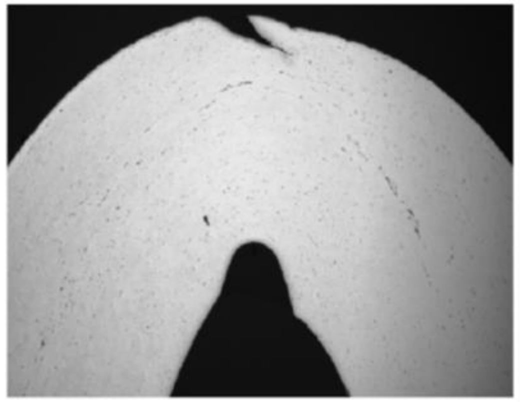
- The Macro-Micro Approach:
  - Using sample scale model to find failure-prone location and the location specific boundaries conditions will be used to drive the micro-model.
  - Can **connect component level simulations with local microstructures**
  - Using this model, the microstructure influences on bendability has been captured *



Macro-Model

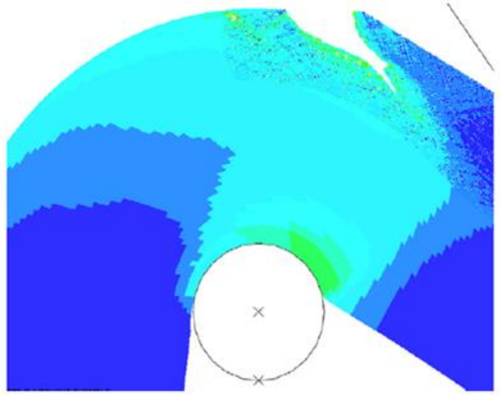


Micro-Model



Exp

Result



Macro-micro Composite Image

*Hu, Jain, Wu, Wilkinson, Mishra, **Journal of Materials Processing Technology** 210 (2010)

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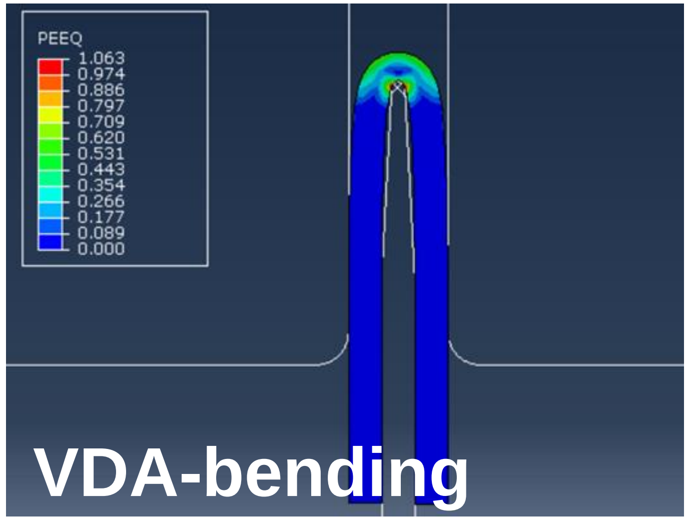
Model for Predicting Influence of local softening on VDA-bending: Preliminary results

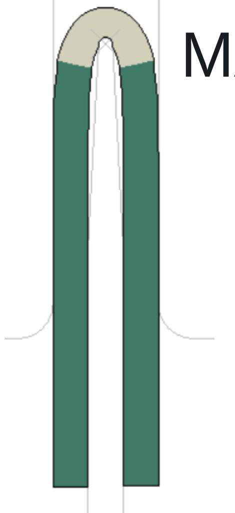
1B/2C

Ying Yang
Alex Plotkowski
Govindarajan Muralidharan
Xiaohua Hu (PI)



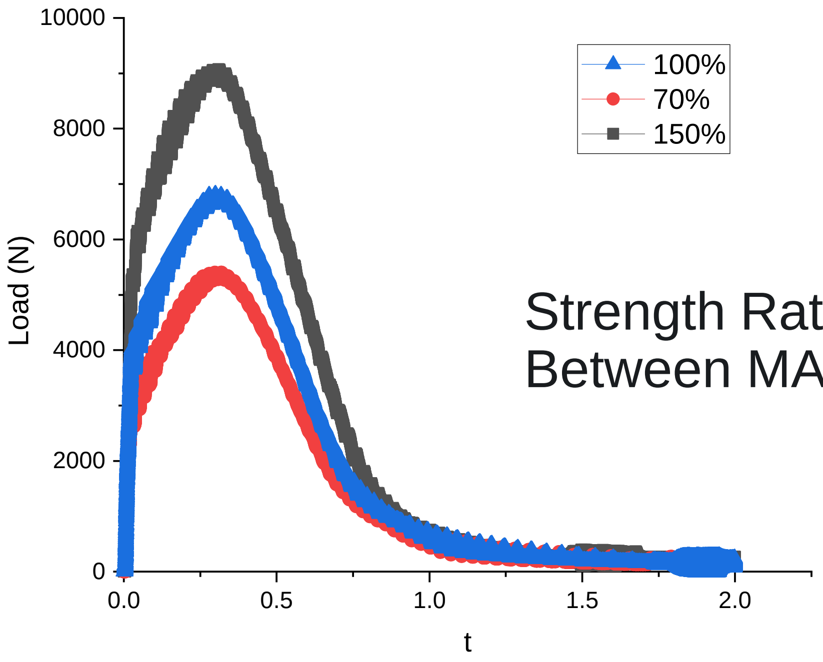
- Macro-models have been established of V-bending and VDA bending
- The influence of local properties on the bending deformation is examined
- Local softening predicted to reduce bending load and potentially increase bendability
- Ongoing effort to implement the multiscale macro-micro models of bending with the use of actual measured local microstructural information.

The model

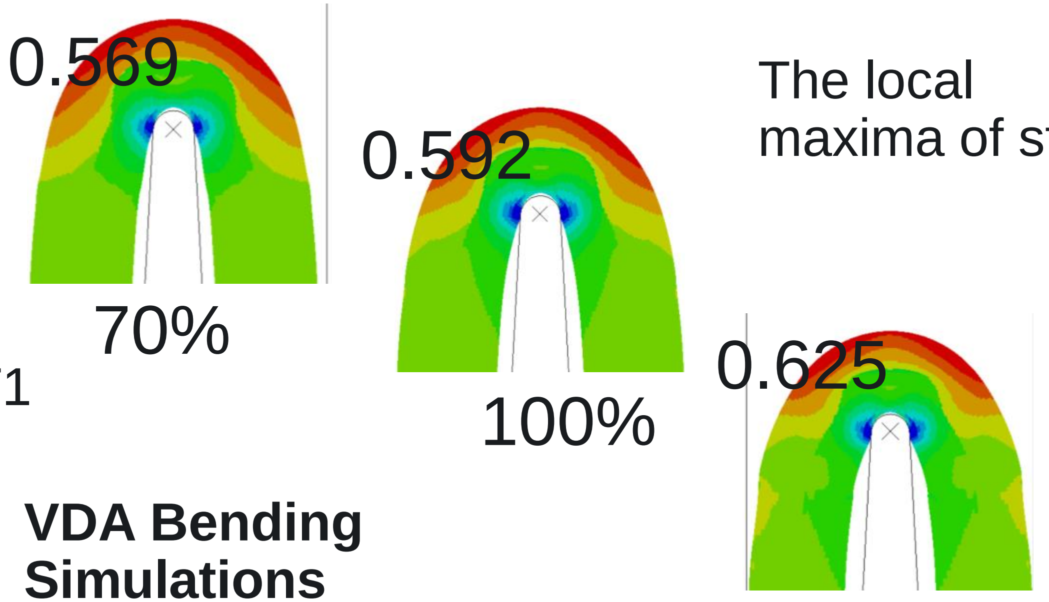


MAT2

MAT1=A7075-T6



Strength Ratio
Between MAT2/MAT1



The local maxima of strain

VDA Bending Simulations

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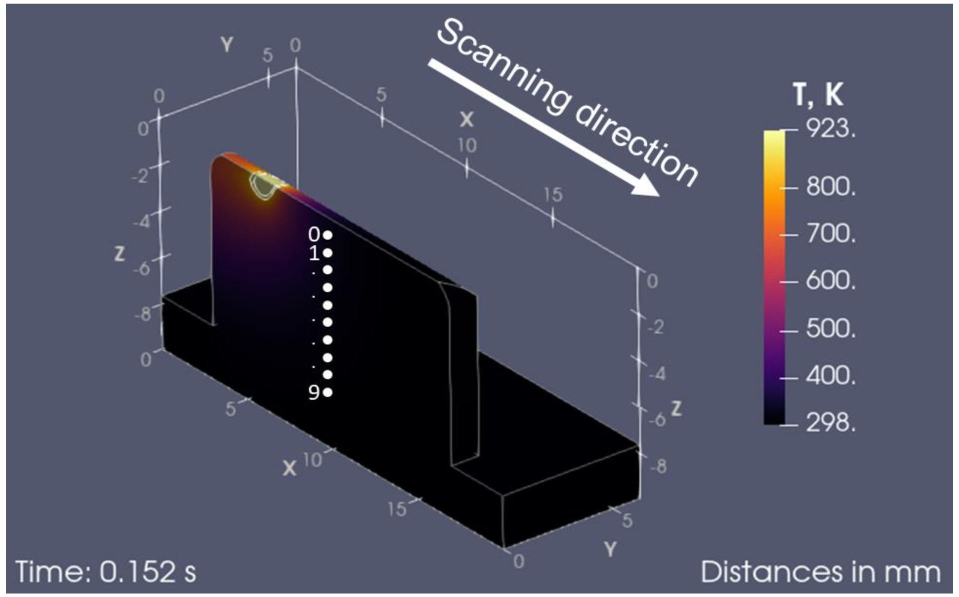
Coupled Thermodynamic & process modeling for AM of aluminum alloys onto dissimilar cast or stamped parts

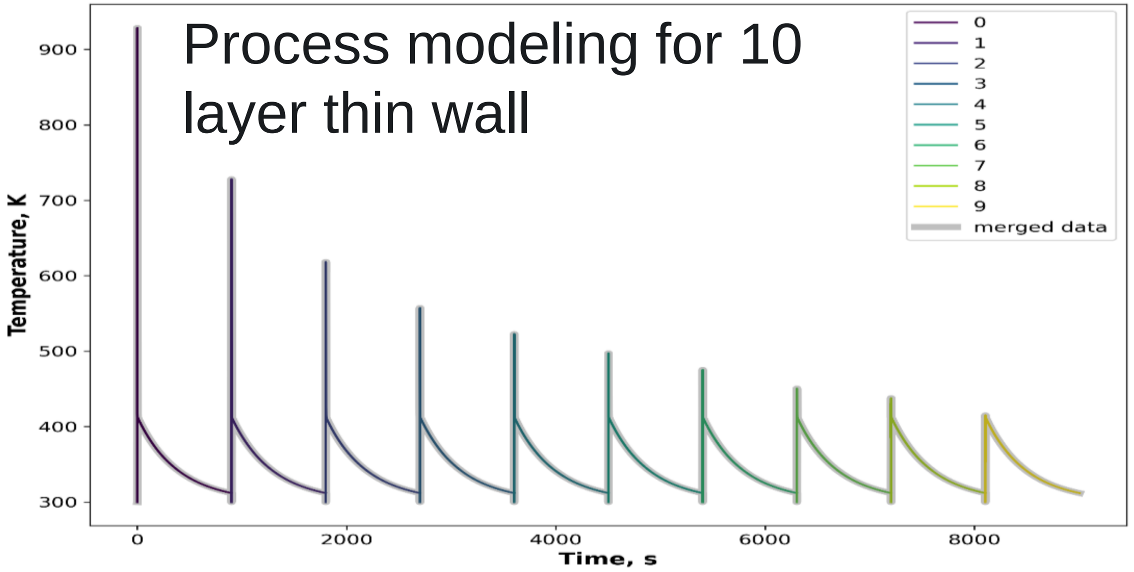
1B/2C

Alex Plotkowski (PI)
Ying Yang
Gerry Knapp
Benjamin Stump

- Processing models developed to simulate thermal history at different thickness of the as-build materials, which is to be used as input for microstructural modeling.
- Simulation: A 10-layer thin wall geometry was melted and allowed to cool. Temperature was measured at probes locations and merged for each layer.
- Results: Representative thermal cycles can be predicted for given process conditions.



Isometric view of simulation domain



Temperature in first layer as a function of time and added layers (e.g., point 9)

TECHNICAL ACCOMPLISHMENTS AND PROGRESS

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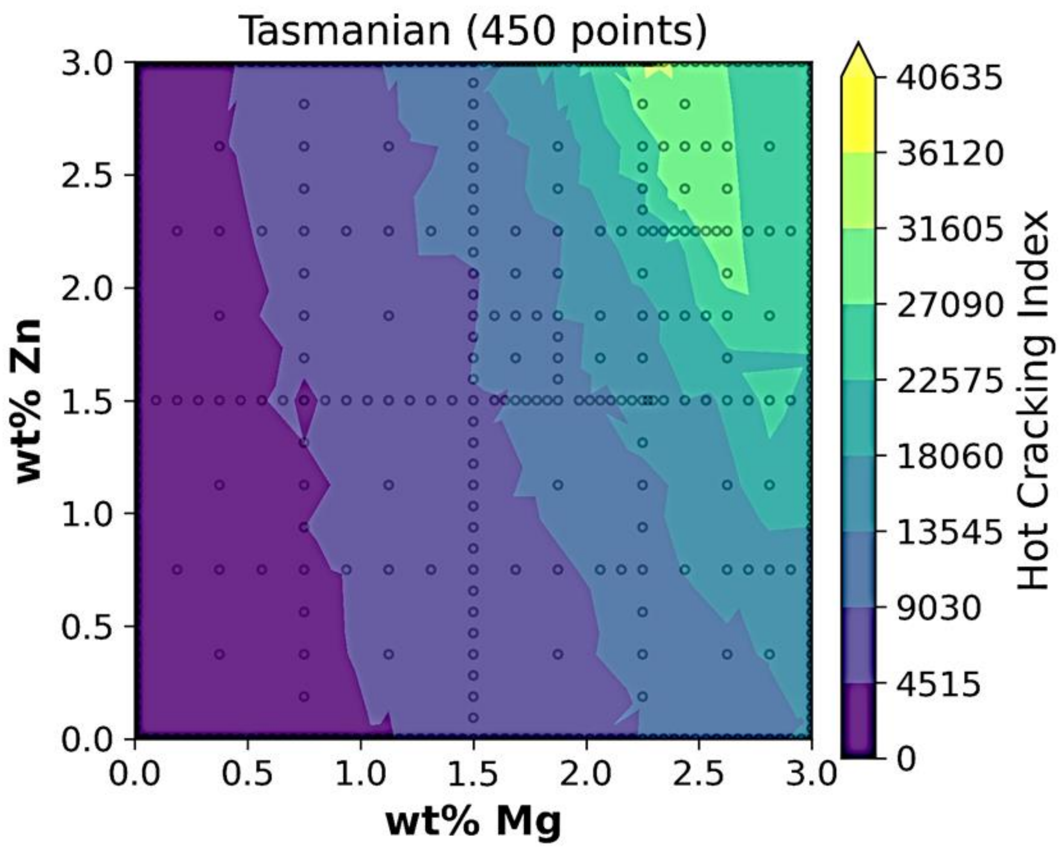
Efficient thermodynamic calculations for multi-component alloy composition space

1B/2C

Alex Plotkowski (PI)
Ying Yang
Gerry Knapp
Benjamin Stump



- **Simulation:** Hot cracking susceptibility across Al-Mg-Zn composition range with both ORNL's Tasmanian adaptive sparse grid mesh.
- **Results:** Adaptive mesh reduces points needed for calculations while preserving accuracy and key features.
- **Planned work:** This scalable calculation method will enable the full utilization of the 8-component aluminum alloy thermodynamic database for material design with Oak Ridge Leadership Computing Facility (OLCF) resources.

- **Ongoing work:** Thermodynamic and kinetic microstructure calculations will use simulated thermal history to predict as-process and heat-treated characteristics for different process parameters.
- The success of this work will help to improve the final properties of the parts by optimizing the processing route and material selection.

TECHNICAL ACCOMPLISHMENTS AND PROGRESS

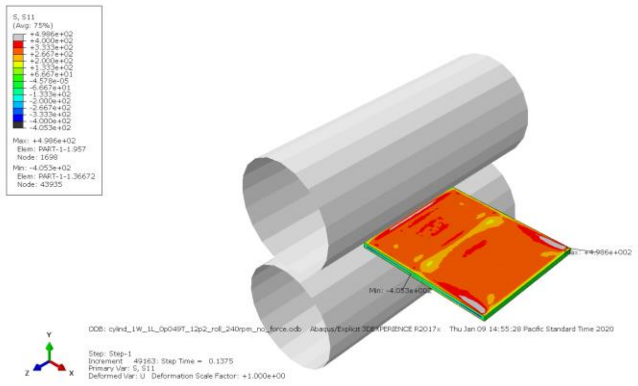
Residual Stress Characterization, Prediction, Optimization

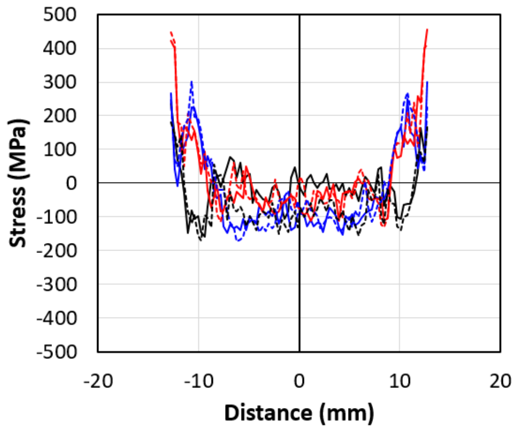
RS

Ayoub Soulami (PI)
Kranti Balusu
Kyoo Sil Choi
Vineet Joshi
Tim Roosendaal
Tingkun Liu
Arun Devaraj

- **Objective:** Investigate residual stresses and provide support to other projects across the various thrusts.
- Develop a combined experimental-computation framework to accurately measure and predict residual stresses resulting from local property enhancement processes.
- Focus on measuring and predicting the residual stresses at the macro-scale.
- Help establish the optimum process parameters to reduce residual stresses and guarantee dimensional stability.
- Assist in developing potential stress relief procedures without altering the strength of the material/part.

Predicted residual stresses during multi-pass rolling





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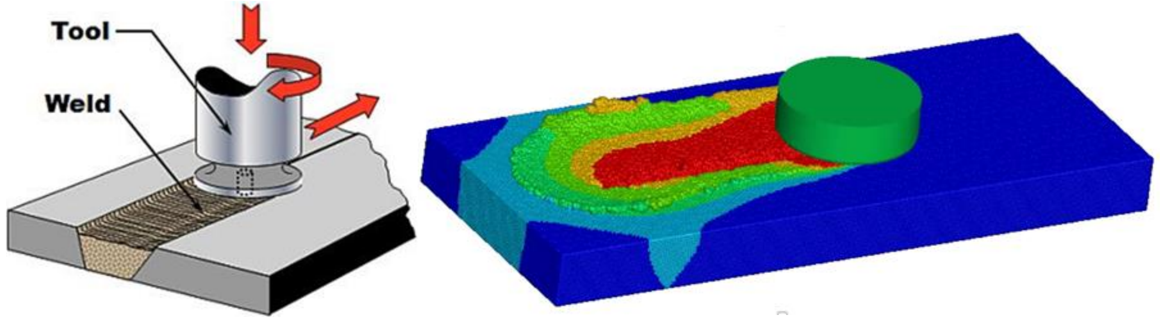
Residual Stress Characterization, Prediction, Optimization and preliminary results

RS

Ayoub Soulami (PI)

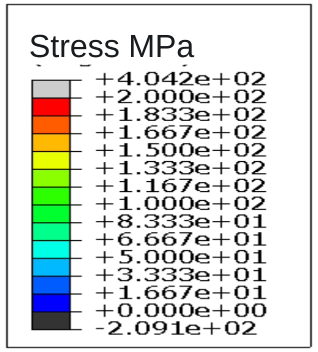
Kranti Balusu
Kyoo Sil Choi
Vineet Joshi
Tim Roosendaal
Tingkun Liu
Arun Devaraj

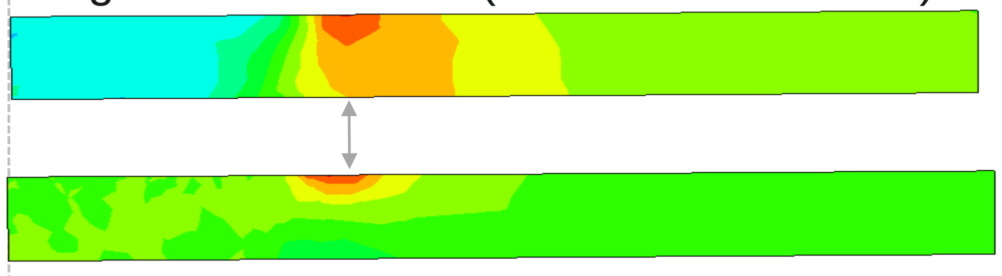
(1) Friction Stir Processing (FSP) of Al sheets and Al/Mg Castings



Temperature and material flow during FSP using smooth particle hydrodynamics (SPH) model

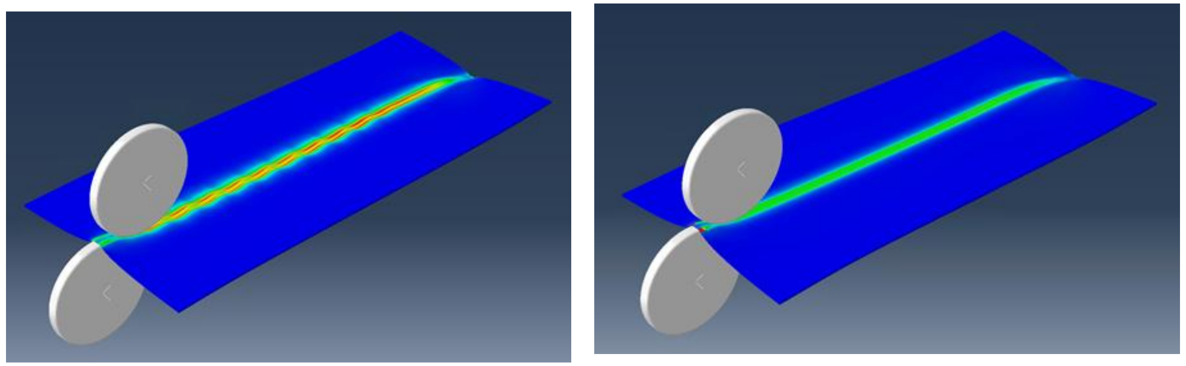
Longitudinal Stresses (in the weld direction)





Transverse Stresses (Normal to the weld line)
Weld center plane

(2) Bending-unbending of Al sheets



Eq. Plastic Strain during Bending-unbending

- Residual stress measurements being conducted both at the macro scale (Hole drilling + Digital Image Correlation (DIC), neutron diffraction) and micro scale

- Models are being developed to predict residual stresses resulting from these 2 processes
  - Finite element analysis (FEA) models for bending-unbending, Thermal Pseudo Mechanical model and Smoothed Particles Hydrodynamics model for FSP of Al sheets and Al/Mg castings

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Material lifecycle

ML
Jeff Spangenberger (PI)
Jessica Durham

Objective:

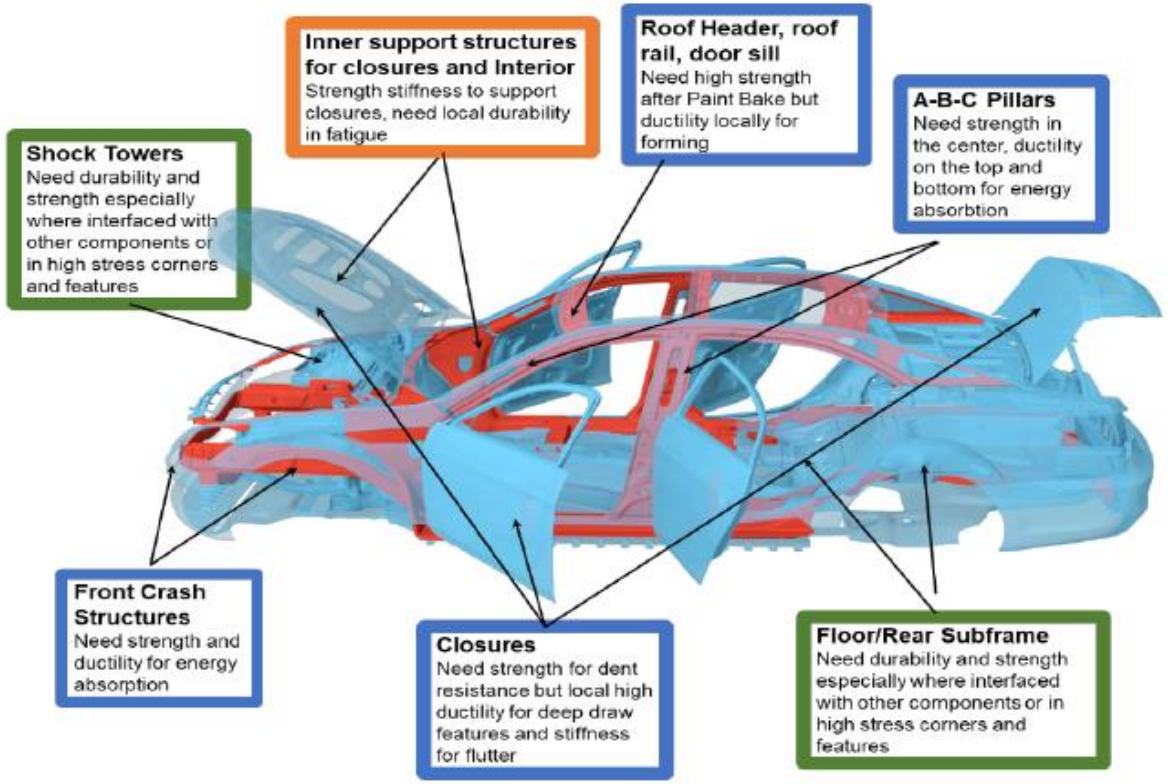
- Evaluate the benefits provided by the lightweight materials core (LMCP) program to the auto shredder and non-ferrous recycling industry
  - Simplification of materials separation due to a reduction in alloys used in vehicles
  - Increased adoption of these materials increase value to the recycler and increase recycling rates

Approach:

- Maintain close communication with domestic auto shredder and non-ferrous processing industries to ensure the maximum benefit from LMCP program derived products
- Use knowledge and tools of the industry to evaluate the potential for usage of more recycled Al/Mg alloys by adopting the processes developed in LMCP

Responses to Previous Years Review Comments

- This project was not reviewed previously



Remaining Challenges and Barriers

- Prioritization plan for experimental and computational resources across all three national labs

Collaboration and Coordination with Other Institutions

- Strong cross-national lab staff expertise and capabilities in advanced characterization, computation, testing, residual stress studies and material life cycle being leveraged through support thrust in LMCP.
- A framework for collaboration between PNNL, ORNL and ANL through thrust 4 has been developed through call for proposals.

Proposed Future Research

Advanced characterization & Computation

- 2nd call for advanced characterization and computation coming up in June for inter-national laboratory collaboration to fully leverage the strength of thrust 4 team
- Supporting thrust 1-3 for understanding how to best characterize, test and predictively model these intentionally heterogeneous materials produced by LMCP

Residual Stress

- Establishment of methods to characterize, predict and optimize micro and macro residual stress in Al and Mg alloys after local processing methods developed in LMCP **(PNNL)**

Material Lifecycle

- Establishing close collaboration with auto shredder industries to quantify the benefits of intentionally heterogenous materials produced in LMCP for recycling of Al and Mg alloys **(ANL)**

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

Summary: Meeting the nations need for scalable manufacturing of next generation light weight materials by close collaboration of three national labs

- **Thrust 4:** Accelerate research and development of intentionally heterogenous light weight materials by leveraging advanced characterization, testing, computational modeling and recycling research expertise and state-of-the-art capabilities across three national labs.
- A convergence of 38+ scientists and world class microscopy capabilities, computational tools and material life cycle research