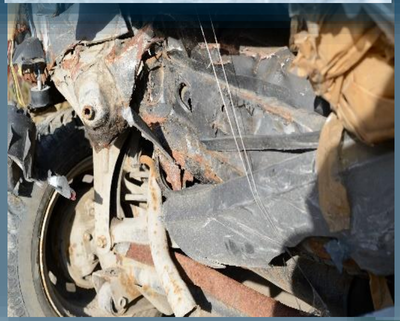

A Multi-Scale Computational Platform for Predictive Modeling of Corrosion in Al-Steel Joints

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University of Michigan

June 23, 2021

2021 DOE Vehicle Technologies Office Annual Merit Review

Project ID: mat153

Overview

Timeline

- Project start: **1/01/2019**
- Project end: **12/31/2021**
- Percent complete: **80%**

Budget

- Total project funding
  - DOE share: **$1,500,000**
  - Contractor share: **$478,431**

Barriers and Technical Targets

- Multi-material systems
- Aluminum – Steel joints
- Corrosion
- Develop predictive models for dissimilar Al-Steel joints (within 10% of experiments) to enable mixed material structures

"USDRIVE Materials Technical Team Roadmap October 2017, section 6"

Partners

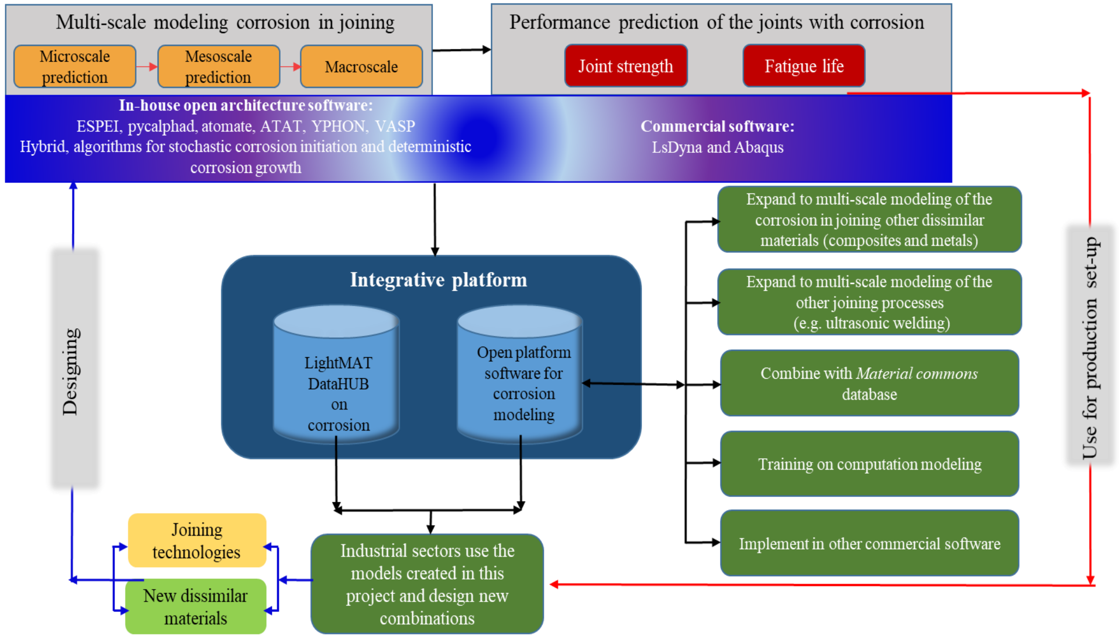
- Pennsylvania State University (Penn State): PI J. Li
- University of Illinois (Illinois): PI C. Shao
- University of Georgia (UGa): PI J. Hu
- General Motors Company (GM): PI B. Carlson
- Optimal Process Technologies (OPT): PI S. Young
- LST, an ANSYS Company (LS-Dyna): PI M. Pigazzini

Project lead: University of Michigan (UM)

Relevance & Objective

Relevance

- The global cost of corrosion was estimated at about 3.4% of the global GDP in 2013. By using available corrosion control practices, it is estimated a saving between 15-35% of the cost of corrosion.
- In the U.S. more than $276 billion is spent repairing corrosion damage.
- Prediction of the corrosion and its impact on performance of the dissimilar material joints is critical for reducing the massive number of the current corrosion-based recalls.
- Corrosion modeling enables predictive maintenance, lifetime extension and end-of-life planning.



Objective

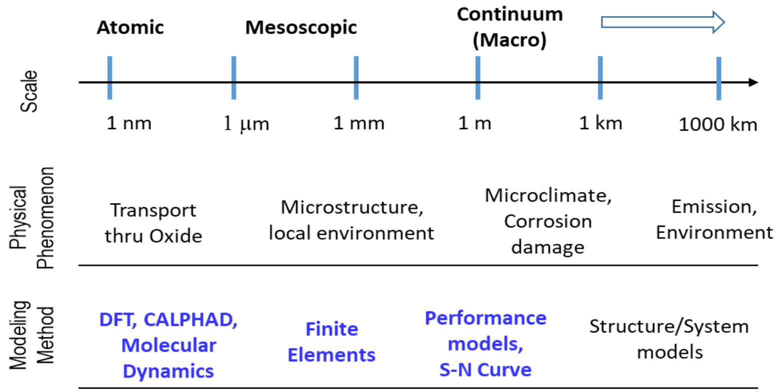
- To develop and validate multi-scale models to predict the location and extent of corrosion in Al-steel joints and its impact on joint strength and fatigue life.

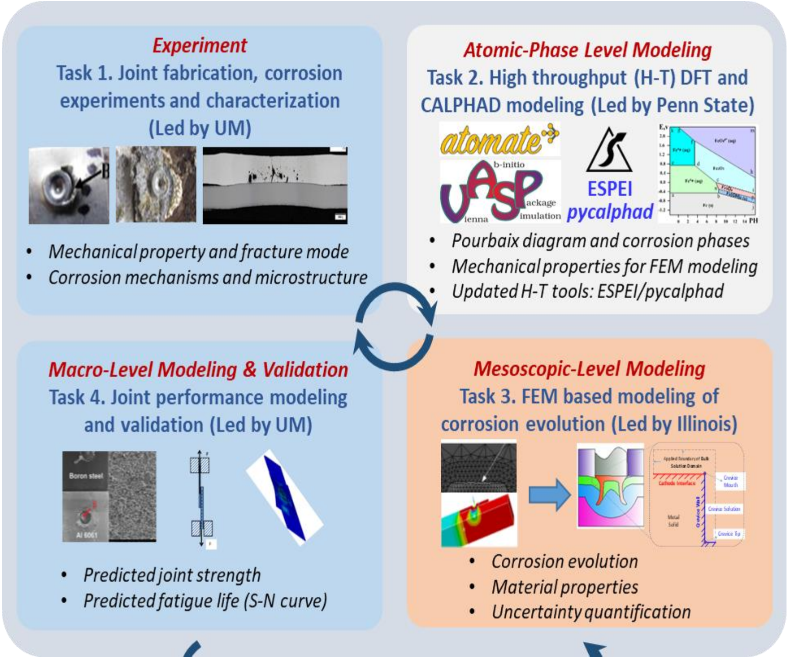
Milestones

Date	Milestone and Go/No Go Decisions	Status	Description
March 2020	Material property parameters	Completed	Physical properties at interface in the corroded areas. Elastic and plastic mechanical properties of the corroded interface. Single crystal stress-strain curves.
June 2020	Material property CALPHAD databases	Completed	Material property databases including by the high throughput CALPHAD modeling technique.
Sept. 2020	Joint performance prediction	Completed	Agreement between experimental and predicted material behavior for corroded areas for constitutive material model coefficients/cohesive layer parameters.
Dec 2020	Ls-Dyna Platform module of material and joint	Completed	LS-Dyna platform module of a constitutive material joint corrosion multiscale model.
Dec. 2020	Go/No Go Decision Extended model of corrosion evolution	Completed	Corrosion evolution model incorporating geometric and environmental factor couplings.
June 2021	Corrosion Evolution Model Verification	On Track	Verification of results from corrosion evolution model incorporating geometric and environmental factor couplings to experimental data.
March 2021	Multiscale Simulation Model Integration	On Track	Integration of microscale and continuum models into the finite element model.
Sept. 2021	Uncertainty quantification Model Integration	On Track	Integration of Probabilistic Confidence-based Adaptive Sampling (PCAS) into the simulation platform.
Sept. 2021	Fatigue Performace Prediction	On Track	S-N curves for fatigue of the joints to be comparable with the existing results.
Dec. 2021	Final report Force-Displacement Prediction	On Track	Obtaining a force-displacement curve prediction for lap-shear test with less than 10% comparative error.

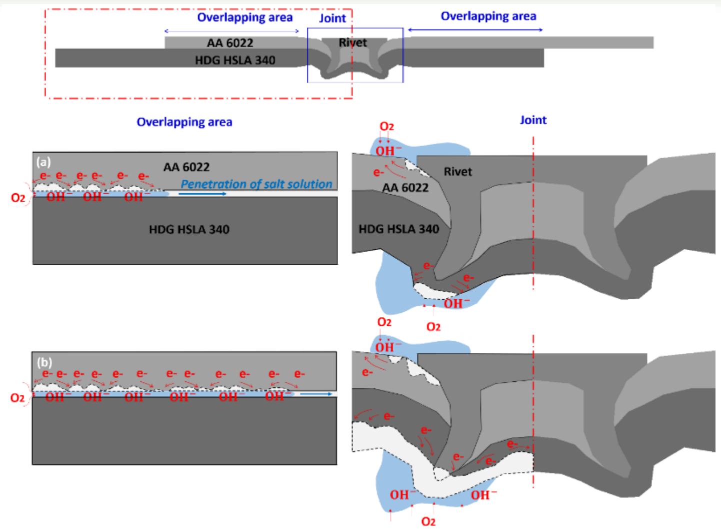
Approach

- Develop **multiscale models for predicting corrosion** rates and their impact on joining performance of aluminum-steel based on structure-property-performance interaction at different scales:
- **Joining processes:** Resistance spot welding (RSW), self-pierce riveting (SPR) and rivet-welding (R-W).
- **Prediction of intermetallic compounds (IMC)** during joining and their evolution in corrosive conditions (atomic-phase level modeling).
- **Prediction of the chemical and elasto-plastic material properties** of the IMCs and their evolution as corrosion products (Young Modulus, Poisson Ratio, ideal shear strength, stacking fault energies.
- **Prediction of corrosion sites, corrosion rates and homogenized mechanical properties** (grain level phase field modeling) in the joining area.
- **Integration of the atomic-phase level and grain level models in prediction of joining performance**: energy absorption, maximum strength with corrosion evolution, fatigue life. Prediction error <10% of experiments.

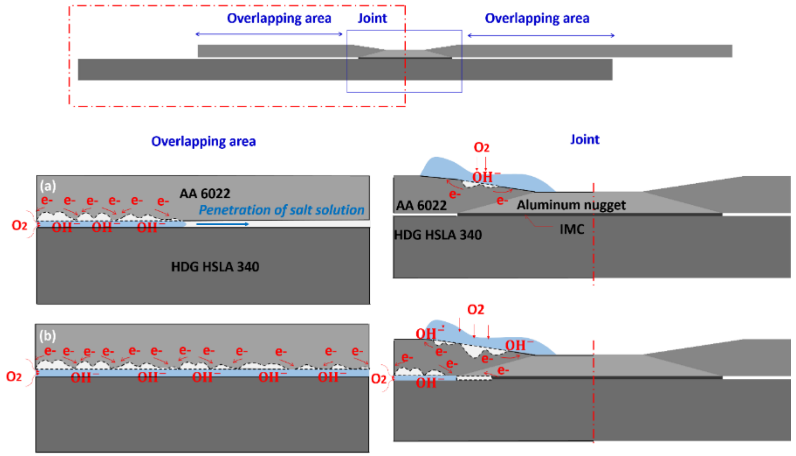




Accomplishment: Depletion mechanisms in corrosion-induced joint failure



Mechanism 1 of corrosion initiation and evolution in SPR joints



Mechanism 2 of corrosion initiation and evolution in RSW joints

- Two depletion mechanisms were formulated based on knowledge extracted from the experimental observations of monitoring corrosion of Al6022-HDG HSLA 340 steel coupons.
  - These mechanisms explain depletion of stiffness and strength in corroded RSW and SPR joints.
  - The two mechanisms enable an accurate formulation/reference for validation of the physic-based and data-driven approaches used in building the multi-scale models for prediction of the joining performance.

Mechanism 1 for rivet-based joints: galvanic corrosion occurs at Al-rivet coupling area and Al-steel overlapping area by pitting AA 6022 surface. Thus, stiffness of the specimen drops significantly. With slight corrosion (~72 cycles), the strength of the joint is not affected. The joint strength decrease significantly under severe corrosion (≥ 104 cycles) in which the rivet will be exposed and corroded.

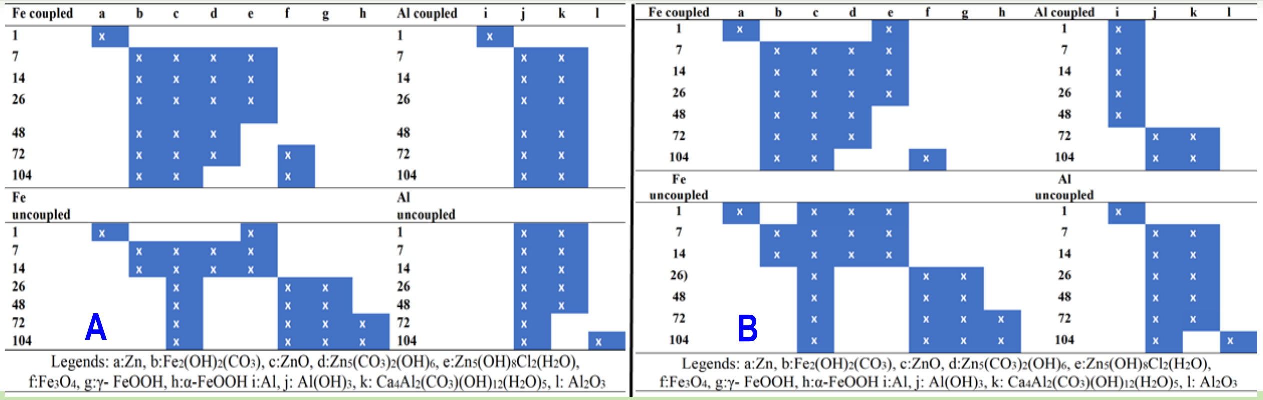
Mechanism 2 for nugget-based joints: galvanic corrosion occurs at Al-steel faying interface. The solution penetrates into the overlapping area by attacking AA 6022 first and then attacking the IMC layer. The joint strength decreases significantly when IMC is corroded. Similar as in SPR joints, pits are formed in AA 6022 at the overlapping area, which results in the decrease of joints stiffness. Since the crevice at Al-steel interface is much larger, galvanic corrosion here in RSW joints are much stronger than that in SPR joints and hence the stiffness reduction is higher.

These two mechanisms are portable for corrosion of other material systems with different electrochemical potentials.

Accomplishment: Prediction of IMC, corrosion products and their elasto-plastic properties

- Two case studies using RSW and SPR joints were carried out to understand and predict the formation of Al-Fe IMCs during welding conditions and the formation of IMCs of Al-Fe joins in corrosion conditions.
- Elastic and plastic properties of the IMCs phases and corrosion products are predicted. The results are included in a Material Property CALPHAD Database which contains:
- List of IMCs for RSW and SPR joints.
- List of corrosion products at different corrosion cycles simulating experimental conditions.
- Thermodynamic properties of Al-Fe IMCs as a function of temperature, pH and pressure together with thermodynamic properties of Al-Fe-based corrosion products at 0 K.
- Mechanical database, i.e., elastic properties of Al-Fe IMCs and corrosion products as well as ideal shear strengths of pure elements in the periodic table. Ideal shear strengths are used in calculation of the plastic properties.

Elastic properties (G_0, B_0, Y_0 Poisson Ratio) and of IMCs are important for modeling the joining constitutive material behavior. The evolution of material properties with corrosion is important for prediction of the joining performance and their fatigue life with and without corrosion.



Material database with predicted corrosion products. Corrosion products (blue colored if can be formed) for the Al coupled region, Al uncoupled region, Fe coupled region, and Fe uncoupled region under different corrosion cycles: **A.** RSW and **B.** SPR joints.

IMCs	B_0 (GPa)	G_0 (GPa)	Y_0 (GPa)	Poisson	B_0/G_0	A^u
Al	77.8	20.9	57.5	0.377	3.73	0.329
Al_6Fe	106.6	53.0	136.4	0.287	2.01	0.694
$Al_{13}Fe_4$	125.6	76.7	191.2	0.247	1.64	0.163
Al_8Fe_5	141.8	73.3	187.6	0.279	1.93	0.001
Al_2Fe ($MoSi_2$-type)	154.7	115.8	278.0	0.201	1.34	0.812
Al_2Fe (structure 1)	134.3	79.8	199.8	0.252	1.68	0.147
Al_2Fe (structure 2)	136.9	83.3	207.8	0.247	1.64	0.134
AlFe	184.0	102.5	259.3	0.265	1.79	0.951
Al_2Fe_5 (structure 1)	132.6	87.8	215.8	0.229	1.51	0.177
Al_2Fe_5 (based on USPEX)	137.0	83.7	208.6	0.247	1.64	0.664
$AlFe_3$ (structure 1)	188.3	56.5	154.1	0.367	3.33	11.040
$AlFe_3$ (structure 2)	197.2	81.0	213.7	0.321	2.43	3.343
Fe	180.6	76.5	201.1	0.315	2.36	0.196

First-principles predicted elastic properties of Al-Fe compounds (IMCs); including bulk modulus (B_0), shear modulus (G_0), B_0/G_0 ratio (> 1.75 for ductile materials), Poisson's ratio, and anisotropic index A^U (A^U = 0 for locally isotropic single crystals)

Accomplishment: Robust capacity of prediction corrosion products

- The atomic-phase modeling can be be applied to predict corrosion products in the joining areas (coupled) as well as adjacent areas (uncoupled).

  - **Pourbaix diagram, i.e., the potential *E* versus pH value diagram,** is a plot of possible thermodynamically stable phases in an aqueous electrochemical system.

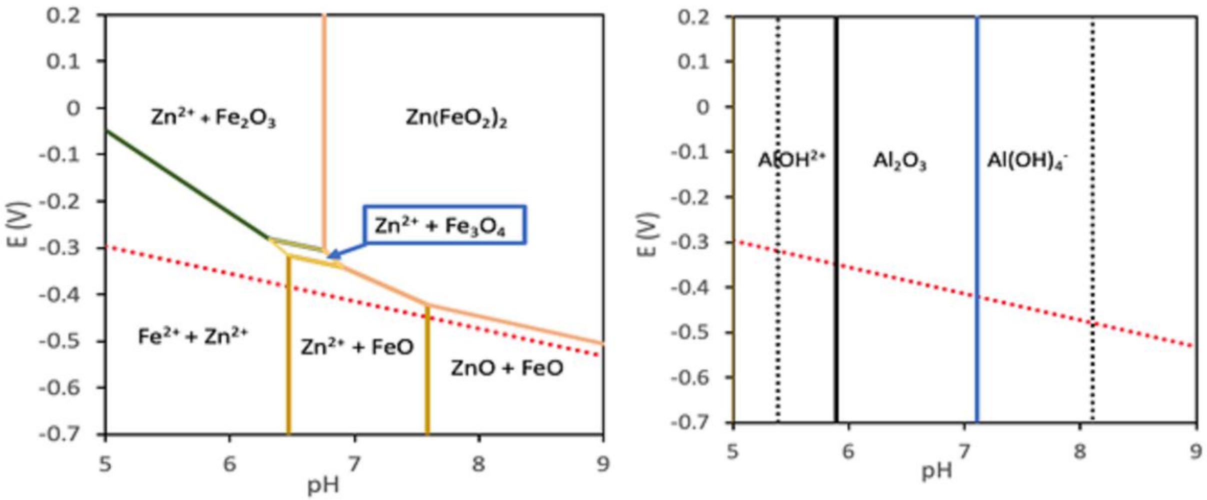
  - The Nernst equation is used to **calculate the equilibrium potential *E* from Gibbs energies** of all solid and solution phases:

$$E = \frac{\Delta G}{nF} - \frac{RT}{nF} ln \frac{[a_p]^p [H^+]^h}{[a_r]^r}$$

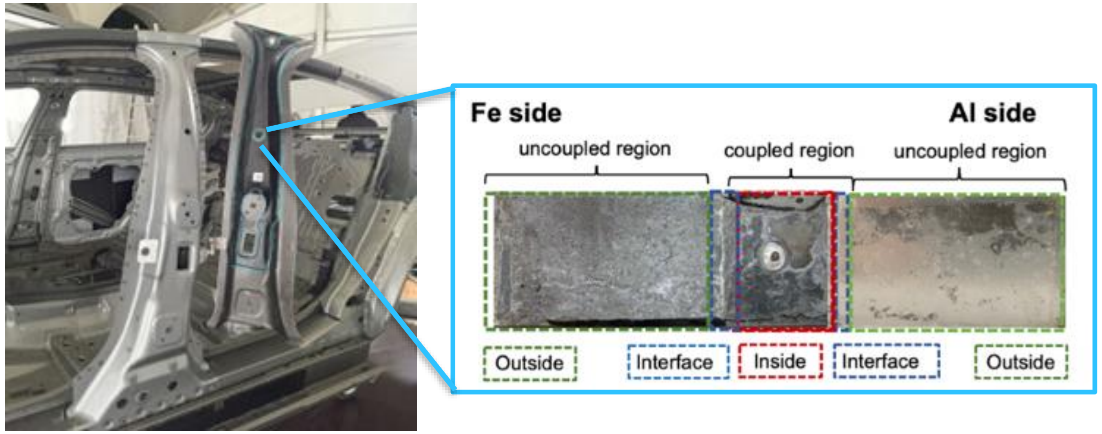
E: Equilibrium potential, ΔG: Standard Gibbs energy of reaction

F: Faraday constant; a_p: Activity of products

a_r: Activity of reagents; NOTE that: $\mathrm{pH} = -\log_{10}(a_{H^+})$



Potential *E* versus pH value diagram calculated using the Pourbaix diagram



Coupled and uncoupled regions in the lap shear Al6022-HSLA 340 joint

Prediction of the corrosion products with 1% error compared with experiments (XRD, HRTEM, SEM analysis). The Pourbaix diagram module is implementing in the open-source code EPSEI/PyCalphad (www.espei.org). The atomic-phase models can be used for prediction of corrosion products in any area of a body-in-white exposed to corrosive conditions.

Accomplishment: Prediction of dynamics of the material behavior under corrosion

Experimental lap-shear tests of RSW and SPR joints with different level of corrosion indicated a change in the behavior from ductile (until 48 cycles) to brittle (from 48-104 cycles). The developed atomic-phase models are able to predict this complex dynamic behavior through calculation of ideal shear strength for dilute Al-based and dilute Fe-based alloys, and stable and unstable stacking fault energy of dilute Al alloys and surface energy.

- Ideal shear strength (τ_{IS}): Yield stress (σ_y) ← τ_{CRSS} ← Peierls stress (σ_P)

$$\sigma_y = \frac{\tau_{CRSS}}{m_{max}},\ \tau_{CRSS} = \tau_P \text{ at 0 K}$$

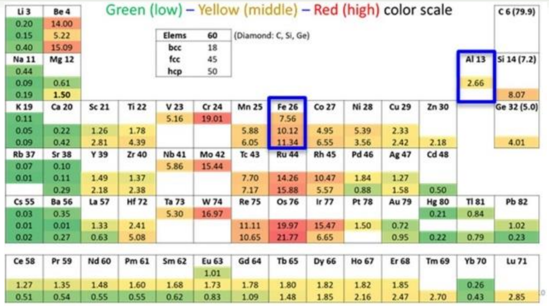
$$\tau_P = \frac{Kb}{a}\exp(-2\pi\zeta/a) \text{ and } \zeta = \frac{Kb}{4\pi\tau_{IS}}$$

CRSS: Critical resolved shear stress
m_{max}: Max value of Schmid factor
K: Elastic factor
b: Burgers vector
a: Spacing distance of slip place

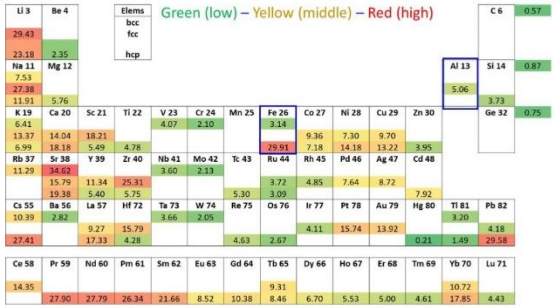
- Unstable stacking fault energy (Υ_{usf}) over surface energy (Υ_S): Ductility of the material ($\frac{\Upsilon_S}{\Upsilon_{usf}}$ ➔ Ductility)
- Fracture toughness
- $K_{Ic} = \frac{\sqrt{\frac{2G\gamma_{usf}}{1-\nu}}}{\cos^2\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)}$ (Rice, 1992)

G or μ - Shear modulus for sliding along slip plane
γ_{usf} - Unstable stacking fault energy
ν - Poisson's ratio
θ – Slip plane inclination angle

σ_P + elasticity + fracture toughness ➔ Input for finite element (FE) simulations of lap shear tests and prediction of the joining performance (force-displacement curves).



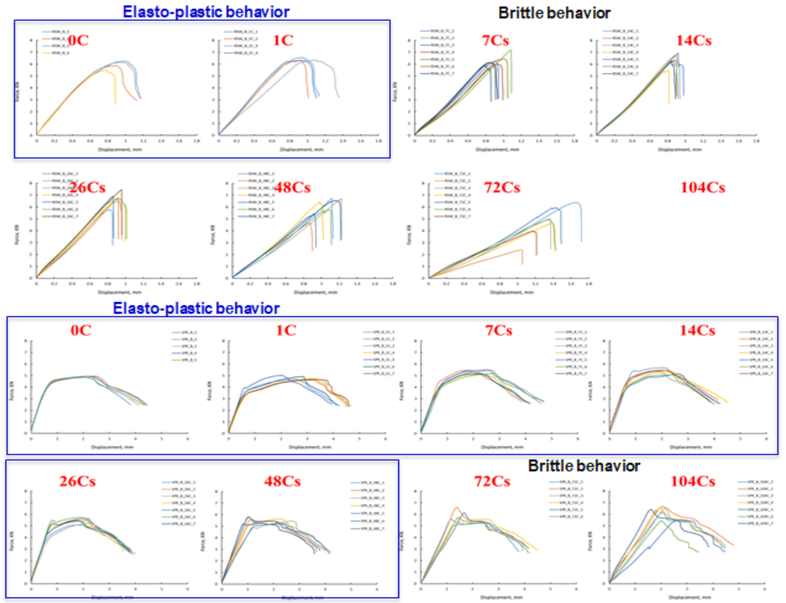
Ideal shear strength of pure elements (GPa)



$\Upsilon_{usf}/\Upsilon_S$

Bare RSW joints with & without corrosion

Bare SPR joints with & without corrosion



Pattern recognition in experimental lap-shear force-displacement curves in RSW and SPR shows that the behavior of the joints changes from ductile to brittle as increasing the corrosion exposure time (from no corrosion (0c cyles) to heavy corrosion (104 cycles).

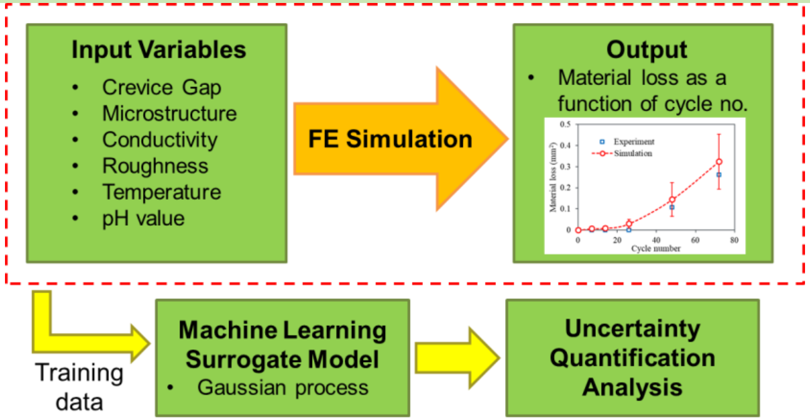
Accomplishment: Uncertainty quantifications in prediction of the material behavior

Identified sources of uncertainty with impact on variation of the force-displacement response of RSW and SPR joints under same loadings and testing conditions, e.g. variation of the thickness of the metal sheets, misalignments of the electrode with the sheets during RSW or SPR leading to crevice gap variations, variation of the coupons exposure position in the chamber.

The mesoscale models are developed for prediction of the corrosion evolution in the joints and in the adjacent areas.

The models include the effects of couplings various geometric and environmental factors, such as:
(i) uneven distribution of the electrolyte
(ii) effects of roughness of Al coupon
(iii) effects of crevice distance
(iv) effects of aluminum crystal microstructure
(v) synergetic effects of the combinations of couplings

Uneven corrosion (material loss) which leads to variations of the force-displacement curves in lap-shear tests of 5% among the 7 replicates



- To quantify the impacts of the input variables it was used a normalized sensitivity (σ) for each parameter calculated using the following formula
- $\sigma = \left\langle \frac{[k_i(q_i+\Delta q_i)-k_i(q_i)]/\bar{k}_i}{\Delta q_i/\bar{q}_i} \right\rangle$ where,
- $\bar{q}_i$ is the value of the *i-th* operation parameter in the baseline design
- $\bar{k}_i$ is the calculated property variation with respect to the *i-th* operation parameter
- Δq_i is the difference of the parameter.

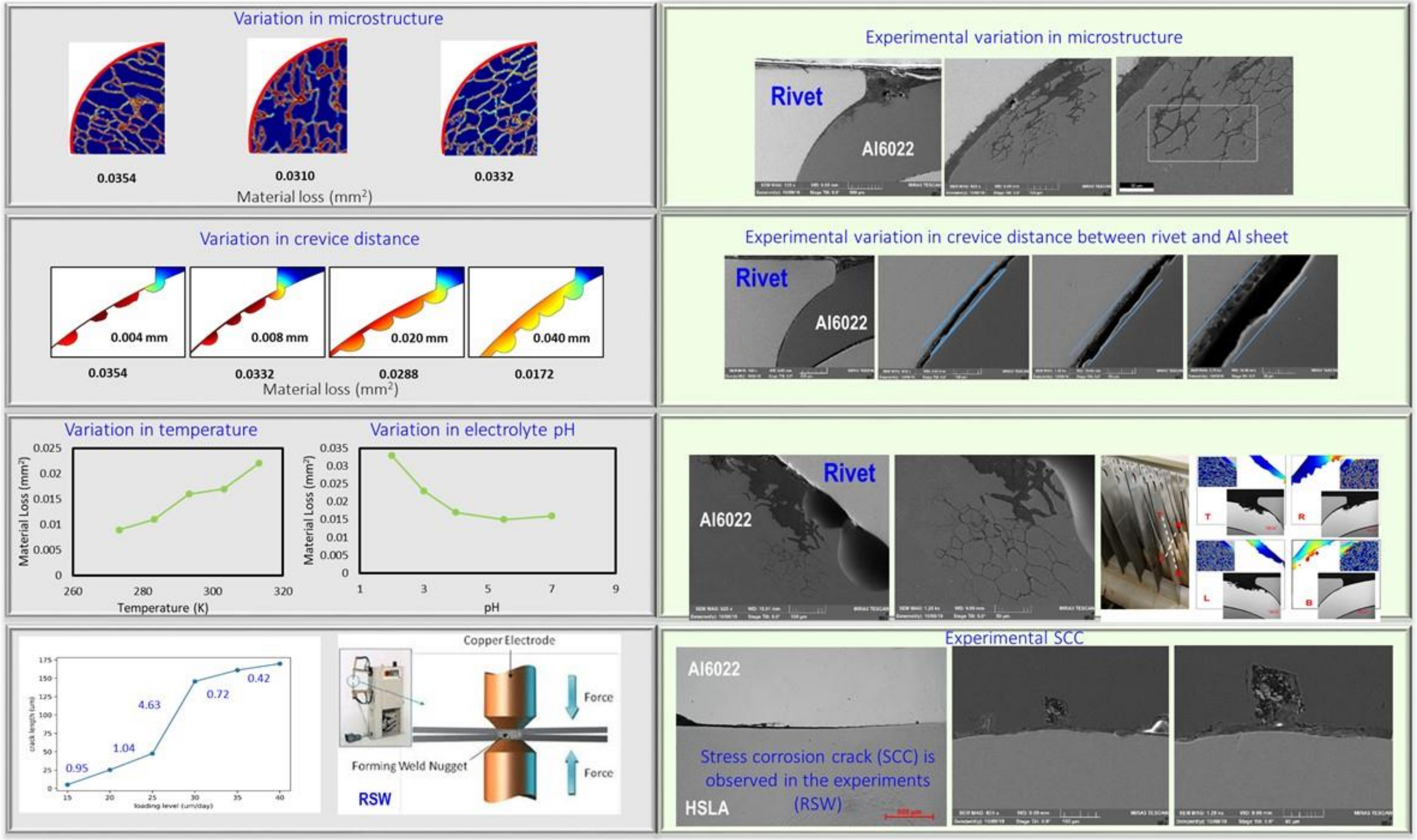
Quantification of uncertainty sources, e.g. grain size, orientation which can be slightly different in the joint due to misalignment of the joining electrode with respect to the stack of the metal sheets (Probabilistic Confidence-based Adaptive (PCAS) algorithm)

Accomplishment: Robust homogenized material models with uncertainty quantification

The effects of the temperature on the corrosion and deposition were investigated. Linear trend between temperature and material loss is predicted because of an increase in the diffusion rate of ions in the electrolyte.

The effects of the pH of the electrolyte on the corrosion and deposition were investigated. Non - linear trend between pH and material loss is predicted. As pH decreases, material loss initially remains constant but increases rapidly below a certain pH value

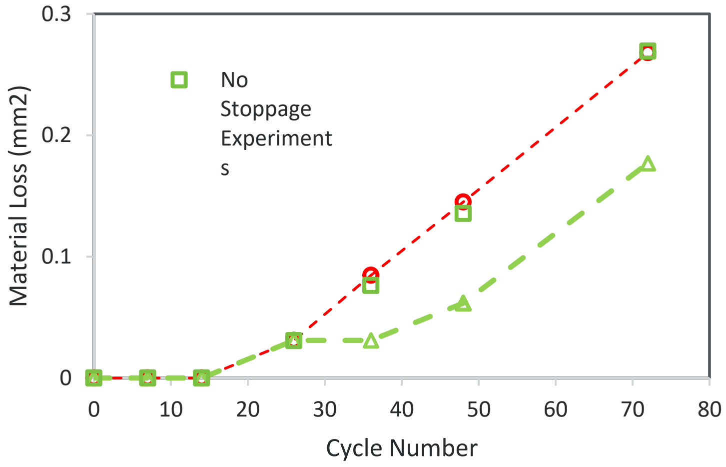
Stress corrosion crack (SCC) is observed in the experiments. SCC is the growth of crack formation in a corrosive environment leading to unexpected sudden failure of the material when subjected to a load. The variation in loading are associated to stress concentration, residual stress, assembly stress.



Influence of individual parameters which influence corrosion (mass loss) in the joining areas and adjacent: prediction versus experimental measurements and observations

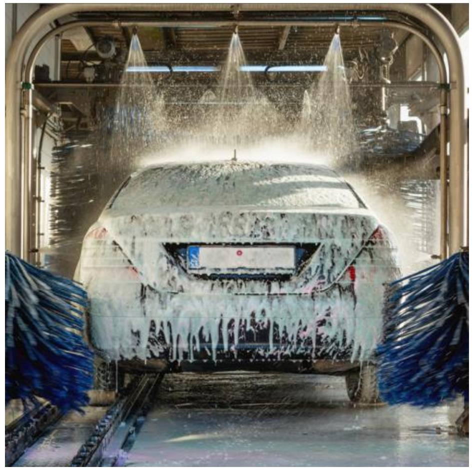
Accomplishment: Prediction of the COVID-related stoppage of corrosion evolution

- GM corrosion chamber was shutdown for 2 months due to COVID 19 leaving SPR coupons at 26 cycles. The procedure involves rinsing with water. After 2 months, the chamber was turned on and continue to expose samples to electrolyte. The results of the 72 cycles coupons shown less corrosion compared with a continuous corrosion until 72 cycles.
- The mesoscale model was used to simulate the COVID-related shutdown.
  - We assumed that the experiments stopped initially at 26 cycles and the simulation ran till this point normally
  - Due to the stoppage, there was a recoating of the joints by the oxidation layer which then acts as a barrier when the experiments were restarted
  - We assume that to get through this layer, 10 corrosion cycles occur without any further material loss. This is seen in the simulation results where the material loss remains constant from cycle number 26 to 36.
  - After these 10 dormant cycles, corrosion starts again with the overall material loss at these stoppage 72 cycles less than the original no stoppage material loss results



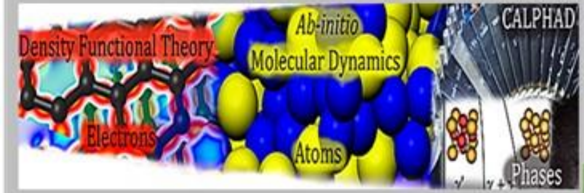
The results shown that the model predicts a significant delay of the corrosion

Often washing cars (especially in winter) has the potential of increasing the life of joints by ~30%.



Accomplishment: Integration of the atomic-phase and mesoscale predictions in in LS-DYNA

Atomic-phase scale modeling

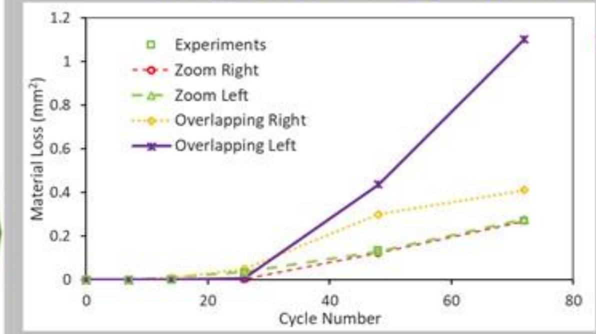


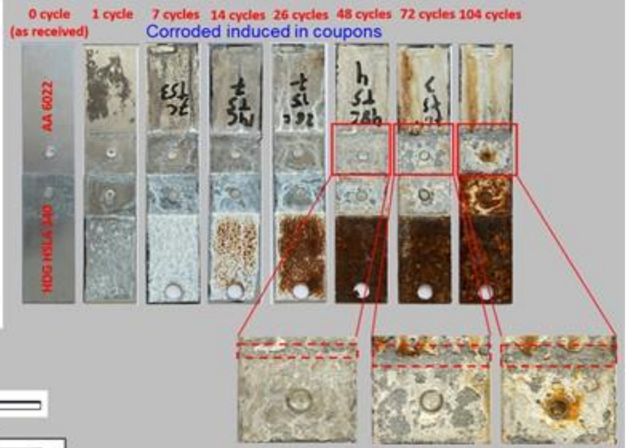
Elastic: G_0, B_0, Y_0 Poisson Ratio

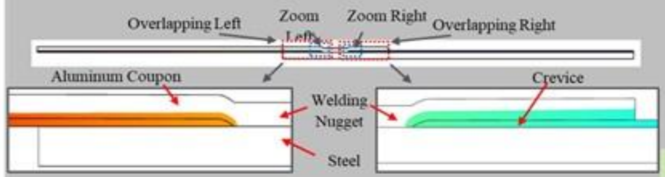
Plastic: Yield stress (σ_y)

Damage: $K_{Ic} = \frac{\sqrt{\frac{2G\gamma_{usf}}{1-v}}}{cos^2\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)}$

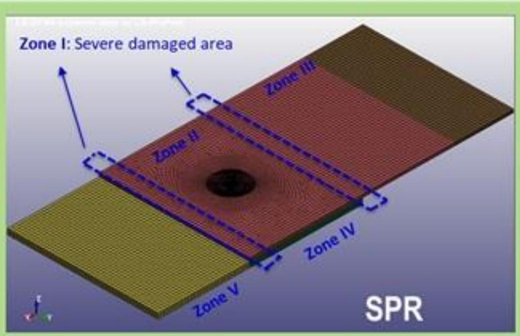
Homogenized methods for global mechanical properties calculation (corrosion rates)





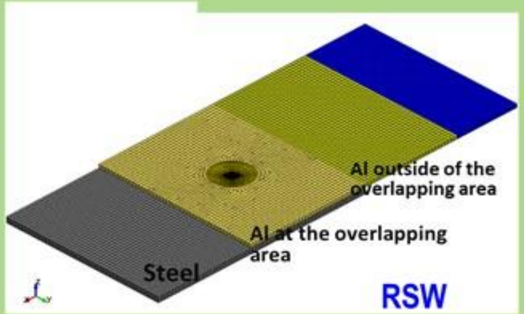


Prediction error of corrosion rates <5% of experiments



LS-DYNA+LS-OPT: Mat120c

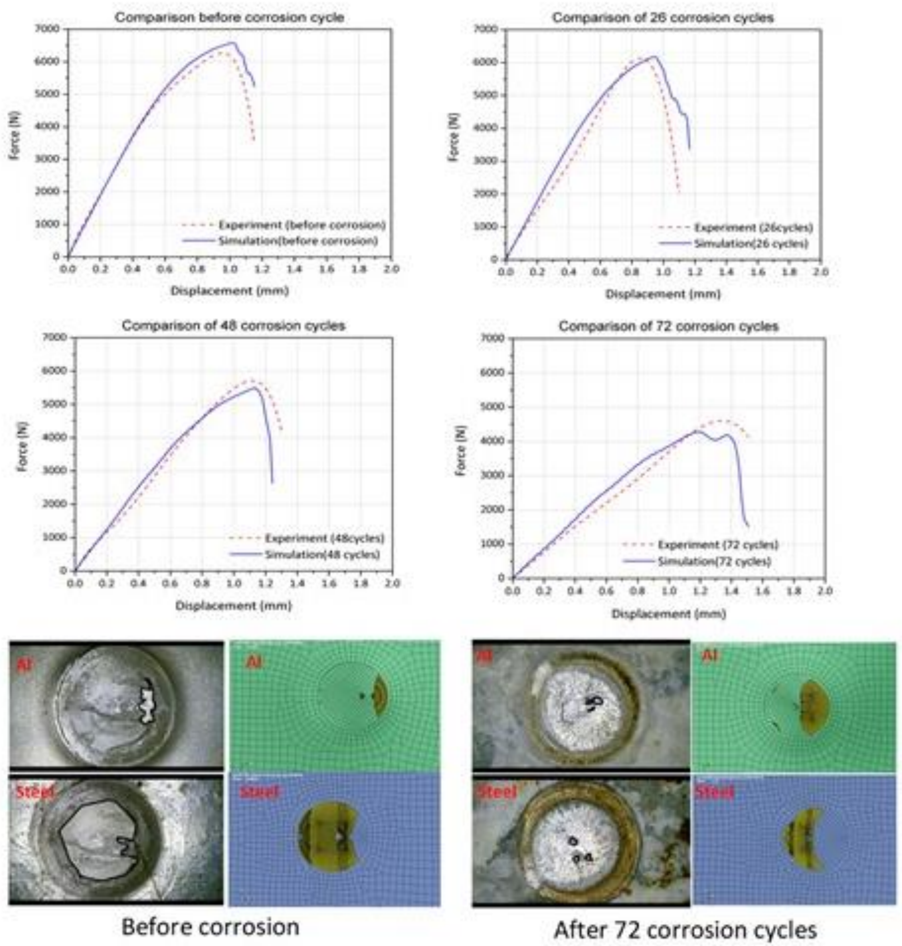
Calculation of the elastic properties and identification of the constitutive material models for plastic area; damage criterion



Finite element simulation of the lap-shear tests

Prediction of the force-displacement curves. Prediction error <10% of experiments

Accomplishment: Prediction of the joining performance RSW



Prediction of the force-displacement response in lap-shear test of RSW joints at different level of corrosion. Comparison with the experimental results.

- Two finite element models were built to predict the mechanical performance of RSW lap shear joining configurations with different levels of corrosion similar with the corrosion induced experimentally.

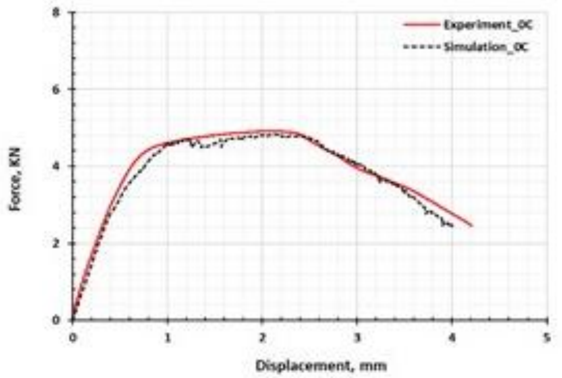
- The key contribution in simulation of the RSW and SPR lap-shear tests under corrosion are:
  - the development of the constitutive material model which is able to simulate changing the behavior of the interface from a ductile to brittle at increasing the number of the corrosion cycles.
  - the material behavior is built upon the ideal shear strength and fracture toughness (atomic-phase level) and corrosion rates predicted at the mesoscale level.

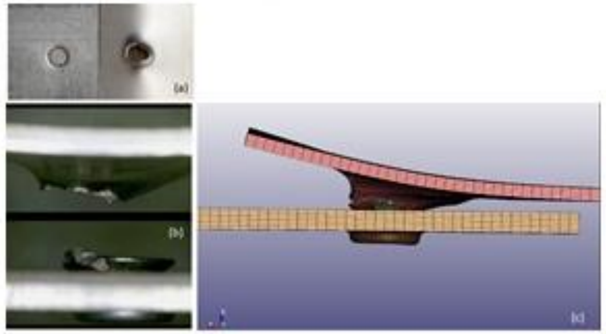
- The resulted force-displacement curves were used for calculation the maximum load capacity, the energy at failure and the energy at the maximum load and compared with the experimental values calculated on the average curves. These three parameters are defining the performance of the joints. The average experimental curve represents an average of 5-7 replicates.

Based on this analysis, the prediction error of the joining performance is 4% comparing with the experiments.

Accomplishment: Prediction of the joining performance SPR

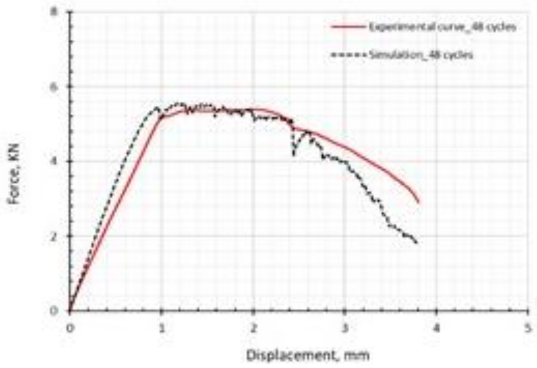
Comparison before corrosion cycles

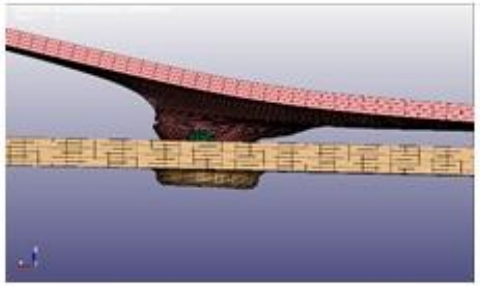




Before corrosion

Comparison of 48 corrosion cycles





After 48 corrosion cycles

Prediction of the force-displacement response in lap-shear test of SPR joints at different level of corrosion. Comparison with the experimental results.

Excellent results were obtained for the most important parameter of joining performance, i.e. energy at failure (0% error) before corrosion and after corrosion. Maximum load was predicted with an error between 2.2% before corrosion, 0% for 48 cycles and 10% error for 72 cycles.

Accomplishment: Computation platforms and open source codes for corrosion prediction

The computation platform for prediction of the corrosion products and the material behavior includes open source and commercial software integrated in a platform.

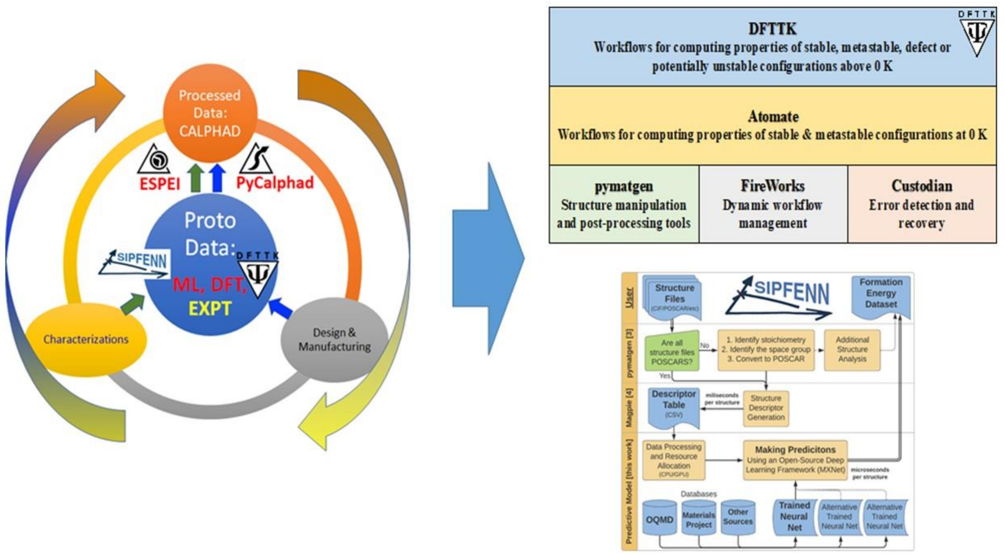
Atomic-phase level

- Machine learning to predict energetics via open source code:
  - **SIPFENN**: Structure-Informed Prediction of Formation Energy using Neural Networks and DFT Data
- High throughput DFT calculations via open source code
  - **DFTTK:** Calculations of thermodynamic and mechanical properties including YPHON code for phonon calculations
- High throughput CALPHAD modeling via open source codes
  - **ESPEI/PyCalphad (ours) + PyMatGen (open source)**: Calculations of phase diagram and Pourbaix (corrosion) diagram
- Web-accessible codes and databases
  - Codes via: espei.org; pycalphad.org; and github.com/PhasesResearchLab
  - Databases via: **Citrine.io** (as well as LightMat, DataHUB: data.lightmat.org – in progress)

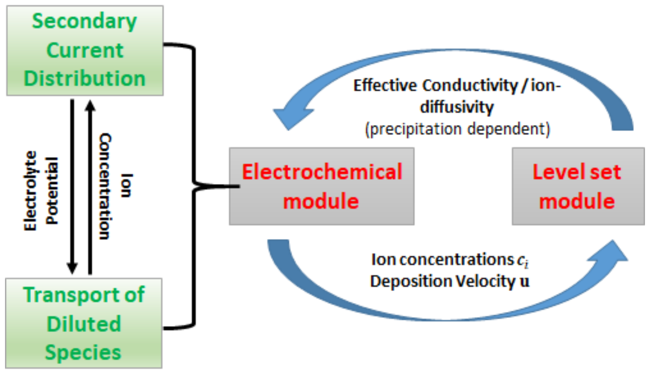
Mesoscale level (homogenized material properties)

- FEA simulation models (Comsol):
  - Modified phase-field model;
  - Decohesion model based on hydrogen embrittlement mechanism;
  - Peridynamics model.
- Data driven models:
  - Combined PCA and SVM (Python library RiskPy available);
  - Deep learning;
- Commercial software:
  - Sysweld is an available software that can accommodate SCC simulation.

Macroscopic level (LS-DYNA Mat120c +LS-OPT (in progress to be finalized)



A summary of the platform for atomic scale modeling and prediction of the material elasto-plastic and fracture toughness

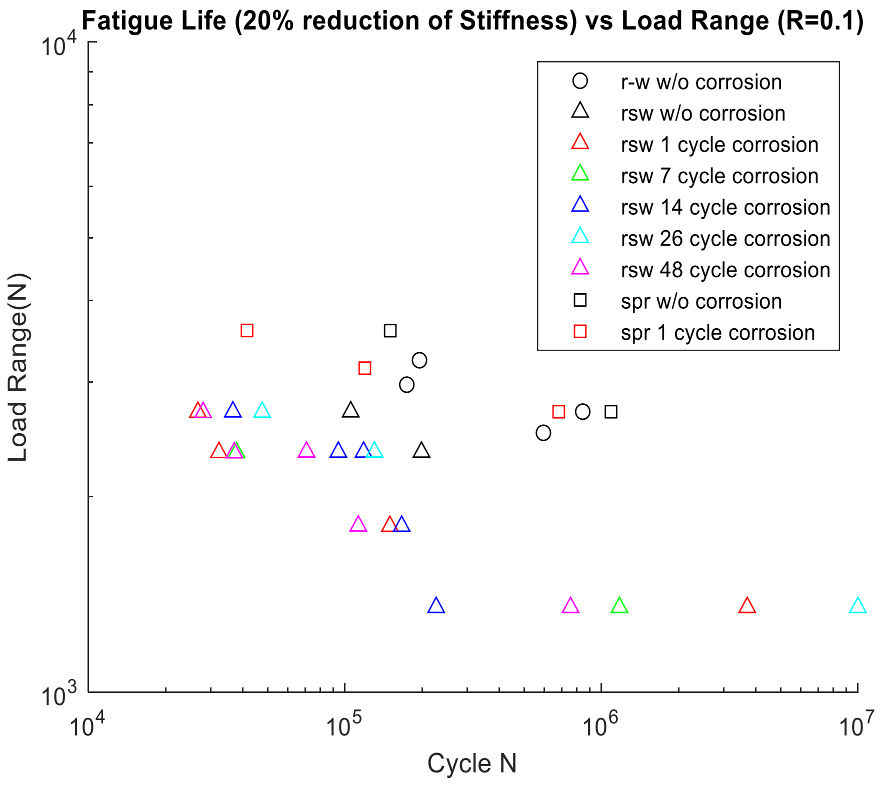


Roadmap for calculation for prediction of the corrosion evolution

Accomplishment: Prediction of fatigue (preliminary results)

Developed a continuum mechanics based spot weld fatigue model for implementation in CAE durability design and life prediction. A mesh-insensitive structural stress method will be used to model the fatigue behaviors.

- 30 fatigue tests were performed under with a load ratio of R=0.1.
- A cyclic load is set to be 50Hz.
- Through a series of preliminary testing and data analysis, a failure criterion (i.e., test stop criterion) is set as either complete separation of a reduction in stiffness of 20%, whichever occurs first. For the latter case, the fatigue life (i.e., cycles to failure) corresponding to the development of noticeable crack in sheet, which is approximately in the same life range as the specimen failed by complete separation
- Further fatigue tests of the RSW corroded coupons between 48-104 cycles SPR and R-W are in progress.



RSW corroded coupons between 1-48 cycles show a significant degradation in fatigue resistance compared to the ones without being corroded.

Response to the reviewers

Reviewers 1 and 2: We thank the reviewers for their appreciative comments on the understanding of the objectives, tasks and achievements reflecting a very good progress of the project. There are no questions to answer.

Reviewer 3 Q1: …The accomplishments currently read as a set of tasks that had been carried out. The project team does not actually describe what was achieved with regard to completion of tasks and how these contribute to the final goal(s).
We thank for this question. We have created a dedicated slide (Slide 13) which shows how the tasks are integrated to achieve the milestones and the final goal – to predict the force-displacement curves of the RSW and SPR joints under corrosion conditions.

Reviewer 3 Q2: …It also appears the tests were both General Motors (GM) and University of Michigan (UM) test protocols. For what does the GM protocol test? Salt exposure could simulate many things; so, what was this test(s) simulating?
We thank for this question. The accelerated cyclic corrosion etsts are performed by GM according to the GM14872 standard which reproduces the environmental conditions for a vehicle exposure. One corrosion cycle is defined and it includes three phases: the first 8 hours of salt spray (Ambient Stage), the second 8 hours of humidity (Humid Stage), and the last 8 hours of drying off (Dry-off Stage). The level of corrosion induced it is up to the complete failure of the joints (104 cycles).

Reviewer 3 Q2: …What is the basis in the stress corrosion cracking (SCC) model for combining the slip dissolution model with a modified phase-field model, a decohesion model for hydrogen embrittlement and a peridynamics model?
We thank for this question. In the current presentation, Slide 11 shows the reason of considering SSC in modeling. RSW is susceptible to developing SCC during corrosion. Consequently, the crack propagates faster in the presence of a an SCC. As shown in the Figure 1 included in this slide.

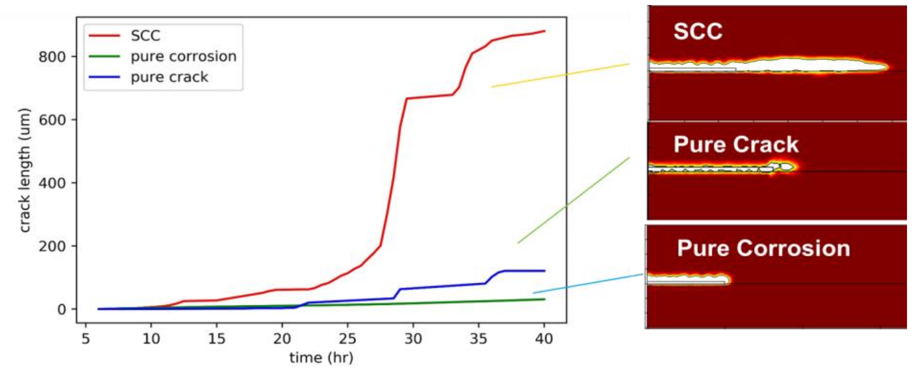


Figure 1 Source: University of Illinois Urbana Champaign

Response to the reviewers

Reviewer 3 Q2: What are the parameters being used to bound the nucleation event and to separate it from propagation? What length scale is the project team working at in the nucleation phase?

We thank for this question.

1. The corrosion nucleation sites are determined through a hybrid model [1] by statistically analyzing the experimental samples, so that the parameters to bound the nucleation events, including number of nucleation sites, their initial locations on the metal surface and corrosion activation sequence and time, can be obtained.

2. The length of the initial nucleation site is set to be 0.1 um.

[1] Z. Zheng, P. Bansal, P. Wang, C. Shao, Y. Li, Corrosion Modeling and Prognosis of the Al-Fe Self-Pierce Riveting Joints, IMECE2020-23597, ASME 2020 International Mechanical Engineering Congress and Exposition (IMECE), Virtual Online, November 16-19, 2020.

Reviewer 3 Q3: The majority of the work reported seems to have been carried out by UM. Perhaps the authors could shed more light on the contribution of the other team members in future presentations.

We thank for this question. Probably it is a confusion. UM is integrating the results from the other partners and have one student supervising the corrosion tests which were done at GM. The atomic-level modeling and mesoscale modeling are entirely done by our partners. To clarify the assignments, we have created a new collaboration/integration figure (Slide 20 or Figure 2 in this slide).

Reviewer 3 Q4: How do the authors propose to use the SN curves they gather to predict failure when there is a likelihood of environment playing a role in fatigue failures with these Al-joints?

We thank for this question. The predicted mass loss (corrosion rates) done using the University of Illinois models will be considered in the continuum mechanics based spot weld fatigue model. Thus, the decay in fatigue performance will be predicted. In the next report, we will demonstrate the performance of the fatigue model in prediction of the S-N curves with corrosion evolution. (Results will be presented in the last report of 2021).

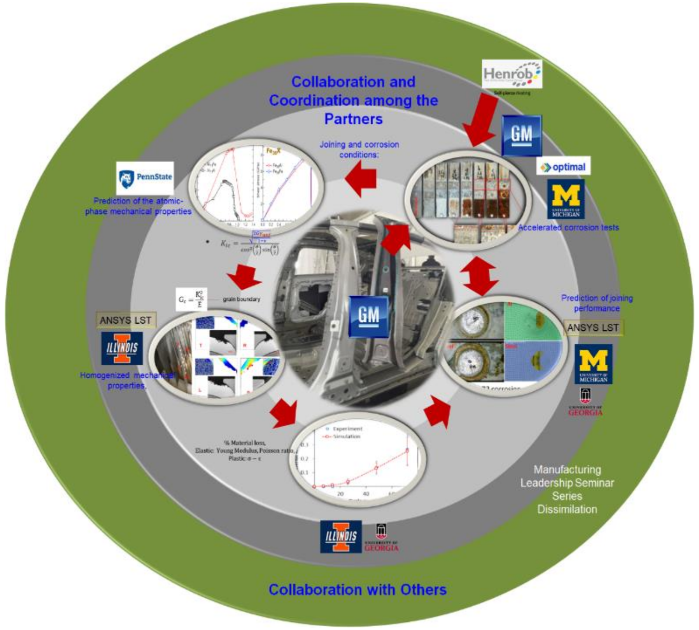


Figure 2 Source: All partners

Collaborations/Interactions

University of Michigan (UM) – characterization of joining and modeling the performance prediction.

Penn State University (PSU) – mechanical behavior and interfacial phenomena, computational thermodynamics and kinetics.

University of Illinois (Illinois) – uncertainty quantification in multiscale modeling and building performance models.

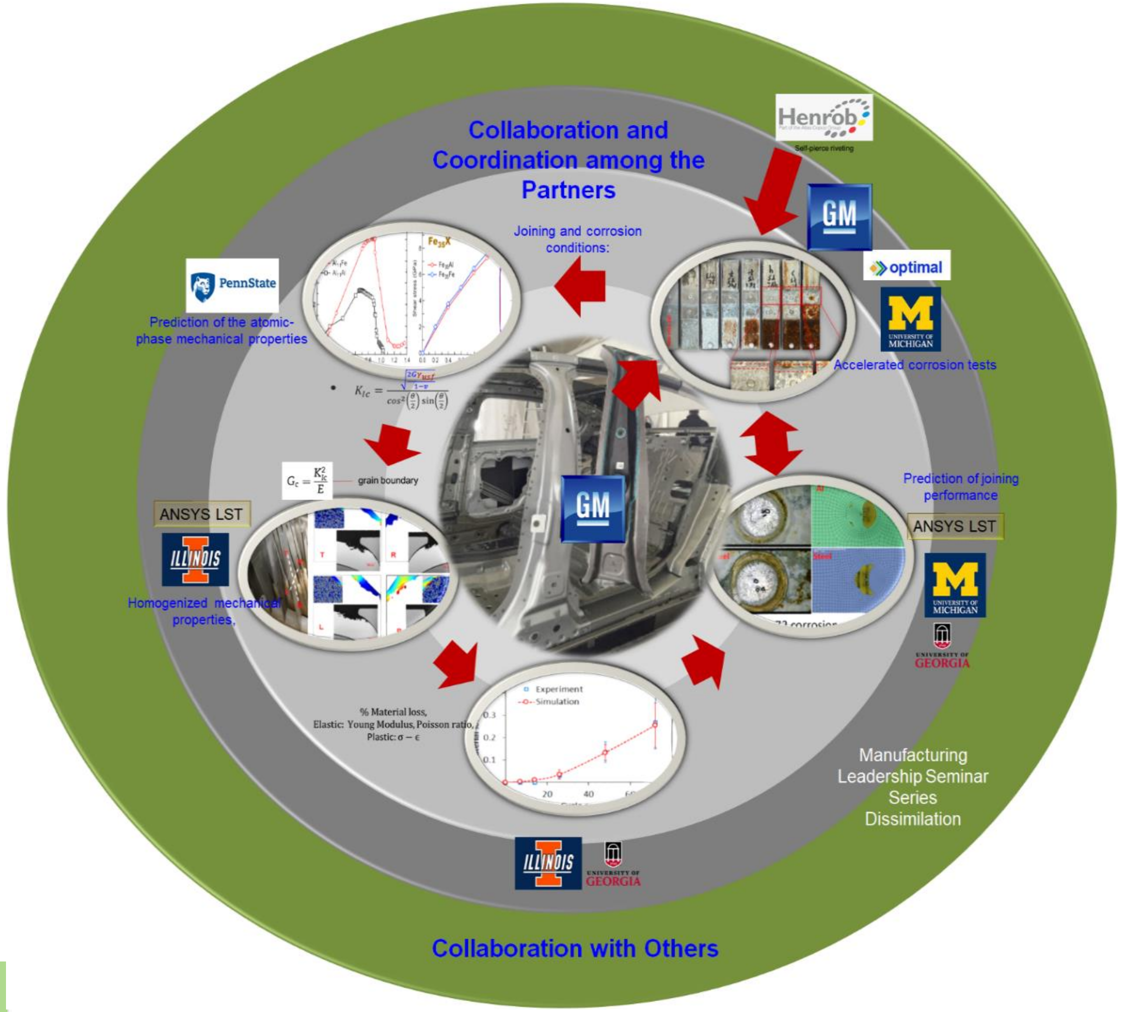
Livermore Software Technology Corp (Ansys-LSTC) – developing a new material card for modeling corrosion.

General Motors (GM) – provide facility for validation and demonstration of the RSW and SPR joints (together with Henrob).

Optimal Process Technologies, LLC (OPT) – provide facility for validation and demonstration of the Rivet-Weld technology.

University of Georgia – advise on design of R-W joint design and fabrication, analyze weld performance and its variation.

The team interacted and share resources in very efficient way. Thus, the project is on track with the expenses and cost-share. Common publications were submitted and others are in progress to be finalized.



Summary

Successful monthly and annual milestones delivered on-time and within budget.

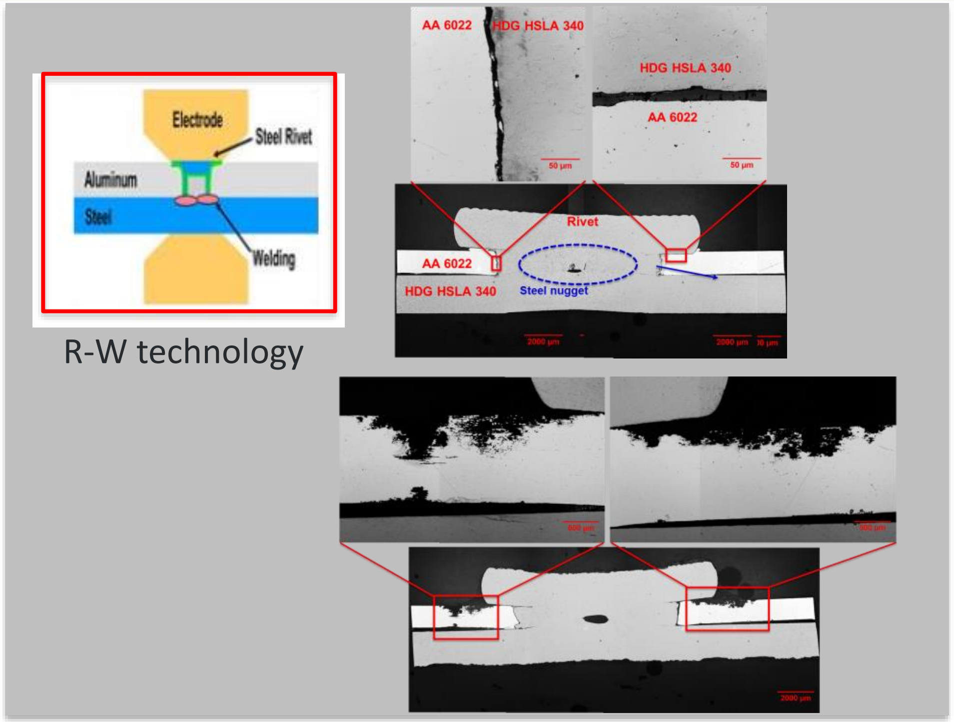
Enable diversity, inclusivity and equity through engaging diverse graduate and undergraduate students.

Enabled opportunities: One student graduated in 2020 and hired by GM.

- Atomic modeling from DFT-based first-principles calculations and phase-scale modeling from CALPHAD approach were developed to predict welding and corrosion products and their mechanical properties (5% error prediction comparing with experiments).
- A material database with the property parameters of the IMC compounds and corrosion products was established.
- Mesoscopic corrosion models were developed based on the finite element method and improved by incorporating SCC modeling and data-driven methods. Material loss and corrosion rates were predicted with an error of <5% compared with the experiments.
- At macroscopic level, FE models were built for simulation of lap shear tests applied to RSW and SPR joints. Thus, the performance of the joints with and without corrosion compare well with results from experiments. An average of 4% error comparing with experiments was achieved for RSW joints. Simulation of the lap shear tests applied to SPR joints are in progress.
- Failure of SPR joints was successfully predicted showing that the model approaches which were developed for RSW and applied to SPR are providing a high accuracy of simulated results. Prediction error <5% up to 48 cycles and 10% for 72 cycles.
- Uncertainty quantification were accounted in predicting the influence of potential source of variation such as: variation of the metal sheets, misalignments of the electrode with the sheets during RSW or SPR leading to crevice gap variations, variation of the coupons exposure position in the chamber.
- Fatigue teste were initiated and a continuum mechanics based spot weld fatigue model for implementation in CAE durability design and life prediction was developed.

Future work

- Continue to validate prediction of uncertainties from the joining processes based on GM input.
- Continue to develop the model for prediction of fatigue tests and validate it with the experimental results (experimental fatigue tests are in progress).
- Apply the multiscale model and run the integrated platform for prediction of the joining performance for rivet-welding
- (R-W) technology.
- Continue to transfer the models in LS-DYNA through training LS-OPT (a data-driven data base created in the LS-DYNA platform) which will be connected to Mat120 library and release Mat120c library containing the result of this project.
- Upload the results of this project on LighDataHub.
- The team plans to formulate guidelines for the automakers in prediction of the corrosion, end-of-life solutions. Also, based on machine learning and using inverse analysis, the team will propose solutions for designing new alloys less susceptible to corrosion when joint in multi-material assembles.



R-W Technology developed by Optimal LLC; Al6022-HDG – HSLa 340 coupons were corroded in the GM chamber and tested. The preliminary results indicate the presence of corrosion.