Integrated Computational Materials and Mechanical Modeling for Additive Manufacturing of Alloys with Graded Structure used in Fossil Fuel Power Plants

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Background and significance

Complex shape manufacturing

Balance between performance and cost

Repair pipeline in a rapid mode

Images from internet
Project objectives

Integrating available computational materials and mechanical engineering tools for graded structure alloy design by WAAM with demonstration.

Figure 1. ICME model framework for additive manufacturing of alloys with graded structure. CALPHAD: Calculation of Phase Diagrams; ICME: Integrated Computational Materials Engineering.
WAAM setup at RTRC

WAAM setup available in RTRC showing the PAW torch, 6-axis robot and wire feeder

(a) Schematic of the PAW torch and (b) in-situ observation during the deposition
(1) Single print and (2) sharp interface print

Design Roadmap

1. Inconel 740H & P91 printing and post-heat treatment
2. Sharp interface builds for deposition sequence and post-heat treatment
3. Computational design on intermediate blocks
4. Post-heal treatment design on graded alloy builds (1st generation)
5a. Data driven ML and GA design for intermediate block (2nd generation)
5b. Interface structure design (2nd generation)
6. 3rd generation printing and testing
Sharp interface print (740H on P91 vs. P91 on 740H)

SEM micrographs across the gradient zone showing a wider HAZ with cracks in P91 over 740H deposit.

Lower hardness at interface between P91 and 740H as well as 740H and substrate.

EDS composition profile along the build direction showing higher dissolution of Fe in 740H observed in 740H over P91 build.

Hardness maps along the build direction.
**Sharp interface print**

740H over P91 is the optimum deposition sequence for P91/740H bimetallic structures

<table>
<thead>
<tr>
<th>740H on P91</th>
<th>P91 on 740H</th>
</tr>
</thead>
<tbody>
<tr>
<td>No detrimental phases or cracks at interface</td>
<td>Cracks observed at the interface</td>
</tr>
<tr>
<td>Smaller gradient zone</td>
<td>Wider gradient zone</td>
</tr>
<tr>
<td>Fine grains at interface</td>
<td>Coarse grains at interface</td>
</tr>
<tr>
<td>Higher dissolution of Fe into 740H for longer distance away from the interface</td>
<td>Lesser diffusion of Ni into P91 away from the interface</td>
</tr>
<tr>
<td>Lower hardness at interface between P91 and 740H</td>
<td>1) Lower hardness at interface between P91 and 740H interface between 740H and mild steel substrate</td>
</tr>
</tbody>
</table>
(3) Computational design of the Gen 1 graded alloy builds

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Computational design of the Gen 1 graded alloy builds

Compositions chosen:
1) 10 wt.% P91
2) 60 wt.% P91
3) 85 wt.% P91
Gen 1 graded alloy builds with interface: 10%, 60%, and 85% P91
As-built alloys with interface: 10%, 60%, and 85% P91 (Hardness Map)

- Predominantly uniform hardness
  - 10% P91
  - 60% P91
  - 85% P91

- Gradient interface has lowest hardness

Colors represent different hardness levels ranging from 139 to 412.
As-built alloys with interface: 10%, 60%, and 85% P91 (Microstructure)

- Gradient interface has an FCC structure.
- The presence of δ-ferrite is in the P91 close to the interface

- Gradient interface has a BCC structure mainly.
- No δ-ferrite exists close to the interface
(4) Post-heat treatment of graded alloy builds

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Homogenization studies for Gen 1 graded alloys (1200°C/1 hour)

Homogenization at 1200°C for 1 hour was chosen based on the post-heat treatment designed for sharp gradient builds.

- Clean interfaces in 85 wt.% P91 graded alloy
- δ-ferrite formation in P91 at P91/gradient interface in 60 wt.% P91 graded alloy
- δ-ferrite formation and Si segregation in P91 at P91/gradient interface in 10 wt.% P91 graded alloy

Presence of δ-ferrite in the P91 side of P91/gradient interface in 60 and 10 wt.% P91 graded alloys.

EDS maps confirming the segregation of Si in the P91/gradient interface in 10 wt.% P91 graded alloy.

IPF and IQ + Phase maps confirming the presence of δ-ferrite in 60 wt.% P91 graded alloy.
Homogenization studies for Gen 1 graded alloys (1150°C/1 hour)

- Homogenization at **1150°C for 1 hour** was found to be the optimum
  - Segregation of Si and δ-ferrite formation was not observed at the interface
  - From the calculated equilibrium phase fraction for P91 steel, it was found that 1150°C is well below the temperature at which δ-ferrite starts to form

**Clean interfaces without δ-ferrite formation and Si segregation after homogenization at 1150°C for 1 hour** in 10 and 60 wt.% P91 graded alloys

**Calculated equilibrium phase fraction as a function of temperature for P91 steel**
(5a) Data driven ML and GA design for intermediate block (2nd Gen)

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Linear build supporting data driven modeling

Composition profile along the build direction for the linear gradient alloy

Composition profile along the build direction for the linear gradient alloy
As-built linear graded alloy

*Inverse pole figure* and *Phase maps* along the build direction

- **P91**
- **Build direction**
- **FCC**
- **BCC**
- **740H**

1mm

Two-phase region

Total length covered ~ 22 mm
Data driven modeling for composition design

Gradient build via WAAM

Microstructure and Hardness

Hardness measurement
3 x 145 indents

EDS measured composition
3 x 145 x 4 point
Pore/Carbides/Phase identification 3 x 145 indents
Data driven modeling for composition design (cont’d)

Measured features:
• Composition
• Matrix phase
• etc.

Calculation features:
• Freezing range
• Phase fractions
• Entropy
• etc.

Measured properties:
• Printability (Porosity)
• Strength (Hardness)
• Ductility (Cracks during hardness test)

SHAP(Shapley Additive exPlanations)

200 Individual With different features

Compositions chosen:
1) 90 wt.% P91 [based on modeling]
2) 26 wt.% P91 [based on entropy]
Data driven modeling for composition design (cont’d)

Based on CALPHAD model, the 26 wt.% P91 has the highest entropy.

Based on ML models, the 90 wt.% P91 has relatively low porosity and high hardness.
Step and Scheil diagrams for selected compositions

TCNI10

26 wt.% P91

90 wt.% P91

TCFE10
As-built 26 wt.% P91 graded alloy

Build dimensions:
Length – 180 mm, Width – 10 mm, Height – 100 mm

26 wt.% P91 build printed using WAAM showing the presence of surface cracks
As-built 26 wt.% P91 graded alloy

- No cracks found in the bottom portion and cracking starts after a certain height (~ 30 mm)
- Crack length increases as the height of the sample increases
As-built 26 wt.% P91 graded alloy

Cracks formed in 26 wt.% P91 build were found to be
• Intergranular
• Surrounded by Laves phase

IPF map confirming the crack to be intergranular and KAM map showing high stress regions near the crack

EDS maps around the crack confirming the presence of Laves phase through clusters of Nb, Ti and Mo

Scheil simulations for gradient compositions between P91 steel and 740H superalloy confirming the formation of Laves phase at 26 wt.% P91
As-built 90 wt.% P91 graded alloy

Successful build without any cracks achieved

Build dimensions:
Length- 190 mm, Width- 15 mm, Height- 105 mm

90 wt.% P91 build printed using WAAM and the sample extracted from the build for analysis
As-built 90 wt.% P91 graded alloy: EBSD – IPF image

Martensite phase observed along the build direction
As-built 90 wt.% P91 graded alloy: Prior Austenite

Prior austenite grain size increases as the build height increases
As-built 90 wt.% P91 graded alloy

Hardness variation predominantly uniform along the build direction
(5b) Interface structure design - 2nd Gen

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Tensile test modeling

• Ductile damage model developed to simulate tensile failure
• Phenomenological model for predicting the onset of damage due to nucleation, growth, and coalescence of voids
• Describes the rate of degradation of the material stiffness once the corresponding initiation criterion has been reached

• By default, an element is removed from the mesh if all the section points at any one integration location have lost their load-carrying capacity

\[
\sigma = \frac{\sum F_n}{A_0}
\]

\[
\epsilon = \frac{\Delta l}{l_0}
\]
Model calibration

JC hardening law $\bar{\sigma} = [A + B(\bar{\varepsilon}^{pl})^n]$
Design comparison

- No improvement between LockingInterface_1 and LockingInterface_3
- Brittle phase property dominates
- Increase of IN740H area/material on side improves ductility
Design comparison: Failure

➢ Both LockingInterface_1 and 3 show more plastic deformation in the IN740H region (lower portion) compared to LockingInterface_2

Damage initiates in P91

\[ \tau_{\text{max}} = 624.7 \text{ MPa} \]
\[ \sigma_{\text{max}} = 1127.36 \text{ MPa} \]

\[ \tau_{\text{max}} = 807.78 \text{ MPa} \]
\[ \sigma_{\text{max}} = 1467.6 \text{ MPa} \]

Cup-cone failure

\[ \tau_{\text{max}} = 815.2 \text{ MPa} \]
\[ \sigma_{\text{max}} = 1473.28 \text{ MPa} \]
Deformation comparison

For sharp interface, load distributes to nearby interface elements and early failure occurs due to reduced ultimate strength in brittle phase compared to P91.

By introducing locking design load gradually transfers from IN740H to Brittle phase to P91.
Summary

• Non-standard ASTM tensile bar designs were studied

• Locking structure design introduced in the interface zone

• Locking interface 3 shows promise w.r.t strength and printability
Future work

- More performance evaluation are undergoing.
- Gen 3 build with mechanical testing will be performed.
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