Crystalline modelling of deformation and recrystallization of an Udimet 720 superalloy during high temperature forging

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Material supplied by Aubert & Duval who cofinance this study with Ecole Centrale Paris.
Outline

Context of the study

I°) The material

II°) The deformation model « Cristalecp »

III°) The recrystallization model « Reclpces »

IV°) The sequential coupling
Context of the study

Improvement of performances and energy efficiency of aircraft engines

Materials with very high mechanical properties

Nickel base superalloy obtained by forging

**Udimet 720**: Superalloy with remarkable mechanical properties at high temperature (Re > 1000 MPa at 800°C, low creep…)

Material of replacement of the well known Waspaloy and Inconel 718 for the manufacturing of turbine discs
Material

- The Udimet 720 belongs to the family of superalloys hardened by $\gamma'$ phase ($\text{Ni}_3[\text{Ti,Al}]$) such as the Waspaloy.
- The strength improvement results in the addition of alloying elements.

<table>
<thead>
<tr>
<th>Alliage</th>
<th>Ni</th>
<th>Cr</th>
<th>Co</th>
<th>Ti</th>
<th>Al</th>
<th>Mo</th>
<th>W</th>
<th>C</th>
<th>B</th>
<th>Zr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waspaloy base</td>
<td>19</td>
<td>13.5</td>
<td>3</td>
<td>1.4</td>
<td>4.2</td>
<td>-</td>
<td>0.04</td>
<td>0.006</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>Udimet 720 base</td>
<td>16</td>
<td>15</td>
<td>5</td>
<td>2.5</td>
<td>3</td>
<td>1.25</td>
<td>0.035</td>
<td>0.035</td>
<td>0.035</td>
<td></td>
</tr>
</tbody>
</table>

- The volume fraction of $\gamma'$ phase reaches 43% instead of 30% for Waspaloy.
- This strength improvement reduces inevitably ductility.
- Sub-solvus forging required.
- Two-phase microstructural evolution during forging.
Material

Two phases microstructure:
- $\gamma$ matrix (FCC)
- $\gamma'$ hardening phase (SC)

Hypothesis: At 1100°C, secondary and tertiary $\gamma'$ are solved

Aims of the work

- Development of a numerical model to reproduce dynamic recrystallization
- Prediction of the microstructural evolution during forging

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Deformation model: « Cristal_ECP »

- **Cristal_ECP**: Crystalline plasticity model implemented in Abaqus® code
- **Large transformation**: \( F = A \cdot P \) where \( P \) plastic contribution
  - \( A = (1 + \varepsilon) \cdot R \) elastic contribution
- **Small elastic distortion** (\( |\varepsilon| << 1 \)) but **large rotation** \( R \)
- **Deformation mechanism**: glide and recovery
- **Modelling on 3D aggregate with real microstructure obtained from EBSD**
- **In each element of the meshing**: - Crystalline orientation (Euler angles)
  - Viscoplastic law
    - 12 slip systems \( \{111\}<110> \) for \( \gamma \) matrix
    - 6 slip systems \( \{100\}<110> \) for \( \gamma' \) precipitates
  - Initial dislocation density

Interaction between neighboring grains and phases are taken into account
Constitutive laws

- Schmid law on each slip system (s), in each element of the mesh
  \[ |\tau^s| = \tau^s_c \text{ et } \dot{\tau}^s = \dot{\tau}^s_c \]

- Viscoplastic law
  \[
  \begin{align*}
  \dot{\gamma}^s &= \left|\tau^{s\text{pl}}\right| \left(\frac{\tau^s}{\tau^s_c}\right) \text{sgn}(\tau^s) \text{ if } |\tau^s| \geq \tau^s_c \\
  \dot{\gamma}^s_0 &= 0 \text{ otherwise}
  \end{align*}
  \]
  Critical shear stress
  \[ \tau^s_c = \tau^s_0 + \mu b \sum a^{su} \rho^u \]

- Hardening law
  \[ \dot{\tau}^s_c = \sum h^{su}\left|\dot{\gamma}^{s\text{pl}}\right| \]

- Hardening matrix
  \[
  h^{su} = \frac{\mu}{2} \sqrt{\sum a^{st} \rho^t} \left(\frac{1}{L^u} - g_c \rho^u\right)
  \]
  \[ \text{with } \frac{1}{L^s} = I + \sqrt{\sum \rho^t} \frac{D}{K} \]

- Dislocation density evolution law
  \[
  \dot{\rho}^s = \frac{|\dot{\gamma}^s|}{b} \left(\frac{1}{L^s} - g_c \rho^s\right)
  \]
  The dislocation density is the state variable in the modelling

- Material parameters determined by compression tests performed at several strain rate and temperature

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Meshing & aggregate

- The meshing is performed from EBSD measurement
  - Aggregate composed by 5 similar layers
  - Element size given by EBSD step (0.6 µm)
  - EBSD map extruded in order to give a thickness of 2 µm

- Two-phases aggregate
  - 165 * 165 * 5 elements (C3D8R)
  - Forging boundary conditions
Deformation results

- 10% of deformation at 1100°C with $\dot{\varepsilon} = 0.01\, s^{-1}$

Initial microstructure

- Hardening voluntarily overestimated
- Creation of sub-boundaries
- Formation of intragranular misorientations (grain 1)
- Heterogeneous dislocation density after deformation
The recrystallization model « Rec_LPCES »

- Model of recrystallization
  - Nucleation-growth approach
- Model based on the cellular automaton method
  - Use of hexagonal meshing (6 neighbors for one site)

Input parameters given by Cristal_ECP for each site:
- New crystalline orientation
- Stored energy: calculated from dislocation density
  \[ E_{\text{stored}} = \frac{1}{2} \mu b^2 \rho \]
- Number to identify phase
Constitutive laws

Nucleation

• Nucleation if \( E_{\text{stored}} > E_{\text{limit}} \)
• Nuclei are near the grain boundaries
• After nucleation \( E_{\text{stored}} = 0 \) and crystalline orientation remains the same

Growth: possible for recrystallized grains

Mobility of grain boundaries

\[
M^{ss'} = M_m \left[ 1 - \exp \left( -\left( \frac{\theta^{ss'}}{10} \right)^3 \right) \right]
\]

Driving force

\[
V = -M \Delta E
\]

\[
\Delta E = E_{\text{stored}} + \gamma
\]

\[
\gamma^{ss'} = \gamma_m \frac{\theta^{ss'}}{\theta^*} \left[ 1 - \ln \left( \frac{\theta^{ss'}}{\theta^*} \right) \right] \text{when } \theta^{ss'} \leq \theta^*
\]

where

\[
\gamma_m \text{ when } \theta^{ss'} > \theta^*
\]

Recrystallized site
- \( E_{\text{stored}} = 0 \)
- Orientation 1

Deformed site
- \( E_{\text{stored}} \neq 0 \)
- Orientation 2

\[ \Delta E \]

Recrystallized site
- \( E_{\text{stored}} = 0 \)
- Orientation 1

Recrystallized site
- \( E_{\text{stored}} = 0 \)
- Orientation 1

If \( \gamma^{ss'} > \) critical value \( \Rightarrow \) réorientation

Probability of reorientation

\[
P^{ss'} = \frac{d}{d_0} = \frac{-M^{ss'} \Delta E t_{inc}}{d_0}
\]

Context of the study  Material Deformation model Recrystallization model Sequential coupling
Recrystallization results

Deformed microstructure (Cristal_ECP)

- Nucleation of all sites near the grain boundaries if $E_{\text{stored}} > 0.3$ mJ.mm$^{-3}$ ($\rho = 1.82 \times 10^8$ mm$^{-2}$)

Recrystallized microstructure

- Growth of grains (grain 2)
- Grains with sub-structure deformation (grain 3)

Context of the study
Material
Deformation model
Recrystallization model
Sequential coupling

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Sequential coupling to simulate dynamic recrystallization

- Sequential coupling of the models « Cristal_ECP » and « Rec_LPCES »
  - Applied to an aggregate:
    - To follow the macroscopic stress variation
    - To study the microstructural evolution

Afterwards, to limit computation time the aggregate is made up of 5 layers where the sequential coupling is applied only to the intermediate layer.
Sequential coupling

Initial microstructure

\( \epsilon = 10\% \)

\( \epsilon + \text{recrystallization} \)

\( \epsilon + \text{recrystallization} + \epsilon \)

- Creation of intragranular misorientation during the first deformation
- Growth of grains and annihilation of sub-boundaries during recrystallization
- Increase of the misorientation of some sub-boundaries and evolution of the crystallographic orientation of some grains (grain 4) during the second deformation
- Evolution of dislocation densities during sequential coupling

Context of the study
Material
Deformation model
Recrystallization model
Sequential coupling

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Sequential coupling

- After two cycles

**Diagram:**
- Material: 99 µm
- Graph showing deformation and stress over deformation.
Sequential coupling

- After two cycles
## Conclusion

- Development of an original simulation procedure for **dynamic recrystallization** on a two-phase material
- Prediction of stress evolution, microstructure, texture, dislocation density, stored energy …

## Prospects

- Improvement of the deformation model for high temperatures
- Introduction of various recrystallization mechanisms identified during experimental analyzes (apparently DDRX for Udimet 720)
- Adjustment of the parameters to obtain a simulated stress-strain curve nearest of the experimental curve
Thank you for your attention!
Sequential coupling

Sequential coupling of the models «Cristal_ECP» and «Rec_LPCES»

Initial state : state 0
- Crystallographic orientation given by EBSD
- Unique dislocation density ($\rho$) per phase

1st Deformation

Deformed state : state 1
- Crystallographic orientation at state 1
- Increase of $\rho$
- $\rho$ heterogeneous in the aggregate

1st Recrystallization

Recrystallized state : state 2
- Crystallographic orientation at state 2
- $\rho$ heterogeneous in the aggregate
  - Recrystallized grains: $\rho=0$
  - Deformed grains $\rho$ : state 1

Input
- Layers at state 0
- Layer at state 2
- Layers at state 0

output
- Layers at state 1
- Layer at state 3
- Layers at state 1

2nd Deformation

Deformed state : state 3
- Crystallographic orientation at state 3
- Increase of $\rho$
- $\rho$ heterogeneous in the layer