Modeling the fragmentation of α lamellae and the subsequent spheroidization of α laths in α/β titanium alloys

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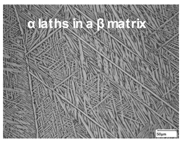
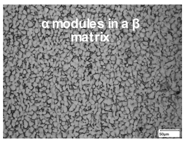
Spheroidization in α/β titanium alloys



Initial microstructure

Hot deformation + Thermal treatment



spheroidized microstructure

Why ?

- α/β titanium alloys show attractive mechanical properties for industrial use.
- Spheroidization is a very important phenomenon for the microstructural control
- Speroidized 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

Experiments

EBSD maps illustrating numerous α colonies inside β grain

Initial state

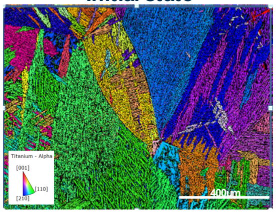
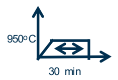


Figure 1: Inverse pole figures map of the α phase in a Ti-64 sample after heat treatment at 950°C.



Deformed state

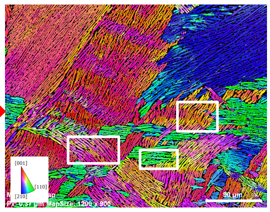
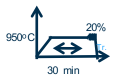


Figure 2: Inverse pole figures map of the α phase in a Ti-64 sample after 20% deformation at 950C



Closer look inside the colonies after deformation

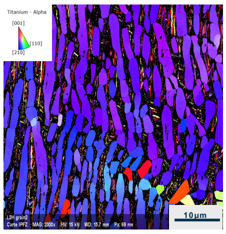


Figure 3: Inverse pole figures map of the α phase in a Ti-64 sample after 20% deformation at 950°C.

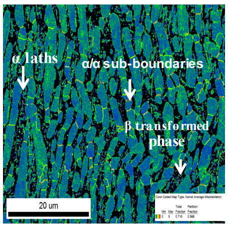


Figure 4: Kernel average misorientation map of the same area

Observations

Applying hot deformation

Local misorientations developed in α lamellae

Formation of α/α sub-boundaries

Governing mechanisms

1) Crystal plasticity
2) Surface diffusion on α/β interfaces
3) α/α interface motion driven by capillarity
3) Coarsening

Modeling surface diffusion in a level set framework

Signed distance function describing the α laths

$$\varphi(x,t) = \pm d(x,\Gamma(t))$$

Outside normal

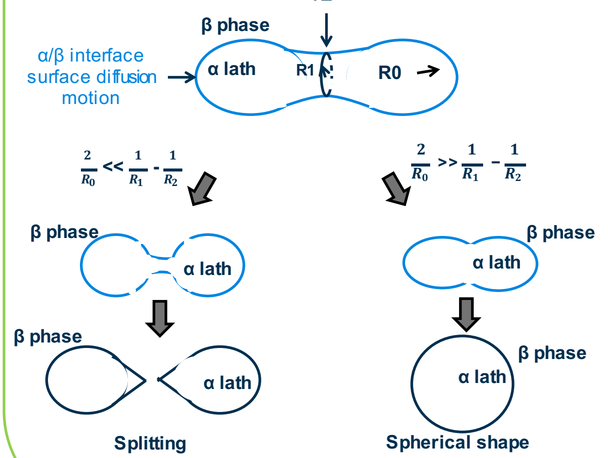
$$\boldsymbol{n} = \frac{\nabla\varphi}{\|\nabla\varphi\|}$$

Mean curvature

$$\kappa = div(\boldsymbol{n}) = \nabla\frac{\nabla\varphi}{\|\nabla\varphi\|}$$

Interface surface velocity

$$\vec{v} = v_n\frac{\nabla\varphi}{\|\nabla\varphi\|} = v_n\boldsymbol{n} = (B(\Delta_s\kappa))\boldsymbol{n}$$



$\frac{2}{R_0} << \frac{1}{R_1} - \frac{1}{R_2}$ (Splitting) ; $\frac{2}{R_0} >> \frac{1}{R_1} - \frac{1}{R_2}$ (Spherical shape)

Simulation of surface diffusion in a α lath

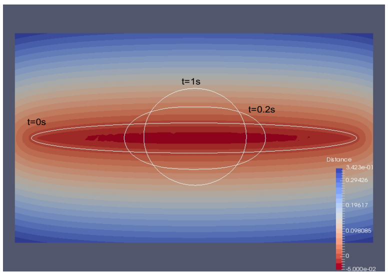
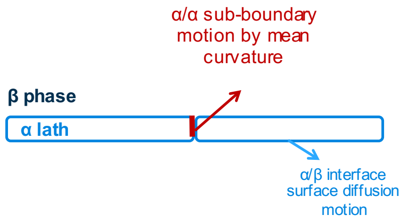


Figure 3: initial distance function field and the obtained interfaces (white lines) at t=0s, 0.2 s and 1s [3]

Time step (ms)	1
CPUs	10
Calculation time	2 min
Volume loss	0.032%

Modeling α/α sub-boundary kinetics



Interface velocity combination [1][2]

$$\vec{v} = v_n\frac{\nabla\varphi}{\|\nabla\varphi\|} = v_n\boldsymbol{n} = (B(\Delta_s\kappa) - Ak)\boldsymbol{n}$$

Conclusions

- A new level set - finite element framework is used to describe the interface kinetics.
- Several mesh adaptation techniques have been tested in order to accurately describe the shape evolution of α laths and to reduce the calculation time.

Future Perspectives

- Coupling between surface diffusion at the α/β interfaces and motion by mean curvature at the α/α grain interfaces.
- An existing crystal plasticity finite element approach developed in a level-set context will also be used to model the deformation of the α lamellae.

References

[1] S. Semiatin and D. Furrer, "Modeling of microstructure evolution during the thermomechanical processing of titanium alloys," *Metals Branch, Metals, Ceramics, and NDE Division,* 2008.
[2] W. Mullins, "The effect of thermal grooving on grain boundary motion," *Acta Metallurgica,* vol. 6, no. 6, pp. 414-427, 1958
[3] D. Polychronopoulou, N. Bozzolo, D. Pino Muñoz, J. Bruchon, M. Shakoor, Y. Millet, C. Dumont, I. Freiherr von Thüngen, R. Besnard, and M. Bernacki, "Introduction to the level-set full field modeling of lath spheroidization phenomenon in α/β titanium alloys, " *In proceedings of NUMIFORM 2016.*