Microstructural evolution prediction during forming processes: towards a modelling by industry

Colloque “La Métallurgie, quel avenir !”

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ABOUT TRANSVALOR SA

- Founded almost 30 years ago
- Pioneer in the world of computer-aided Material Forming Simulation
- High performance industry-leading 3D solutions for process design and analysis technologies to the Material Forming Industries.
- Today we stand as a World Leader in our industry
Our DNA

- Rooted in research
- Driven by innovation
- Designed for industrial results

Colloque « La Métallurgie, quel avenir ! » – June, 27th / July, 1st 2016
OUTLINE

• Introduction

• Microstructural evolution modelling: different approaches

• Mesoscale modelling in a Level-Set framework
  • DIGIMU®: mesoscale computations in an industrial context
  • Generation of polycrystals in a finite element context
  • Recrystallization and grain growth modelling

• Application examples

• Conclusion
INTRODUCTION

- A growing interest for microstructure modelling throughout the whole process chain...
INTRODUCTION

... and particularly during hot forming processes

For the parts made, hot forging scheme must ensure:
- the required shape and size
- the mechanical performance requirements (strength, toughness, corrosion resistance, high-temperature properties...)

Decisive effect of the grain size

Properties

Microstructure

Process

Adapted thermomechanical processing route
**INTRODUCTION**

- **Microstructural evolution**
  - Governed by the process parameters (temperature, strain and strain rate)
  - Given by reduction of the internal energy

*Necessity to model the different metallurgical phenomena to predict the microstructural evolution*

*The way to return to equilibrium*
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**DIFFERENT APPROACHES**

- **Phenomenological approach**
  - Results of observed phenomena expressed mathematically
  - Coefficients obtained by a regression method based on experimental observations

*Example: Description of the recrystallized fraction*

*In constant conditions (strain rate and temperature)*
- Sigmoidal shaped curves
- Kinetics described by the analytical Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation:

\[ X(t) = 1 - e^{-b \cdot t^n} \]
DIFFERENT APPROACHES

- Phenomenological approach

**Low CPU time**
- Easy coupling with FE methods (metallurgical computation at each integration point of a FE mesh)
- Investigation of the process parameters on recrystallization fraction and grain size

**Lack of physical background**

**Extensive experimental observations required**
- Can only be used within a specified range
- Necessary to update the model parameters according to the forging scheme

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ASTM grain size after an orbital forging process on Inconel718
Comparison experiments / FORGE® simulation (courtesy Tecnalia, ES)
DIFFERENT APPROACHES

- **Physically-based approach**
  - Models taking into account elementary physical phenomena

![Diagram of different approaches]

- Initial microstructure
- Modelling of the elementary physical phenomena
- Actual microstructure

**Macroscopic description of the microstructure**

- Definition of “averaged” representative material parameters
  - *i.e.* dislocation density, grain diameter...

**Output**

- “Updated” microstructure given by the evolution of these parameters
DIFFERENT APPROACHES

-Physically-based approach

**Microstructure-based constitutive model**
- Coupling metallurgy and rheology (update of the material behaviour with the current microstructural state)

**Low CPU time (analytical laws)**
- Integration in FE software possible

- Homogenized quantities
  - Unable to capture local phenomena

- Calibration
  - Large number of material constants
DIFFERENT APPROACHES

- **Mesoscale modelling – Full field approach**
  - Modelling the evolution of the grains (microstructure components fully modelled)
  - Simulations performed on Representative Volume Elements (RVE)

- **Realistic description of microstructural features**
  - Topological aspects taken into account
  - Help for understanding microstructural phenomena
  - Modelling local and heterogeneous phenomena

- **Concept of numerical tests (scale transition)**
  - Improvement of higher scale models usable for macroscopic simulations
  - Calibration of these models

- **Computation time**
  - Simulation performed on specific locations of an industrial workpiece (thermomechanical and thermal history as boundary conditions applied to the RVE)
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DIGIMU®: MESOSCALE COMPUTATIONS IN AN INDUSTRIAL CONTEXT

- From simulations for industry towards simulations by industry

Development of an industrial solution for simulating microstructural evolutions at the grains scale during thermomechanical processes

Our industrial partners
GENERATION OF POLYCRYSTALS IN A FE CONTEXT

- Definition and construction of a Representative Volume Element (RVE)

From purely experimental description

- Feasible but heavy experimental devices necessary in 3D
- Representativeness of the chosen volume?

From random processes

- Must respect grains topology and a given grain size distribution

![Experimental micrograph](image1)

![Initial polycrystal considered](image2)
GENERATION OF POLYCRYSTALS IN A FE CONTEXT

- Microstructure immersion in a FE mesh

Explicit approaches:
- Body-fitted mesh (may be hard to obtain)
- No mixing laws
- Contact handling

Implicit approaches:
- Fixed mesh
- Easy handling of topological changes
- Complicated contact conditions

Problem of tracking the interfaces avoided
**GENERATION OF POLYCRYSTALS IN A FE CONTEXT**

- **Microstructure immersion in a FE mesh**
  
  Implicit description of the interfaces using a level-set framework

  - What is a level-set function?

    - Signed distance function
      
      \[
      \begin{aligned}
      \psi(x,t) &= \pm d(x, \Gamma(t)), \ x \in \Omega, \\
      \Gamma(t) &= \{ x \in \Omega, \psi(x,t) = 0 \}.
      \end{aligned}
      \]

  - Evolving interfaces

    - Transport of a LS function
      
      \[
      \begin{aligned}
      \frac{\partial \psi(x,t)}{\partial t} + \vec{v} \cdot \nabla \psi &= 0, \\
      \psi(x,t = 0) &= \psi^0(x)
      \end{aligned}
      \]

  - Extension to several LS functions

    - Multiphase calculations
      
      \[ \psi_\rho(x,t) \text{ with } \rho \in \{1, \ldots, N_p\} \]

  - Adaptative anisotropic remeshing
RECRYSTALLIZATION AND GRAIN GROWTH MODELLING

Normal velocity of a grain boundary

\[ \vec{v} = m (\tau \Delta \rho - \gamma \kappa) \vec{n} \]

- $m$: grain boundary mobility
- $\gamma$: grain boundary energy
- $\kappa$: grain boundary mean curvature
- $\tau \Delta \rho$: stored energy
- $\vec{n}$: outward normal unit vector

Thermodependent

Driving force for grain boundaries motion
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APPLICATION EXAMPLES

- Deformation step modelling (CPFEM & DRX)

CPFEM (crystal plasticity FE modelling)
- Deformation of the RVE
- Evolution of dislocation densities, stored energy in each grain (dependent on grains orientation)
- Determination of preferential nucleation sites for new grains

Coupling CPFEM and dynamic recrystallization
- Nucleation and growth of new recrystallized grains
- Influence on local orientation and dislocation densities

R. Boulais-Sinou’s talk
(June, 28th – 9:20am, Amphi F2)
APPLICATION EXAMPLES

- Post deformation modelling (MDRX & SRX)

Static and metadynamic recrystallization

- Microstructural evolution driven by grain boundaries curvature and differences in stored energy
- Nucleation conditions (site-saturated, random)
APPLICATION EXAMPLES

- Post deformation modelling (MDRX & SRX)

Determination of the recrystallization parameters: a multi-scale approach
- Critical dislocation density for nucleation
- Number of nuclei
- Critical germ radius

Evaluation of different SRX configurations

APPLICATION EXAMPLES

- Post deformation modelling (MDRX & SRX)


Evolution of the surface ReX fraction measured on 10 slices and comparison with the volume information and experimental data.
APPLICATION EXAMPLES

- Grain growth modelling

Normal grain growth
- Microstructural evolution driven by grain boundaries (GB) curvature
- Uniform GB mobility (thermodependent)
- Uniform and isotropic GB energy
- Influence of initial grain size distribution

Inconel 718 heat treated 75min at 1040 °C \( (d_0=20\mu m) \)

M. Bernacki’s talk
(June, 27th – 5:00pm, Amphi F2)
APPLICATION EXAMPLES

- Grain growth modelling

Smith-Zener pinning phenomenon
- Dragging effect exerted by second phase particles (SPP) on GB
- Enable to control the final grain size by slowing down the GB kinetics

B. Scholtes et al., “Full field modeling of the Zener pinning phenomenon in a level set framework - Discussion of classical limiting mean grain size equation”, 13th International Symposium on Superalloys, Sept. 11-15 2016, Seven Springs, Pennsylvania
APPLICATION EXAMPLES

• Grain growth modelling

Understanding of the abnormal grain growth phenomenon
- Growth of a limited number of grains much faster than the rest
- Decrease of mechanical properties

A. Agnoli et al., Strain induced abnormal grain growth during δ sub-solvus annealing in inconel 718. Accepted in Metallurgical and Materials Transactions A, 2015
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CONCLUSION

Will to propose industrial solutions for simulating microstructural evolution during forming processes. A help for:

- Predicting local material properties
- Optimizing the process route

Microstructural evolution modelling at the mesoscopic scale

- Simulate heterogeneous and local phenomena
- Improve mean field models for macroscale computations
- Numerical developments already available
- Step by step introduction in the DIGIMU® software

Future developments

- Continuous improvements of the physical models (dynamic recrystallization, anisotropy, phase transformations...)
- Towards full 3D simulations: intensive work to reduce computation times
Thank you for your attention

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