Phase-Field Modeling of Corrosion for Design of Next-Generation Magnesium-Aluminum Vehicle Joints

Presenter:
Adam Powell
Worcester Polytechnic Institute (WPI)

Project ID: mat151

Overview

WPI

Timeline

Start Date: October, 2018

End Date: July, 2022

Budget

Total Project Funding: $ 1,899,462
- DOE: $ 1,499,612
- Participants: $ 399,850 (21%)

Actual Costs Incurred: $ 1,370,943
- DOE: $ 1,068,359
- Participants: $ 302,584 (22%)

As of March 31, 2021

Status: 65% of time, 71% of DOE budget

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

Barriers & Technical Targets

- Barrier: limited understanding of multi-material joint corrosion & fracture – Mg-Al, friction stir welds (FSW)
- Target: validated model of microgalvanic corrosion and mechanical failure based on joint microstructure

Accomplishments

- Model of pitting corrosion and galvanic oxidation
- Verified model of Mg-steel FSW joint lap shear failure
- Developed model of Al-Mg FSW joint lap shear
- Characterized Mg-Al FSW joint using many tools

Technology Partners

Worcester Polytechnic University (WPI)

Pacific Northwest Laboratory (PNNL)

Oak Ridge National Laboratory (ORNL)

Magna International, Inc. (Magna)

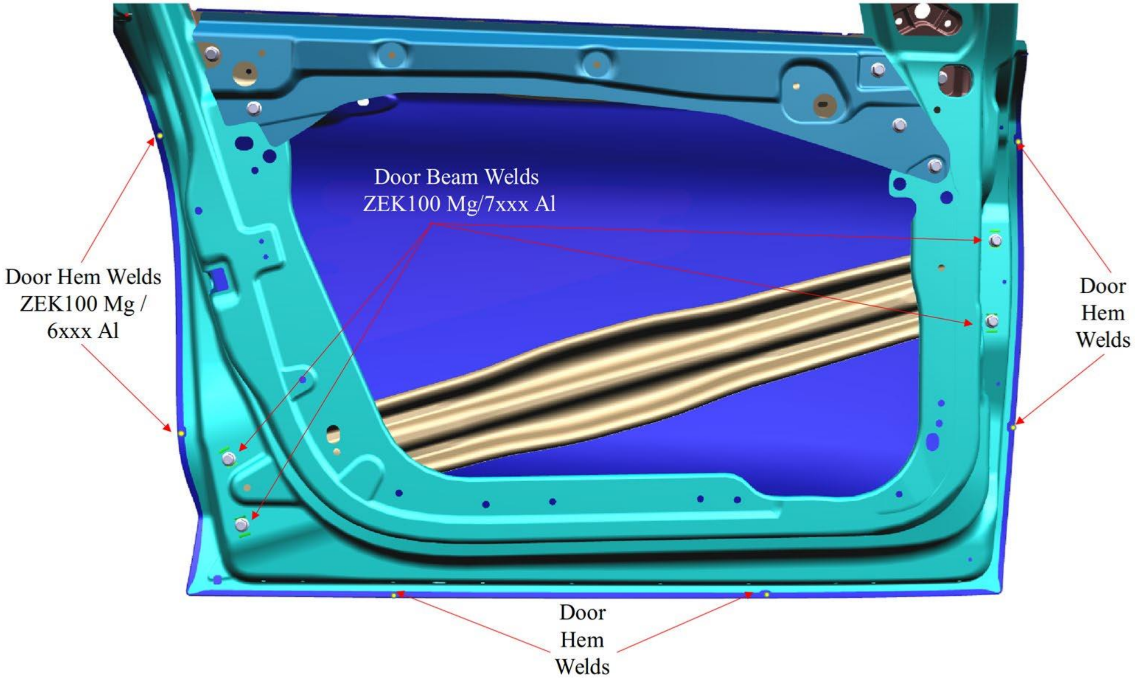
Relevance and Project Objectives

Relevance DOE Vehicle Technologies Office Mat'ls Team Roadmap Multi-Material Systems Enablers: high-volume joining, corrosion, predictive modeling

Objective Develop and validate phase field corrosion model and coupled mechanical failure model in magnesium-aluminum alloy joints

End-of-Project Goal Predict tensile & fatigue strength of corroded joints within 10% of measured values

Challenge problem FCA-Magna ultralight door



Magna – Joint application requirements, materials

PNNL – Friction stir welding, diffusion bonds (Task 1); modeling consulting (Task 4)

ORNL – Advanced characterization (Task 3)

WPI – Corrosion and mechanics testing (Task 2), corrosion and mechanics modeling (Task 4)

Deliverables:
7/2020 Validated 2D galvanic corrosion model
7/2021 Validated model of coupled corrosion and mechanical failure
7/2022 Accurate model of corroded joint tensile & fatigue strength

Project Approach and Milestones

Time	Goal	Bond (PNNL)	Tests (WPI)	ORNL	Model (WPI)
BP 1: 10/2018-7/2020	Initial phase field corrosion model: diffusion bond	Diffusion-bond Al-Mg sheet, 6022-ZEK100	Galvanic corrosion - ASTM G71	SEM-EDS, EBSD, FIB, STEM	2-D diffusion bond & galvanic corrosion models
	Go/No Go	**Predict corrosion pit depth within ±2x**			
BP 2: 8/2020 - 7/2021	Refine corrosion & initial strength model	FSW 6022-ZEK100 sheet	Cyclic Corrosion Testing (CCT), tensile strength	SEM, STEM, FIB, neutron scattering	3-D corrosion & tensile failure models
	Go/No Go	**Predict corroded joint strength within ±2x**			
BP 3: 8/2021 - 7/2022	Refine tensile and fatigue strength models	FSW 6022-ZEK100 sheet	Cyclic Corrosion Testing (CCT), tensile strength	SEM, STEM, neutron scattering	3-D corrosion & tensile and fatigue models
	Go/No Go	**Corroded joint tensile & fatigue strength ±10%**			

S(T)EM: Scanning (Transmission) Electron Microscopy
EDS: Energy-Dispersive X-Ray Spectroscopy
EBSD: Electron Backscatter Diffraction
FIB: Focused Ion Beam (milling)

Project Accomplishments & Progress

Phase field corrosion model results are similar to experiments

- 4-component Cahn-Hilliard electrochemistry formulation
- Modeled pitting rate is faster than observed
- Galvanic oxidation model qualitatively agrees with experiments

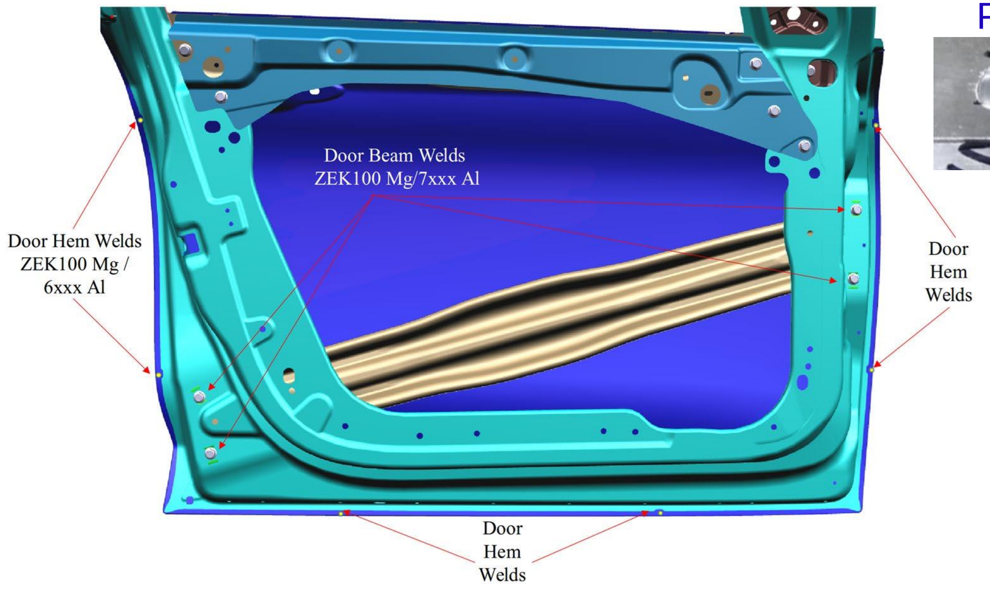
Model of Mg-Al FSW joint failure requires better fracture data

- Verified model using published Mg-steel FSW joint strength data
- Model of Al-Mg FSW joint shows higher strength than observed
- Nanohardness maps and 3-D characterization indicate bands of grain refinement and intermetallic compound formation
- Model refinement is ongoing to include these effects

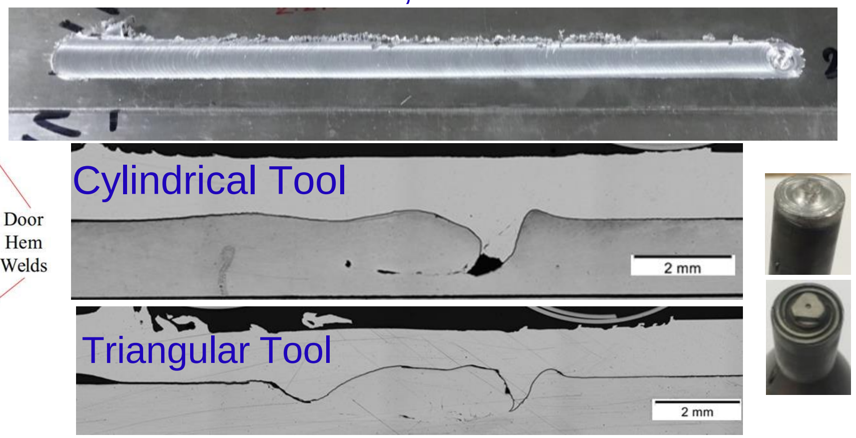
Friction Stir Welding

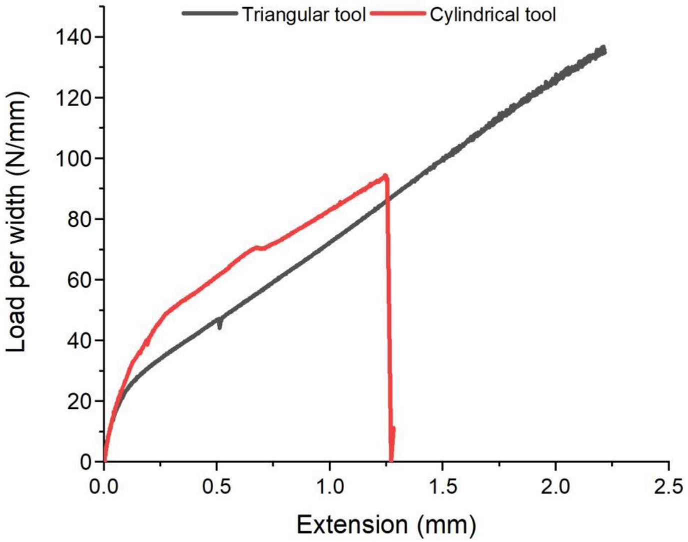
Pacific Northwest NATIONAL LABORATORY

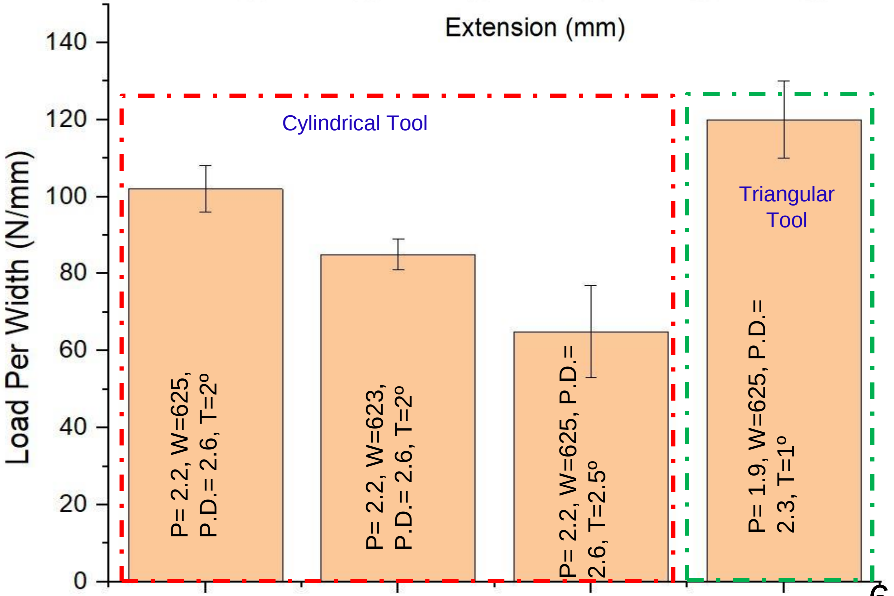
Need to weld through hard 6022 Al into soft ZEK100 Mg – most FSW lap joints go through soft into hard



Power Control Welds, no surface defects







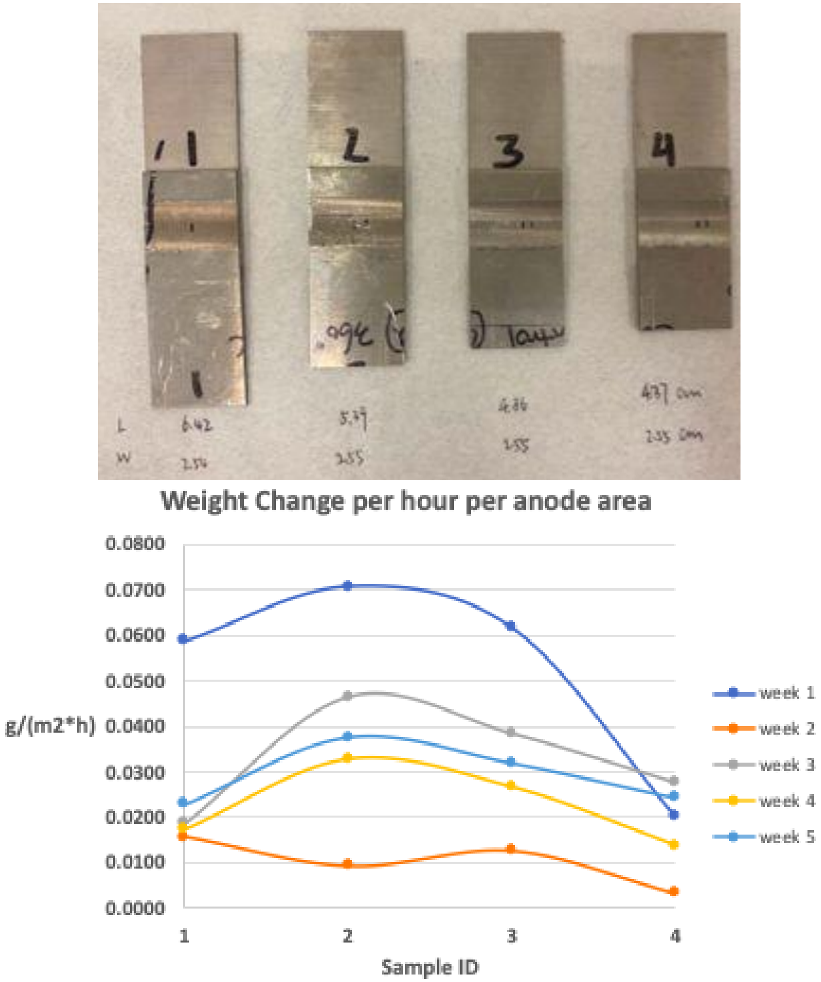
PNNL team developed FSW tool, control strategy, and parameter set for Mg-Al towards greater strength and repeatability:

- Triangular tool instead of cylindrical or others
- Power control instead of RPM, Temperature, etc.

Result: 120 N/mm strength = 80 MPa in ZEK100 cf. 140 MPa yield stress

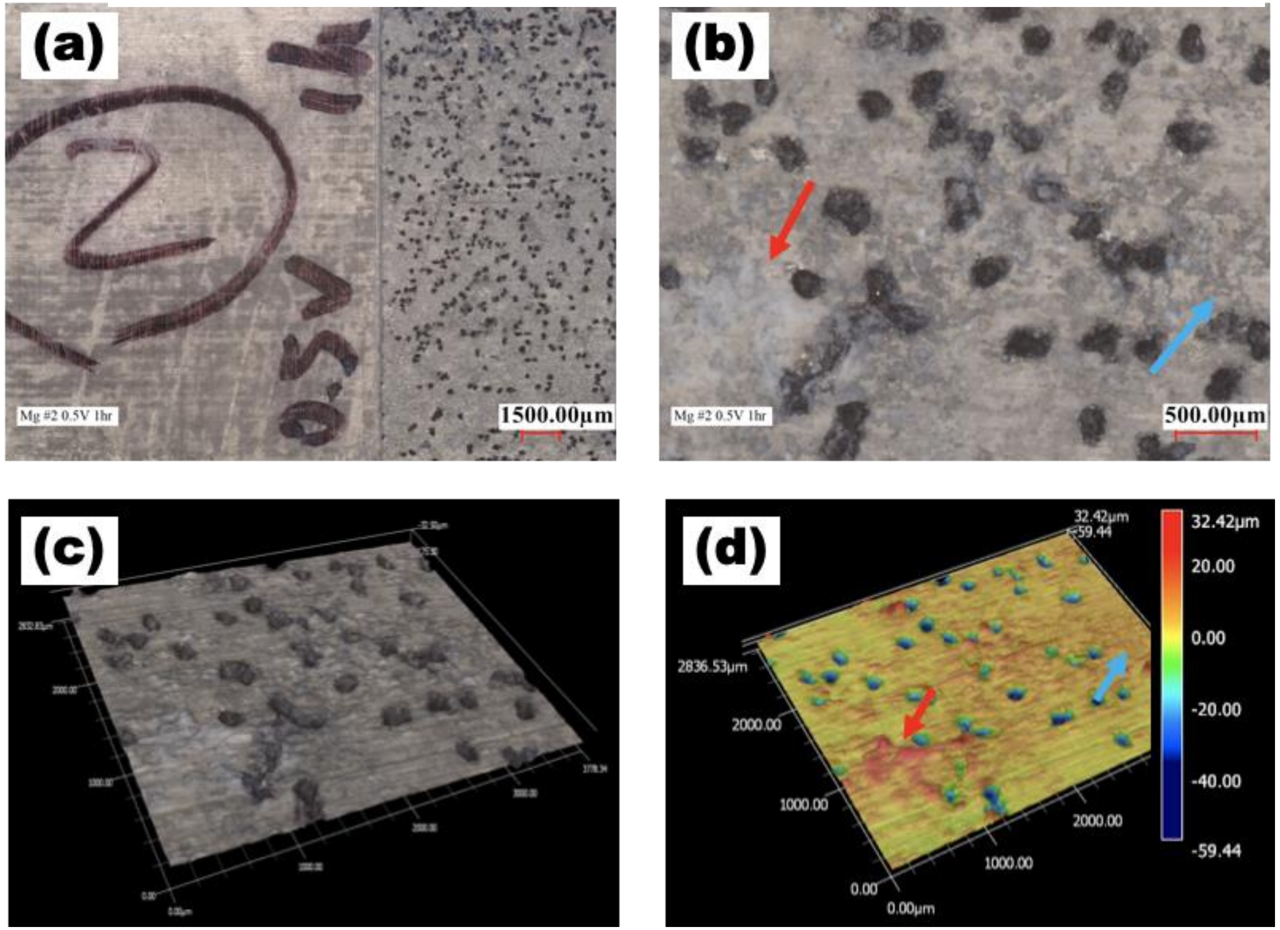
Corrosion Experiments

SAE J2334 Cyclic Corrosion Testing



Corrosion rate dependence on Al:Mg surface area ratio shows cathode-limited behavior in line with expectations

ASTM G71 Galvanic Corrosion Testing



(Surface characterization by ORNL)

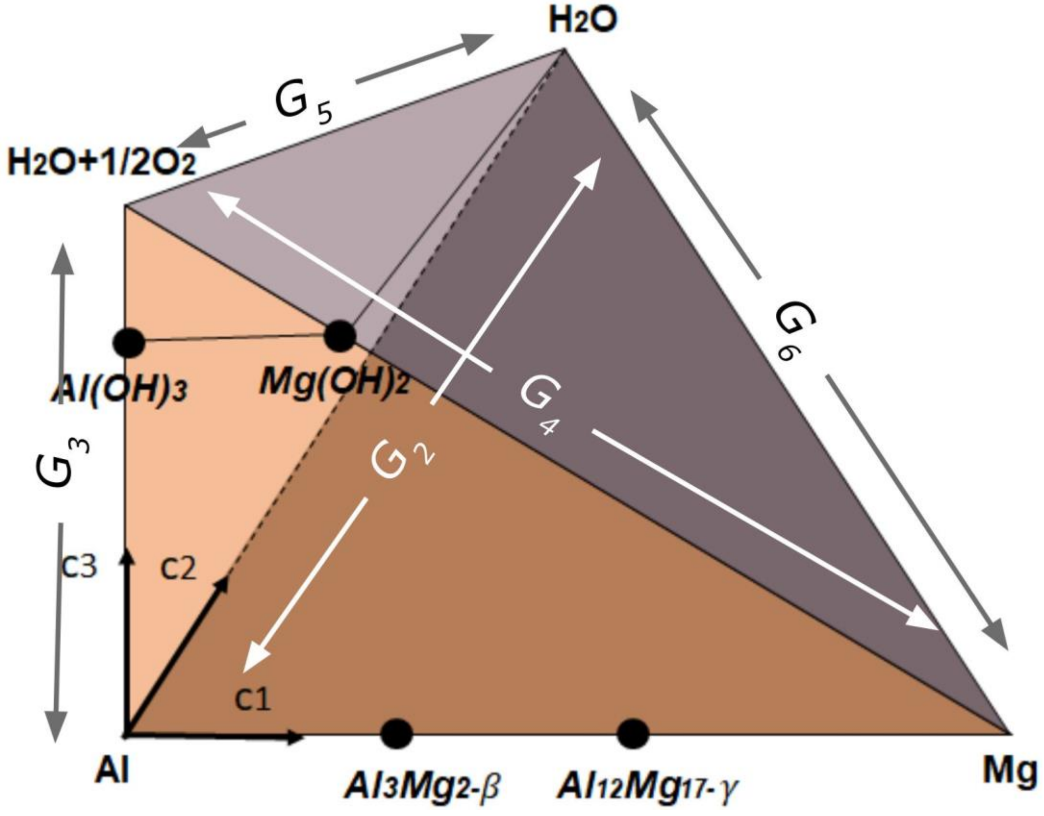
Galvanic corrosion tests → Mg pitting

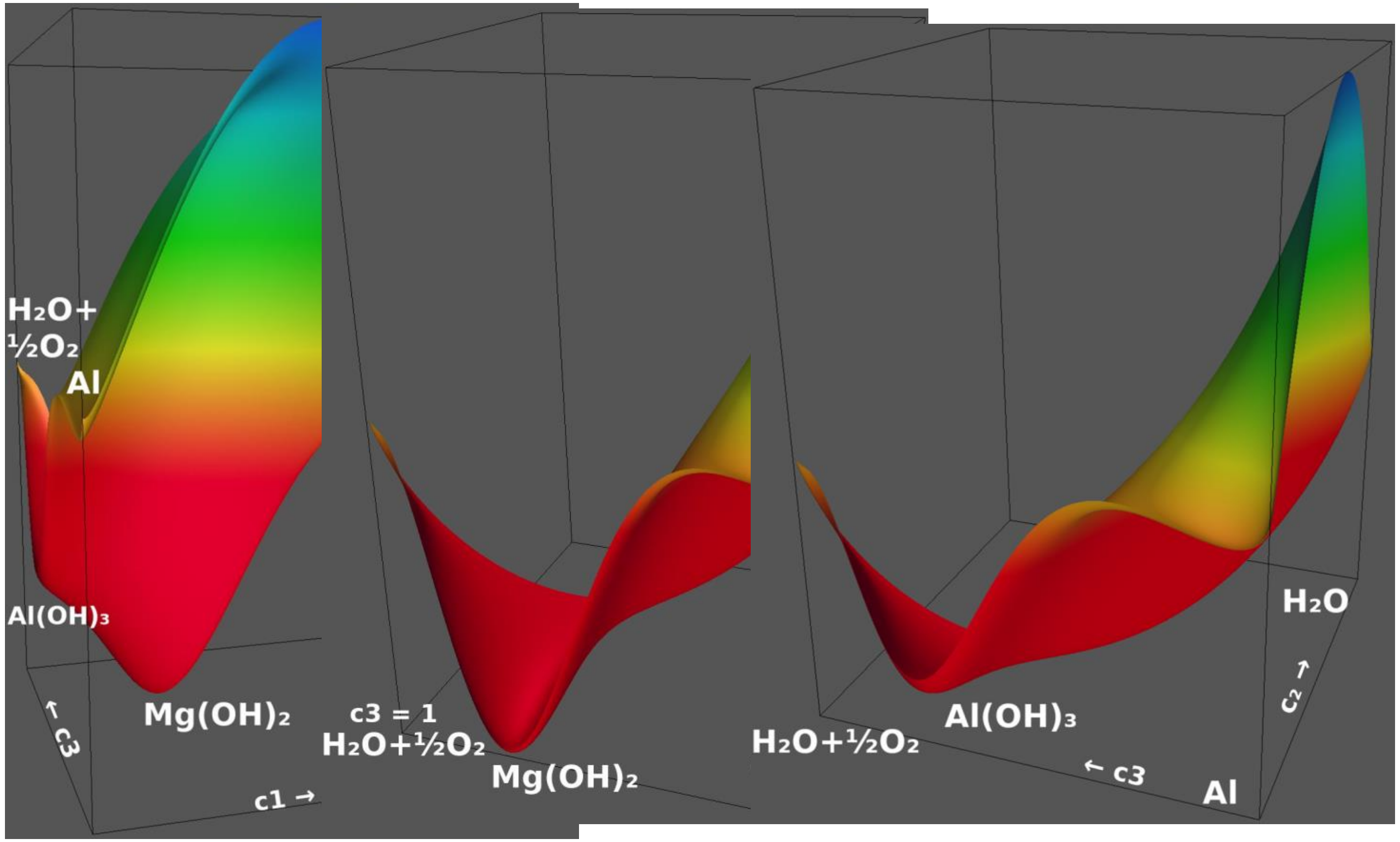
Literature: Mg anodic polarization → pitting

1 hr pit diameters 200-300 µm, depths 30-65 µm

Corrosion Model Formulation

Phase field model begins with Al-Mg-H-O quaternary subsystem free energy



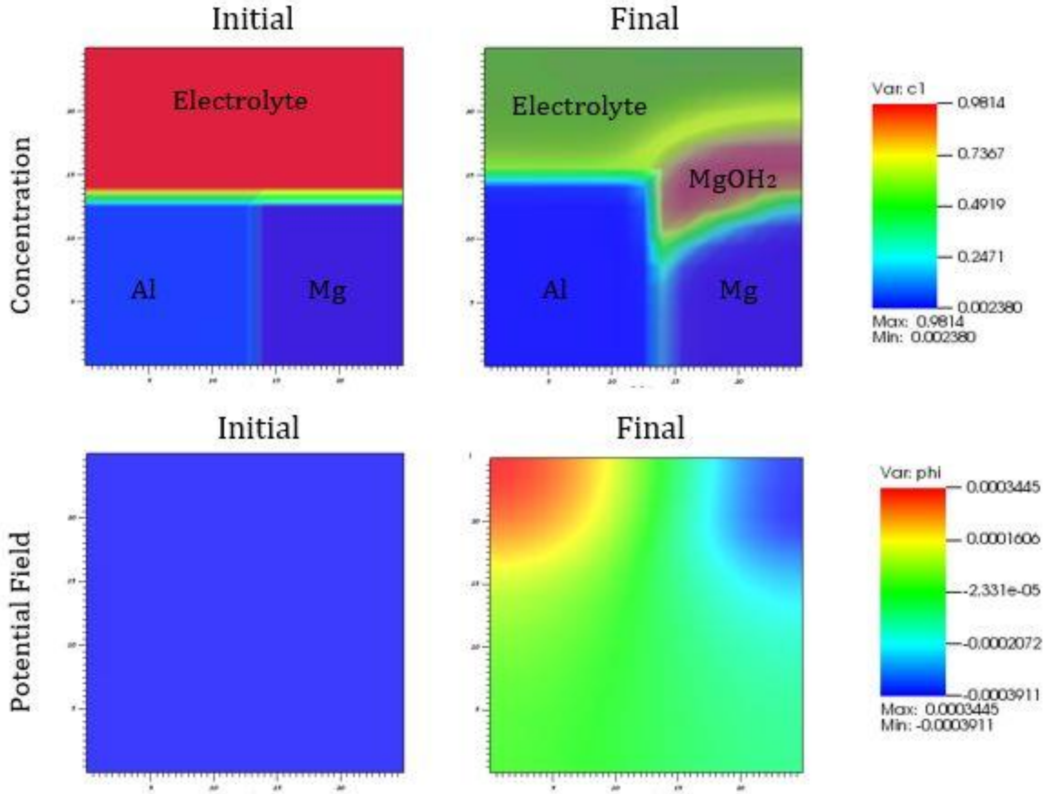


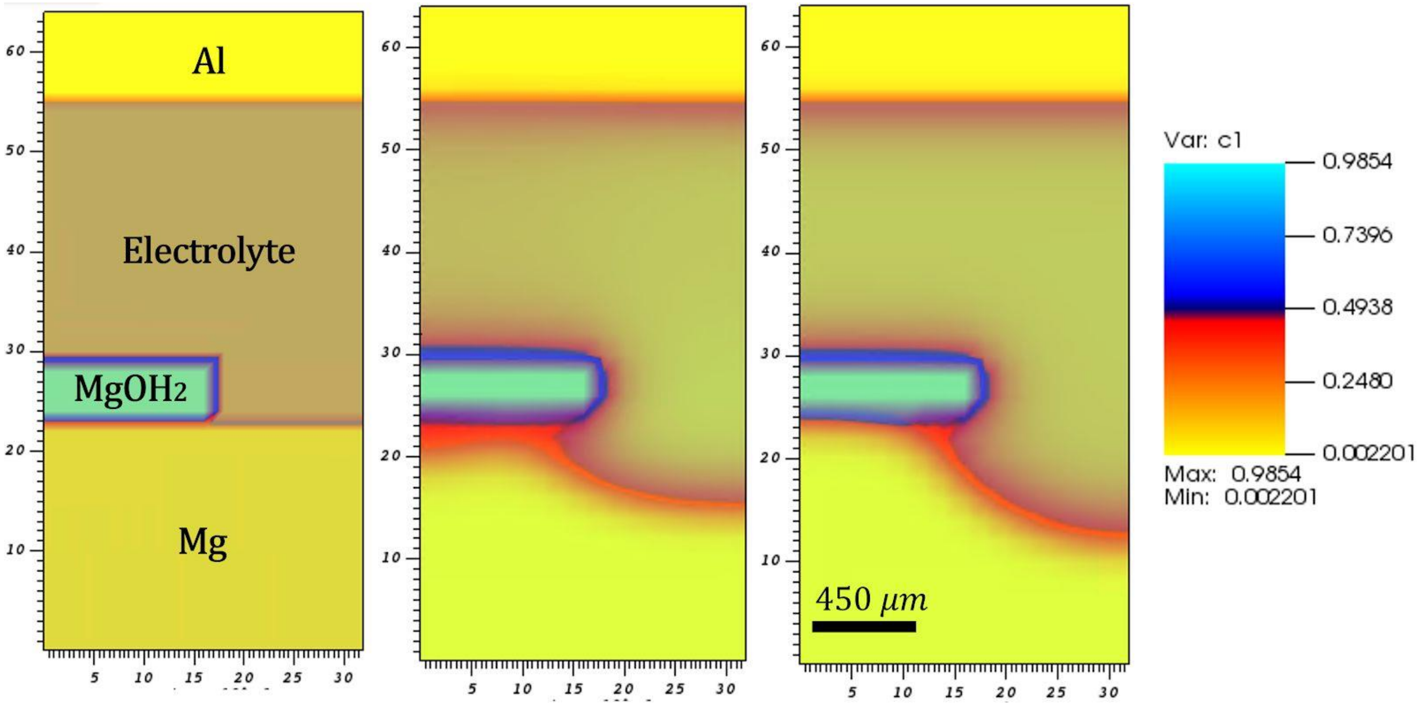
Need 4-component system for hydroxides interaction and water oxidation cathode reactions:

$Mg + Al(OH)_3 \rightarrow Mg(OH)_2 + Al$ $\frac{1}{2} O_2 + H_2O + 2\, e^- \rightarrow 2\, OH^-$

Corrosion Model Results

Prediction of magnesium galvanic oxidation and pitting reaction





Both driven by galvanic potential difference

Oxidation: $Mg + H_2O + ½\ O_2 \rightarrow Mg(OH)_2$

Pitting: $Mg + H_2O + ½\ O_2 \rightarrow Mg^{2+} + 2\ OH^-$

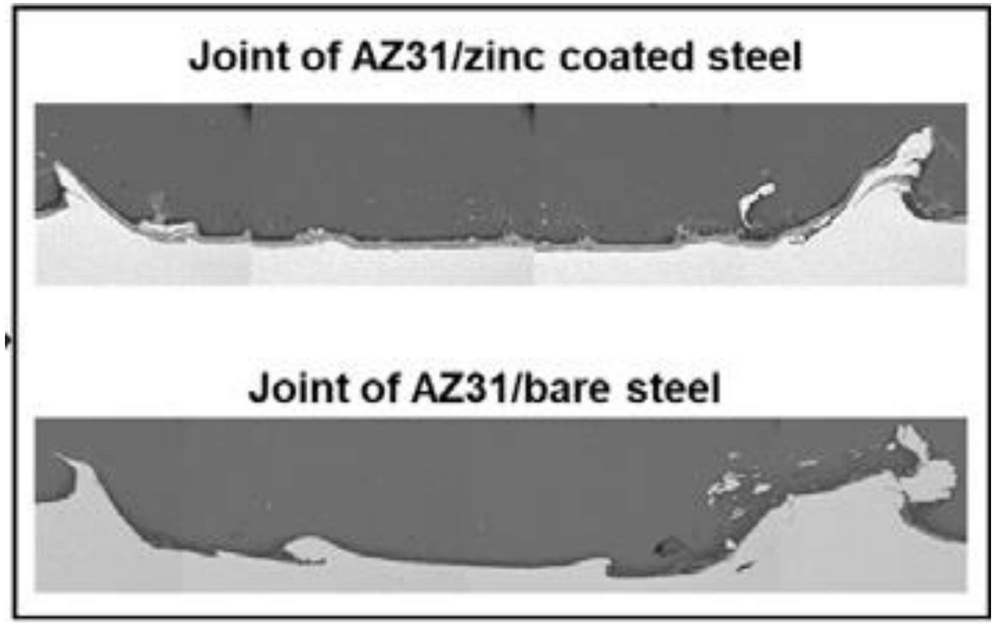
Pitting result 1 hr: 400-500 μm depth

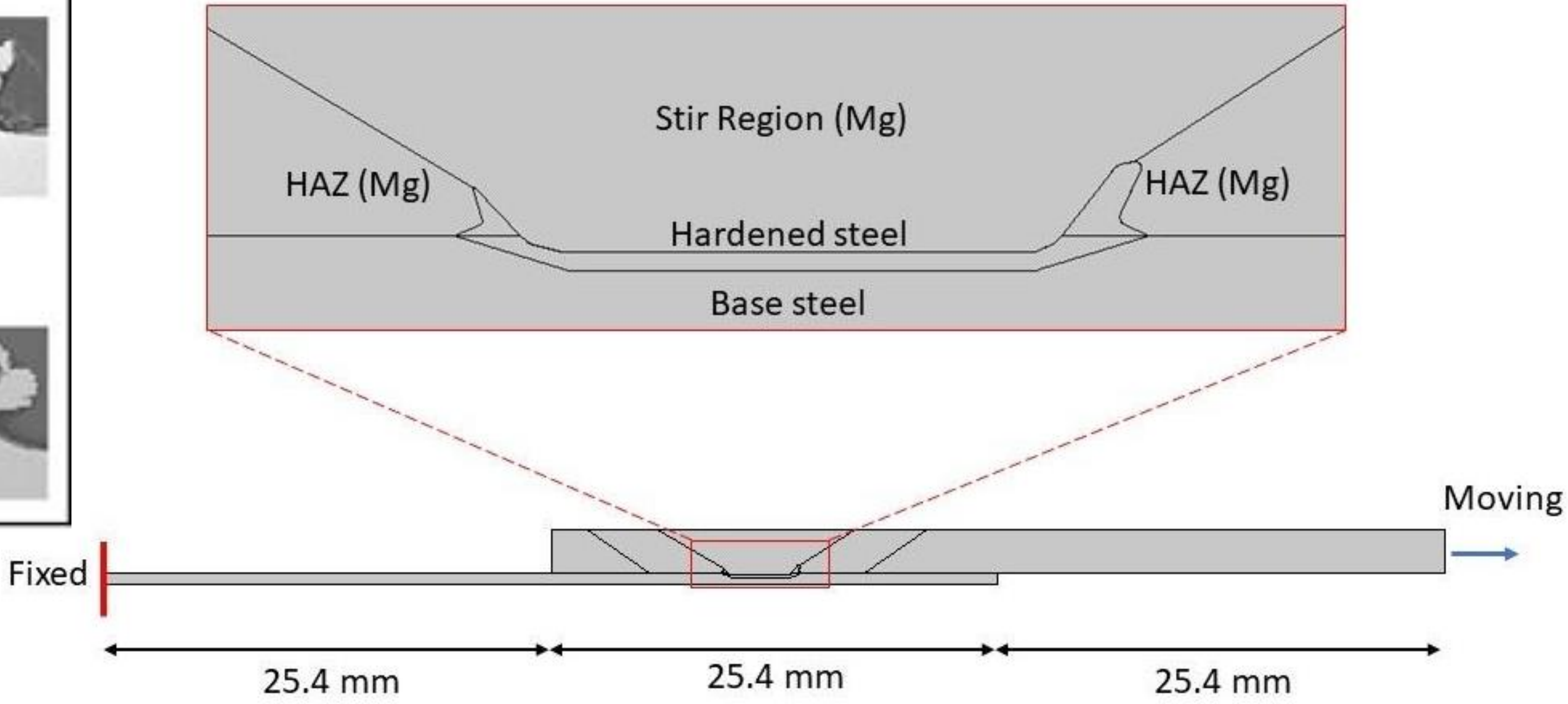
Why so high? 2-D vs. axisymmetric, missing charge transfer resistance

High-performance 3-D model with charge transfer resistance is nearly complete

Mechanical Deformation Model Verification

Literature model of lap shear failure of steel-magnesium sheet FSW



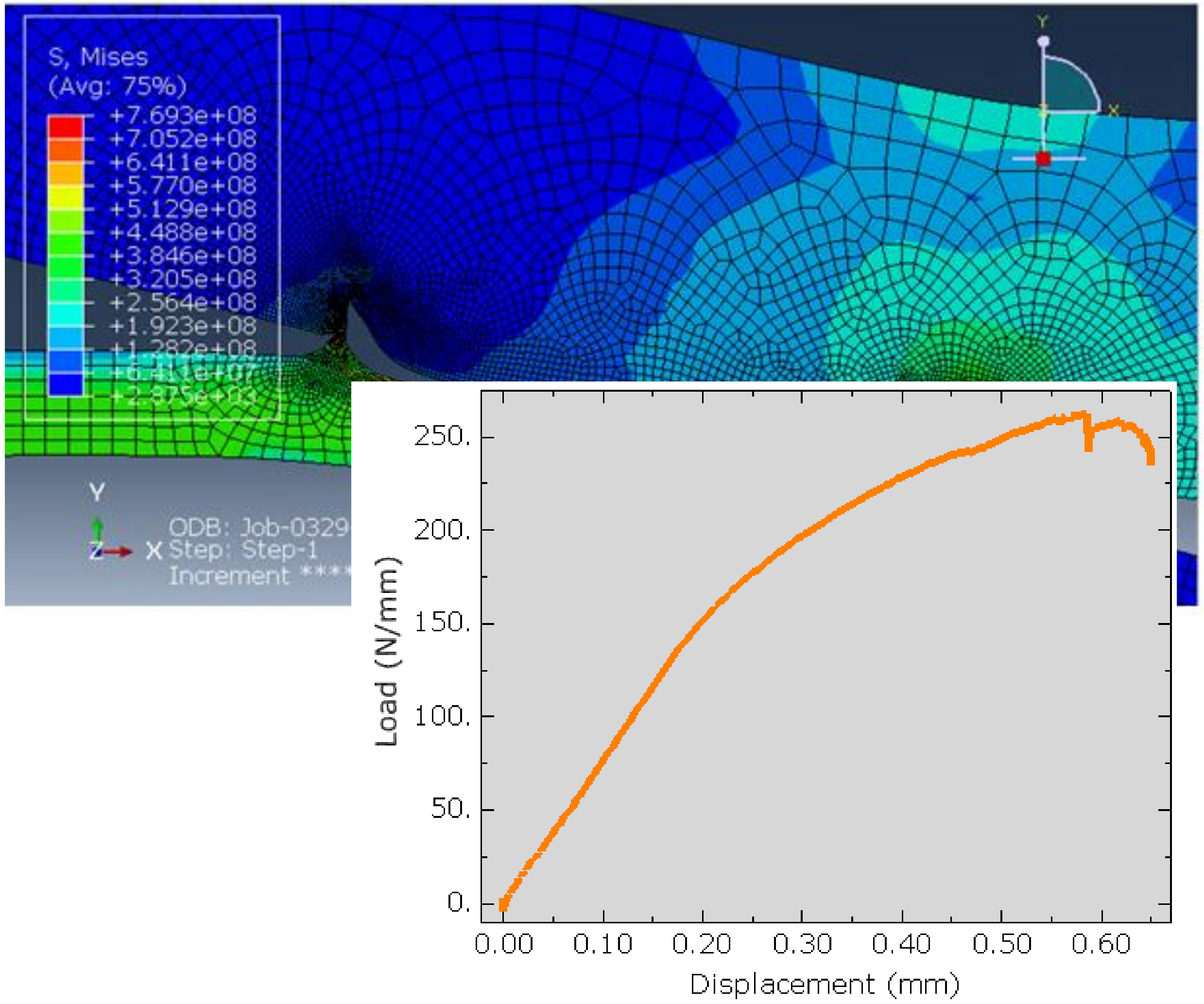


Wang et al., Materials & Design 192 (2020) 108697

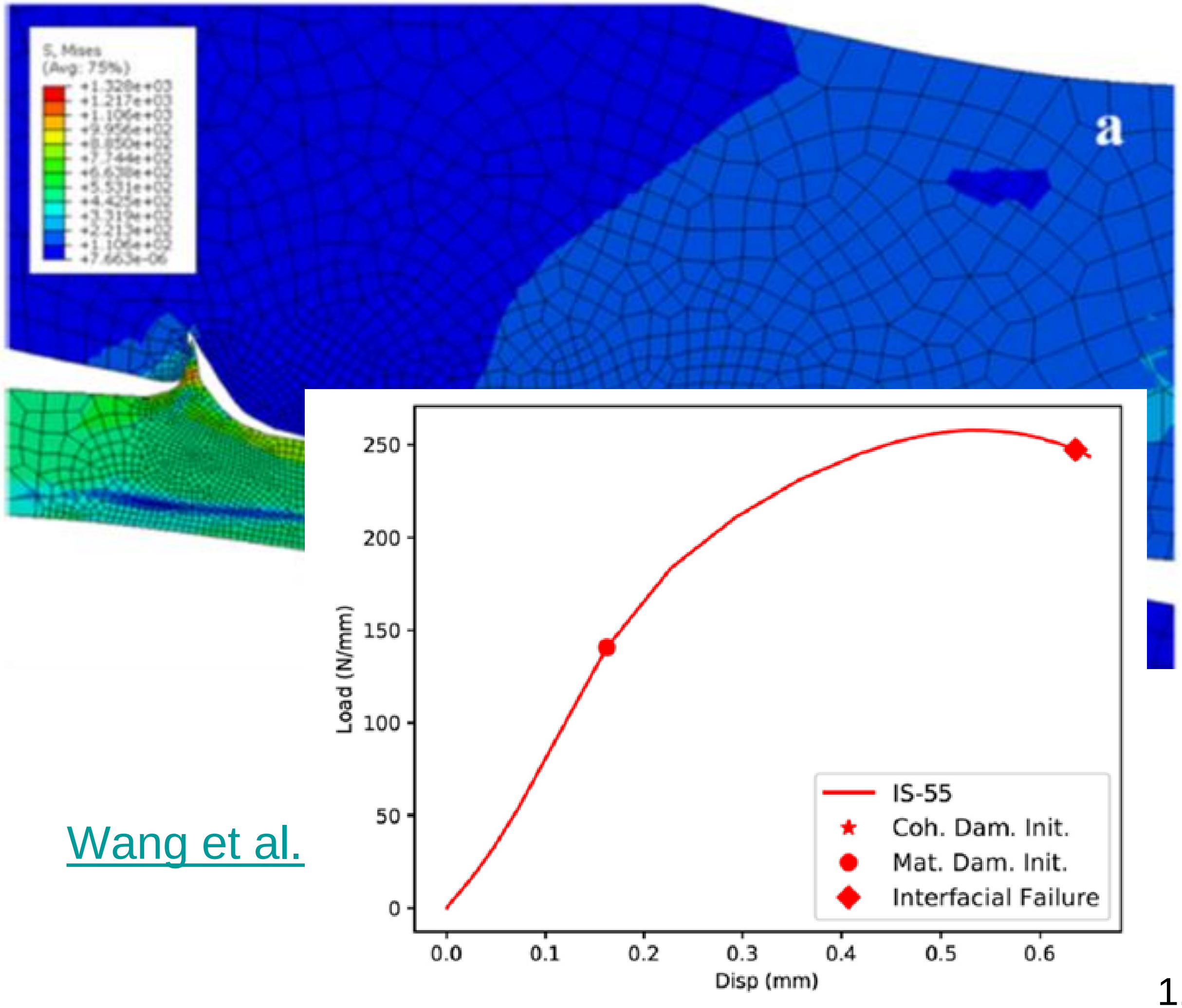
Mechanical Deformation Model Verification

Model of lap shear failure of steel-magnesium sheet FSW

WPI team



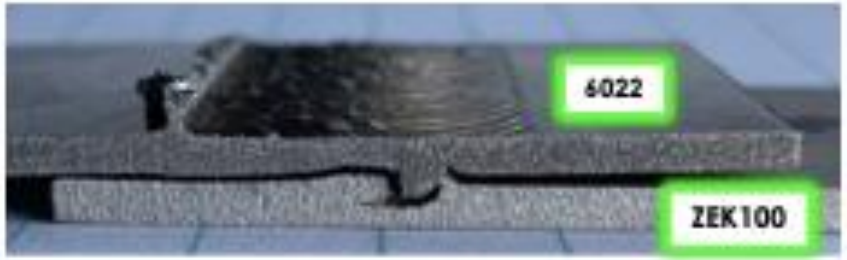
Wang et al. 2020



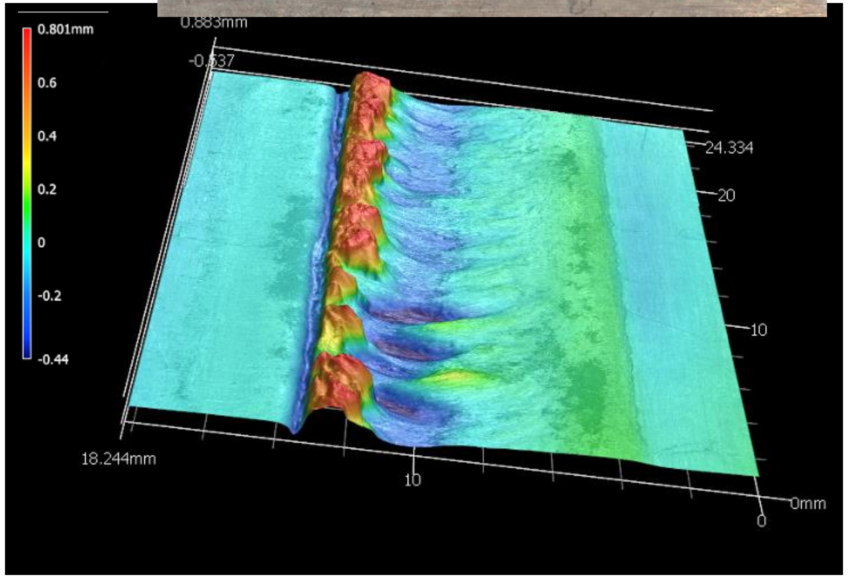
Wang et al.

Al-Mg FSW Joint Geometry

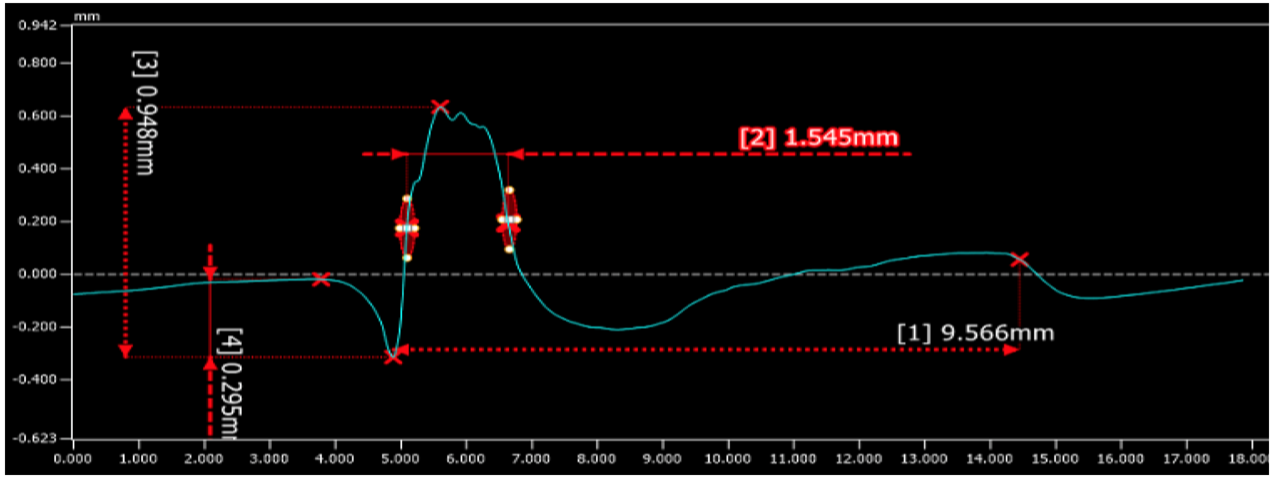
In lap shear, joint fractures roughly on Al-Mg boundary



Al fracture surface,
Scanned topography

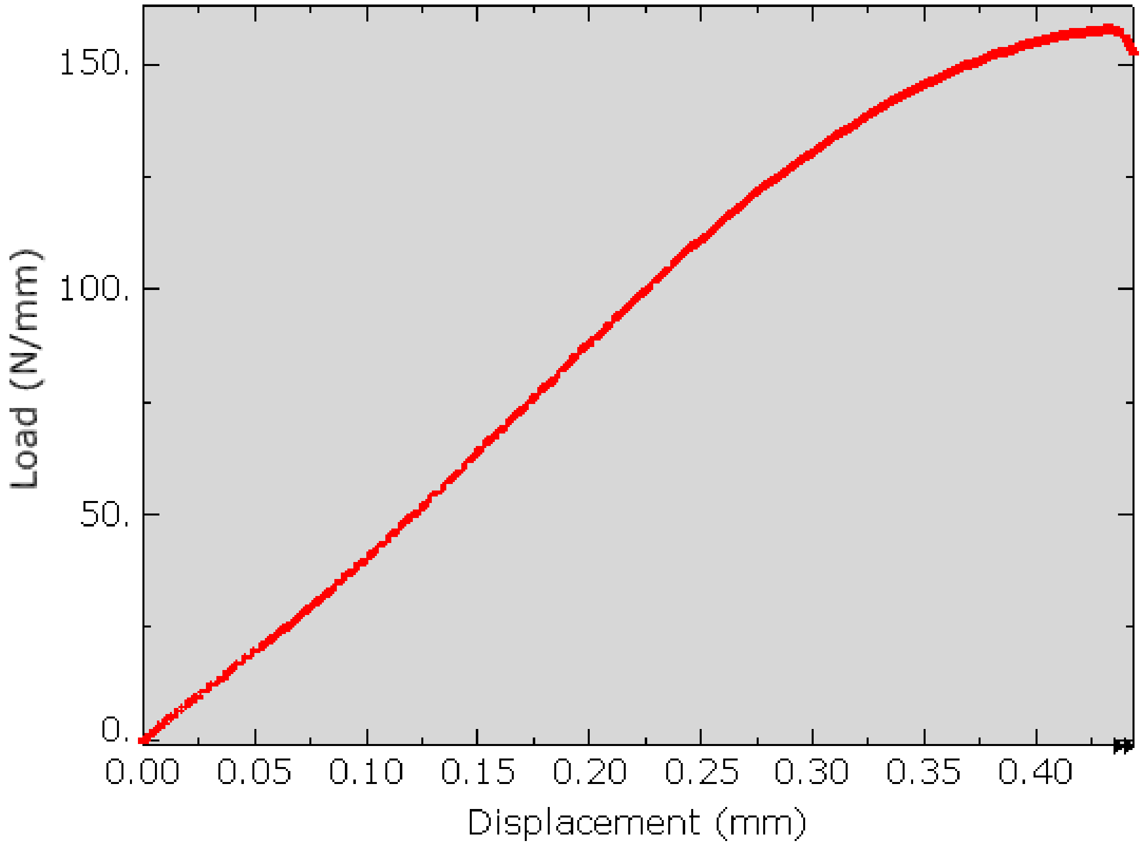


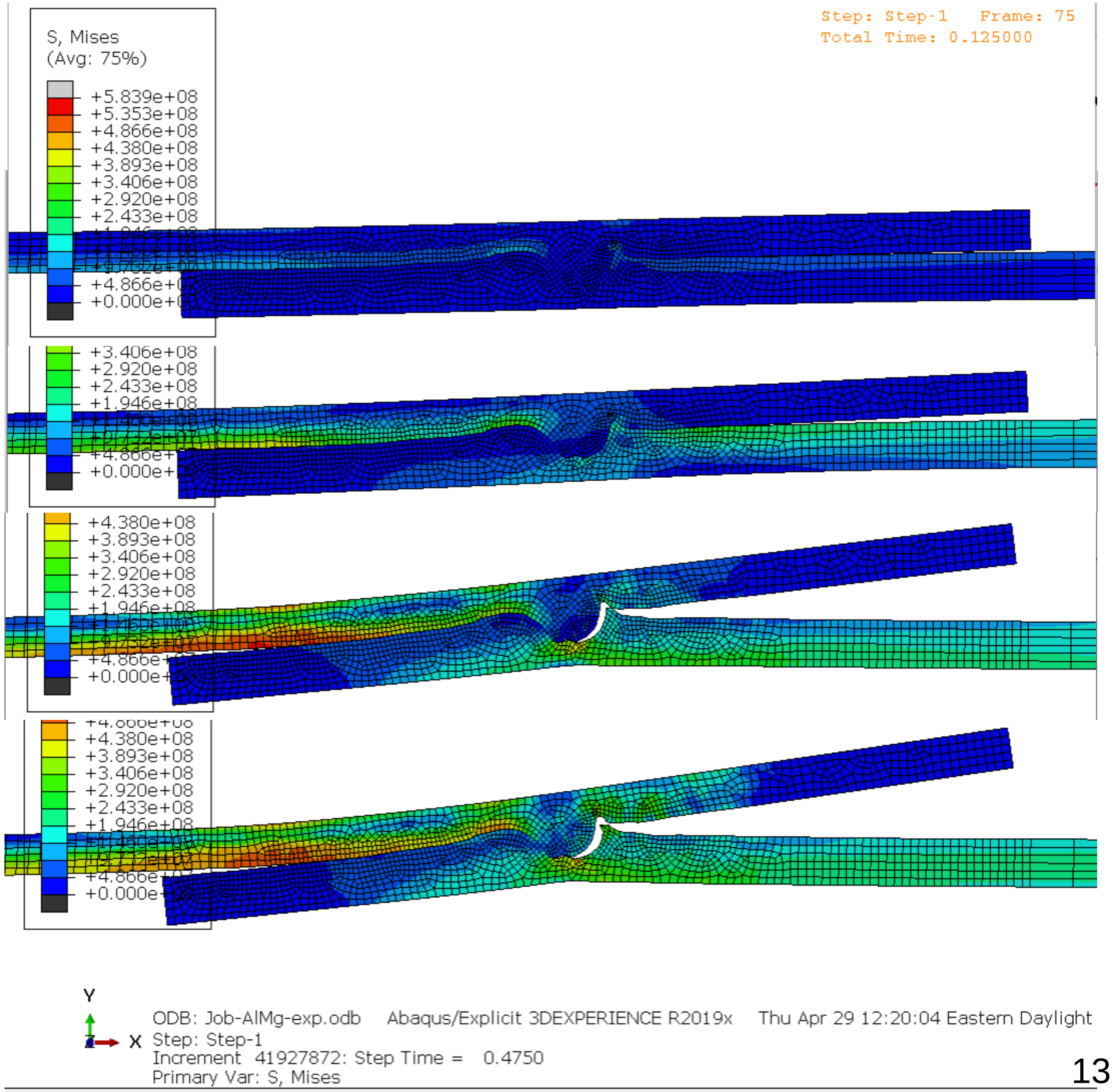
Computed average interface shape



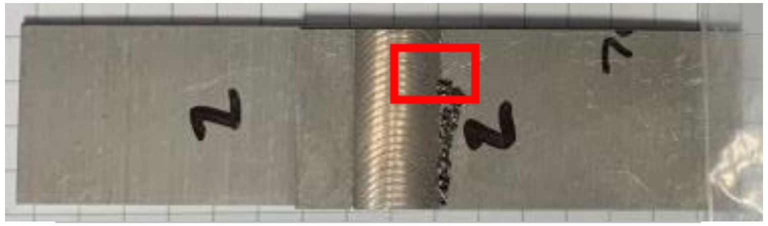
Al-Mg FSW Mechanical Deformation Model

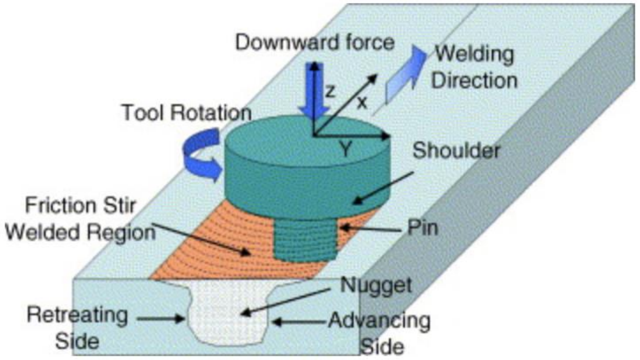
Model predicts joint strength > 150 N/mm
Cf. 110-120 N/mm measured joint strength

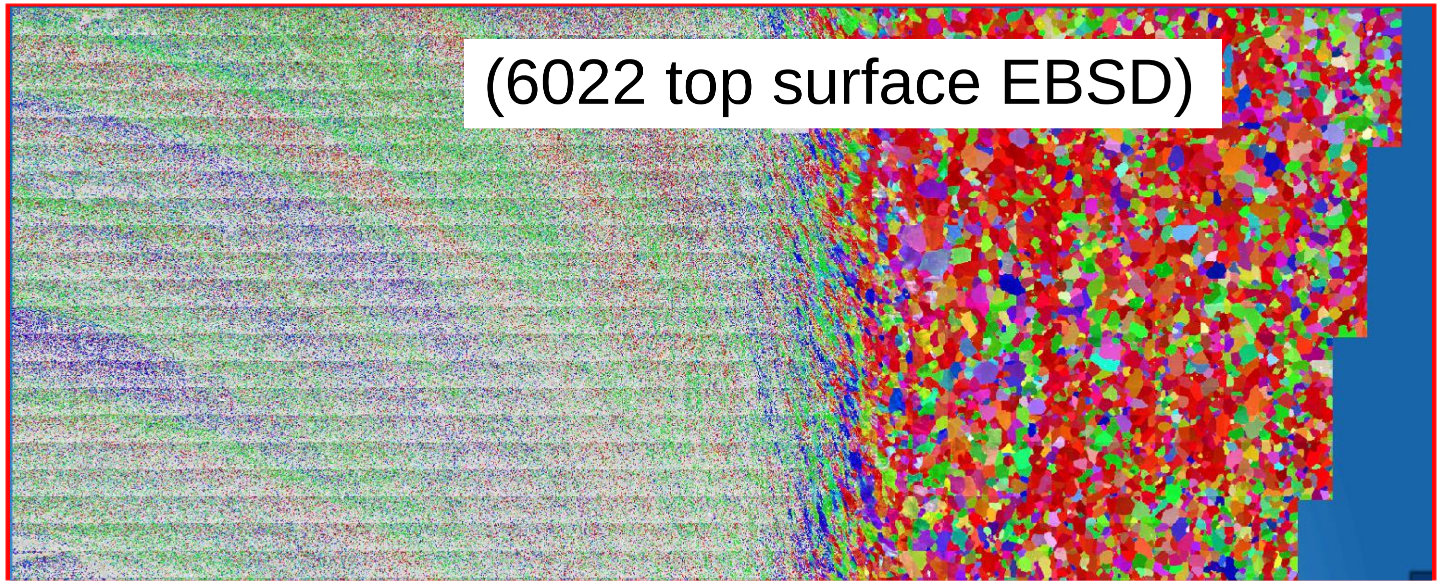


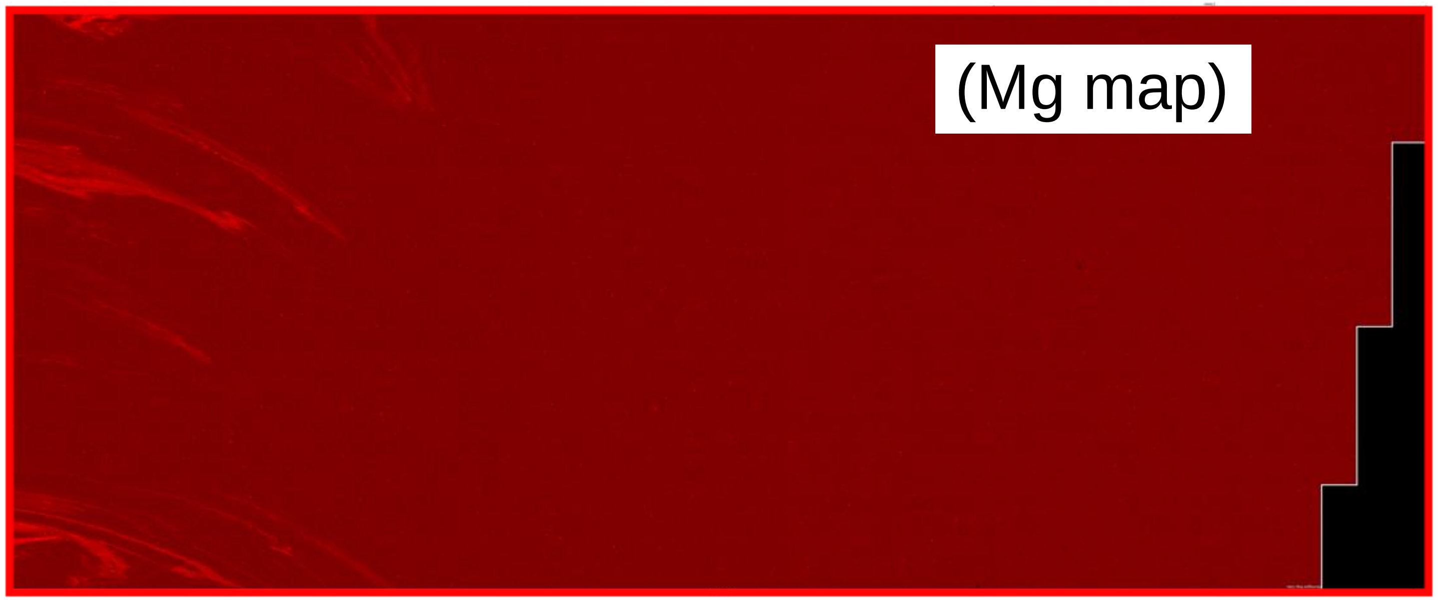


FSW Joint SEM Large Area Maps (LAM)





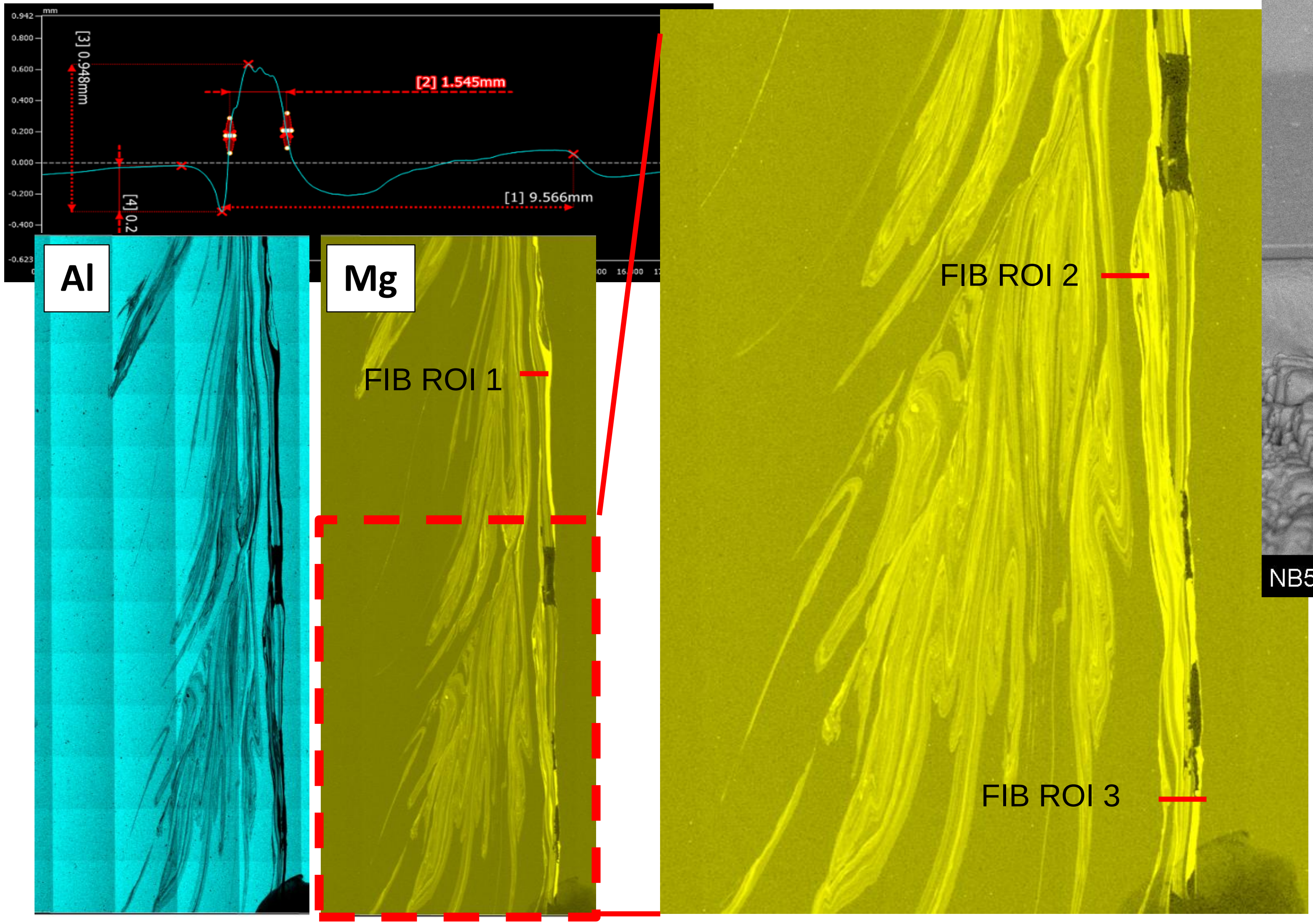


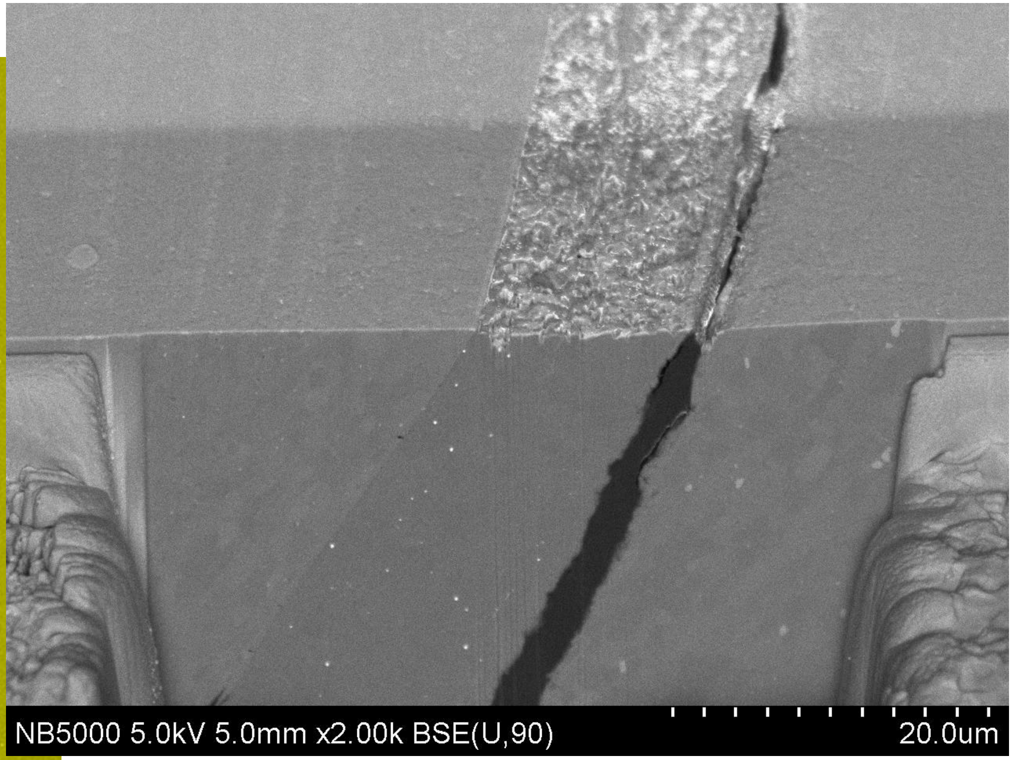


Detailed Characterization/Near Hook Region

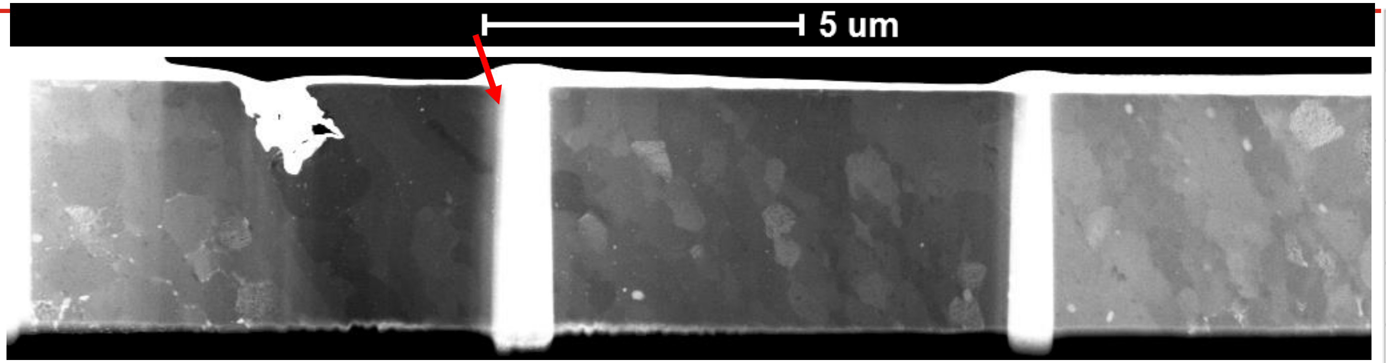
Polish down through Al into peak/hook region

SEM EDS Large Area Map (LAM) shows Mg "swirls" into Al

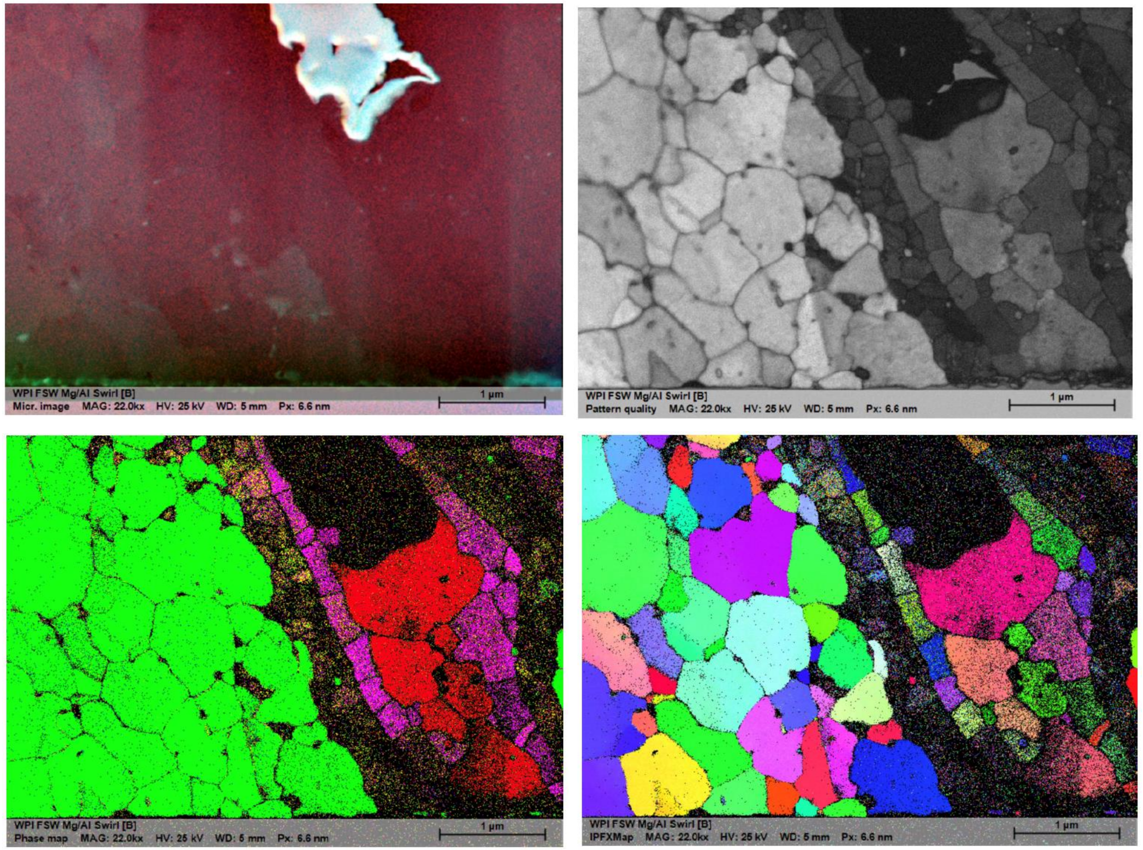


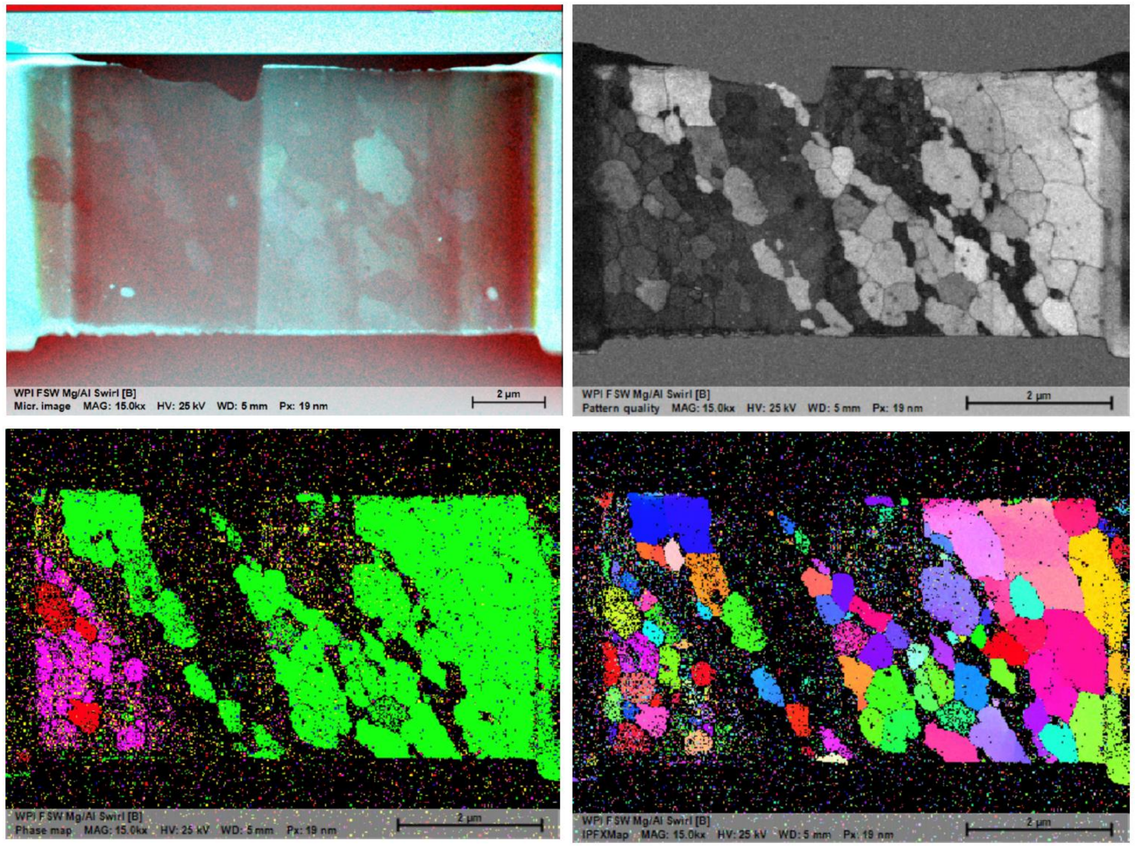


25kV SEM Transmission Kikuchi Diffraction



No	PhaseName
1	Magnesium
2	Aluminium
3	Aluminium magnesium (3.7/0.3)
4	Aluminium magnesium (30/23)
5	Aluminium magnesium (12/17)

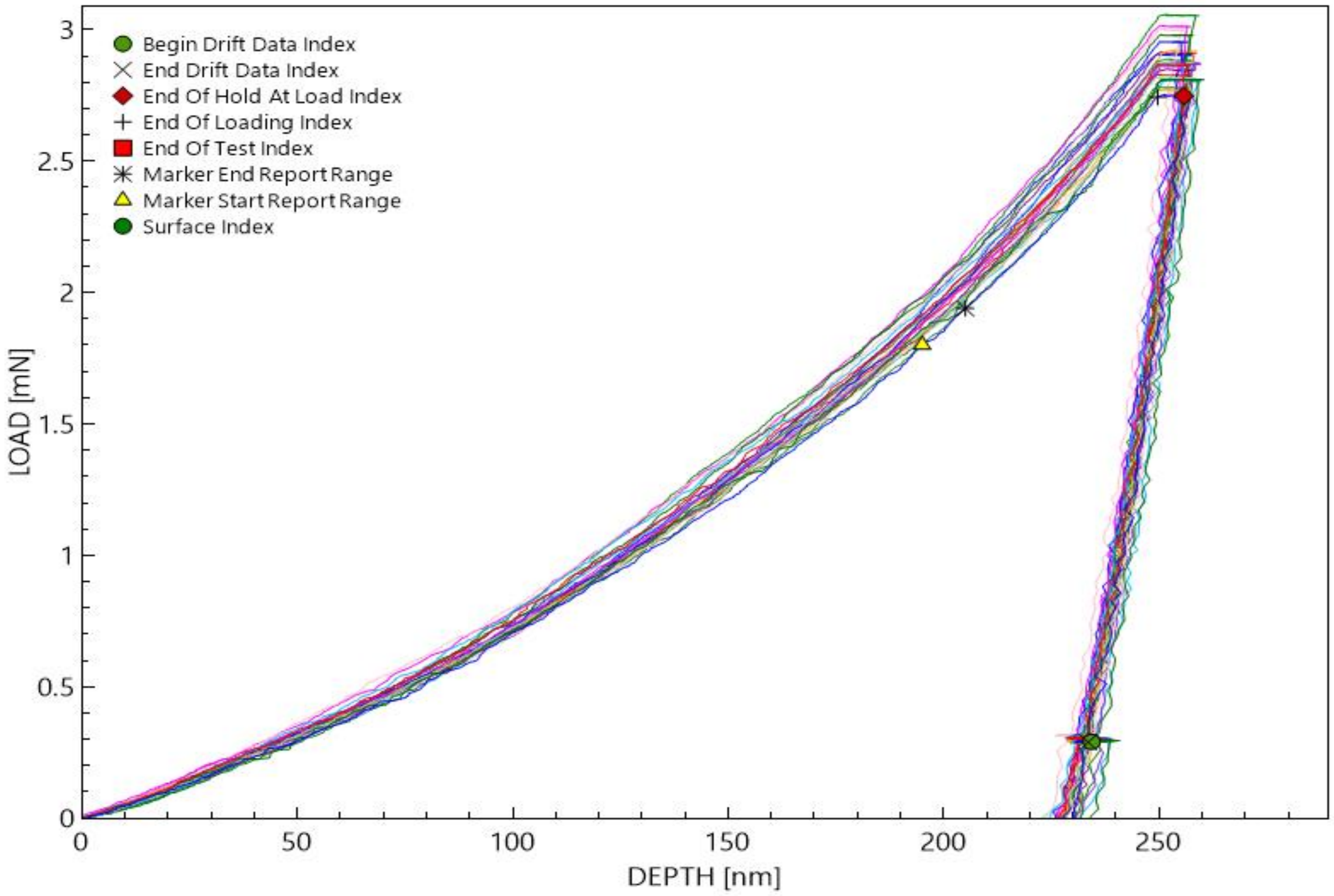




Nanohardness Testing

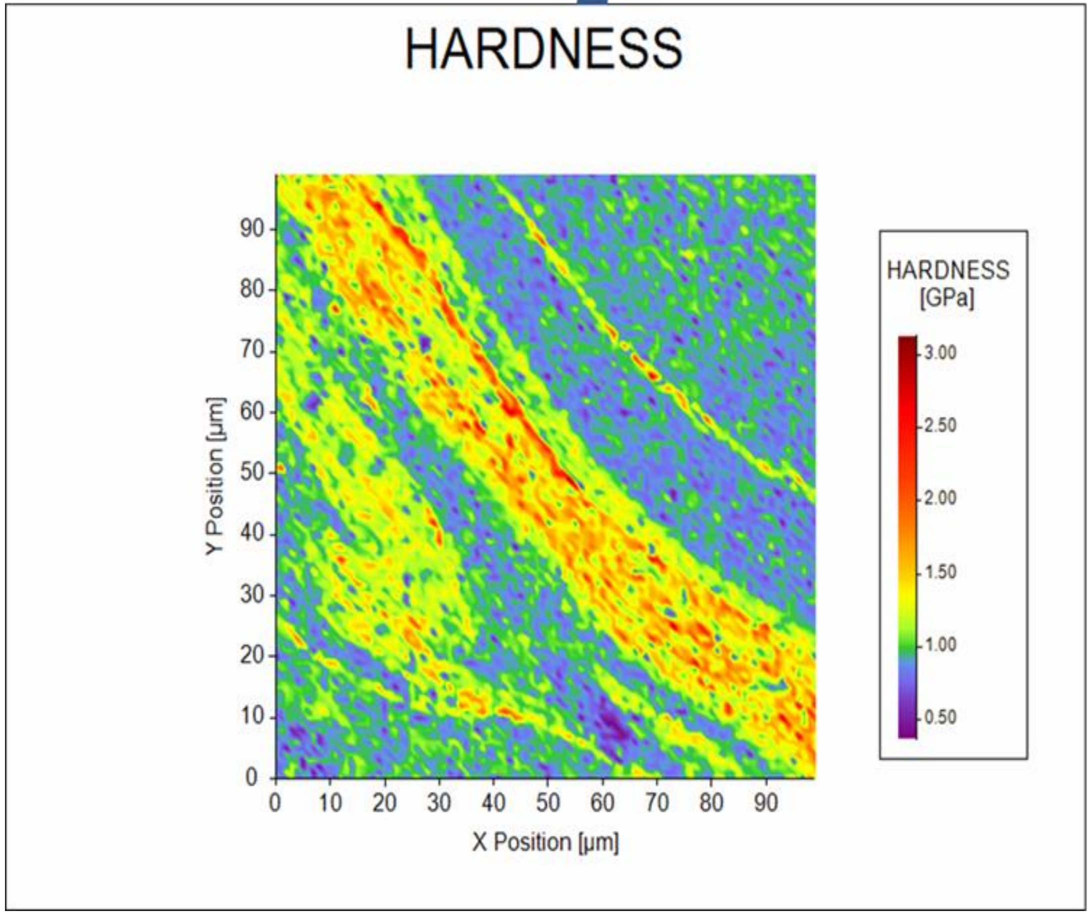
Nanoindentation local stress-strain curve

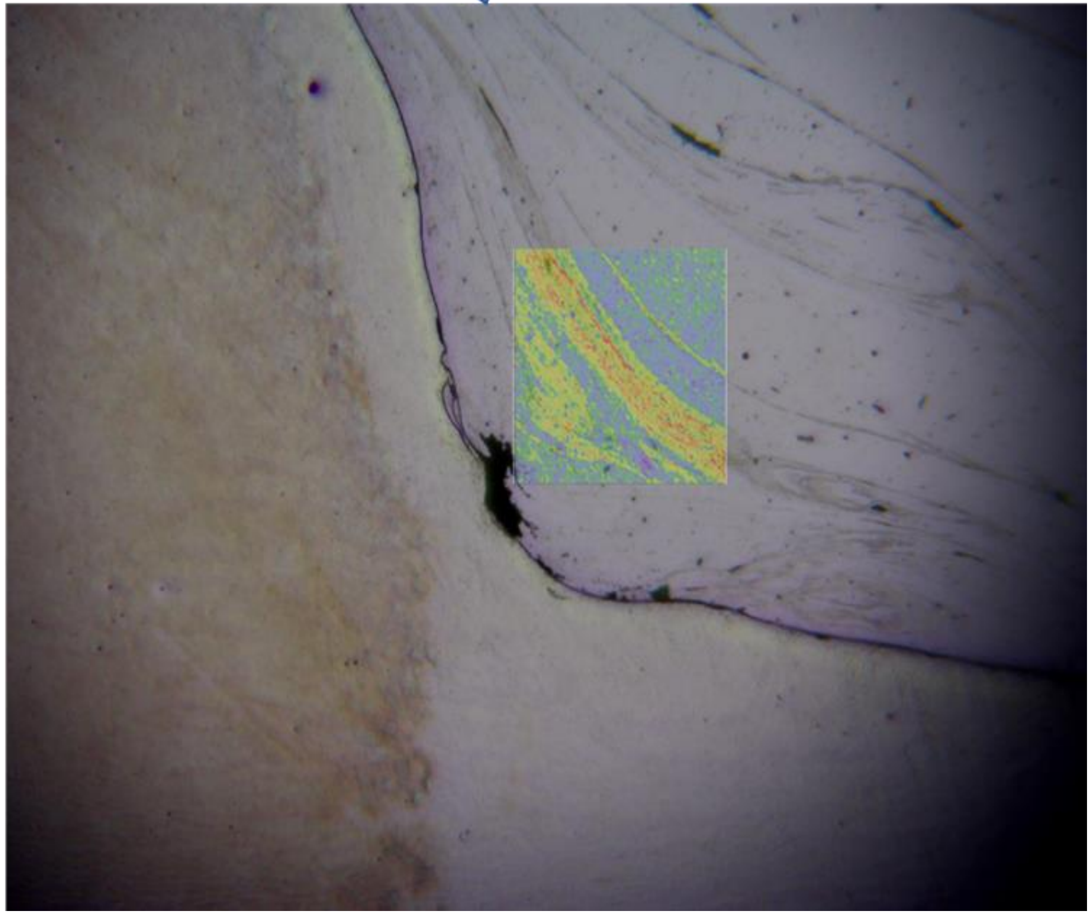
- Use nanoindentation to further characterize weld
- Fine indenter, 1 μm spacing without interference
- 1 indentation per second, 100×100 array in ~4 hrs
- Develop FEA constitutive relationships from load-depth curves



Nanohardness Mapping

"Swirl" regions show strong variations in hardness,
likely due to small grain size and intermetallic compounds





Response to Previous Year Reviewer Comments

How does this phase field model address grain size effects on corrosion?

- The present model does not address grain size effects
- We continue to investigate corrosion behavior, and will include grain size as we measure and understand its effect

Will the model address strength variations across the joint?

- Yes, these effects (strength, intermetallics) are part of the model

Metrics for evaluating corrosion at joints are not well defined

- True, we are still investigating how corrosion affects joint strength

In the corrosion model, does the electric potential field vary with time?

- Yes, it is re-calculated at each time step along with composition

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

Team Collaboration & Coordination

P.I. Adam Powell of WPI leads the technical team comprised of:

WPI

- Brajendra Mishra, Qingli Ding } Corrosion & mechanics exp'ts
- Kübra Karayağız – Modeling lead

PNNL

- Piyush Upadhyay, Darrell Herling } Joint fabrication & data mgt.
- Erin Barker – Modeling consultant

ORNL

- Donovan Leonard – Materials Characterization

Magna

- Tim Skszek - Application, materials

Cost-Effective Collaboration

- Zoom - at least monthly, sometimes weekly
- One annual two-day face-to-face Project Meeting (COVID-permitting)
- Team meetings at other events: TMS Annual Meeting, VTO AMR

Remaining Challenges/Barriers and Future Work

Complete corrosion model implementation and validation

- Accelerated 3-D Cahn-Hilliard model
- Add charge transfer resistance to electrochemistry model

Continue mechanics model using new characterization insights

- Understand fracture based on nanohardness maps

Model: couple phase field corrosion with mechanical deformation

- Understand corrosion in FSW joint microstructure
- Model fracture of corroded sample

Continue FSW development for strength and repeatability

Model cyclic loading based on published models of FSW fatigue

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

Summary

Friction stir welding through 6022 Al into ZEK100 Mg

- Conducted extensive parametric study of FSW through Al into Mg
- Established protocol with good repeatability and strength

Nearly complete model of galvanic oxidation and pitting corrosion

- Corrosion is limited by cathode reaction
- 4-component Cahn-Hilliard formulation with water oxidation

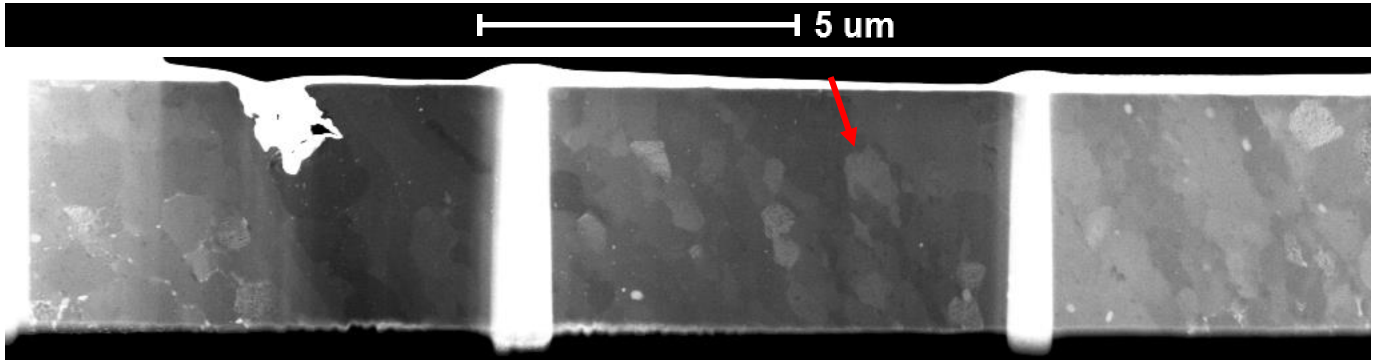
Developing the ability to model microgalvanic corrosion reactions

Potential impact on VTO objectives: Method and open source tool for modeling in a key enabler for multi-material systems

Thank You

Technical Back-Up Slides

FSW 6022/ZEK100: 3 Phases Evolved, Beta, Gamma, Mg_2Si



- TKD confirmed Beta and Gamma present in swirled regions
- STEM/EDS shows Mg_2Si also present in these swirled regions (purple dots in combo map below)