SAND2024-07015C

Multiscale Modeling of Active Brazing

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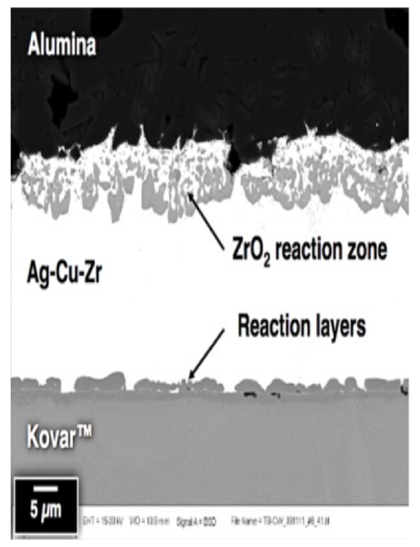
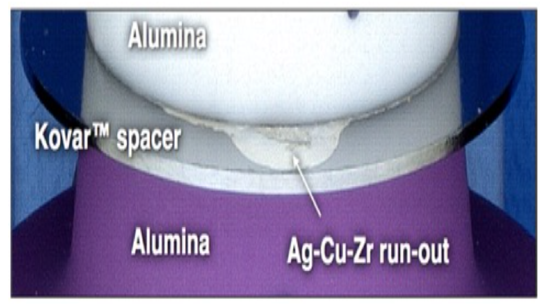
Introduction

- Brazing
  - Method of joining materials
  - Braze alloy melts to join parts
- Active Brazing
  - Ceramic/metal joining (alumina to Kovar™)
  - Redox reaction aids wetting of ceramic

$$4\,Al_2O_3 + 3\,Zr \rightleftharpoons 3\,ZrO_2 + 4\,Al$$

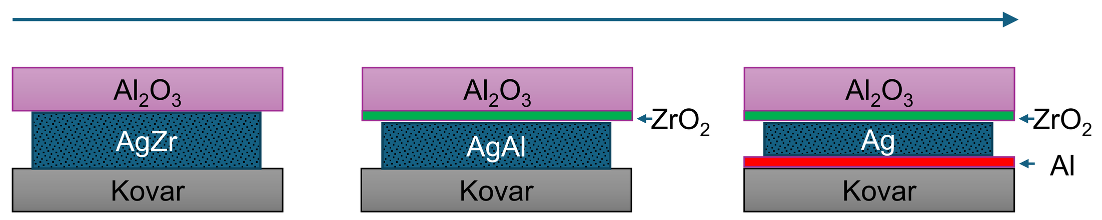
- Braze run-out causes parts to be scrapped
  - Physical origins unclear
  - Possible wetting transition
  - Likely brought on by Al in braze alloy



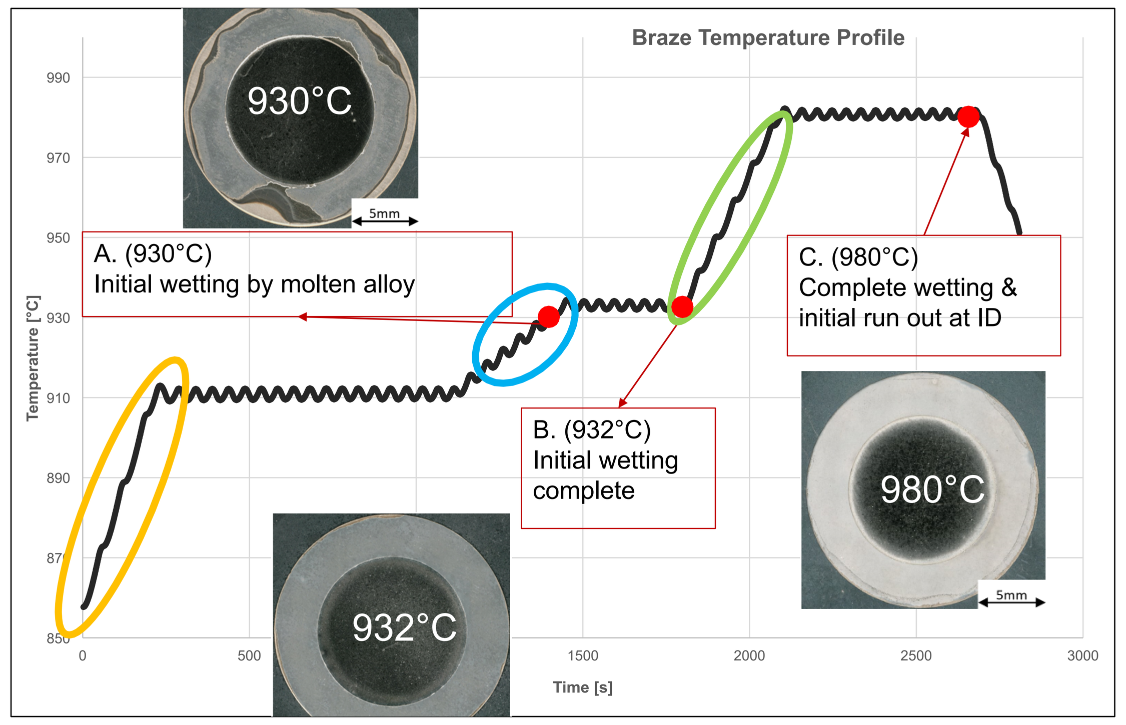


P. Vianco et al. Welding Journal, 97 (2018)

Schematic of Process



Ramp/Hold Temperature Profile

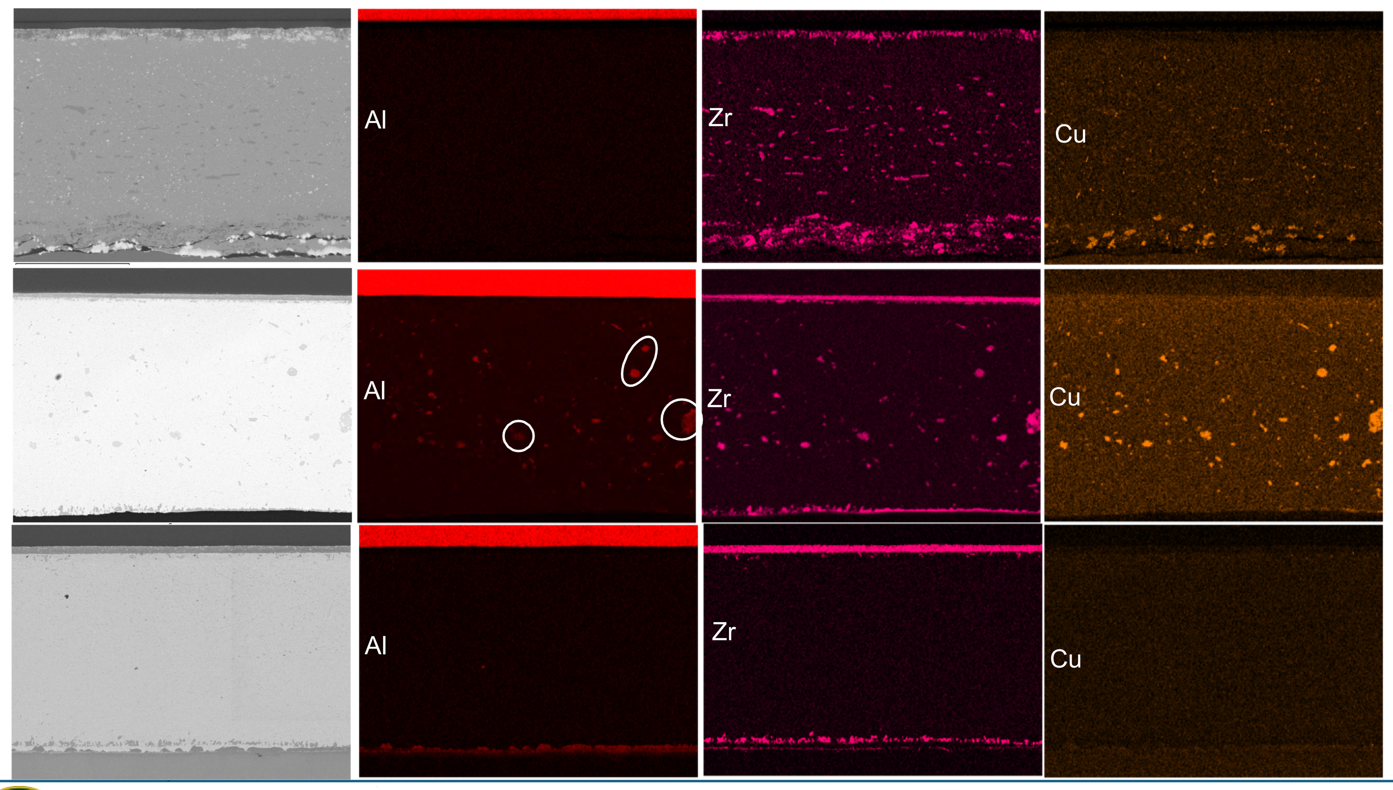


EDS of quenched samples

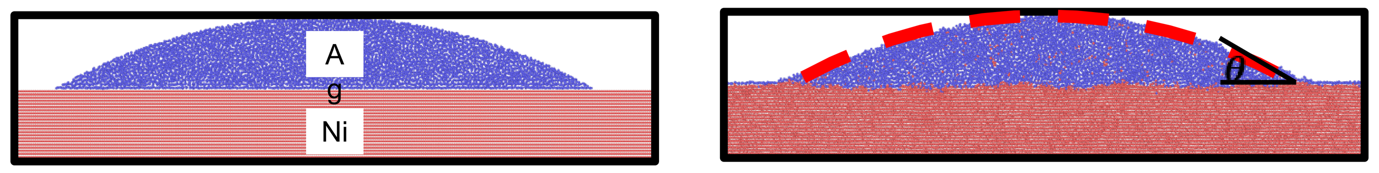
930°C initial wetting

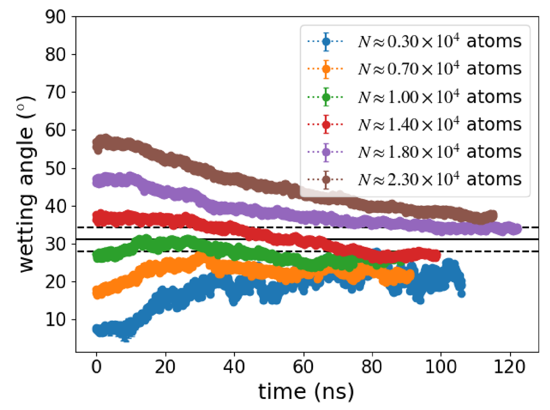
932°C after hold

980°C complete wetting

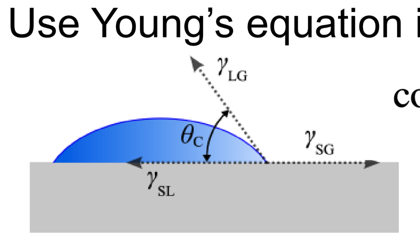


Wetting Simulations with Molecular Dynamics (sample system)



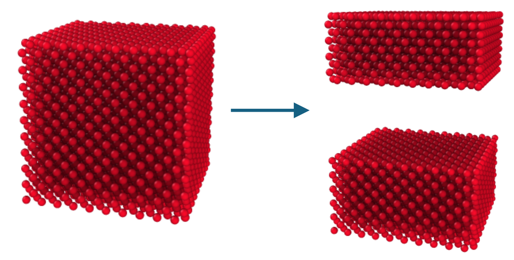


- Metal with ceramic requires reactive potential.
- Developed new reaxFF potential
- Too slow to run for 100 ns
- Use Young's equation instead

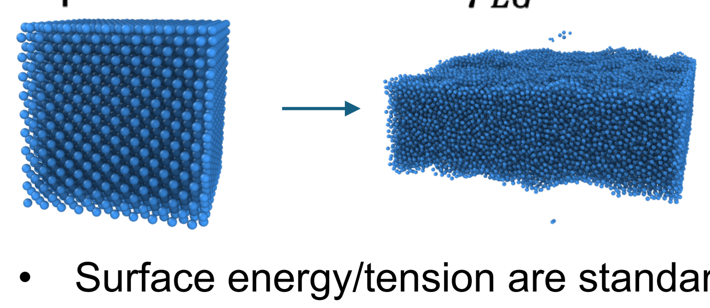


$$\cos\theta = \frac{\gamma_{SL} - \gamma_{SV}}{\gamma_{LV}}$$

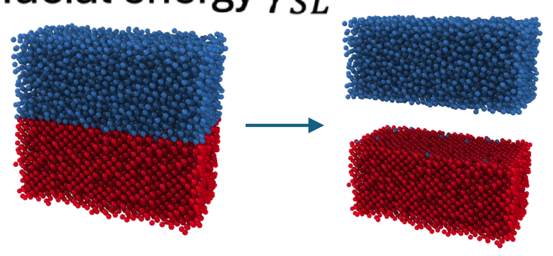
Solid surface energy γ_{SG}



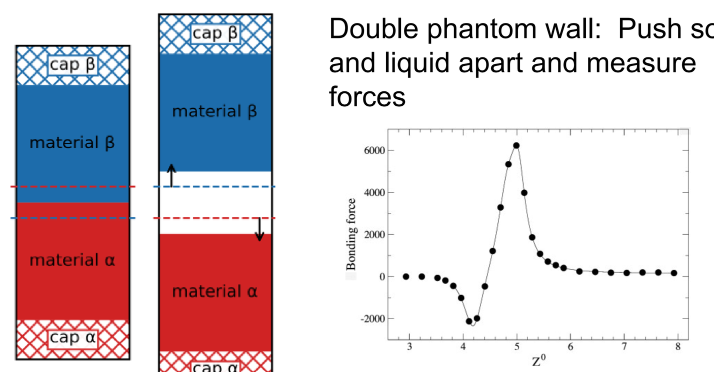
Liquid surface tension γ_{LG}



Interfacial energy γ_{SL}

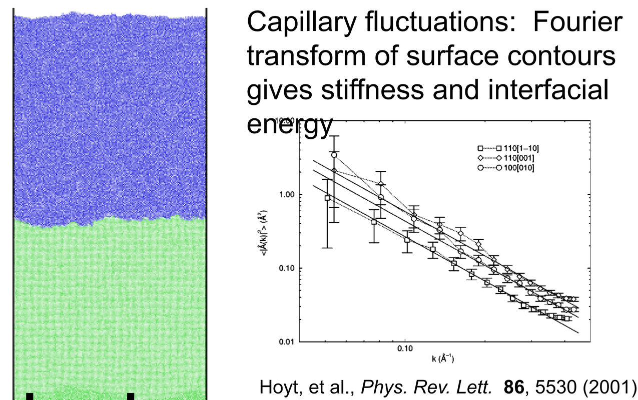


- Surface energy/tension are standard calculations
- Solid/liquid interfacial energy is more difficult
- Using two methods
  - Double phantom wall
  - Capillary fluctuations



Double phantom wall: Push solid and liquid apart and measure forces

Lacey & Muller-Plathe, J. Chem. Phys. 133, 044110 (2010)



Capillary fluctuations: Fourier transform of surface contours gives stiffness and interfacial energy

Hoyt, et al., Phys. Rev. Lett. 86, 5530 (2001)

Creating Constitutive Equations from Molecular Dynamics

- Model forms for wetting angle (θ) and surface tension (σ)
- $\Theta = w_0 + w_1 t + w_2 y + w_3 y^2 + w_4 y t$

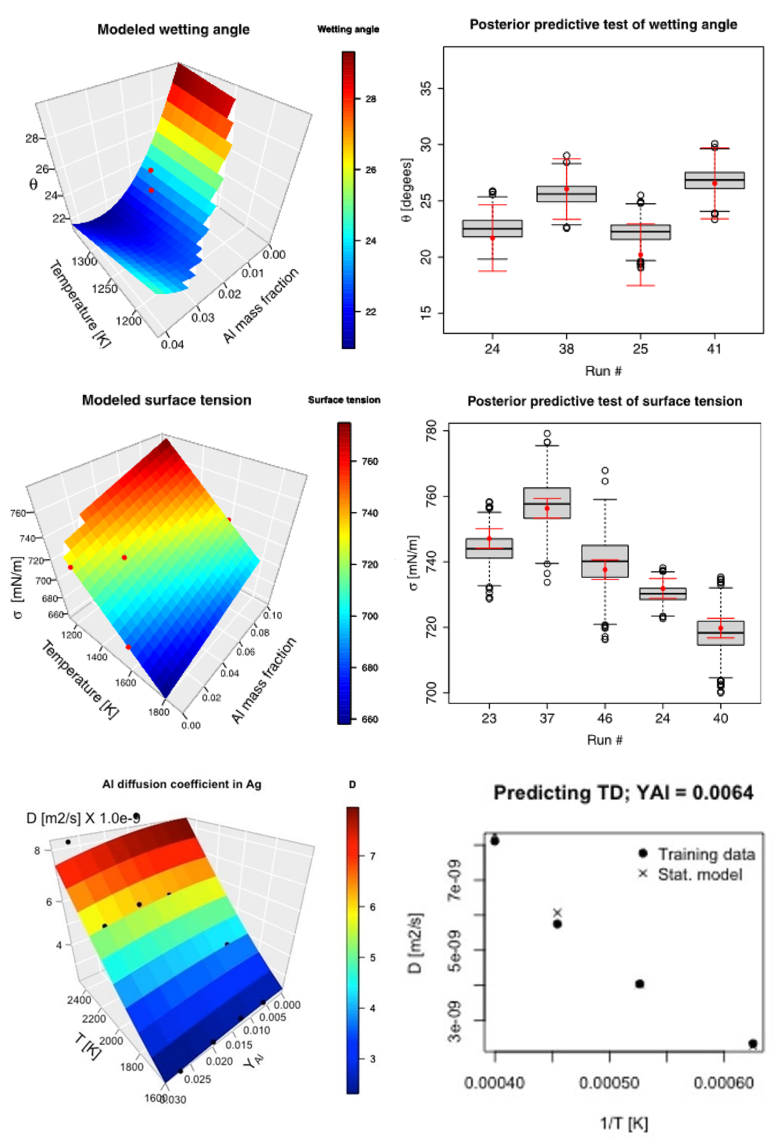
$$\Theta = \frac{\theta - \mu_\theta}{\sigma_\theta};\ t = \frac{T - \mu_T}{\sigma_T};\ y = \frac{Y_{Al} - \mu_Y}{\sigma_Y}$$

$$\sigma = aT + bY_{Al} + cT^2$$

- Several runs were not included in training data set for posterior predictive analysis
- Predictions showed good agreement with excluded data indicating reliability of the model
- Model form for diffusivity (Arrhenius):

$$D(Y,T) = D_0(Y)\,e^{T_0/T}$$

- T_0 = -5732, ln(D_0) = -16.31 – 128.2 * Y_{Al}^2
- 128.2 is uncertain, p value = 0.05, R^2 = 0.9895



Finite Element Modeling: Details

- Conformal decomposition with arbitrary Lagrangian-Eulerian mesh
- Alloy/atmosphere interface uses level set (ϕ)

$$\frac{\partial\phi}{\partial t} + \vec{v}\cdot\nabla\phi = 0$$

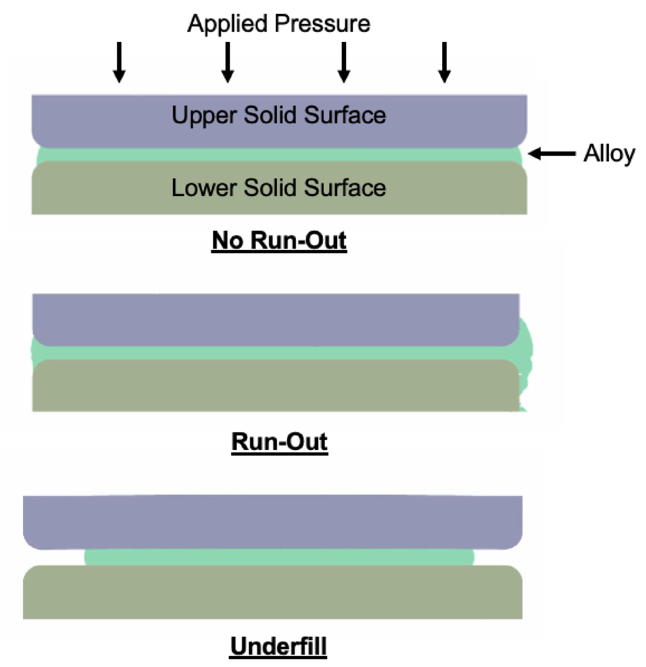
- Slip boundary condition with wetting angle (θ)

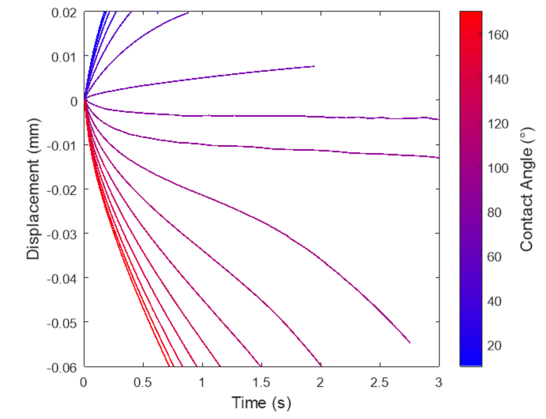
$$\vec{t}_w \cdot \bar{\bar{T}} \cdot \vec{n}_w = \frac{\mu\beta}{\Delta x}(\vec{v}_w - \vec{v})\cdot\vec{t}_w$$
$$\vec{f}_\theta = \gamma(\vec{t}_w \cos\theta + \vec{n}_w \sin\theta)$$

- Surface tension (γ) is additional liquid/atmosphere boundary condition

$$\vec{n}_{int}\cdot(\bar{\bar{T}}_l + \bar{\bar{T}}_g) = -\gamma\vec{n}_{int}\nabla\cdot\vec{n}_{int}$$

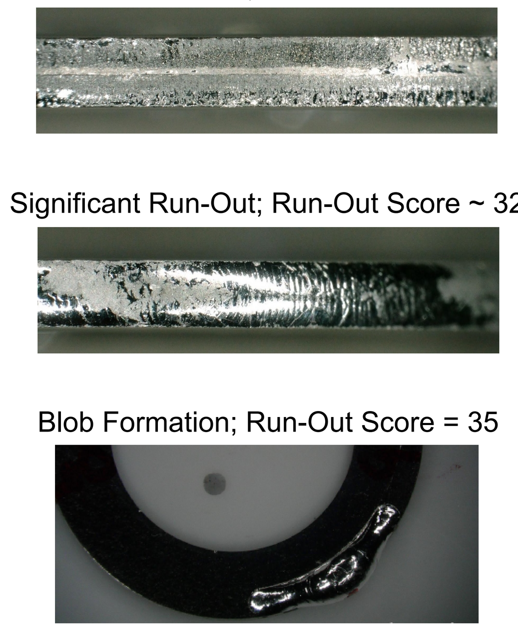
- Runout is defined as displacement of the top surface by > 10%



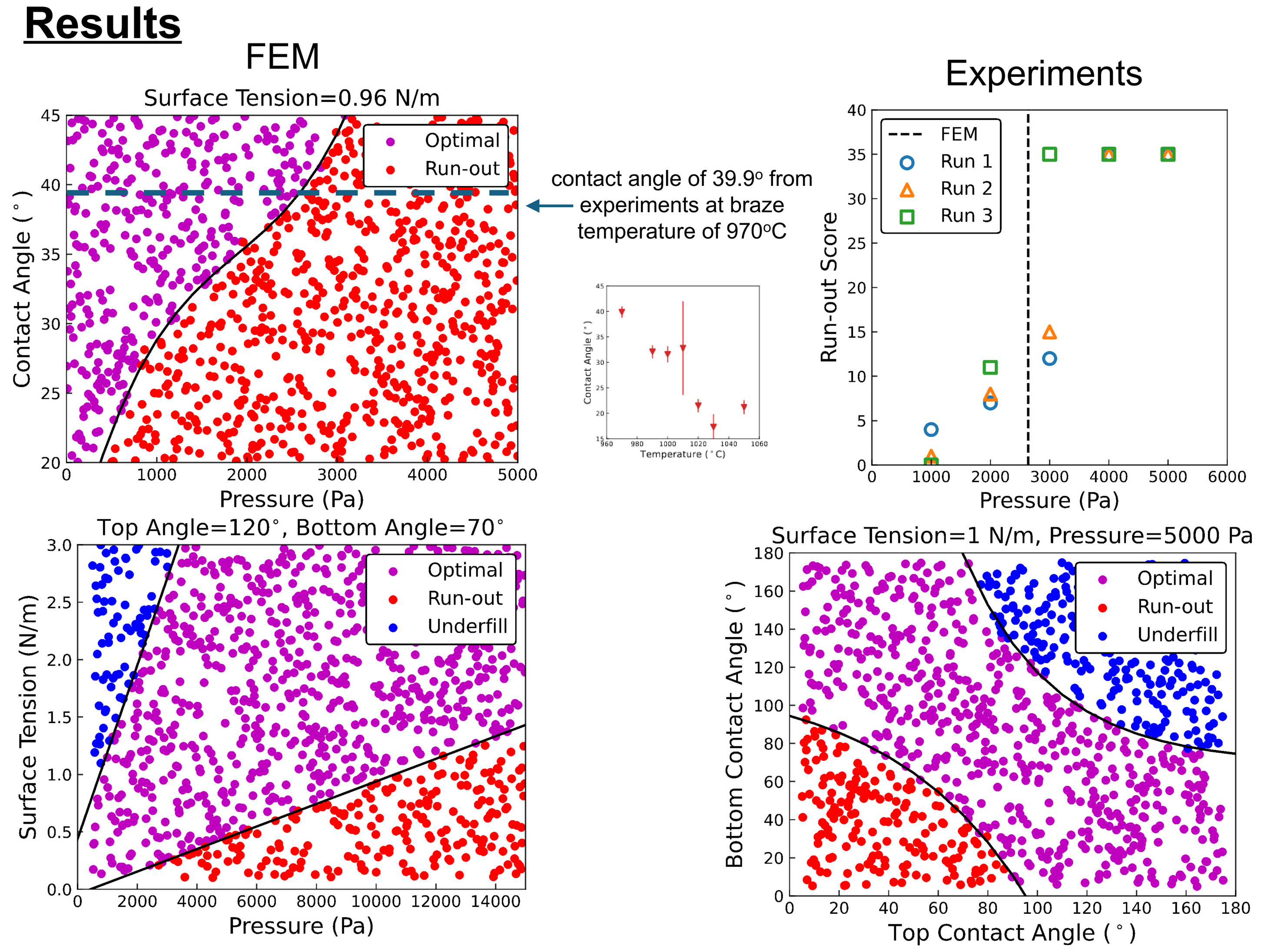


Experimental Validation

- Experimental measurement of wetting angle of silver on Kovar™
- Quantified by summing observations at 32 regions of the edge
  - 1 = runout
  - 0 = no runout
- Full runout arbitrarily set to 35



Results



- FEM results match experiments well
- Boundary is linear with surface tension, curved with surface tension
- Currently working to include results from new, more accurate MD simulations

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