Full-field modeling of spheroidization phenomenon in α/β titanium alloys during hot-deformation and subsequent annealing at a given temperature.

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What is spheroidization in α/β titanium alloys?

Why?

• α/β titanium alloys show attractive mechanical properties for industrial use.

• Spheroidization is a very important phenomenon for the microstructural control

• Spheroidized microstructure shows enhanced strength and ductility

Goals

To develop a global experimental and numerical framework in order to understand and simulate the phenomenon of spheroidization.
Which are the main governing mechanisms?

- β Grains Size ≈ 0.25 – 0.7mm
- Laths thickness ≈ 1-2 µm

Initial state

Deformed state

Short annealing state

Longer annealing state
Microstructural evolution

Before deformation

+ 15min annealing

Conclusions
The higher the strain the quicker is the evolution during annealing

+ 1h annealing
Quantification of microstructural evolution

0.36 strain
350 laths measured

0.36 strain
350 laths measured

1.34 strain
450 laths measured

Binarization with ImageJ

We want to measure
- Aspect ratio
- Particle area

Aspect ratio = \( \frac{\text{major radius}}{\text{minor radius}} \)
Quantification of microstructural evolution

![Graph showing the quantification of microstructural evolution with time (min) on the x-axis, mean aspect ratio on the y-axis, and mean surface area on the y-axis. The graph includes data points for 1.34 strain.]
Overview of the physical mechanisms

Governing Mechanisms
- Crystal plasticity
- Surface diffusion in α/β interfaces
- Motion by mean curvature in α/α interfaces
- Coarsening

Observations
- Applying hot deformation
  - Local misorientations developed in α lamellae
  - Formation of α/α subboundaries

Splitting of lamellae
- Motion driven from surface diffusion at the α/β interface
- Motion driven by mean curvature at the α/α interface
**FE/ Level-Set Method**

**Simulating Grooving**

Distance function

\[ \varphi(x, t) = \pm d(x, \Gamma(t)) \]

Outside normal

\[ \vec{n} = -\frac{\nabla \varphi}{\|\nabla \varphi\|} \]

Mean curvature

\[ \kappa = -\nabla \frac{\nabla \varphi}{\|\nabla \varphi\|} \]

**Mathematical formulation**

coupling of two different motion velocities

\[ \vec{v}_n = (-C_0 \Delta_s \kappa) + A \kappa \vec{n} \]

**Coupling coefficients**

\[ C_0 = \begin{cases} -\gamma_{\alpha\beta} v \Omega^2 D_{\alpha\beta} & \text{at the } \alpha/\beta \text{ interface} \\ \frac{kT}{kT} & \text{everywhere else} \end{cases} \]

\[ A = \begin{cases} \gamma_{\alpha\alpha} b f \Omega e^{-\frac{Q}{RT}} & \text{at the } \alpha/\alpha \text{ interface} \\ \frac{kT}{kT} & \text{everywhere else} \end{cases} \]
FE/ Level-Set Method

Calculation of curvature $\kappa$ and velocity $v_n$ (use of the surface diffusion estimation solver developed by Bruchon, Pino Muñoz et al. *)

Enhanced Lagrangian framework

$$\mathbf{v}_n = [-C_0(\Delta_S \kappa) + A\kappa]\mathbf{n}$$

Analytical exact reinitialization**

$$\|\varphi(x) = 1\|$$

- No validation/calibration of unphysical parameters necessary to reinitialize
- It enables the exact description of $\mathbf{n}$ (no P1 interpolation of LS)


Immersion of microstructure

Extraction of real $\alpha$ colonies from experimental images and application of surface diffusion

- Binarization and image treatment with “Image J”
- Extract of the distance function with “Image J”

Experimental picture of LN$x_4$ deformed
Enhanced Lagrangian framework

New topological mesher (Fitz)

- Body fitted meshing and remeshing is possible with this technic

Necessary use of adaptive mesh

- Efficient representation of the $\alpha$ laths
- Following the shape evolution of the interfaces
- More efficient regarding volume loss

Mesh quality

**Extraction of real $\alpha$ colonies from experimental images and application of surface diffusion**

Motion by surface diffusion

\[ \vec{v}_n = (C_0 \Delta \kappa) \hat{n} \]

Zero iso-surface evolution

Mesh adaptation technique

<table>
<thead>
<tr>
<th>Mesh adaptation technique</th>
<th>Method 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step (ms)</td>
<td>10</td>
</tr>
<tr>
<td>Time (s)</td>
<td>1</td>
</tr>
<tr>
<td>( h_{el} ) close to surface (( \mu m ))</td>
<td>1</td>
</tr>
<tr>
<td>time calculation (12CPUs)</td>
<td>2min</td>
</tr>
<tr>
<td>Volume loss</td>
<td>1.5%</td>
</tr>
</tbody>
</table>
Motion by mean curvature

\[ \overrightarrow{v_{curv}} = (A\kappa)\overrightarrow{n} \]

**simple case of triple junction in a Lagragian Framework**
Calculation time: 8 min
Coupling of surface diffusion and motion by mean curvature

\[ \overrightarrow{v_{\text{curv}}} = (A\kappa)\overrightarrow{n} \]
\[ \overrightarrow{v_{\text{surf}}} = C_0 (\Delta_s \kappa)\overrightarrow{n} \]
Surface diffusion in real microstructure
Motion by surface diffusion coupled with motion by mean curvature
Comparison

Surface diffusion

Surface diffusion
+ motion by mean curvature

Volume loss approximation: 2.8%

No unphysical coalescence
Volume loss approximation: 0.1%
Conclusions

1. Governing mechanisms for the first stages of annealing

Motion driven from surface diffusion at the \( \alpha/\beta \) interface

\[
\vec{v}_n = (-(C_0 \Delta_s \kappa) + A \kappa) \vec{n}
\]

Motion driven by mean curvature at the \( \alpha/\alpha \) interface

2. Efficiently simulated the splitting of the lamellae

3. Simulated the coupling of the mechanisms on real microstructure

Perspectives

- Estimation of the right values for coefficients \( C_0 \) and \( A \)  
- Simulating coarsening
- Simulating crystal plasticity during deformation for the formation of sub-boundaries
Thank you for your attention!