Microstructure-based Multiscale Analysis of Hot Rolling of Duplex Stainless Steel by using Various Simulation Software

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Background ~Multi-physics problem~

Continuous Casting

Solidification
- Evolutions of δ-ferrite and austenite
- Thermal conductivity

Hot rolling
- Large plastic deformation
- Recrystallization

http://www.nisshin-steel.co.jp/saiyo/process/process03.php
http://www.nisshin-steel.co.jp/saiyo/process/process04.php
Simulation procedure

Microscale

1. Solidification simulation
   - Thermo-Calc Software
   - FINAS/STAR TPS edition
   - Distribution of microstructure

2. Step 4 Hot rolling simulation
   - ABAQUS
   - Strain energy for nucleation and growth of Rex. grains

3. Step 5 Recrystallization simulation
   - micress

Nanoscale

4. Virtual material test
   - VASP
   - LAMMPS

5. Experimental material test
   - Nanoindentation, Tensile test
   - Elastic constants stress properties of δ and γ phases

6. Calc. of microscopic properties
   - FINAS/STAR TPS edition
   - HOMAT
   - Elastic constants
   - Stress-strain curves

Macroscopic

- Macroscopic Stress-strain curves
  - Elastic constants
  - Stress-strain curves
  - HOMAT/ABAQUS

Micro-to-Macro scale

- More detailed in poster session

Simulation procedure

**Microscale**

- Solidification simulation
  - Thermo-Calc Software
- Distribution of microstructure

**Nanoscale**

- Virtual material test
  - Thermo-Calc Software
- Experimental material test
  - Nanoindentation, Tensile test
- Elastic constants, stress properties of δ and γ phases

**Macroscale**

- Step 4 Hot rolling simulation
  - ABAQUS
  - Strain energy for nucleation and growth of Rex. grains
  - Macroscopic Stress-strain curves

**Micro-to-Macro scale**

- Calc. of macroscopic properties based on microstructure
  - Elastic constants
  - Stress-strain curves
  - HOMAT/ABAQUS

Additional resources:

- http://www.micress.de/
- http://www.thermocalc.com/
- http://www.3ds.com/simulia/
- http://www.vasp.at/
Hot rolling slab model

Chemical composition: Fe-18wt%Cr-8wt%Ni-0.08wt%C (SUS304 Duplex stainless steel)
Cooling curve estimation

Thermal conductivity analysis by EM with **FINAS/STAR TPS edition**

- Initial temperature: 1733 K
- Cooling rate at the surface of the slab: 25 K/s

Temperature profile at the center of the slab

Input information of equiaxed solidification

Temperature gradient on the surface is 400 K/cm

Input information of columnar solidification
Columnar solidification simulation

• Computational domain and grid sizes
  Grid size : 0.5 μm
  Number of grids: 128 × 128 × 256
  Domain size: 64μm × 64μm × 128μm

• Cooling conditions
  Cooling rate $Q$: 25 K/s
  Temperature gradient $G$: 400 K/cm

• $\delta$ and $\gamma$ nucleation conditions
  $\delta$: initially placed in the four corner on the bottom surface
  $\gamma$: random nucleation on $\delta$ and liquid interface by time between checks, 0.01s, and nucleation distance, 3μm
Equiaxed solidification simulation

- Computational domain and grid sizes
  
  Grid size: 0.5 μm  
  Number of grids: 128 × 128 × 128  
  Domain size: 64μm × 64μm × 64μm

- Cooling conditions
  
  Variation of temperature at the center of the slab calculated by FINAS/STAR

- δ and γ nucleation conditions
  
  δ: randomly initially placed in the region by nucleation distance, 30μm  
  γ: random nucleation on δ and liquid interface by time between checks, 0.01s, and nucleation distance, 3μm
Material constants

• Interfacial energy (cf. MICRESS example)
  Liquid/δ interface: $\sigma_{L-\delta} = 2 \times 10^{-5} \text{ J/cm}^2$ (Strength of anisotropy: 0.2)
  Liquid/γ interface: $\sigma_{L-\gamma} = 3 \times 10^{-5} \text{ J/cm}^2$ (Strength of anisotropy: 0.2)
  γ/δ interface: $\sigma_{\gamma-\delta} = 7 \times 10^{-5} \text{ J/cm}^2$ (Isotropic)

• Interface mobility
  Liquid/δ interface: $K_{L-\delta} = 1 \times 10^{-2} \text{ cm}^4/\text{J/s}$, (Strength of anisotropy: 0.2)
  Liquid/γ interface: $K_{L-\gamma} = 1 \times 10^{-2} \text{ cm}^4/\text{J/s}$, (Strength of anisotropy: 0.2)
  γ/δ interface: $K_{\gamma-\delta} = $ depending temperature (Isotropic)

• CALPHAD DATABASE
  Thermo-Calc TCFE7

• Diffusion DATABASE
  Thermo-Calc(DICTRA) MOBFE3

<table>
<thead>
<tr>
<th>Temperature / K</th>
<th>$K_{\gamma-\delta} / \text{ cm}^4/\text{J/s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1733.0</td>
<td>2.0e-04</td>
</tr>
<tr>
<td>1700.0</td>
<td>1.51e-04</td>
</tr>
<tr>
<td>1600.0</td>
<td>5.94e-05</td>
</tr>
<tr>
<td>1500.0</td>
<td>2.07e-06</td>
</tr>
<tr>
<td>1400.0</td>
<td>6.21e-07</td>
</tr>
<tr>
<td>1300.0</td>
<td>3.05e-07</td>
</tr>
</tbody>
</table>
Phase distribution

Columnar solidification

Fractions of residual $\delta$: 12.3%

Equiaxed solidification

Fractions of residual $\delta$: 11.9%
Carbon composition distribution

Columnar solidification

Equiaxed solidification

Mol.%
Simulation procedure

**Microscale**

- Solidification simulation
  - Thermo-Calc Software
  - FINAS/STAR TPS edition

- Distribution of microstructure

**Step 4 Hot rolling simulation**

**ABAQUS**

- Strain energy for nucleation and growth of Rex. grains

**Step 5 Recrystallization simulation**

**Nanoscale**

- Calc. of microscopic properties
  - Virtual material test
  - Experimental material test
    - Nanoindentation, Tensile test

- Elastic constants stress properties of δ and γ phases

**Macroscale**

- Calc. of macroscopic properties based on microstructure

- Elastic constants
- Stress-strain curves

**Micro-to-Macro scale**

- HOMAT/ABAQUS

Elastic constants of FCC structure in Fe-Ni-Cr alloy

Molecular dynamics simulation for obtaining elastic constants of FCC structure in Fe-18wt%Cr-8wt%Ni alloy

Calculation condition
- Software: LAMMPS
- Force field: EAM potential
  “FeNiCr_Bonny_2013_ptDef.eam.alloy
- Number of atoms: 4000
- Temperature: 0 K
- Model case: 11 cases (Fe, Cr and Ni are randomly located.)

<table>
<thead>
<tr>
<th>Elastic constant [GPa]</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FCC</td>
<td>229.71</td>
<td>154.30</td>
<td>126.92</td>
</tr>
</tbody>
</table>
Elastic constants of FCC structure in Fe-Ni-Cr-C alloy

As the interatomic potential for metal and C atoms, LJ potential was used. For Fe-Ni-Cr-C alloy, the hybrid potential (EAM + LJ) was used.

**Fe-18wt%Cr-8wt%Ni**

<table>
<thead>
<tr>
<th>Elastic constant [GPa]</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FCC</td>
<td>229.71</td>
<td>154.30</td>
<td>126.92</td>
</tr>
</tbody>
</table>

**C doped**

**Fe-18wt%Cr-8wt%Ni-0.08wt%C**

<table>
<thead>
<tr>
<th>Carbon concentration</th>
<th>Elastic constant [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.08wt%</td>
<td>$C_{11}$</td>
</tr>
<tr>
<td></td>
<td>261.87</td>
</tr>
</tbody>
</table>

- The elastic constant value of C-doped alloy is larger than one of no doped alloy.
Elastic constants of BCC structure in Fe-Ni-Cr alloy

First-principles calculation for elastic constants of BCC structure in Fe-22wt%Cr-5wt%Ni alloy

Calculation condition
- Software: VASP
- Pseudopotential: PAW_PBE Fe 06Sep2000, PAW_PBE Cr 06Sep2000, PAW_PBE Ni 02Aug2007
- Number of atoms: 54
- Temperature: 0 K
- Model case: 11 cases (Fe, Cr and Ni are randomly located.)

<table>
<thead>
<tr>
<th></th>
<th>Elastic constant [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_{11}$</td>
</tr>
<tr>
<td>BCC</td>
<td>239.22</td>
</tr>
</tbody>
</table>
Temperature dependency

FCC

Elastic constants becomes smaller with increasing temperature.

BCC

These elastic constants are used for hot rolling simulation using ABAQUS/Explicit.
Simulation procedure

**Microscale**
- Solidification simulation
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- ABAQUS
  - Strain energy for nucleation and growth of Rex. grains
  - Macroscopic Stress-strain curves

**Step 5 Recrystallization simulation**
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**Nanoscale**
- Virtual material test
  - Nanoindentation, Tensile test
- Calc. of microscopic properties

**Experimental material test**
- Elastic constants stress properties of δ and γ phases

**Mesoscale**
- Calc. of macroscopic properties based on microstructure
  - Elastic constants
  - Stress-strain curves

**Micro-to-Macro scale**
- HOMAT/ABAQUS

**Additional Resources**
- http://www.micress.de/
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- http://www.3ds.com/simulia/
Nanoindentation test for obtaining stress-strain curve of single δ ferrite

- Berkovich triangular pyramid indenter
- Maximum load: 100 mN
- Displacement velocity: 13.324 m/s

Parameters at room temperature

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [GPa]*</td>
<td>224.5</td>
</tr>
<tr>
<td>$\sigma_y$ [MPa]</td>
<td>114.1</td>
</tr>
<tr>
<td>$R$ [GPa]</td>
<td>1.723</td>
</tr>
<tr>
<td>$n$</td>
<td>0.358</td>
</tr>
</tbody>
</table>

Estimation of stress-strain curve of single $\gamma$ phase

Nanoindentation of $\gamma$ phase is very difficult due to the deformation-induced martensitic transformation.

We assume the following relation

$$\sigma_M = f_\gamma \sigma_\gamma + f_\delta \sigma_\delta \quad (f_\gamma + f_\delta = 1) \quad \rightarrow \quad \sigma_\gamma = \frac{\sigma_M - (1 - f_\gamma)\sigma_\delta}{f_\gamma}$$

$\sigma_M$: Experimental data of stress-strain curves SUS304 stainless steel* (*JAEA, PNC TN941 85-128, (1985) )

$f_i$: Volume fraction of $i$ ($i = \gamma$ and $\delta$ ) phase calculated by MICRESS

Estimated parameters at room temperature

<table>
<thead>
<tr>
<th>Parameter</th>
<th>(SUS304)</th>
<th>$\delta$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [GPa]</td>
<td>237.5</td>
<td>224.5</td>
<td>239.3</td>
</tr>
<tr>
<td>$\sigma_\gamma$ [MPa]</td>
<td>140.3</td>
<td>114.1</td>
<td>145.7</td>
</tr>
<tr>
<td>$R$ [GPa]</td>
<td>0.589</td>
<td>1.723</td>
<td>0.487</td>
</tr>
<tr>
<td>$n$</td>
<td>0.193</td>
<td>0.358</td>
<td>0.162</td>
</tr>
</tbody>
</table>
Estimation of stress-strain curves of δ and γ phases at 900°C

We assumed logarithmical scaling for yield stress and stress hardening exponent between room temperature (RT) and high temperature (900°C) as:

\[
\frac{\log \sigma_{M,900} - \log \sigma_{\delta,900}}{\log \sigma_{M,RT} - \log \sigma_{\delta,RT}} = \frac{\log \sigma_y}{\log \sigma_y} \cdot \frac{n_{900}}{n_{RT}}
\]

\(\sigma_{M,900}\): Experimental data of stress-strain curves SUS304 stainless steel at 900°C* (*JAEA, PNC TN941 85-128, (1985) )

Estimated parameters at 900°C

<table>
<thead>
<tr>
<th>Parameter</th>
<th>(SUS304)</th>
<th>δ</th>
<th>γ</th>
</tr>
</thead>
<tbody>
<tr>
<td>E [GPa]*</td>
<td>172.5</td>
<td>180.3</td>
<td>171.4</td>
</tr>
<tr>
<td>(\sigma_y) [MPa]</td>
<td>60.8</td>
<td>58.6</td>
<td>61.2</td>
</tr>
<tr>
<td>R [GPa]</td>
<td>0.0771</td>
<td>0.0885</td>
<td>0.0752</td>
</tr>
<tr>
<td>n</td>
<td>0.030</td>
<td>0.051</td>
<td>0.026</td>
</tr>
</tbody>
</table>

*C11 from nano-calculation
Simulation procedure

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  - Elastic constants
  - Stress-strain curves
    - HOMAT
    - HOMAT/ABAQUS

**Micro-to-Macro scale**
- FINAS/STAR TPS edition
- Elastic constants stress properties of δ and γ phases
- Stress-strain curves
  - HOMAT
  - HOMAT/ABAQUS

Elastic constants of equiaxed and columnar microstructures

- We calculated elastic constants for microstructures simulated by MICRESS.
- Elastic constants of $\delta$ and $\gamma$ phases in the microstructures estimated by LAMMPS and VASP were used.

\[ H_{ijkl}^h = \frac{1}{|Y|} \int_Y \left[ H_{ijkl}(y) - H_{ijrs}(y) e_{rs}(\zeta^{kl}) \right] dy \]

Elastic constants for columnar microstructure
- $C_{11} = 205.31$, $C_{22} = 205.32$, $C_{33} = 172.36$
- $C_{12} = 74.13$, $C_{13} = 107.08$, $C_{23} = 107.09$
- $C_{44} = 53.63$, $C_{55} = 95.05$, $C_{66} = 95.05$

Elastic constants for equiaxed microstructure
- $C_{11} = 219.64$, $C_{22} = 211.20$, $C_{33} = 205.55$
- $C_{12} = 80.59$, $C_{13} = 86.29$, $C_{23} = 94.71$
- $C_{44} = 60.33$, $C_{55} = 66.14$, $C_{66} = 70.83$
Stress-strain curve by virtual test

- Virtual tensile tests were performed by ABAQUS using HOMAT interface for columnar and equiaxed microstructures.
- Elastic constants calculated by HOMAT were considered.

Stress-strain curves for columnar and equiaxed microstructures
Simulation procedure

**Microscale**
- Solidification simulation
  - Thermo-Calc Software
  - FINAS/STAR TPS edition
- Distribution of microstructure
- Step 4: Hot rolling simulation
  - ABAQUS
  - Strain energy for nucleation and growth of Rex. grains
- Step 5: Recrystallization simulation
  - micress

**Nanoscale**
- Calc. of microscopic properties
  - Virtual material test
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    - FINAS/STAR TPS edition
  - Experimental material test
    - Nanoindentation, Tensile test
- Elastic constants stress properties of $\delta$ and $\gamma$ phases
- Calc. of macroscopic properties based on microstructure
  - Elastic constants
    - HOMAT
  - Stress-strain curves
    - HOMAT/ABAQUS

**Macro-to-Micro scale**

Hot rolling simulation using ABAQUS/Explicit

- Simulation conditions
  - Roller diameter: 160 mm
  - Roller surface velocity: 18 m/min
  - Rolling reduction: 8mm
  - Initial temperature: 900°C
  - Number of pass: 1

Equiaxed solidification zone

Columnar solidification zone

Rolling direction

Symmetry surface

20 mm
3 mm
40 mm
50 mm
Simulation results

Roller passing time: 0.4s

Maximum plastic energy in columnar region: 195.5 [MPa]

Maximum plastic energy in equiaxed region: 116.7 [MPa]
**Simulation procedure**

**Microscale**

- **Solidification simulation**
  - FINAS/STAR TPS edition
  - Thermo-Calc Software

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  - ABAQUS
    - Strain energy for nucleation and growth of Rex. grains

- **Step 5 Recrystallization simulation**
  - micress

**Nanoscale**

- **Calc. of microscopic properties**
  - Virtual material test
    - Atom simulation
  - Experimental material test
    - Nanoindentation, Tensile test

- Elastic constants stress properties of δ and γ phases

**Macroscale**

- Distribution of microstructure

**Micro-to-Macro scale**

- Calc. of macroscopic properties based on microstructure
  - Elastic constants
  - Stress-strain curves

- Macroscopic Stress-strain curves
- HOMAT/ABAQUS

**Additional Software**

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- http://www.thermocalc.com/
- https://www.vasp.at/
- http://www.3ds.com/simulia
Modeling and assumptions

- 2D simulation of REX of $\gamma$ phase using MICRESS
- Recrystallization is driven by plastic energy stored during the hot rolling process for 0.4s.
- Before the REE, the residual $\delta$ phase is transformed to $\gamma$ phase.

Plastic energy density: 116.7 MPa

Plastic energy density: 195.5 MPa
Interface and nucleation conditions

- **Interfacial energy**
  \[ \sigma_{\gamma-\gamma} = 5 \times 10^{-5} \text{ J/cm}^2 \]

- **Interfacial mobility**
  \[ K_{\gamma-\gamma} = 7.5 \times 10^{-3} \text{ cm}^4/\text{J/s} \]

- **Model of interfacial anisotropy**
  - Threshold misorientation: ±15 Deg.
  - Interfacial energy: Read-Shockley
  - Interfacial mobility: Humphreys

- **\( \gamma \) grain nucleation**
  - Position: \( \gamma-\gamma \) interface
  - Grain crystal-orientation: ±15Deg. of parent relation to substrate
  - Time between checks: \( 5 \times 10^{-5} \text{s} \)
  - Shield distance: 2.5μm
Recrystallization behavior

Columnar $\gamma$ phase

Equiaxed $\gamma$ phase

Deg.
Conclusions

Summary

• We have successfully performed multi-scale simulation of hot rolling process of duplex stainless steel based on microstructure by using various computational tools and software.
• Our methodology enables us to simulate solidification, hot rolling and recrystallization process seamlessly.

Future issues

• We have to improve accuracy and reliability of each simulation, especially estimation of properties of single phase and homogenization method.
• Crystal plasticity models will give us more useful information for multiscale simulation.