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Full field simulation of dynamic and post-dynamic recrystallization in 304L steel

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Abstract

This paper describes a level-set framework for the full field modeling of dynamic and post-dynamic recrystallization in a 3D polycrystalline material submitted to large deformation. Topological evolutions are simulated based on a kinetic law linking the velocity of grain boundaries to the thermodynamic driving forces. Recrystallization is modeled by coupling a level-set approach to phenomenological laws describing strain hardening and nucleation. The proposed formalism enables to reach outstanding dynamic recrystallization computations in a front-capturing finite element framework comparatively to the state of art.

Introduction

During hot deformation, plasticity increases the dislocation density while dynamic recovery decreases the dislocation density in the microstructure. Globally, the dislocation density increases. When a critical dislocation density is locally reached, nucleation which is the appearance of new grains free of defects can occur. In parallel, grain boundary migration occurs due to stored energy gradients across interfaces and due to capillary effects. These mechanisms lead to the so-called dynamic recrystallization (DRX) mechanism. When plastic deformation stops, the material is still at high temperature, thus grain boundary migration is still active under the same thermodynamic driving forces. Furthermore, nucleation can also occur in the most hardened grains. These mechanisms appearing right after hot deformation lead to the so-called post-dynamic recrystallization process (PDRX). In the present work, a 3D finite element (FE) model based on the level-set (LS) method in the context of unstructured tetrahedral mesh is proposed to model the DRX and PDRX phenomena in austenitic stainless steel 304L submitted to large deformation and with relatively low computational costs. The LS approach coupled to a remesher provides an accurate tracking of interfaces (i.e. grain boundaries) all along the simulation while phenomenological laws are used for controlling nucleation, work hardening and recovery.

Constitutive laws of the model

Representation of the digital microstructure

The model is based on a LS description of the interfaces within a FE framework (Bernacki et al. 2008; Bernacki et al. 2009). First, grain interfaces are virtually generated by

using the Voronoï (Weaire, Kermode, and Wejchert 1986) or Laguerre-Voronoï (Fan et al. 2004) method. The virtual interfaces are then described into an unstructured FE mesh thanks to LS functions. Furthermore at the initial stage of the simulation, an energy field considered constant per grain is defined in the microstructure.

Grain boundary migration

At high temperatures, grain interfaces migrate driven by stored energy gradients across interfaces and by capillarity forces induced by grain boundary mean curvature. To simulate grain boundary migration, the strategy presented in (Scholtes et al. 2016) is adopted.

Strain hardening and recovery

The strain hardening and recovery mechanisms appearing during hot deformation can be modeled at different scales: at a local scale with crystal plasticity algorithms or at a higher scale with phenomenological laws. In this model, phenomenological laws are used in order to limit the computational cost of the 3D simulations. Considering N_G grains in the microstructure, the averaged dislocation density field in each grain j noted $\langle \rho_j \rangle$ is assumed to evolve according to the Yoshie-Laasraoui-Jonas law (Yoshie et al. 1987) :

$$\dot{\langle \rho_j \rangle} = (K_1 - K_2 \langle \rho_j \rangle) \dot{\varepsilon}_{eff}^p,$$

where $\dot{\varepsilon}_{eff}^p$ denotes the rate of effective plastic strain, K_1 and K_2 are two constants which represent respectively the strain hardening and dynamic recovery term. A superposed dot denotes differentiation with respect to time.

Nucleation mechanism

In the considered model, a nucleus can appear where the averaged dislocation density reaches a critical value noted ρ_{cr} . Concerning the computing of ρ_{cr} , a first approximation is made and an iterative calculation is done according to the following equation (Beltran, Huang, and Logé 2015):

$$\rho_{cr} = \left[\frac{-2\gamma_b \dot{\varepsilon} M_b \delta(\dot{\varepsilon}) \tau^2}{\ln \left(1 - \frac{K_2}{K_1} \rho_{cr} \right)} \right]^{1/2},$$

where τ is the dislocation line energy, $\delta(\dot{\varepsilon})$ is a strain rate dependent parameter, M_b is the grain boundary mobility and γ_b is the grain boundary energy.

When a new nucleus appears in the microstructure, its critical radius must be high enough so that the growth

driving force resulting from the difference in stored energy with the neighborhood compensates for the shrinkage driving force induced by capillarity forces. This condition is approximated by the so-called Bailey-Hirsch criterion (Bailey and Hirsch 1962):

$$r^* = \omega \frac{2\gamma_b}{\rho_{cr}\tau},$$

where $\omega > 1$ is a safety factor ensuring that the created nucleus has the required driving force for growth.

The nucleation rate \dot{V} , representing the volume of created nuclei per unit of time, is calculated according to a variant of the proportional nucleation model of Peczak and Luton (Peczak and Luton 1993):

$$\dot{V} = K_g \Phi \Delta t,$$

where K_g is a probability coefficient related to the thermo-mechanical conditions (i.e. temperature and effective plastic strain rate) and Φ represents the total boundary area (for necklace-type nucleation) or total volume (for bulk-type nucleation) of grains verifying $\rho_i > \rho_{cr}$.

Simulation of a hot compression

A simulation has been launched on 4*24 CPU processors using the above-described model. Results are presented on Fig. 1. The simulated process is a channel-die compression at 1000°C up to 1.90 strain, at a strain rate of 0.01s⁻¹. The number of initial grains is 64 while the final number of grains is around 50.000. The final recrystallized grain radius predicted by the model is 6.1µm while experimental investigations have predicted 5µm at the same instant and in similar thermomechanical conditions (Beltran, Huang, and Logé 2015). The microstructure is recrystallized at 96% after 190s of process. The same framework is able to account for post-dynamic evolutions as well.

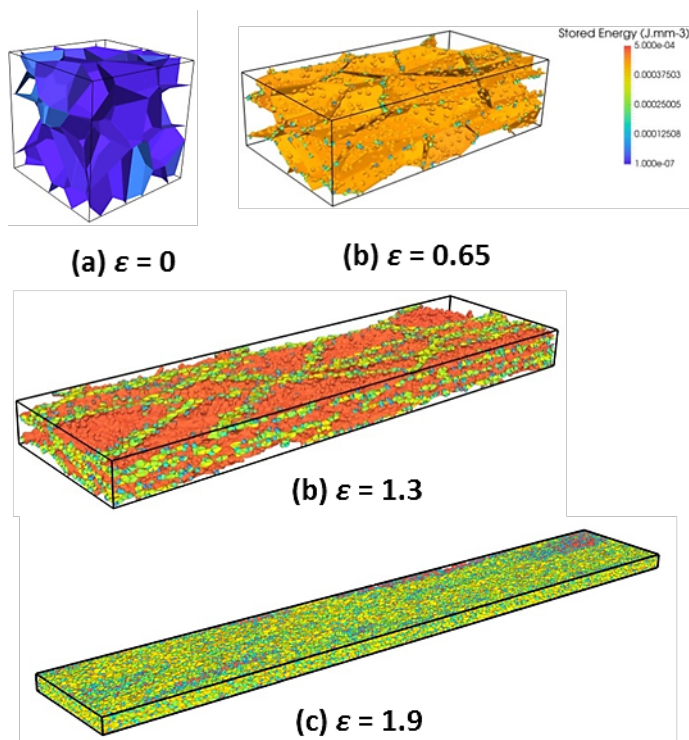


Figure 1. Simulation of a channel-die compression of the 304L steel at 1000°C and at a strain rate of 0.01s⁻¹. Four different instants are represented: (a) $\varepsilon = 0$, (b) $\varepsilon = 0.65$, (c) $\varepsilon = 1.3$, (d) $\varepsilon = 1.9$. The initial number of grains is 64 and the final number of grains is around 50.000.

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