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Pacific Northwest
NATIONAL LABORATORY

Simulations of Coarse-grained Materials

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CIVA North American User Group Meeting, August 19, 2020

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Carol Nove, NRC COR

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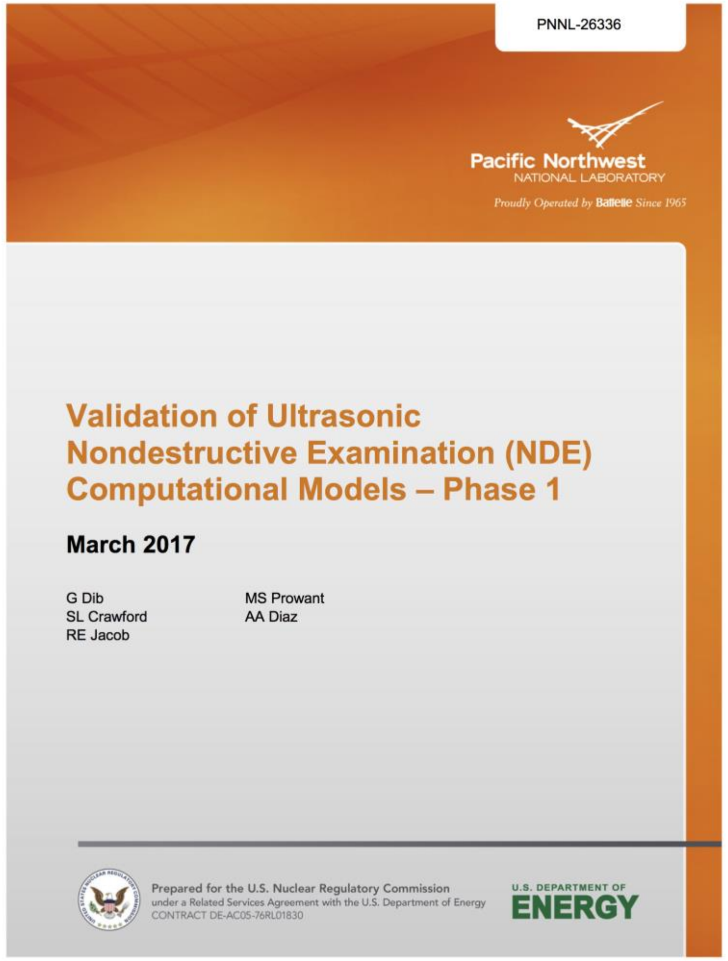
Purpose

Goal of this Research: Provide a solid technical basis to guide NRC staff in conducting, interpreting, and applying ultrasonic modeling to assess the effectiveness of inspections of NPP components.

This presentation will focus on PNNL's recent work to evaluate the usability of CIVA for predicting beam coverage in granular structures, such as austenitic welds and cast austenitic stainless steel.

Recent PNNL Reports on Modeling and Simulation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Validation of Ultrasonic Nondestructive Examination (NDE) Computational Models – Phase 1

March 2017

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RE Jacob
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AA Diaz

Prepared for the U.S. Nuclear Regulatory Commission
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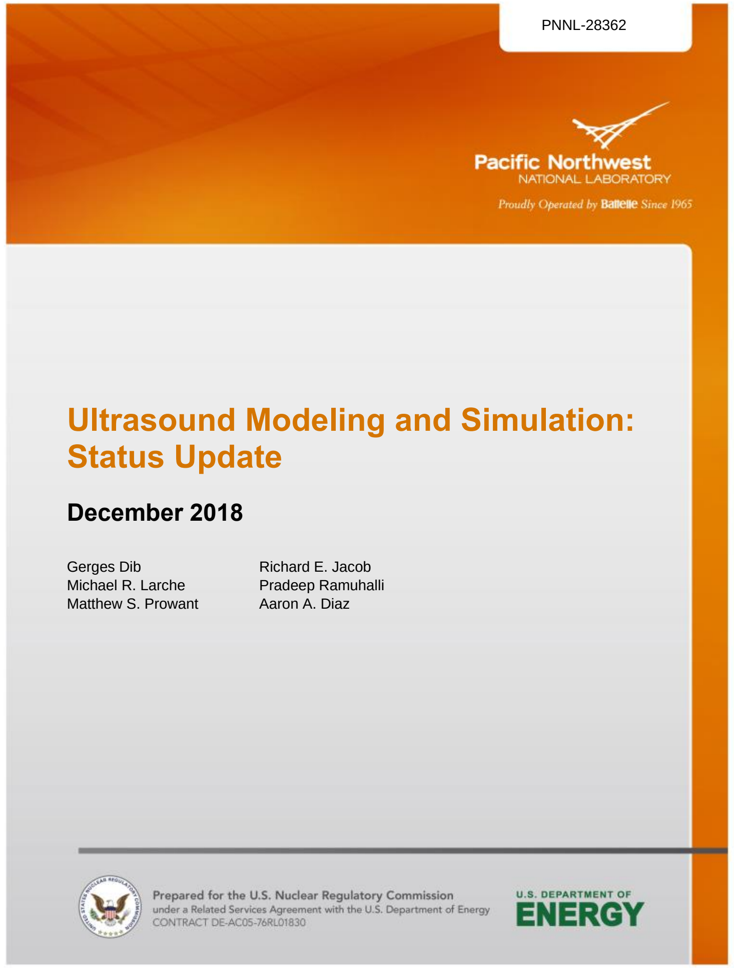
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Ultrasound Modeling and Simulation: Status Update

December 2018

Gerges Dib
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PNNL-29899

Modeling and Simulation of Austenitic Welds and Coarse-grained Specimens

May 2020

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Reports are freely available from https://adams.nrc.gov/wba/

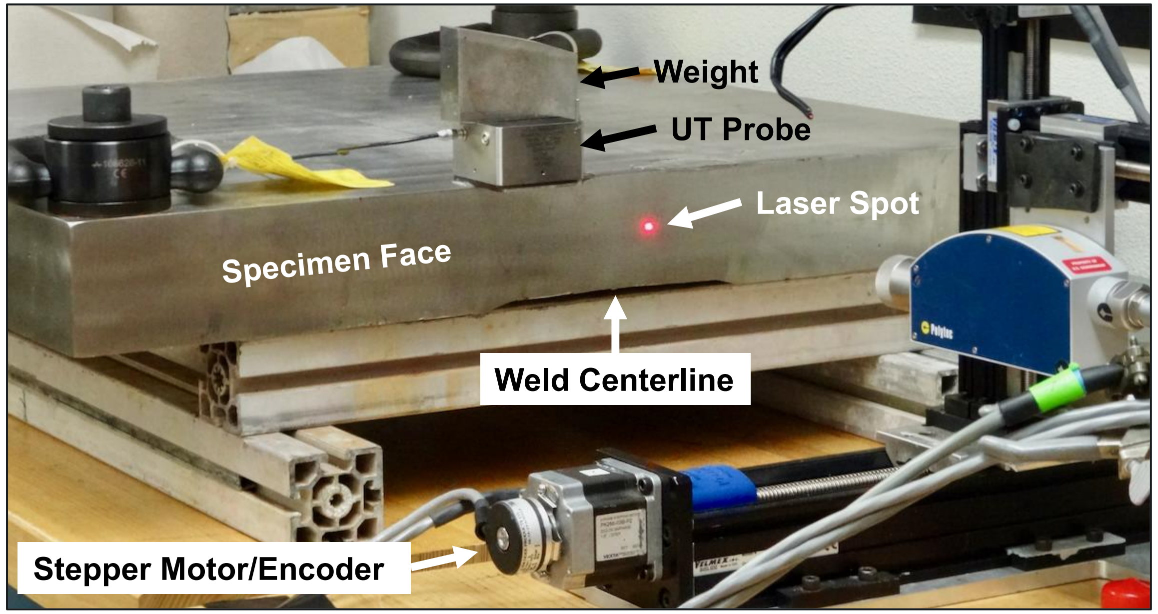
Approach

- Generate realistic models of austenitic welds and coarse-grain materials, including crystalline orientations (Euler angles).
- Evaluate beam simulations in CIVA, and compare results to empirical beam maps.
- Compare the beam simulations from realistic specimen models to those from simple structural models that are included with CIVA.

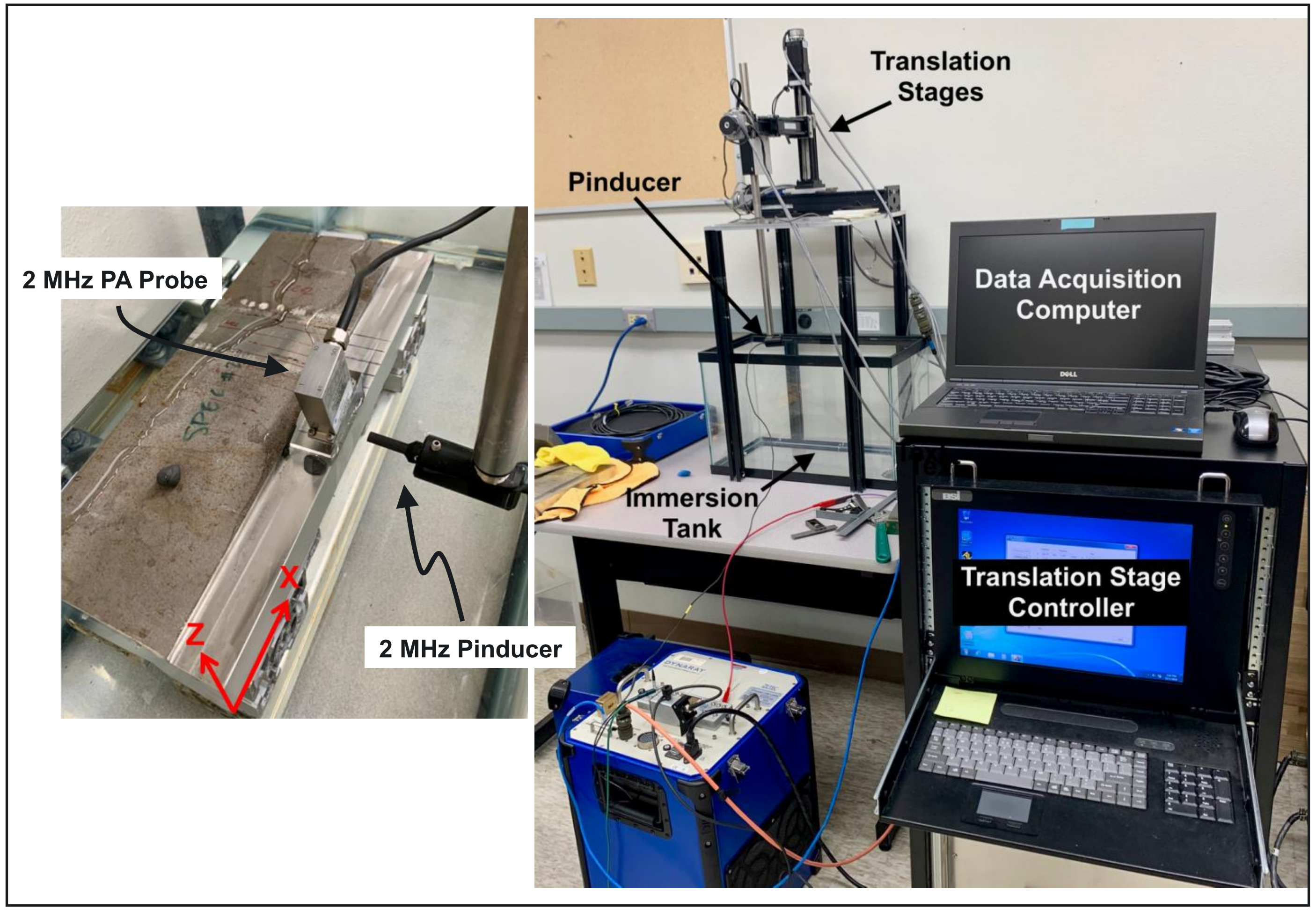
Effects of Weld Microstructure on Ultrasonic Beams: Empirical Measurements

- Beam maps were acquired on several stainless steel specimens through welds and through parent material.
- Beam maps were acquired with a laser vibrometer or with a pinducer in an immersion tank.

Laser Vibrometer

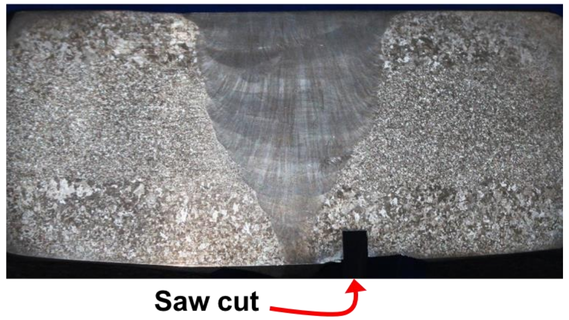


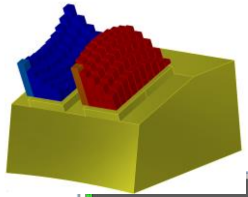
Immersion Tank



Empirical Beam Maps

- Wrought-to-wrought specimen, 36 mm thick
- Images acquired through parent material (left) and through a weld (right)
- 2 MHz TRL probes with 36 mm focal depth and 45° or 60° refraction angle – laser vibrometer
- 2 MHz PA probe with 24 mm focal depth and 30°, 45°, and 60° focal laws – immersion tank



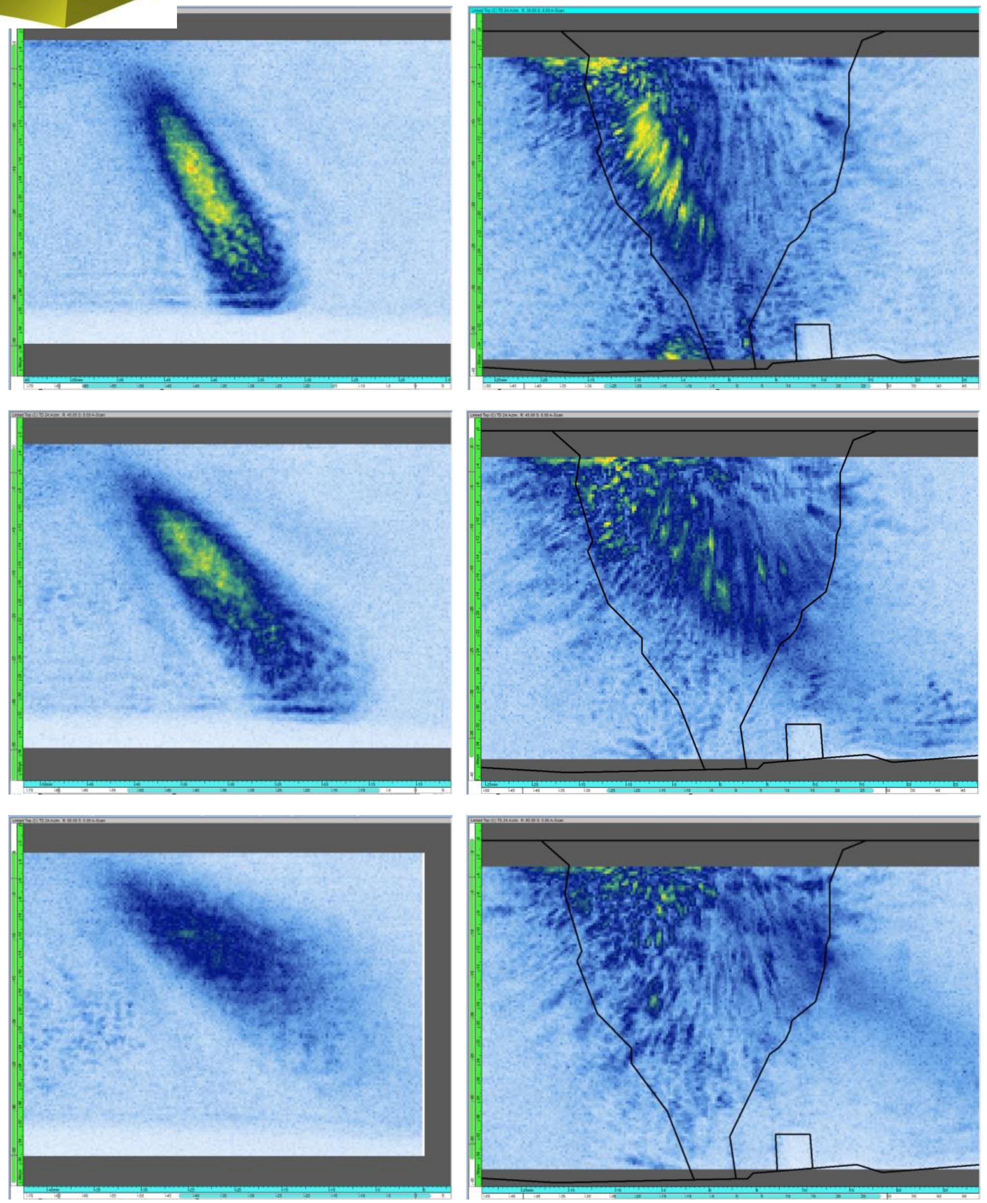


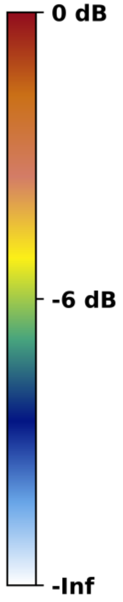
PA Probe

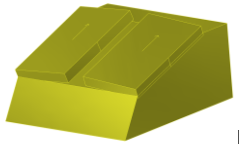
30°

45°

60°



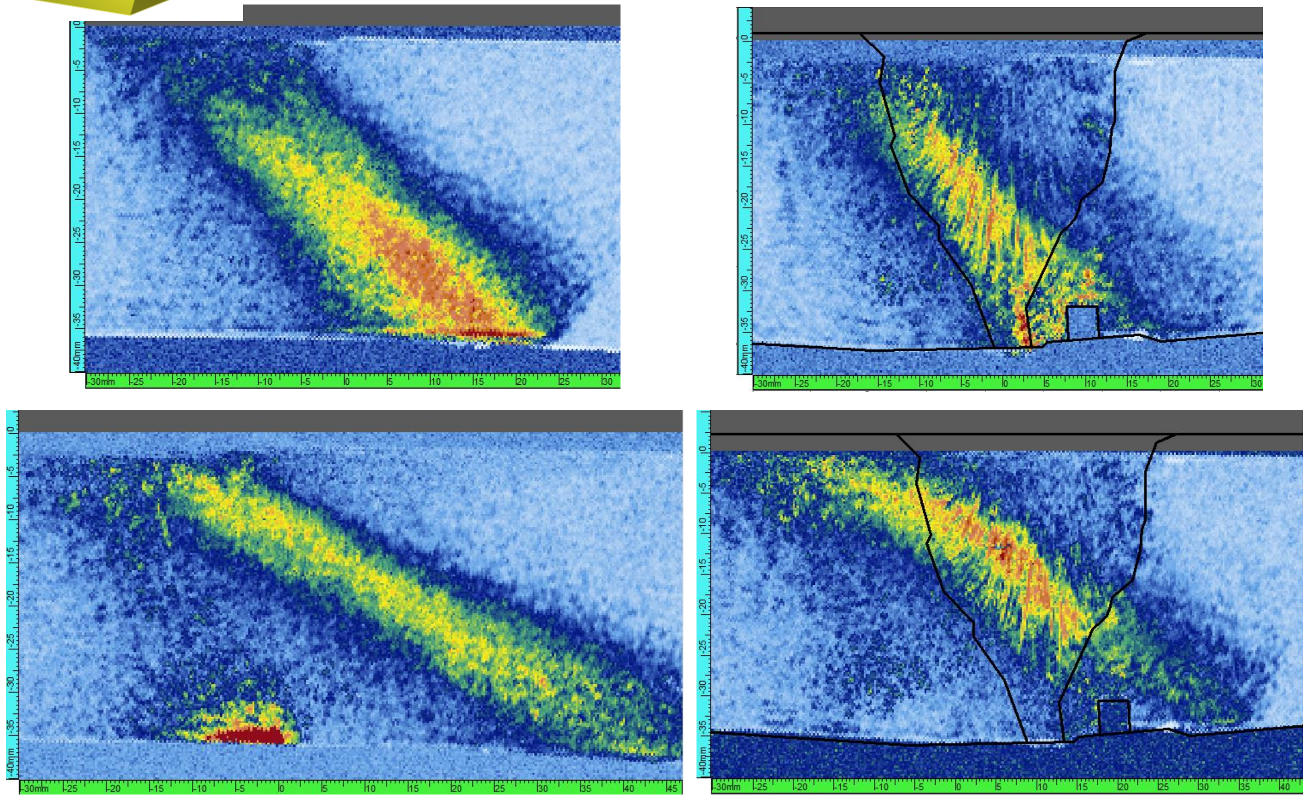




TRL Probes

45°

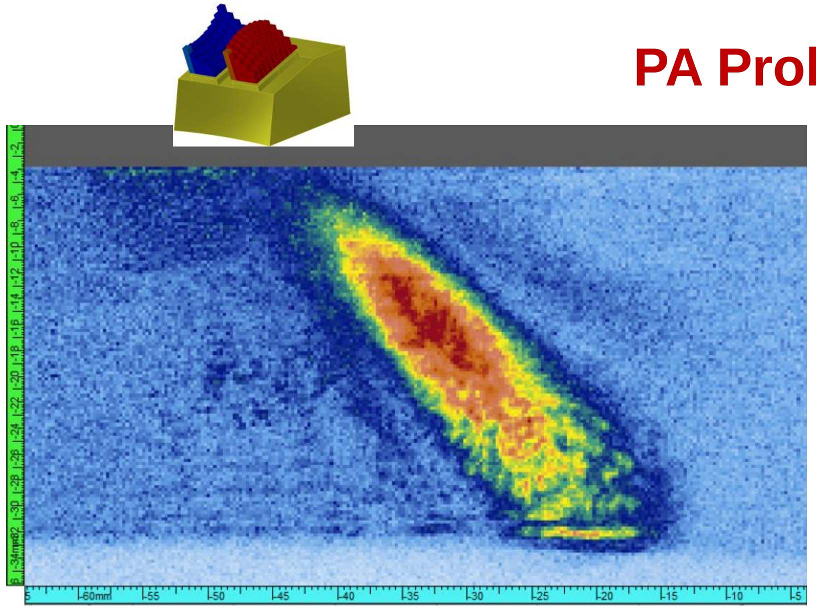
60°

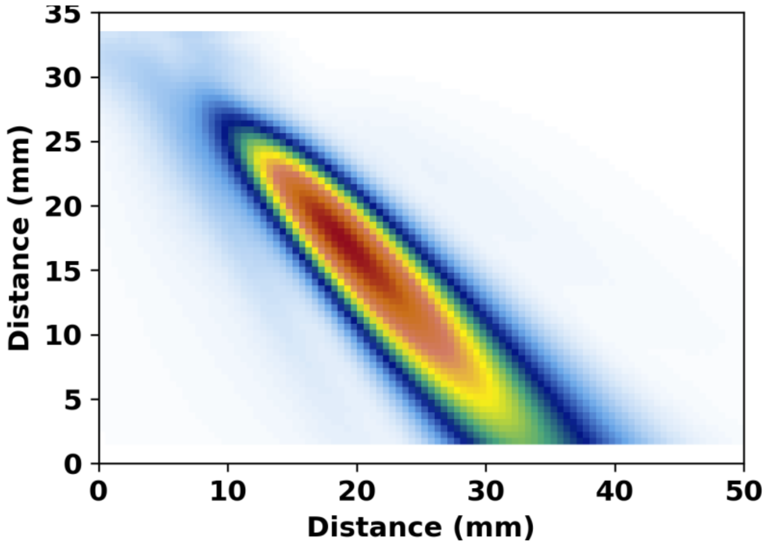


Qualitative Comparison of Simulated and Empirical Beam Maps

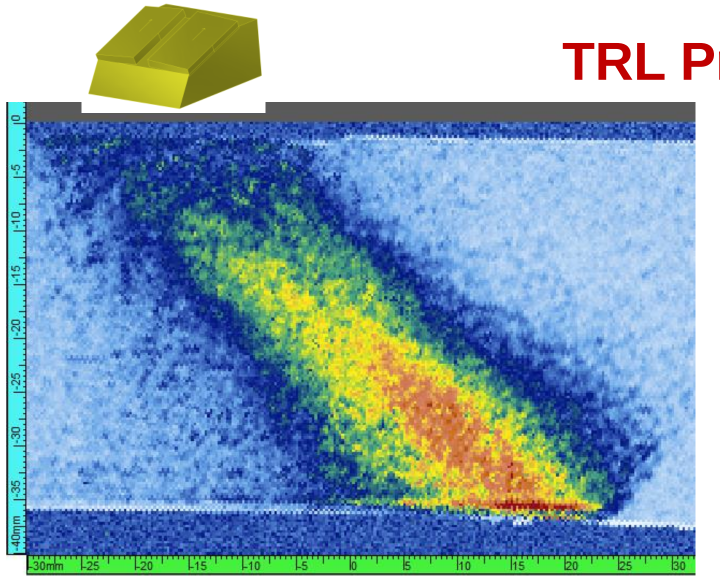
- Empirical beam maps (left) were acquired through wrought stainless steel.
- CIVA simulations (right) used a “simple isotropic” specimen model.
- Probe and specimen parameters from the empirical work were used in CIVA.
- Results show strong qualitative similarities between the scans and the simulations.

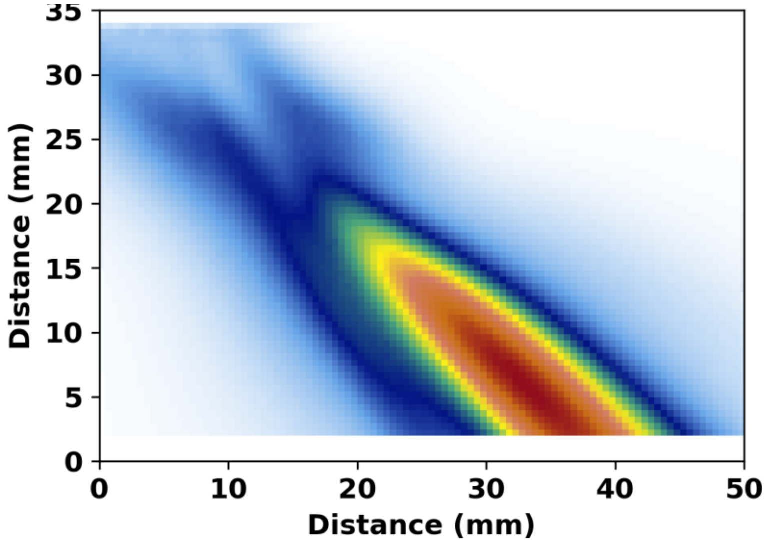
PA Probe, 45°





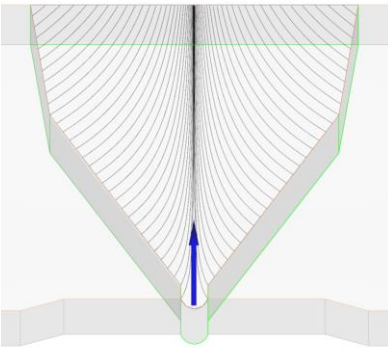
TRL Probe, 45°





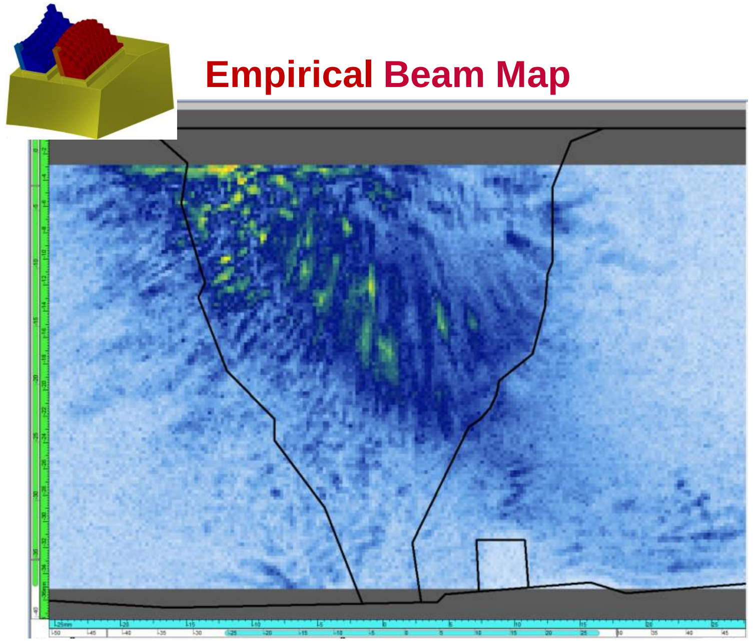
The Ogilvy Weld Model for Austenitic Beam Simulations

- The Ogilvy model is commonly used to approximate grain structures in austenitic welds because it is easy to implement and it simulates some beam redirection.
- However, the Ogilvy model generates grains with smoothly varying crystalline orientations.
- Seven simulations were run with the same Ogilvy model but using different stiffness matrix values taken from the literature.
- The Ogilvy model tends to bend or distort the beam. Beam focusing still occurs, and scatter is not present.

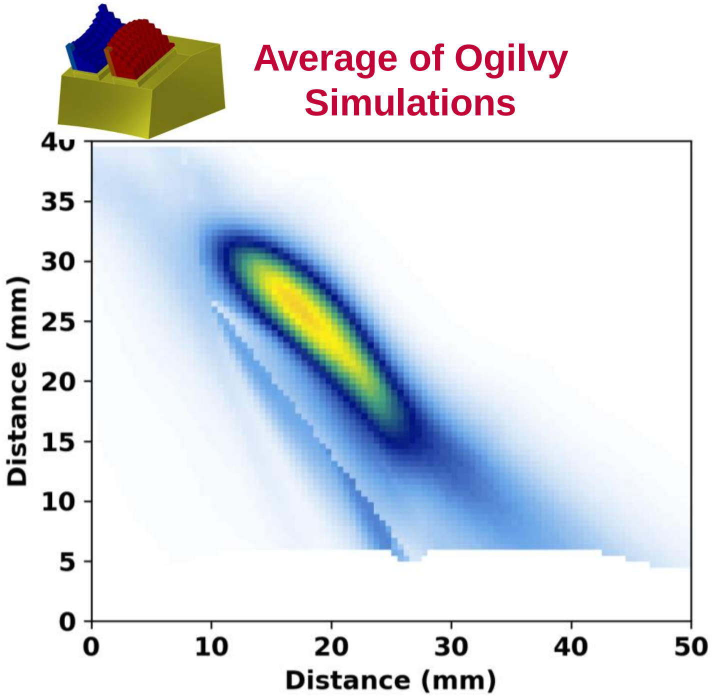


The Ogilvy model used for simulations

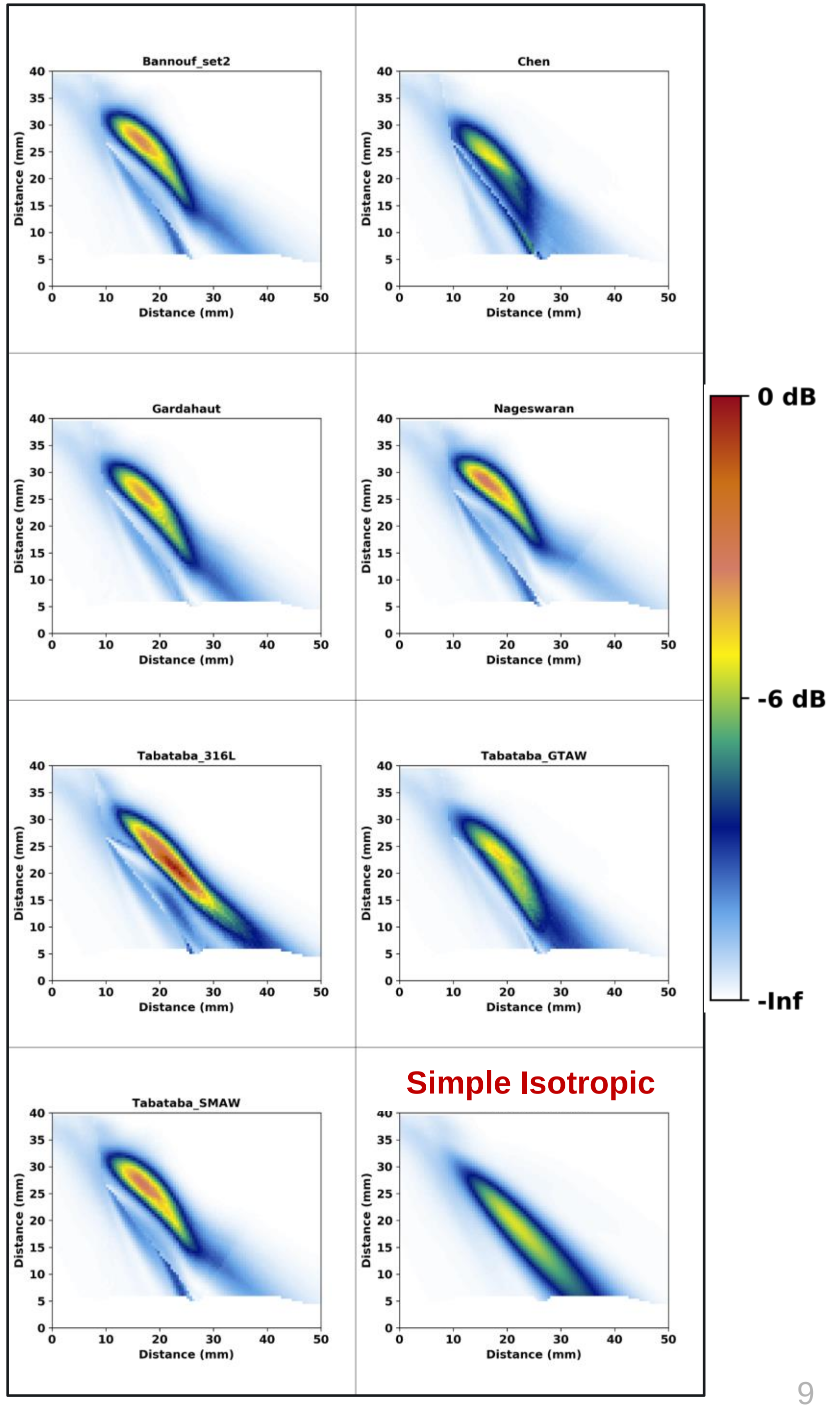
Empirical Beam Map



Average of Ogilvy Simulations



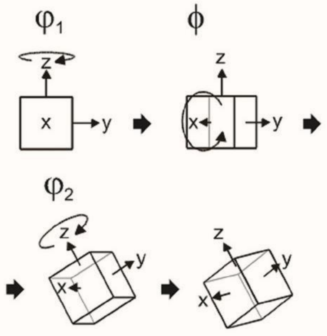
Ogilvy Model Simulations



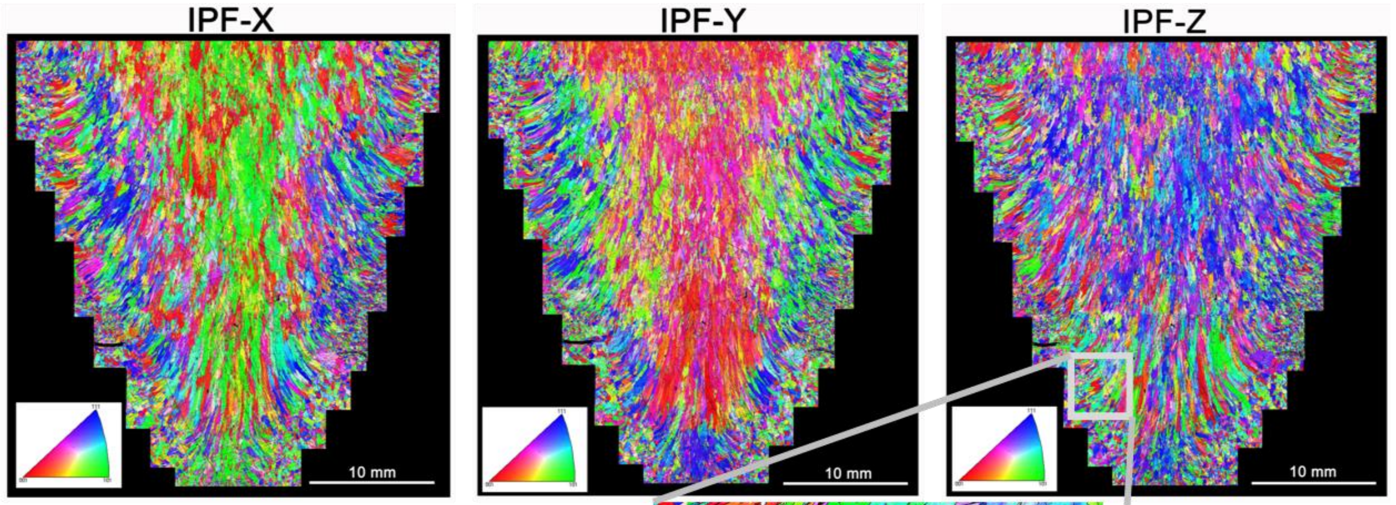
Towards a More Realistic Weld Model

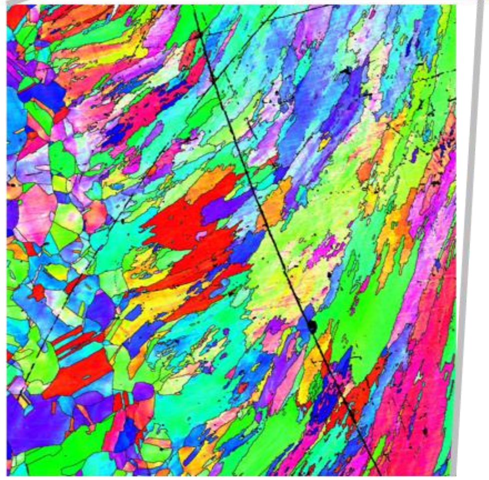
- A more realistic representation of weld microstructure was needed to provide a basis, or true-state, for weld models.
- An austenitic weld sample was polished and etched to characterize the weld microstructure.
- Electron backscatter diffraction (EBSD) was used to measure grain size and orientation.
  - The grain sizes were measured to 4 µm resolution.
  - Grain crystal orientations (Euler angles) were also measured.

Euler angles are used to define grain orientations



Electron Backscatter Diffraction Results



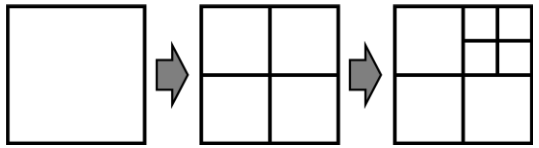


Each color represents a different grain orientation

Weld Photograph

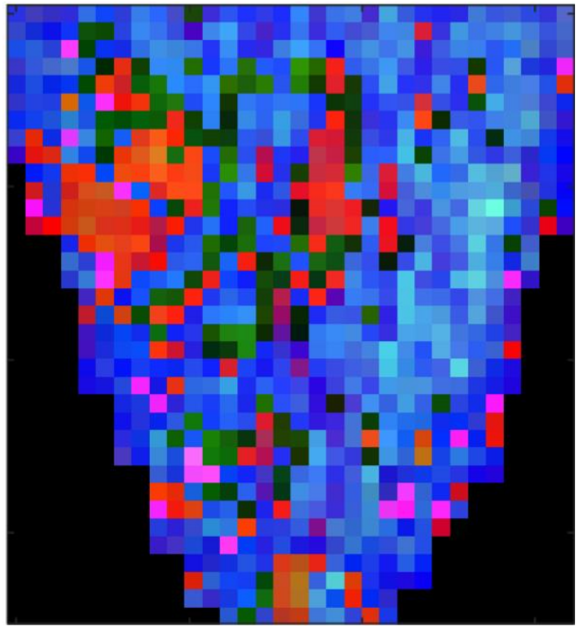
Weld Microstructure Downsampling

- 4 μm resolution is way too high for a specimen model. What grain resolution is required to simulate the weld microstructure with sufficient accuracy while balancing simulation runtime?
- Data were downsampled using a quadtree decomposition to varying levels of resolution (1 pixel = 4 μm):
  - 256 pixels (about 1.2 mm, ≈ 40% λ at 2 MHz),
  - 128 pixels (about 0.6 mm, ≈ 20% λ),
  - 64 pixels (about 0.3 mm, ≈ 10% λ).

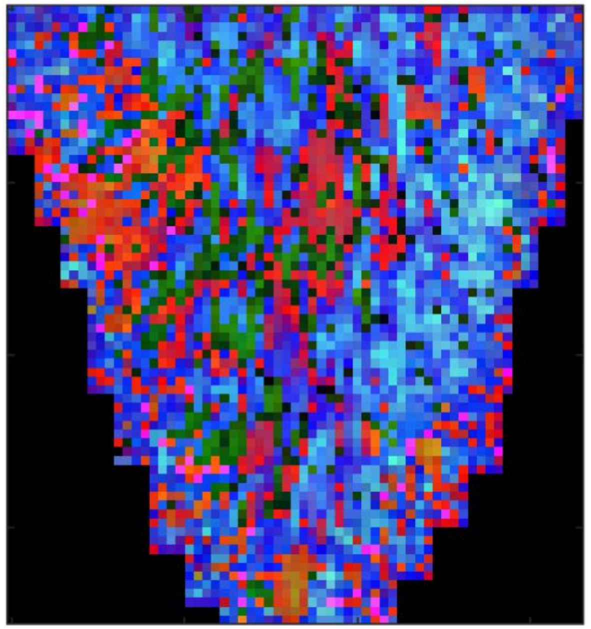


- Several weld cartograms of varying resolution were generated to test simulation sensitivity to weld microstructure parameters. Each color represents a different set of Euler angles.

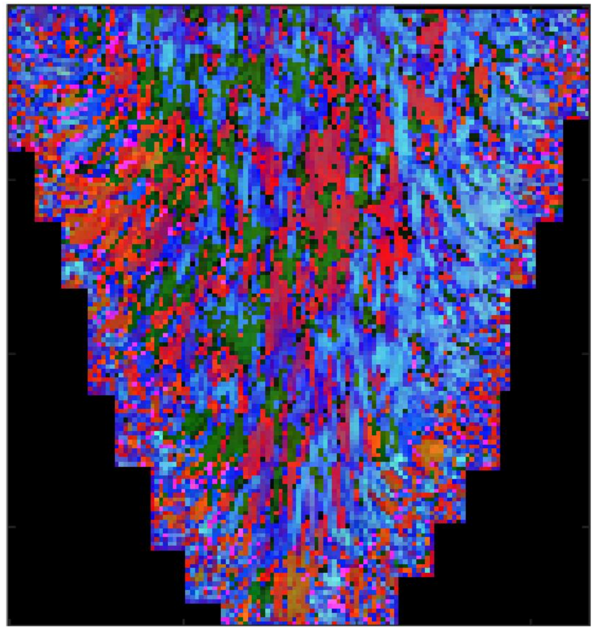
256 pixels (≈1.2 mm)



128 pixels (≈0.6 mm)



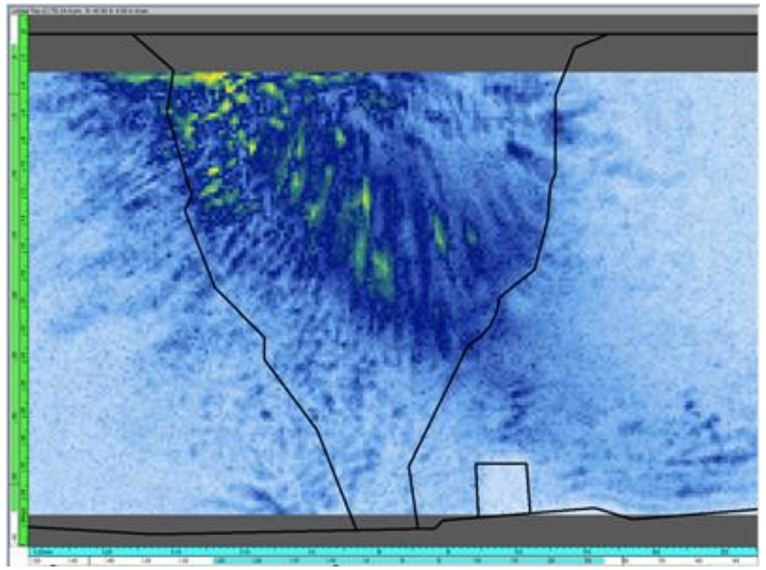
64 pixels (≈0.3 mm)

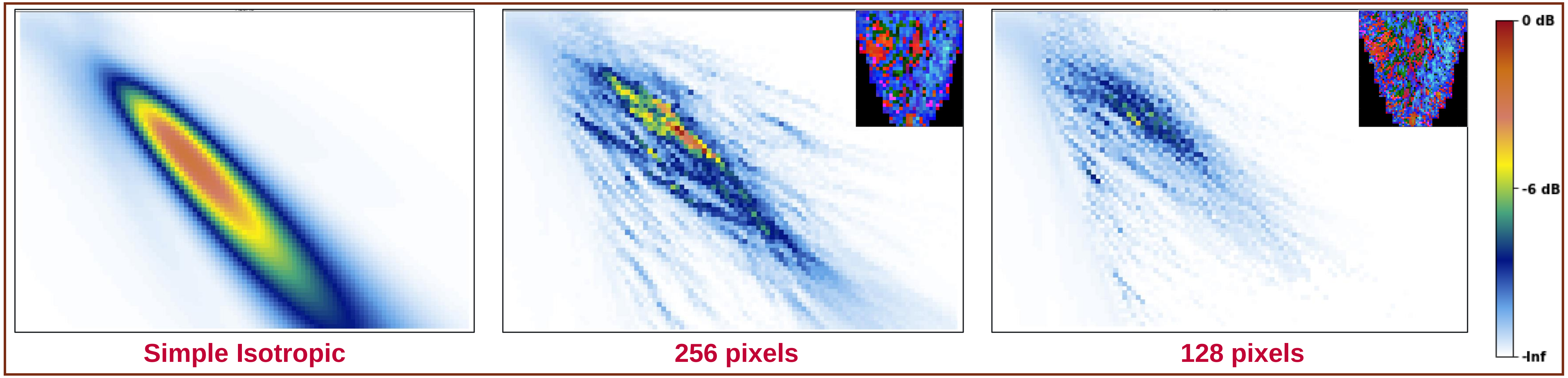


Comparing Beam Simulation Results

- 2 MHz phased-array probe at 45°, 24 mm focal depth
- Empirical and simulated beams show almost no far-side backwall insonification, little insonification of the inner 1/3 inspection volume, and significant beam scatter.
- The empirical beam shows a granular scatter pattern in the weld and significant near-OD scatter, effects not observed in simulation results.
- Identified model shortcomings:
  - 256-pixel grain sizes are too large
  - Mode conversions or interface interactions were not included due to long simulation times
  - Attenuation was not included
  - The 64-pixel model was too complex, the simulation did not finish after >6 weeks

Empirical Scan

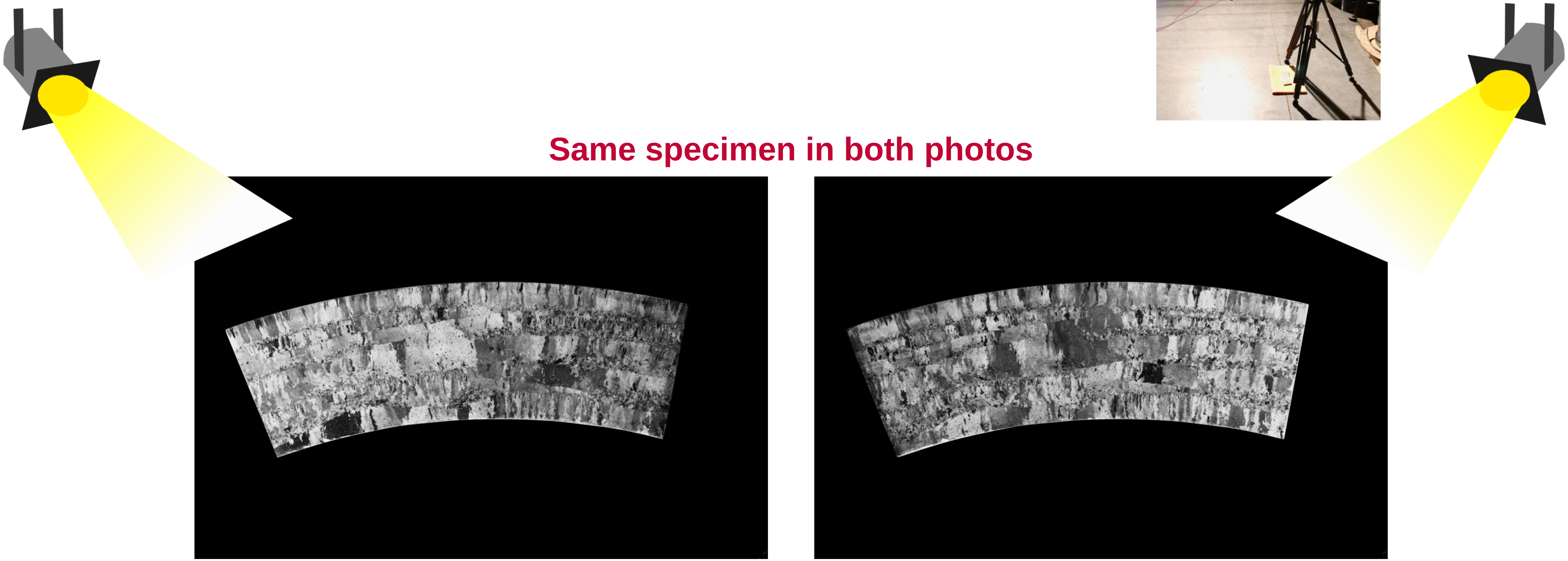




Simulations with Coarse-Grained Materials

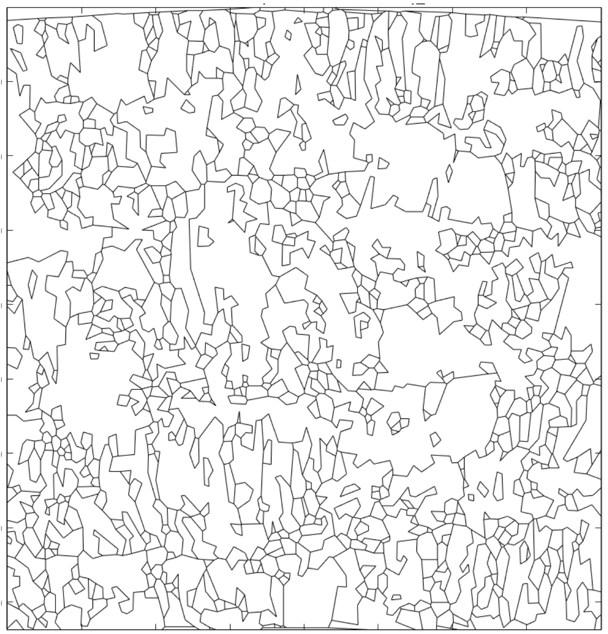
- Simulations in coarse-grained cast austenitic stainless steel (CASS) materials require grain boundary definitions
- Photographs from multiple illumination angles capture the grain boundaries of polished and chemically etched sections
- Appearance of grain reflections depends on incident light angle

Same specimen in both photos

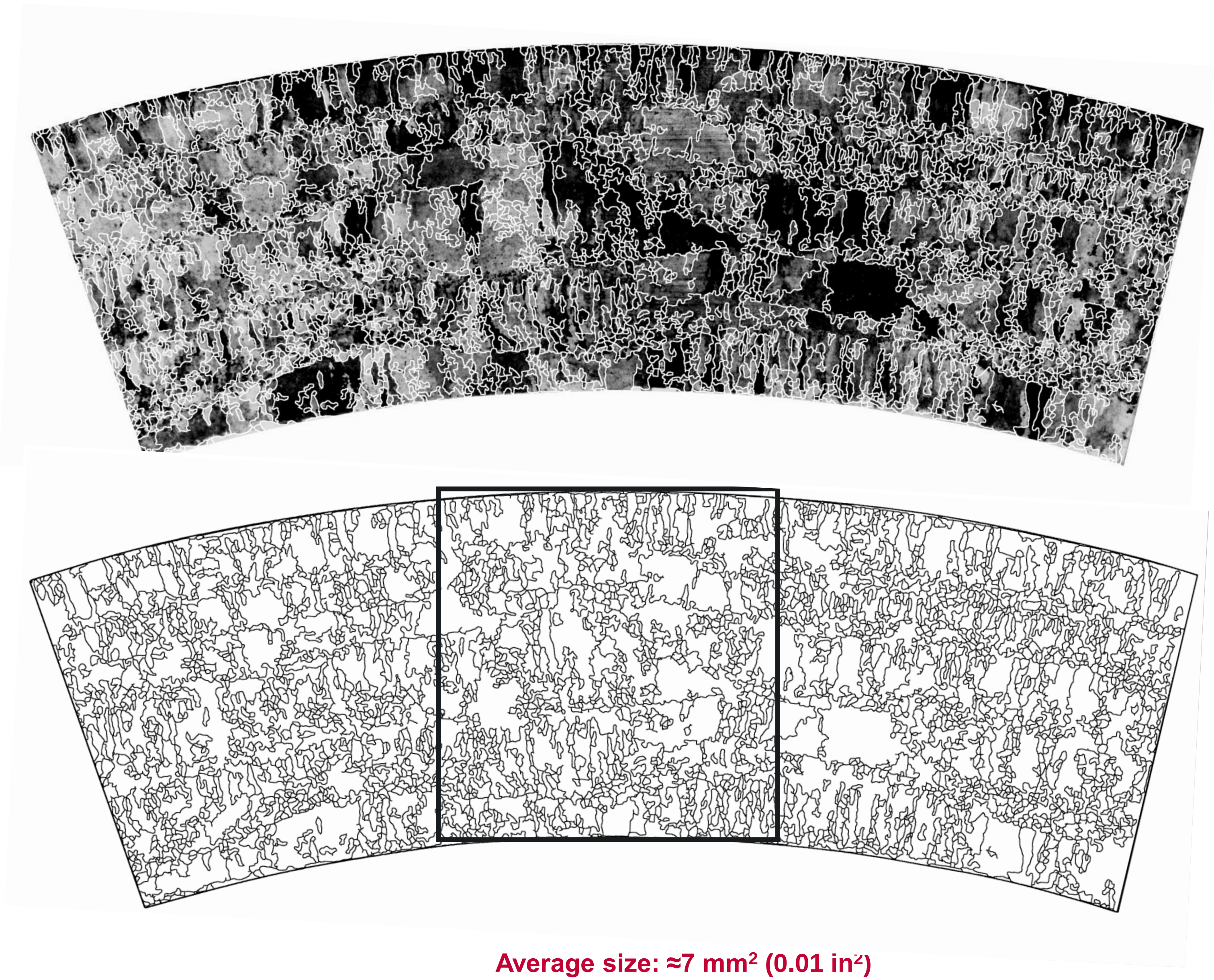


Identify and Outline the Grain Boundaries

- Photos were processed and filtered to highlight and outline grain boundaries.
- Grains smaller than ≈0.5 mm were removed.
- Curved grain boundary outlines were made into straight line segments to generate a 2D CAD file.
- The CAD file can be imported into CIVA.



Subsection of specimen with straight line segments used in simulations

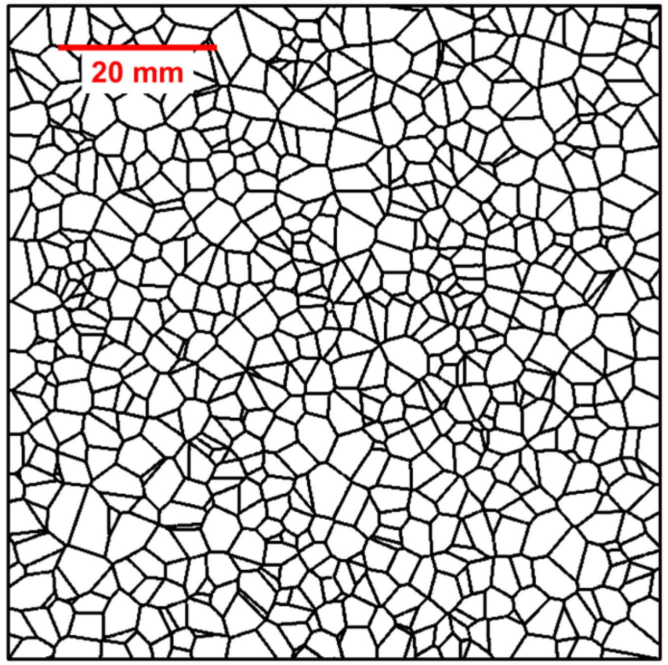


Average size: ≈7 mm^2 (0.01 in^2)
Median size: ≈2 mm^2 (0.003 in^2)

Realistic Geometries vs CIVA-generated Models

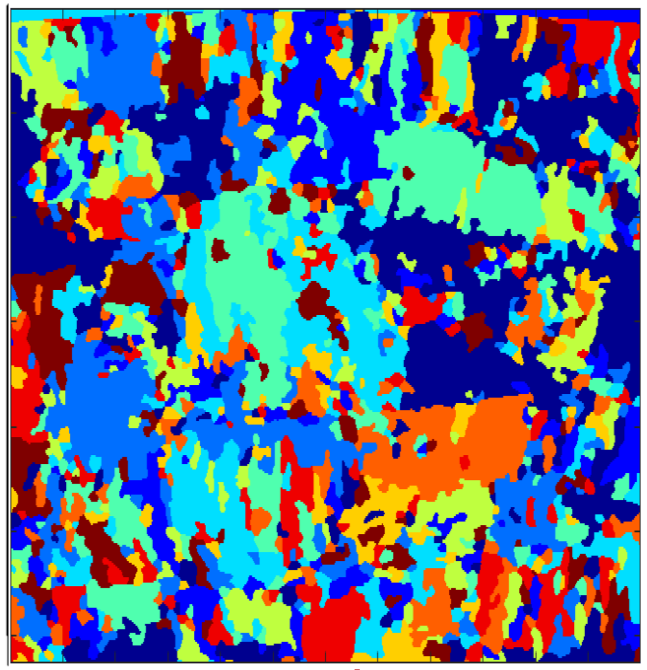
- CIVA can automatically generate random Voronoi regions to imitate coarse-grained geometries.
- The number of Voronoi regions and coarse-grained regions was the same, and both models comprised 2D grains extruded in the third dimension.
- For the coarse-grained model, 10 Euler angles were assigned at random, and stiffness matrix values were taken from the literature.
- CIVA does not assign Euler angles to the Voronoi regions; instead, it assigns different propagation velocities within a selected range.

Voronoi, Equiaxed



Voronoi:
- **810 regions**
- **7 mm^2 avg.**
- **26 mm^2 max.**

Coarse-grain Equiaxed

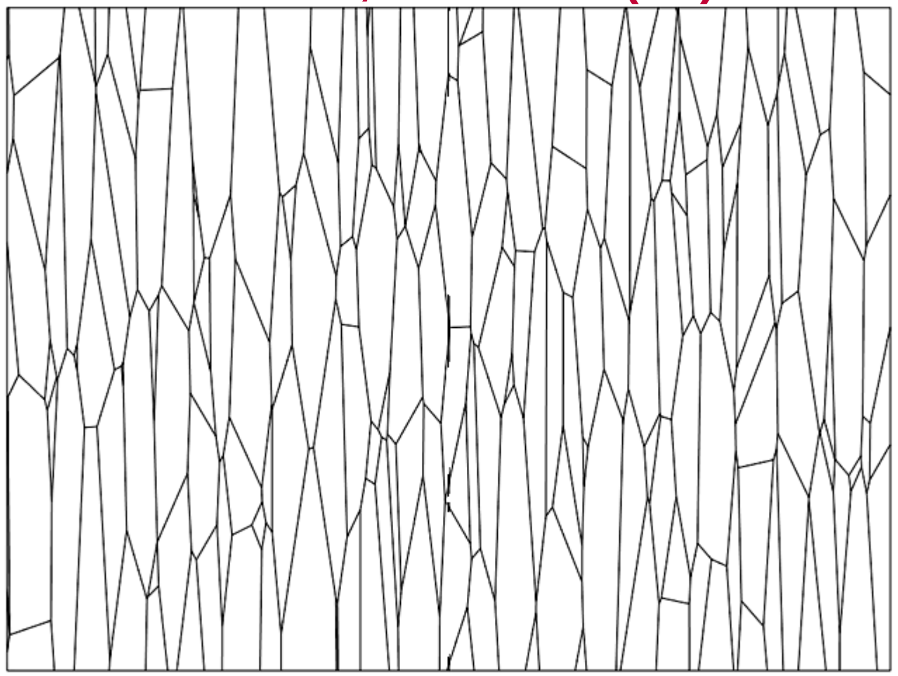


Coarse grain:
- **810 regions**
- **7 mm^2 avg.**
- **430 mm^2 max.**

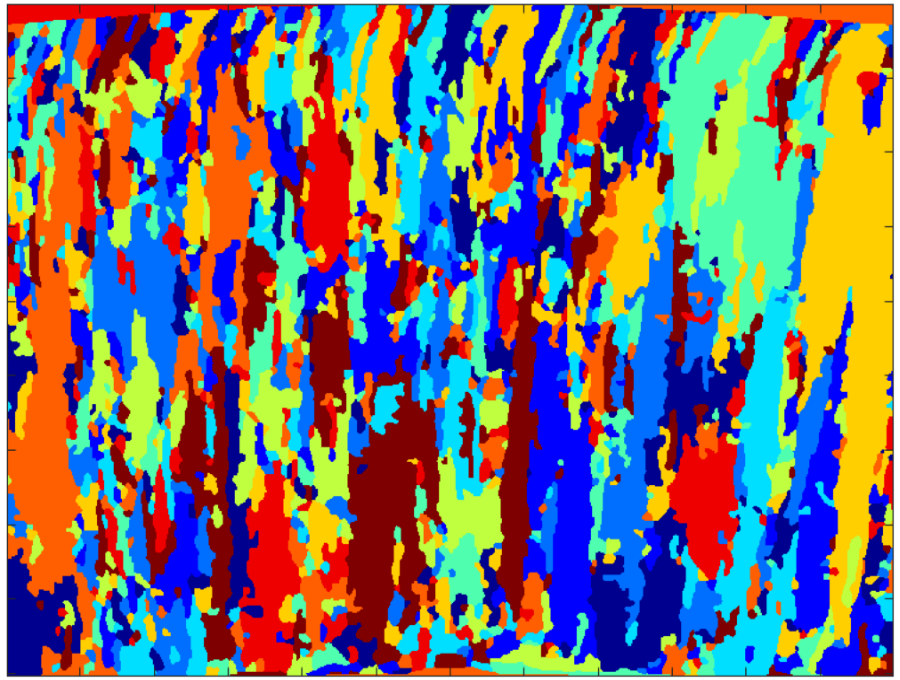
A Columnar Specimen was also Modeled

- A columnar specimen model was generated in the same manner as the equiaxed model.
- The columnar model comprised 2D grains extruded in the third dimension. The Voronoi model comprised 3D grains, because Voronoi regions cannot be elongated in two dimensions in CIVA.
- The number and size of Voronoi regions were approximated.

Voronoi, Columnar (3D)



Columnar (2D)



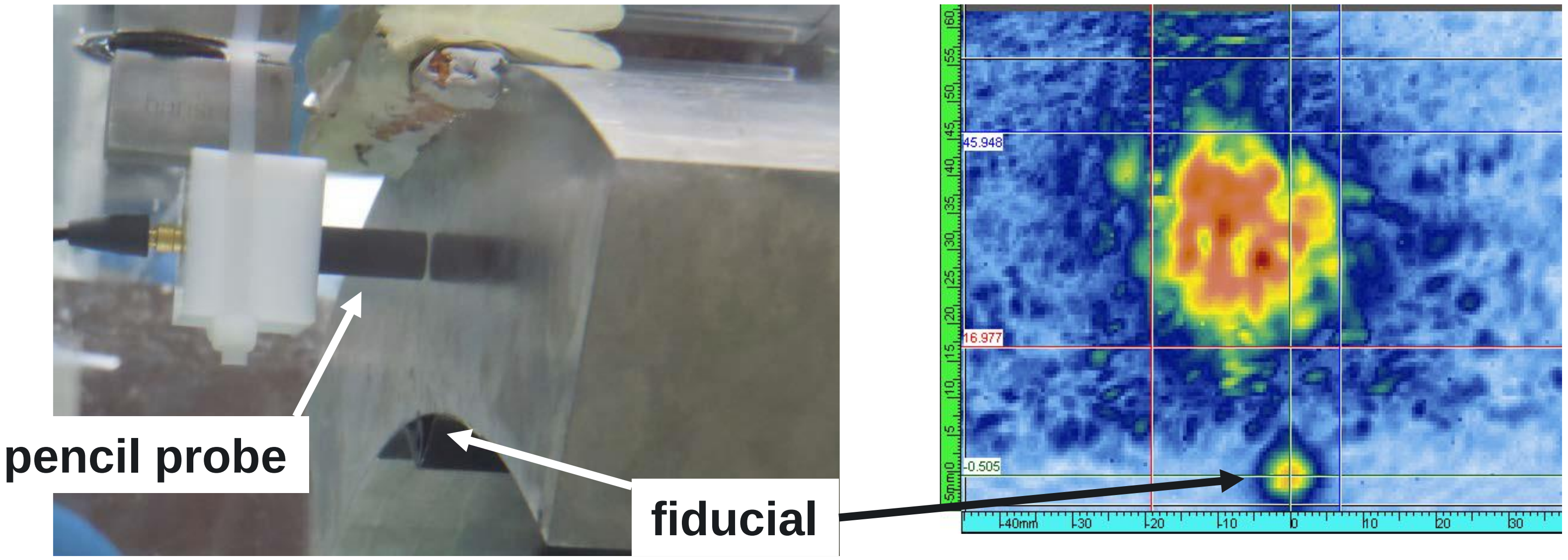
Columnar:

- **1034 regions**
- **5 mm^2 avg.**

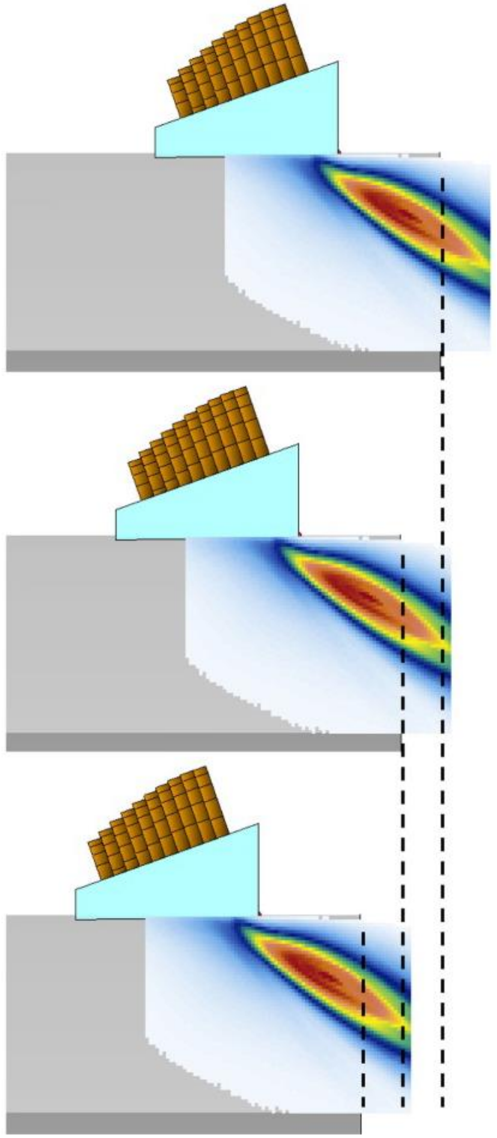
Acquisition of Empirical Beam Maps

- Beam maps were acquired through cast austenitic stainless steel specimens using a pencil probe.
- Serial slicing allowed multiple beam maps to be acquired on each specimen.
- Each slice was polished and etched to reveal the grain structure.
- Two of the slices were used to generate the CASS models.
- Figures and experimental details can be found in Crawford, et al. (2014), “Phased Array Ultrasonic Field Mapping in Cast Austenitic Stainless Steel.” ML14155A165.

Experimental Setup **Beam map example**

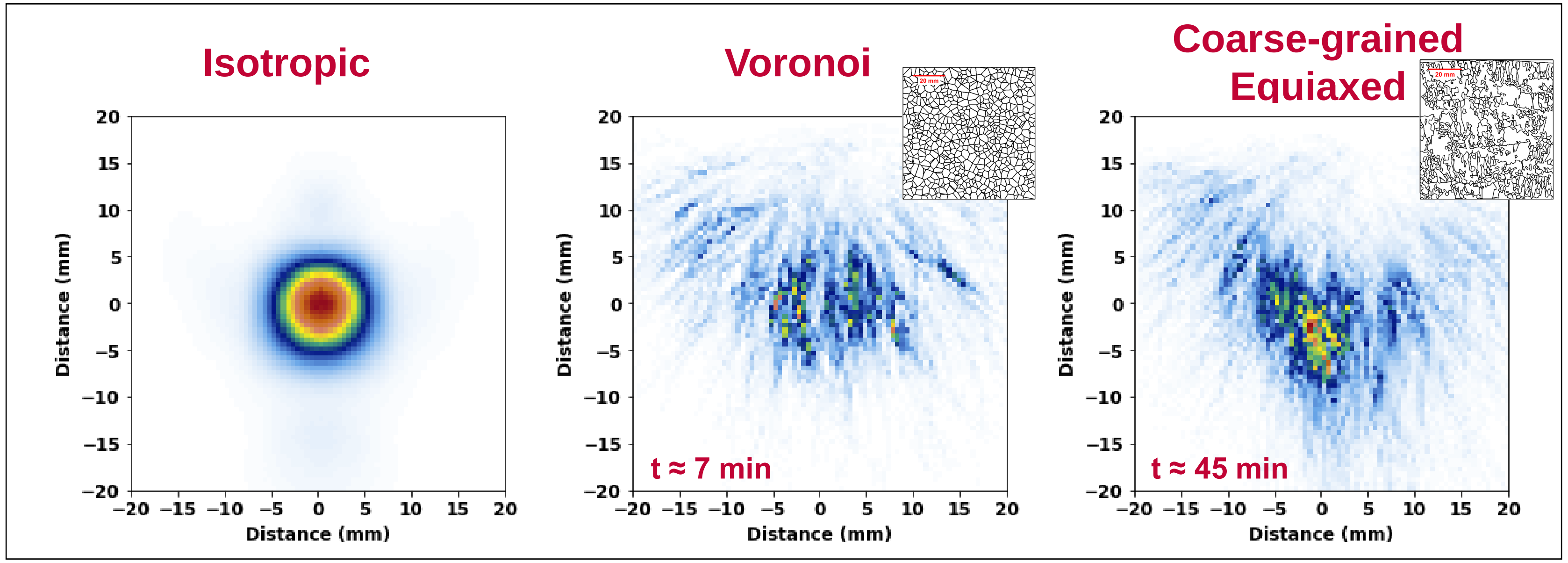


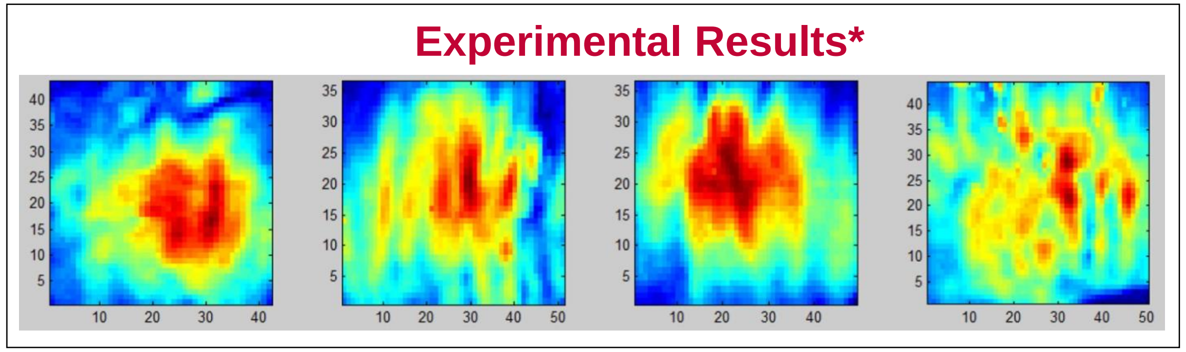
Multiple beam maps were acquired through the same block after slices were removed



Beam Simulation Results, Equiaxed

- CIVA simulations were run with a 1 MHz phased-array probe and a 45° refraction angle. The beam was focused in the simulation plane to be consistent with experimental setup.
- Simulations results show significant beam scatter in both coarse-grained scenarios.
- Beam scatter in the Voronoi case is qualitatively similar to that in the simulated coarse-grain case.
- Simulation results are qualitatively consistent with experimental results on the same specimen.

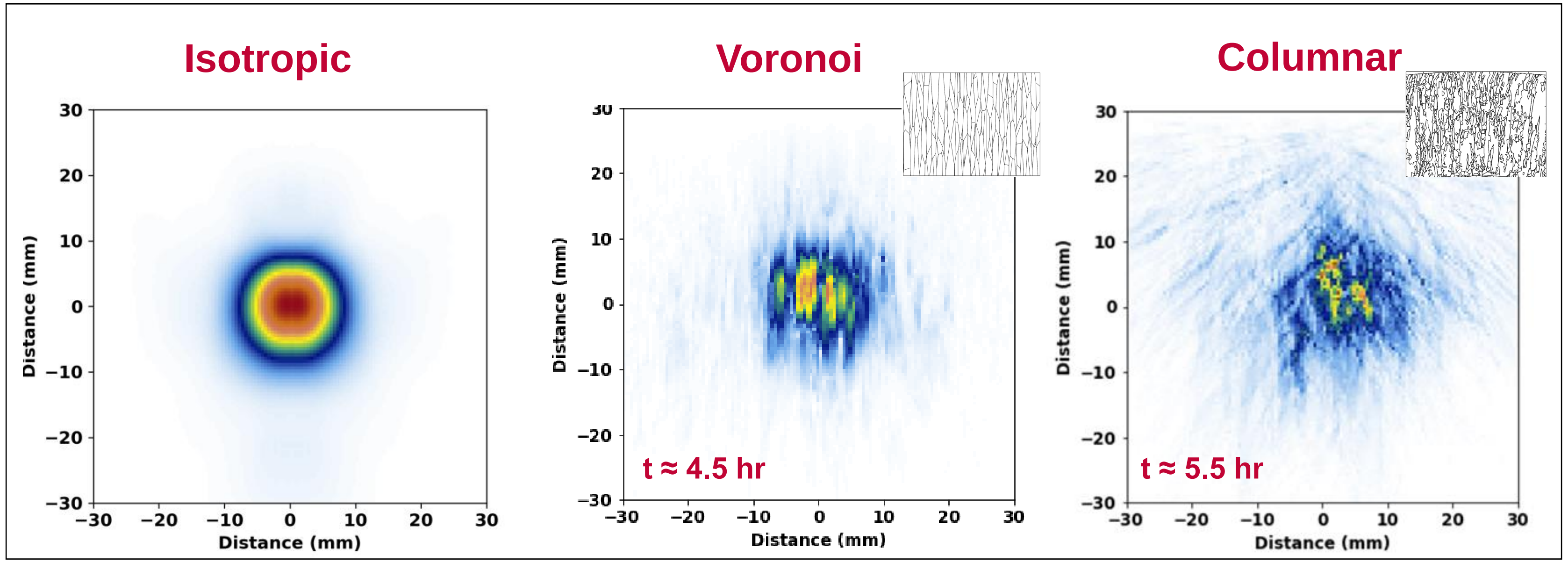


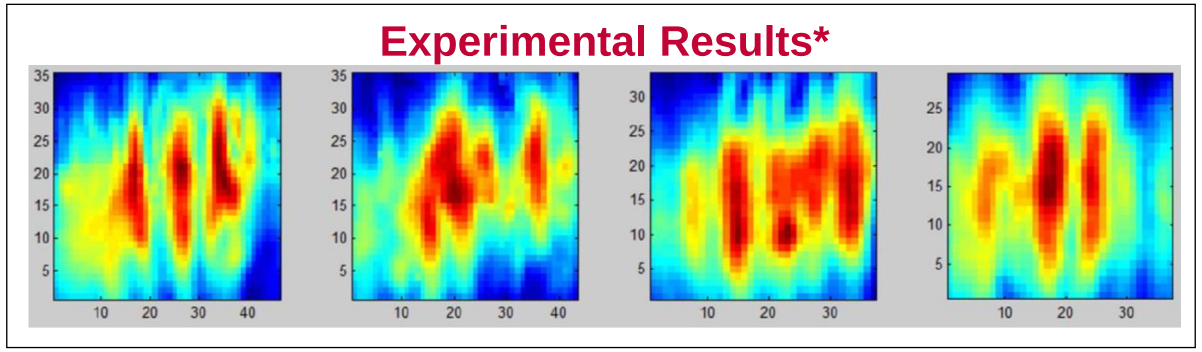


*From Crawford, et al., "Phased Array Ultrasonic Field Mapping in Cast Austenitic Stainless Steel." ML14155A165. 2014.

Beam Simulation Results, Columnar

- The same simulation parameters were used, although higher accuracy factors were needed.
- Simulated results show beam scatter in both columnar scenarios but considerably different scatter patterns, probably due to the 3D nature of the Voronoi grains vs 2D-extruded for the columnar model.
- The Voronoi-based model appears to agree better with experimental results.





*From Crawford, et al., “Phased Array Ultrasonic Field Mapping in Cast Austenitic Stainless Steel.” ML14155A165. 2014.

Summary

- Empirical beam maps suggest that idealized weld geometries (e.g., Ogilvy) do not realistically represent beam scatter and beam formation through weld microstructure.
- Simulated beam profiles through realistic welds are qualitatively in agreement with experiments, showing scatter, reduced beam formation, and poor penetration through the weld, though experimental scans generally show more scatter, less beam formation, and less sound penetration.
- Equiaxed Voronoi grains appear to provide results comparable to realistic CASS models, but much more quickly and efficiently.
- Columnar Voronoi grains appear to be superior to realistic CASS models, although with less advantage in simulation times due to higher accuracy factors needed.

Overall, modeling is a valuable tool for predicting beam coverage, but results should be validated with empirical studies whenever possible and appropriate model parameters are critical.

Thank you