A full-field model for dynamic recrystallization

Anna Ask*†1, Christophe Bovet1, Pauline Stricot1, and Jad Doghman

1DMAS, ONERA, Université Paris Saclay [Châtillon] – DMAS ONERA – France

Abstract

The macroscopic properties of metals and metallic alloys are strongly influenced by the crystalline microstructure. It is natural then that thermomechanical processing to control the microstructure is an important aspect of metal manufacturing. One such process is recrystallization, whereby an existing microstructural arrangement is replaced by another one. This can be a sequential process, typically including a first step of plastic deformation such as cold rolling, and then a second step of annealing where the elevated temperature allows a release of the stored deformation energy by grain boundary rearrangement. Concurrent recrystallization processes may also take place during deformation at elevated temperature. In the latter case, a typical feature is the nucleation of new grains along existing high angle grain boundaries or deformation bands. These newly nucleated grains are not work hardened and a temporary softening can therefore be observed in the macroscopic stress-strain curve as the new grains grow. Recrystallization, whether static (sequential) or dynamic (concurrent), changes the morphology of the microstructure in terms of grain shape and size, and also the crystalline orientation distribution. Both of these microscopic properties strongly influence the macroscopic mechanical response.

Many approaches have been proposed to model recrystallization. At the scale of a polycrystal, the most common approach seems to be to combine a continuum model of crystal plasticity with some method that can account for grain boundary migration. In recent years both level-set and phase-field models have been used successfully to model grain boundary migration in polycrystals. In this study, a phase-field model is favored due to the straight-forward way to integrate it together with the crystal plasticity model in one thermodynamically consistent formulation. Specifically, an orientation-based phase-field model, originally proposed by (1,2), is used because this gives a great degree of freedom for heterogeneous evolution of the crystal orientation everywhere in the microstructure including in the interior of existing grains. The crystal orientation is also an important descriptor of the microstructure and in crystal plasticity simulations must be considered when the resolved shear stress is calculated in a material point. In standard crystal plasticity the grain orientation is however not a degree of freedom but a tabular quantity that is updated as deformation produces elastic reorientation of the crystal lattice. The model used in this work is formulated in a Cosserat continuum description which does contain local orientation as a degree of freedom. This local Cosserat rotation is associated with the crystalline orientation in the constitutive model by a penalty approach.

Earlier, a small deformation version of the model has been implemented in two (3) and three (4) dimensions. However, a small deformation formulation is not in general adequate to model recrystallization since the deformations that are involved are large. Furthermore,

---

*Speaker

†Corresponding author: anna.ask@onera.fr

the small deformation model is also restricted to small misorientations and this is not representative of general crystalline microstructures. A large deformation model (5) is therefore necessary but numerically challenging both to the inherent nonlinearity of the coupled equations and also because large rotations are involved. Unlike the displacement degrees of freedom, the rotational degrees of freedom do not belong to a vector space and cannot be added incrementally in the finite element treatment. A dedicated numerical treatment is therefore necessary that (a) correctly handles the rotational degrees of freedom and (b) adopts high performance computing methods. In this work, a staggered scheme that partly decouples the mechanical part from the phase-field part is adopted. Parallelization of the resulting systems of equation is performed using AMPFETI (Adaptive MultiPreconditioned Finite Element Tearing and Interconnecting) (5).

The large deformation coupled crystal plasticity and phase-field model allows the study of polycrystalline systems. The focus here is not on very large polycrystals where other models already exist that can predict average properties such as grain size distribution and orientation texture with good precision, but rather on smaller systems and a quantitative prediction of the microstructure evolution.

(1) R. Kobayashi, J. A. Warren, W. C. Carter, A continuum model of grain boundaries, Physica D: Nonlinear Phenomena 140 (1-2) (2000) 141–150.

(2) J. A.Warren, R. Kobayashi, A. E. Lobkovsky,W. Craig Carter, Extending phase-field models of solidification to polycrystalline materials, Acta Materialia 51 (20) (2003) 6035–6058. d

(3) A. Ask, S. Forest, B. Appolaire, K. Ammar, O. U. Salman, A Cosserat crystal plasticity and phase field theory for grain boundary migration, Journal of the Mechanics and Physics of Solids 115 (2018) 167–194.

(4) F. Ghiglione, A. Ask, K. Ammar, B. Appolaire, S. Forest, Cosserat-phase-field modeling of grain nucleation in plastically deformed single crystals, Journal of the Mechanics and Physics of Solids 187 (2024).

(5) A. Ask, S. Forest, B. Appolaire, K. Ammar, A cosserat–phase-field theory of crystal plasticity and grain boundary migration at finite deformation, Continuum Mechanics and Thermodynamics 31 (2019) 1109–1141.

(6) C. Bovet, A. Parret-Fréaud, N. Spillane, P. Gosselet, Adaptive multipreconditioned feti: Scalability results and robustness assessment, Computers & Structures 193 (2017) 1–20