Validating a Model for Welding Induced Residual Stress Using High-Energy X-ray Diffraction

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Abstract

Integrated Computational Materials Engineering (ICME) provides a pathway to advance performance in structures through the use of physically-based models to better understand how manufacturing processes influence product performance. A particular challenge for ICME is predicting residual stresses induced during fabrication that directly impact the life of structures. As one particular challenge, consider that residual stresses induced in fabrication are pervasive, and they directly impact the life of structures. For ICME to be an effective strategy, it is essential that predictive capability be developed in conjunction with critical experiments. In the present work, simulation results from a multi-physics model for gas metal arc welding (GMAW) are evaluated through X-ray diffraction techniques using synchrotron radiation. A test component was designed with intent to develop significant gradients in residual stress, be representative of real-world engineering application, yet remain tractable for finely spaced strain measurements with positioning equipment available at synchrotron facilities. The experimental validation lends confidence to model predictions, facilitating the explicit consideration of residual stress distribution in prediction of fatigue life.

Introduction

Like many industries today, the heavy equipment sector has a need for developing lighter-weight and more durable structures to compete for best in-class fuel efficiency, payload/performance, and owning/operating cost. One way to support product development in this environment is to understand the effects of manufacturing processes on material properties and state, and how these properties and state influence the performance of structures.

Residual stresses that result from manufacturing processes are pervasive, and they directly impact the life of structures. Welding is no exception to this phenomenon, and traditional design practices for welded structures do not explicitly account for the local residual stress field. Advanced methods for fatigue analysis attempt to account for residual stress, however, providing the needed input – the initial residual stress field – becomes a daunting task even for a relatively simple engineering component.

Often, the only way to obtain these data on a large welded structure is to simulate the welding process, predict the residual stress and perform analysis for the fatigue life. Integrated Computational Materials Engineering (ICME) provides a framework for predicting the performance of a welded component [2]. Models of the welding process are built upon materials information including thermal properties, kinetics of plasticity, work hardening response and material anisotropy. This information is built into detailed manufacturing process simulation procedures for heat transfer coupled with mechanical response, leading in this particular application to a prediction of the state of residual stress. Finally, the in-service performance of the product rests upon models for fatigue life. Success of ICME relies on validation of the modeling foundation. *Validation of welding residual stress predictions from a simulation of the welding process is the primary goal of this work.*

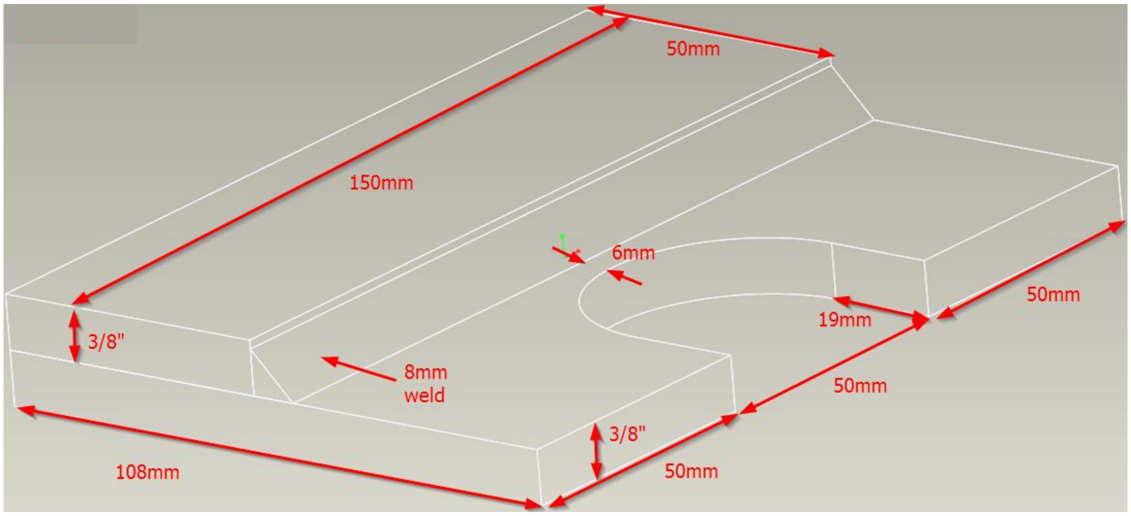
A common method for residual stress characterization in an industrial setting involves a lab-source x-ray diffraction (XRD) machine. Ease-of-use and automated post-processing of data are attractive features of lab XRD machines. However, lower energies of the X-rays generated by the lab source can only penetrate to depths on the order of tens of microns for the traditional reflection geometry. Thus, obtaining a full picture of the overall residual stress state becomes difficult and one may have to resort to relaxation-based methods.

Synchrotron x-ray sources can provide higher energy X-rays (enabling increased penetration) and higher brilliance, providing shorter collection times and finer spatial resolution. Depending on the technique and material under study, use of high energy radiation enables study through thicknesses on the order of tens of millimeters. In this work, two different techniques are applied to measure residual stress in a welded steel component. Energy Dispersive Diffraction (EDD), utilizing a polychromatic X-ray beam, offers the high energy and flux to penetrate cm-thick steel plate with collection times on the order of a minute per interrogated location on the plate. Alternatively use of a monochromatic beam in Angular Dispersive Diffraction provides a bridge to traditional methods of x-ray stress analysis used in the industrial laboratory. Results of the two x-ray diffraction techniques are applied in the validation of a model for Gas Metal Arc Welding (GMAW) of steel.

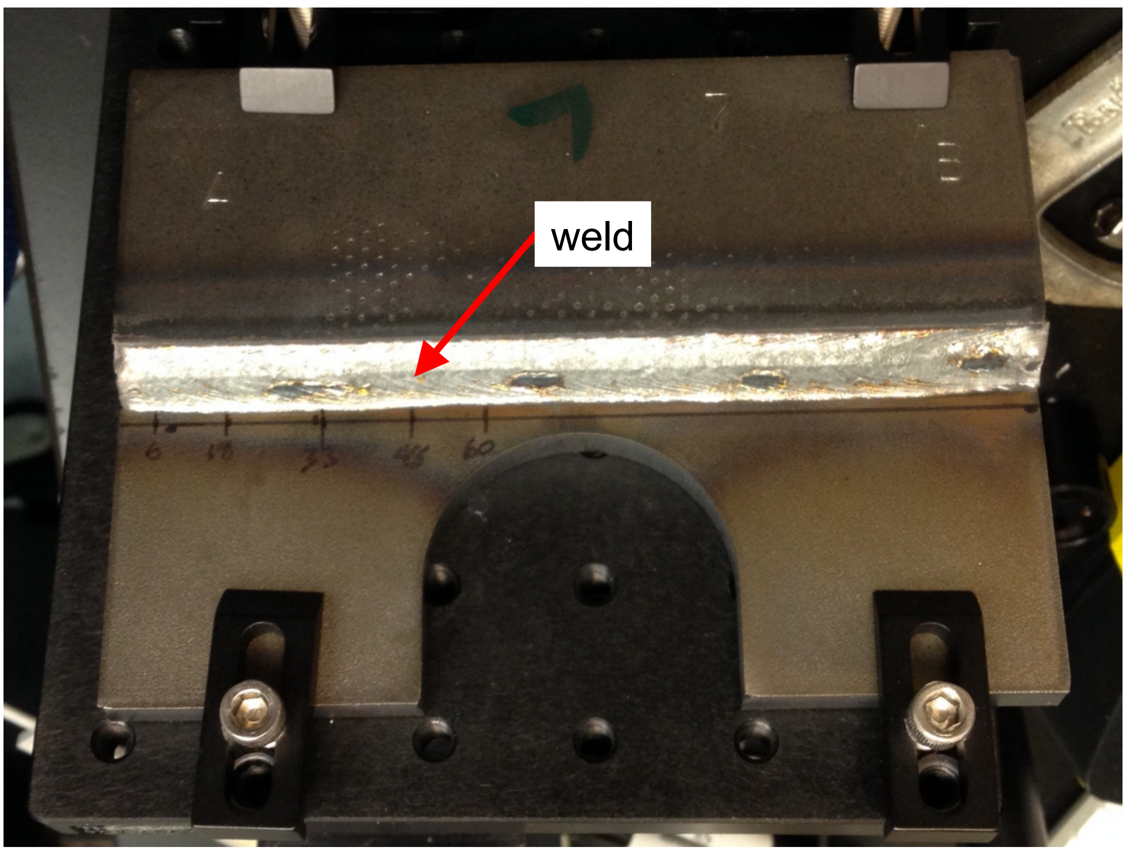
Method

Welded Lap-Joint Sample

A single weld pass lap-joint geometry (shown in Figure 1) with a "U"-shaped cutout was designed for its amenability to a reflection measurement technique and for large variations of residual stress magnitudes transverse to the weld. The transverse stress magnitude varies from compressive to tensile to compressive across half the length of the weld, i.e. this pattern is nearly symmetric about the cutout. The plate material is a low carbon structural steel similar to ASTM A572 Gr 42 or 50.



(a) 8mm single pass lap-joint weld on 3/8” thick steel plate.



(b) Sample A in fixture for reflection experiment.

Figure 1: Lap-joint sample

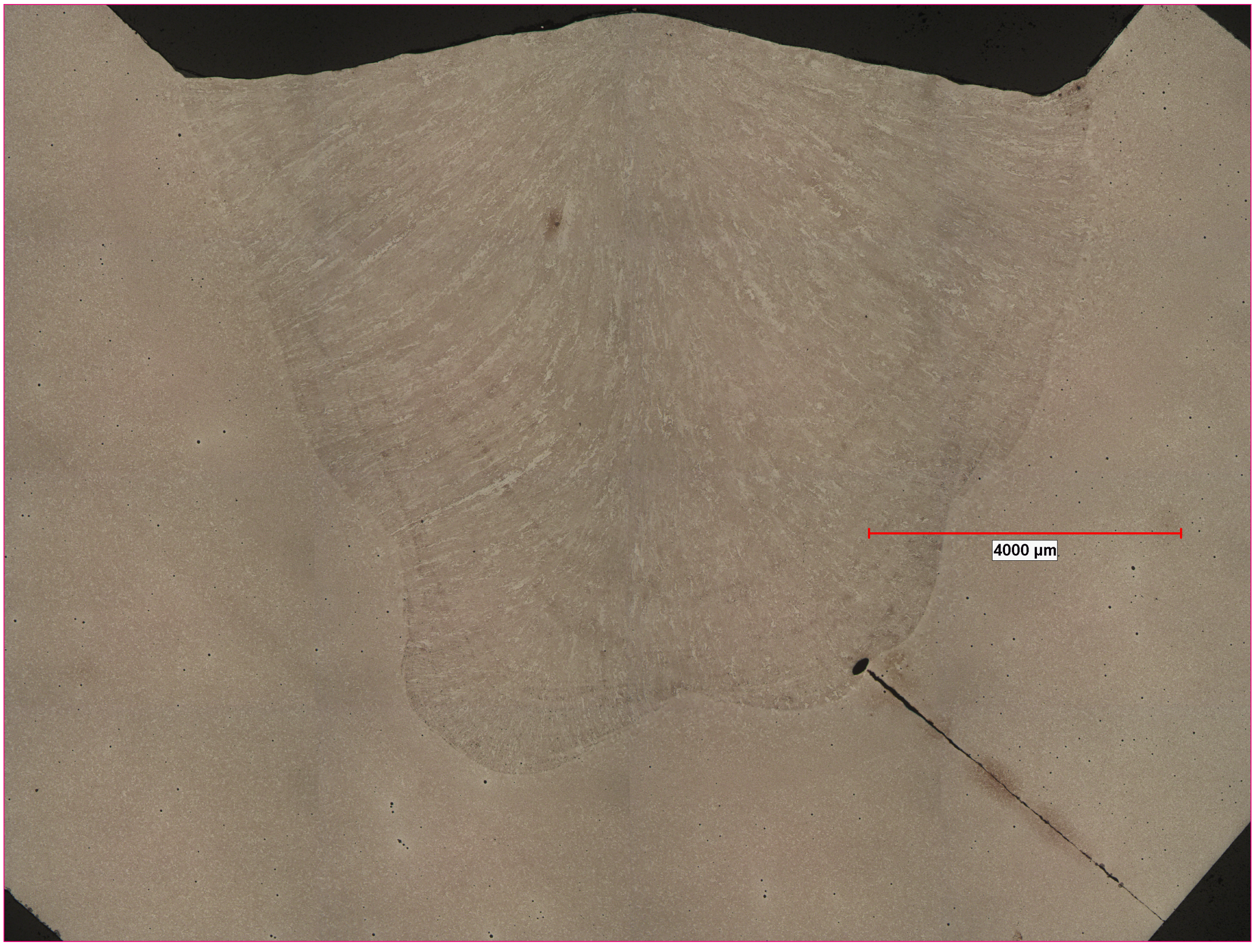


Figure 2: Mosaic image of weld at edge of sample.

The image in Figure 2 is an etched micrograph (25x) that shows the cross-section of the weld at the mid-point of the weld length. The lower plate with the U-shaped cutout and the upper plate are shown in the left and right sides of the images, respectively. The samples were welded in the horizontal position, so there is a slight asymmetry and deeper penetration of the fusion zone that is biased toward the lower plate (due to the gravitational effect). We can also see that this is a partial penetration weld, which was captured in the model through tuning of the thermal parameters and contact between the plates. The heat affected zone (HAZ) surrounding the weld (where the microstructure is altered by the thermal cycle) is less visible in this image, but it does have an effect on measurements near the weld. Grain size and phase change are the two main factors that will affect measurements in the HAZ and fusion zones. The strain measurements were conducted in the parent plate material outside of the HAZ to facilitate more efficient data collection and to reduce sample/material variability in the measurements.

Welding process model

Simulation of the gas metal arc welding (GMAW) process is routinely used to predict distortion and residual stress in welded structural fabrications. Distortion predictions have been repeatedly validated using factory measurement data, however it can be more difficult to validate

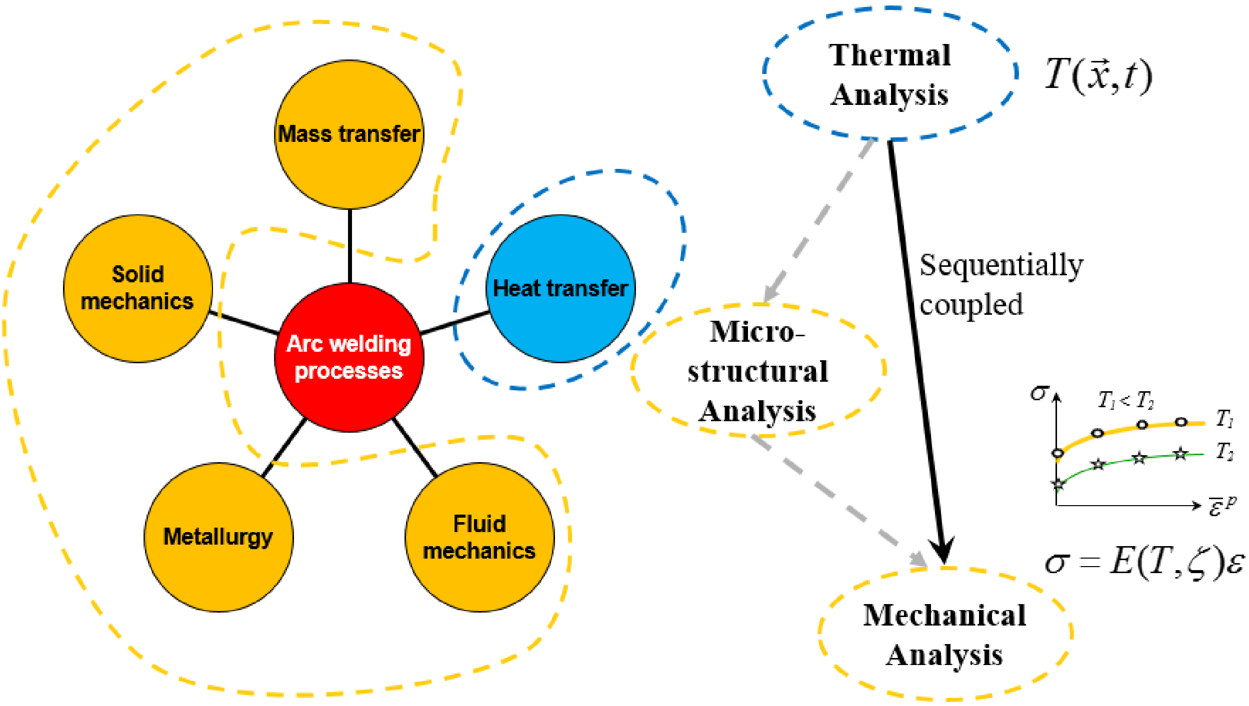
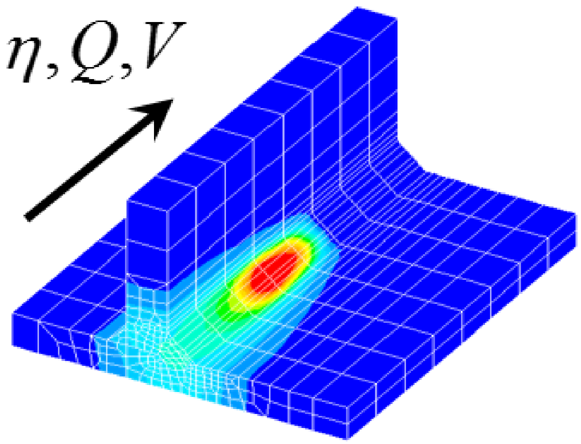


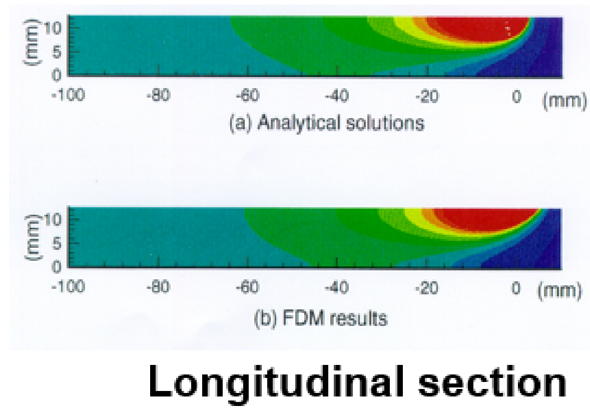
Figure 3: General approach to modeling arc welding processes using VFT®.

residual stress predictions due to inherent variability and lack of capability in residual stress characterization techniques used in the industrial laboratory. A welding process simulation was used to predict the residual stress distribution to help guide the experiments in selecting locations of interest, in addition to verification of the process model. In the late 1990s, in partnership with Battelle Memorial Institute, Caterpillar developed a welding simulation software framework known as VFT® (Virtual Fabrication Technology) [1, 10, 4]. This software was developed to simulate the GMAW process for structural fabrications with the objective of improving manufacturing processes through knowledge of the as-manufactured geometry (distortion) and material state (residual stress and microstructure). Figure 3 outlines the general approach to modeling arc welding processes using VFT®.

The simulations are completed using sequentially coupled thermal-mechanical models, where the thermal load history is provided to the mechanical solver at time increments commensurate to the mesh size. The material properties in the mechanical analysis are a function of temperature (and optionally micro-structural state variables), which allow for the displacement and stress to be solved for throughout the entire thermal history. The thermal history is typically solved using either an analytical solution (modified for finite geometry) or transient-thermal FEA with a user subroutine to describe the shape of the heat source—typically a double ellipsoid for GMAW. The analytical solution is based on a point heat source traveling in a semi-infinite body [8] and it has the advantage of improved computational efficiency, but the heat source and boundary condition modeling is less flexible than the FEA solution. However, the FEA solution typically requires a finer mesh and time step to obtain a stable, converged solution. Figure 4a shows a temperature contour plot for a single pass t-joint fillet weld where the efficiency η, power Q, and travel speed V describe the welding process parameter inputs for the model.



(a) typical temperature contour plot for a single pass t-joint fillet weld



(b) temperature field comparison between analytical and numerical solutions

Figure 4: Temperature solution

Figure 4b is a temperature contour comparison between the analytical solution and a numerical (finite-difference method) solution for a longitudinal (along weld direction) section of the weld pass.

For regular weld joint geometry and normal GMAW conditions, the analytical solution provides a thermal load history similar to the numerical solution. Both thermal solution methods were utilized in the present study, however only results using the FEA solution are presented.

The VFT® mechanical analysis utilizes a user material subroutine (UMAT) to model the material response to the thermal load history. This UMAT can be used with either the commercial general-purpose nonlinear FEA software ABAQUS® or the open-source nonlinear FEA software WARP3D. A summary of the physical deformation mechanisms that can be modeled in the mechanical analysis is summarized in Figure 5.

All mechanisms except for microstructure / phase transformation were active in the UMAT for the simulations in this study. The sample material is a low-carbon structural steel (similar to ASTM A572) where the phase transformation mechanism is often considered to be of secondary importance in welding simulation predictions. However, the microstructure-based material models included in the UMAT may be leveraged for such materials in the future if more accurate residual stress predictions or detailed information about the evolution of the microstructural phases are required. A pure isotropic hardening model and a pure kinematic hardening model were used in this study; these hardening models tend to bracket the upper and lower bounds of residual stress predictions, respectively, according to [9]. A mixed isotropic-kinematic hardening model is also available, given sufficient cyclic stress-strain data for a fit of the Lemaitre and Chaboche model for mixed hardening [7].

The overall simulation workflow is described in Figure 6. The model is defined by the structural plates and weld joint geometry, and it is meshed with linear hexahedral elements. The thermal load history is calculated and passed to the mechanical analysis using a UFIELD-type of user subroutine, where the deformation and stress are then solved for through the duration of the thermal load history. The residual stress solution is simply the final stress state after removal of fixture constraints (boundary conditions) and complete cool-down of the welded

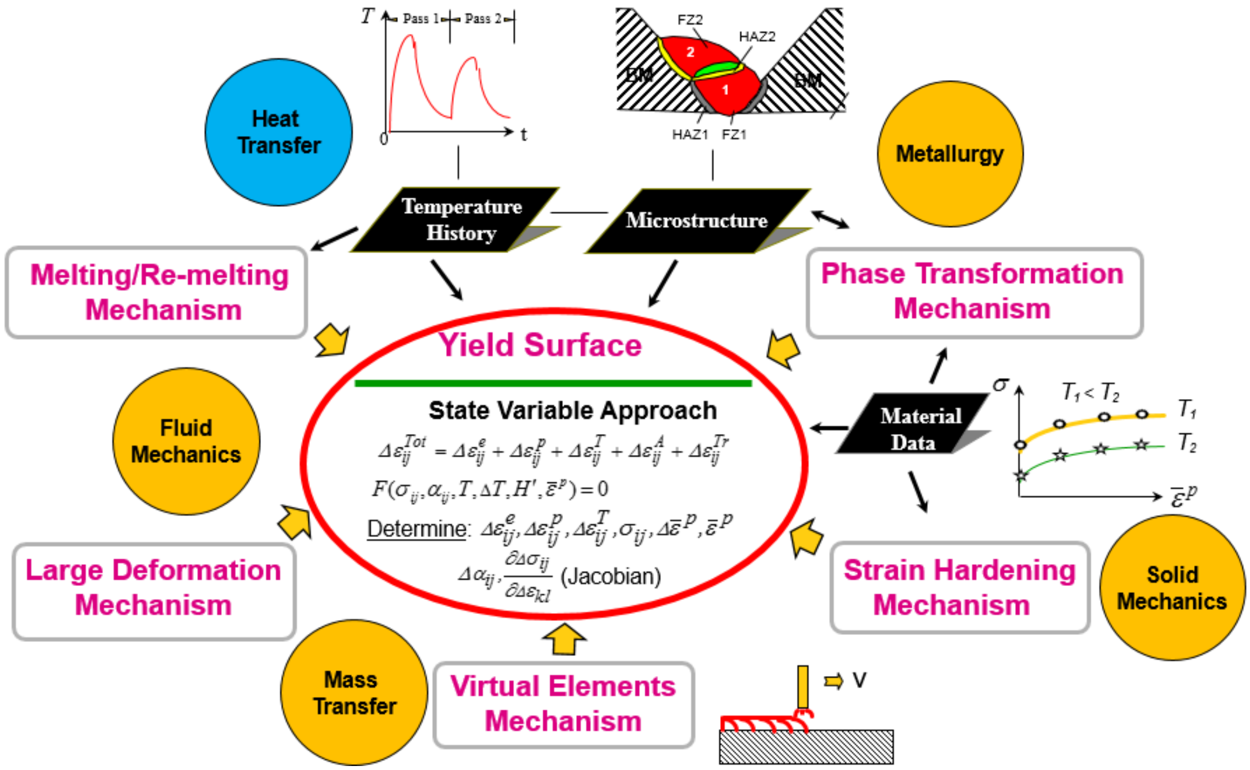


Figure 5: Summary of approach to modeling deformation mechanisms in mechanical analysis.

structure.

Characterization of residual stress using synchrotron radiation

Two diffraction techniques are used to characterize residual stresses in the welded component. The EDD technique in transmission geometry leverages a high energy polychromatic (white) beam. It is capable of non-destructively probing an internal volume in an engineering component and measuring the lattice strains. As a complement to the EDD technique, the Angle Dispersive Diffraction (ADD) technique utilizing monochromatic X-ray beam and reflection geometry is employed as a cross-check to the EDD measurements – and serve as a connection to lab source based measurements typically used in industrial setting.

EDD technique in transmission geometry

In the EDD technique, the angle of diffraction is fixed by the experimental geometry [3]. High-energy x-rays, greater than 30 keV, provide high penetration power to investigate thick samples. Through the use of slits, a volume of material in a sample on the order of $1mm^3$ can be probed and the lattice strains in the volume can be measured. The sample can be translated with respect to the beam such that different volumes of material can be probed to obtain the strain gradient information. Multiple point detectors can be placed strategically to measure several strain components simultaneously.

Experiments were carried out at the 1-BM-B beamline of the Advanced Photon Source (APS). Figure 7a shows a schematic of a typical setup for the technique at 1-BM-B. A pair of

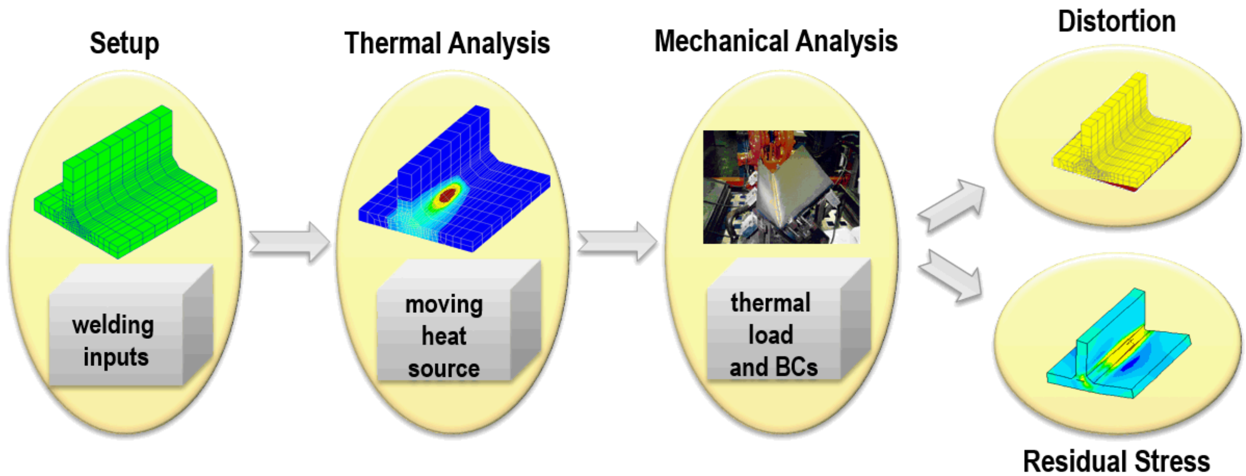


Figure 6: Welding simulation workflow.

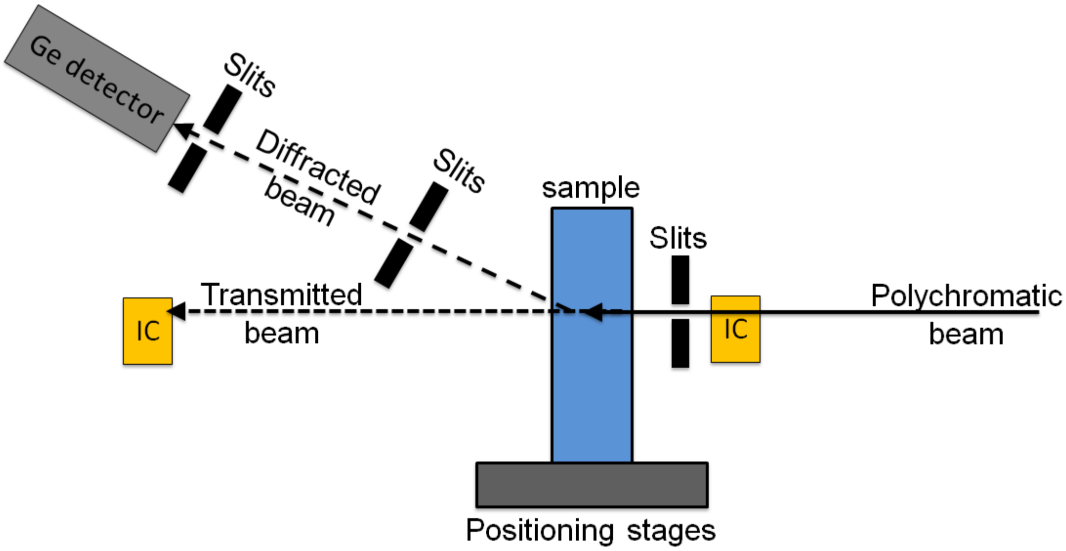
Ge single crystal photon detectors were placed at a fixed angles with respect to the incoming beam to measure the lattice strains from an aggregate of crystallographic planes aligned with directions of interest on the sample – more specifically, so as to recover strains perpendicular and parallel to the weld. Combined with the small 2θ angles, the internal strains in a large sample can be measured non-destructively with approximately 1×10^{-4} strain uncertainty. Figure 7b shows a picture of the detector arrangement used to measure two components of strain in the sample simultaneously. The horizontal and vertical detectors were positioned at take-off angles of 6.970° and 6.886°, respectively. The slits had a spacing of 200μm; following Croft [3], the through-thickness extent of the gauge volume (the diffracting volume) is 3.3 mm. Measurements were carried out for two samples, A and B.

The {211}, {220} and {310} lattice planes were used to evaluate strain. Strains were computed for each reflection independently; the averaged strain is considered as the strain at the continuum length scale. The plate was positioned along the beam such that the gauge volume was just within the plate surface. The strain field was mapped on a regular grid, perpendicular to the beam, with a 3mm spacing between points. The lattice parameter was taken as 2.868 Å.

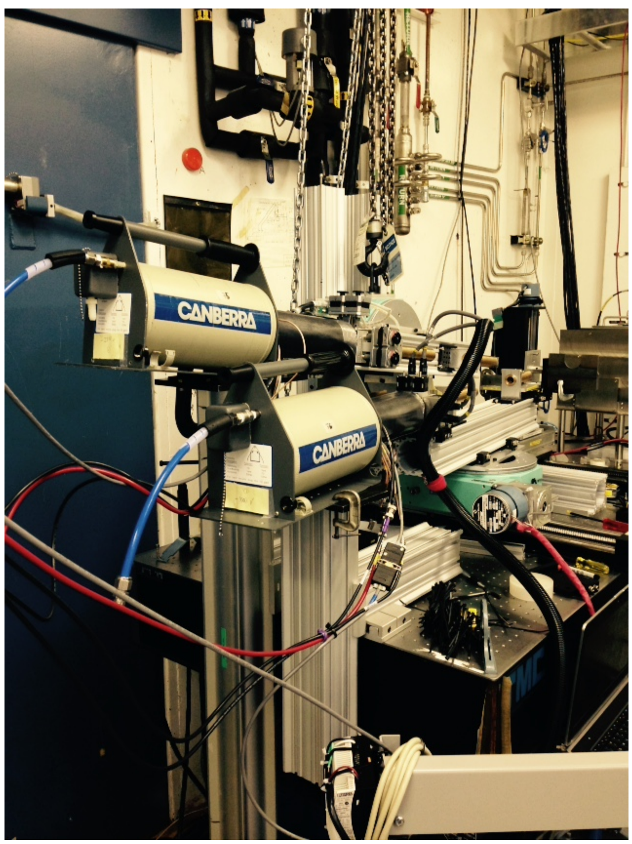
Monochromatic X-ray diffraction with reflection geometry

Measurements using a monochromatic x-ray beam in a reflection geometry [5, 6] were performed for sample A, using the A2 beamline located at the Cornell High Energy Syncrotron Source (CHESS). The lap joint sample was placed in a four circle goniometer fitted with translation stages. Translation perpendicular and parallel to the weld in the plane of the steel plate provided for a mapping of stress in the vicinity of the weld. In addition, use of a laser distance sensor and positioning normal to the plate surface was performed during scan to maintain the diffraction geometry during mapping of the strain. Measurements were taken in 4mm steps.

The energy was set to 15.845 keV. Diffraction images were collected using a Pilatus 300K detector. The {211} reflection was used to evaluate stress using the $\sin^2\psi$ procedure [5, 6].



(a) Schematic of the EDD setup.



(b) Two Ge single crystal photon detectors are used to measure two different components of strains in the sample.

Figure 7: Energy Dispersive Diffraction at the 1-BM beamline of the Advanced Photon Source

Results

The stress distribution following from the model for welding is shown in Figures 8 and 9 for the top and bottom surfaces, respectively. In these Figures, the welding pass progresses from left to right. However, it is evident that the stress distribution is relatively symmetric about a vertical centerline. The S11 and S22 components of stress – taken in the x and y directions, respectively – show relatively high values, around the yield stress of $\sim$ 300 MPa. The shear stress, S12, is comparatively small. From the standpoint of practical application, the S22 component of stress on the top surface of the sample, acting perpendicular to the length of the weld (Figure 8b) is of particular interest.

This S22 stress component is highlighted in Figure 10, with the welding path proceeding vertically from top to bottom (the image is rotated 90 degrees with respect to 8, with S22 acting horizontally). There is a local minimum (compressive stress) at the edges of the part and a local maximum (tensile stress) acting at the weld between the edge and the circular cut-out. For the region of tension between the upper edge and the cut-out, the stress value developed through EDD appears to be lower in magnitude than in the model – particularly for Sample A. This may be due to the relatively large ($\sim$ 3mm) through-thickness region that is sampled in EDD. The reflection measurement for sample A, where the diffracting volume is well within 100 μm of the surface, shows a bit higher stress perpendicular to the weld as compared to EDD.

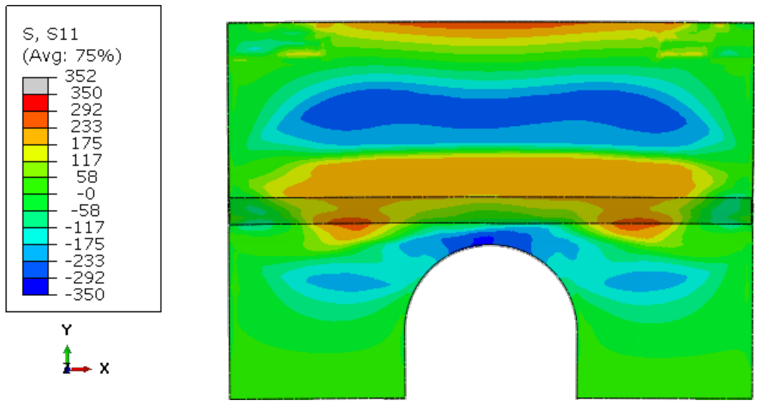
The component of stress parallel to the weld is shown in Figure 11. The model result indicates a region of tension adjacent to the weld and compression along the same horizontal position to the left of the weld. Results for samples A and B show distinctly different trends: sample A has a tendency toward greater compression away from the weld and sample B has elevated tensile stress acting along the weld. The compressive stress of sample A is confirmed by the reflection measurement. It appears that the welding operation places the 150mm $\times$ 50 mm upper plate in a bending-like state, with the tension along the weld and compression along the middle of the upper plate (Figure 8). This bending-like state is also apparent on the bottom surface (Figure 9). The x-ray measurements provide indication that the stress parallel to the weld,in the bottom plate with cut-out, is sensitive to the state of bending in the upper plate.

Discussion

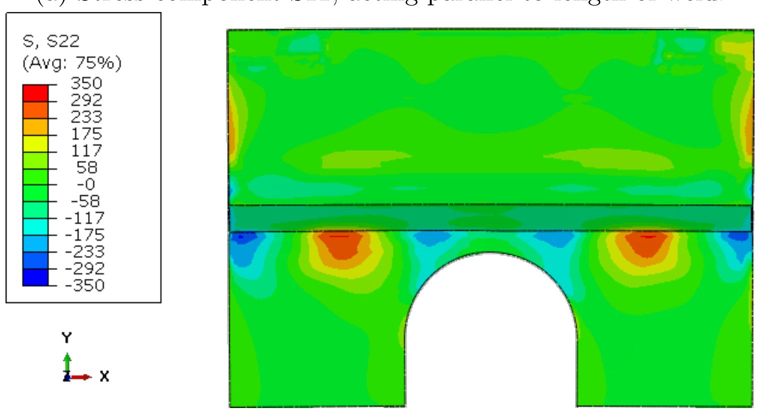
The EDD technique provides a means of mapping stress in components of practical dimension relevant to application, yet with resolution necessary to provide a path to model validation. In the present work, EDD is complemented by measurements using a monochromatic beam in a reflection geometry. The use of the traditional $\sin^2\psi$ technique provides a link to x-ray techniques used in the industrial laboratory.

The present results provide a validation of the model prediction of stresses acting perpendicular to the weld. These are stresses of concern to application, and play into the prediction of fatigue life. The end result is guidance in strategies for light-weighting of large structures in heavy equipment.

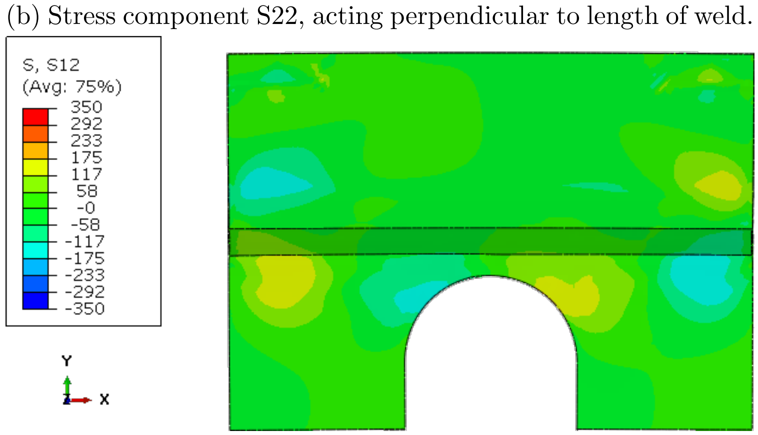
The experimental results indicate sensitivity of stress parallel to the weld to the process. While the stress perpendicular to the weld was consistent between the two samples, the parallel component varied considerably. The x-ray measurements directed interpretation of the model results toward the development of a bending like state, supported by the upper plate. While



(a) Stress component S11, acting parallel to length of weld.

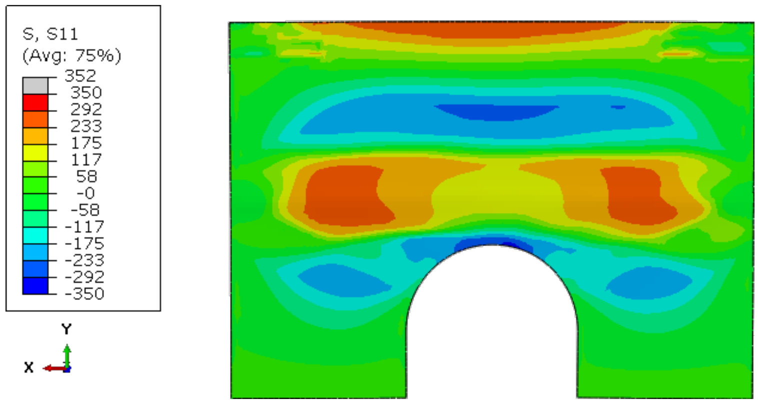


(b) Stress component S22, acting perpendicular to length of weld.

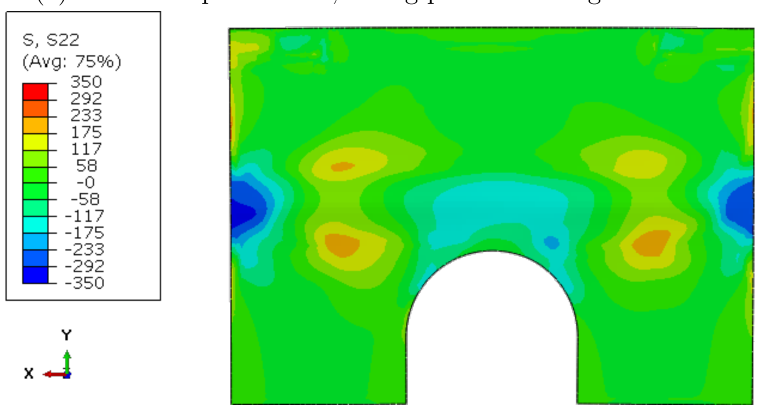


(c) Shear stress component S12, acting perpendicular to length of weld.

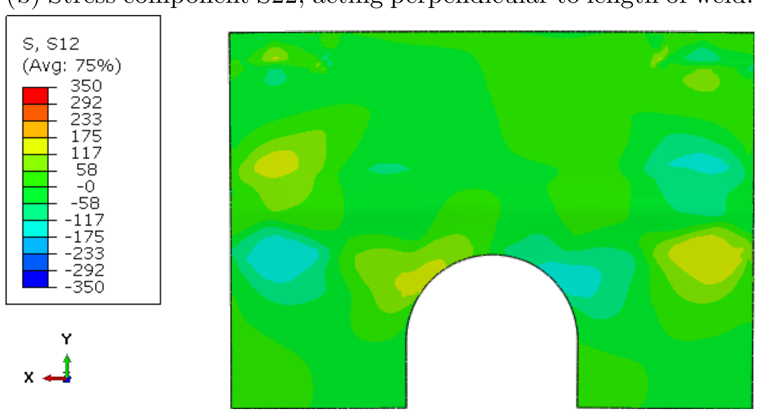
Figure 8: Model prediction of stress on top surface of lap sample.



(a) Stress component S11, acting parallel to length of weld.



(b) Stress component S22, acting perpendicular to length of weld.



(c) Shear stress component S12, acting perpendicular to length of weld.

Figure 9: Model prediction of stress on bottom surface of lap sample.

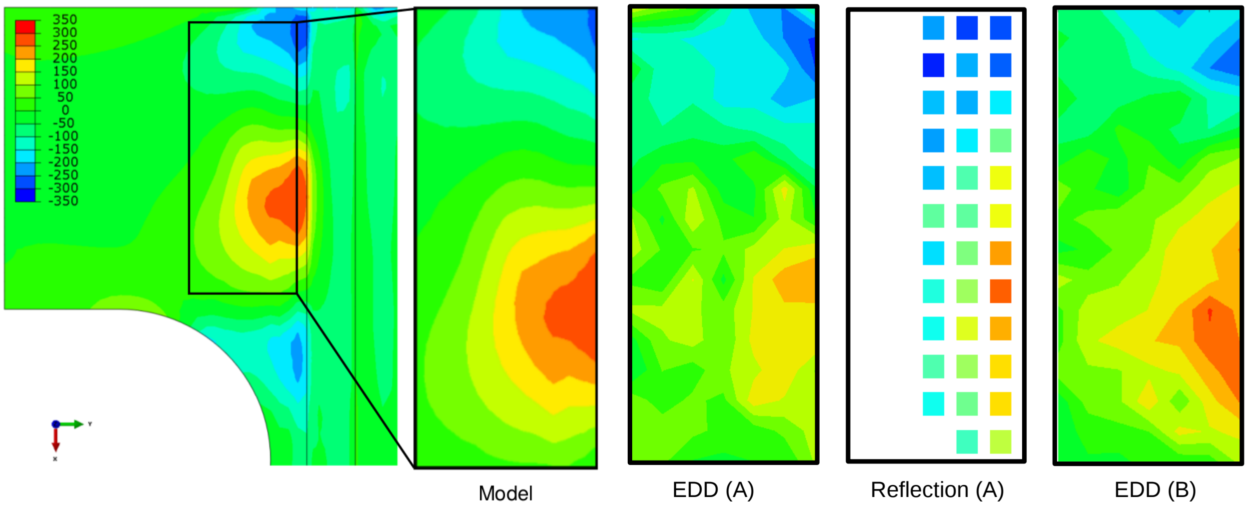


Figure 10: Stress component perpendicular to the weld.

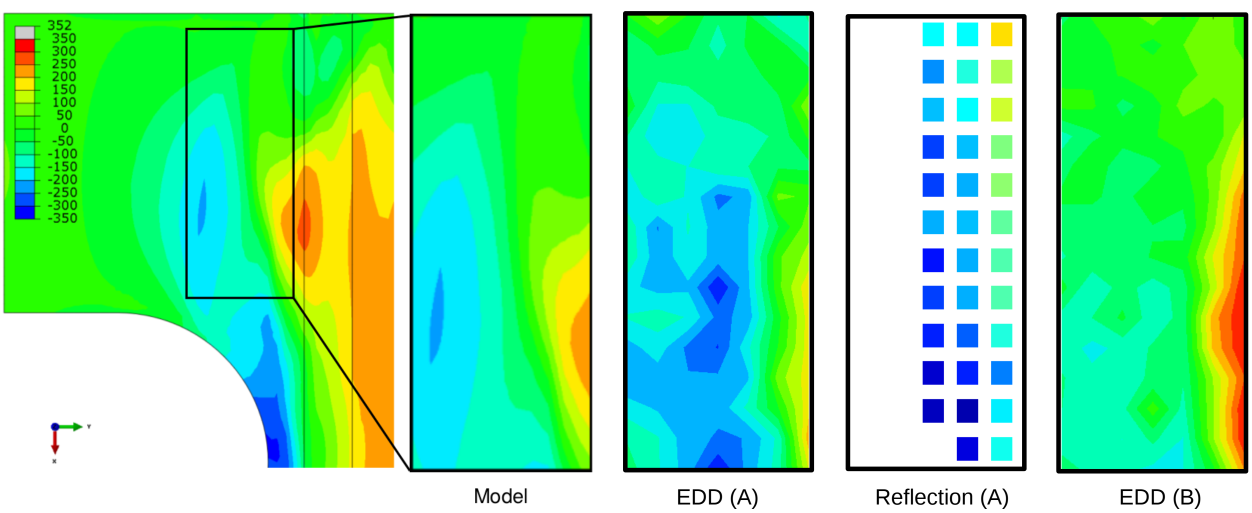


Figure 11: Stress component parallel to the weld.

this is not the stress component of primary concern, this observation offers the opportunity for exploring the sensitivity of the GMAW model to process conditions.

Outlook

Use of high-energy synchrotron radiation will play an increasingly large role in validation of models for structural metal alloys at many length scales. As discussed, the unique capabilities of these sources enable the full field measurements necessary for validation of the ICME approach, critical for its success.

As facilities such as the APS and CHESS go through upgrades and new detector technologies and instrumentation come on-line, both the EDD and ADD techniques for residual stress characterization will be greatly improved. Endstations will be equipped with improved sources and optics capable of providing increased flux densities. This will improve both penetration and collection times allowing for detailed mapping of large parts in reasonable time. For the ADD technique, large high resolution area detectors that are efficient at higher energies combined with diffracted beam apertures will allow strain mapping with sub-mm spatial resolution. For the EDD technique, multiple volumes and measurement directions can be probed simultaneously with area detectors with energy resolving capability.

As part of an upgrade effort presently underway at CHESS, the EDD technique will be able to be performed at beamline utilizing a wiggler source where electrons in the synchrotron storage ring are oscillated to produce radiation of high energy and intensity in comparison to a bending magnet source. The shifting of the emitted X-ray spectrum to higher energies and increased flux will improve both penetration and collection times, allowing for detailed mapping of the strain state of large components in reasonable time. In addition, the EDD technique will be advanced further by detector technology, including the adoption of CdTe detectors with increased counting efficiencies at high energies and two-dimensional energy resolving detectors that can collect multiple projections of probed strain state simultaneously.

The techniques outlined in the present work provide only a small subset of those available at various facilities that can be of great use to ICME. For example, the 1-ID beamline at the APS and F2 station at CHESS offer state-of-the-art capability to non-destructively obtain orientation maps (refs) and lattice strain on a grain-by-grain basis (refs) during in-situ thermo-mechanical loading. With simultaneous in-situ wide angle X-ray scattering (WAXS) / small angle X-ray scattering (SAXS) technique, researchers can investigate the aggregate behavior of a polycrystalline material at several length scales (ref). These scattering techniques can also be combined with tomographic techniques thereby obtaining a more complete snapshot of the material state (refs). More generally, capabilities of assessing the performance of structural materials using synchrotron radiation are advancing rapidly and stand ready to serve in the validation of models that underlie ICME.

Acknowledgments

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