Coupled crystal plasticity and phase field approaches for modeling grain boundary migration during viscoplastic deformation

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ABSTRACT

Viscoplastic deformation plays a crucial role in recrystallization and grain growth occurring in metallic materials during thermo-mechanical processing. In addition to grain boundary curvature and misorientation, the energy stored in the grains during deformation is an important driving force for grain boundary migration. Information about crystalline orientation, dislocation content and stored energy are therefore important parameters in a coupled modeling approach dealing with both viscoplastic deformation and subsequent or even concurrent recrystallization and grain growth,

Several modeling approaches exist that deal with grain boundary migration. In the current work, a phase field model developed by Kobayashi, Warren and Carter [1] is used. The KWC model treats the crystalline orientation as a phase field variable with an associated evolution law, accounting for the fact that a sweeping grain boundary will leave behind it a region with a different orientation than before. Since the orientation is treated as a field, the KWC model also allows for heterogeneities in the orientation within a grain. Crystal plasticity approaches on the other hand are well suited to calculate heterogeneous orientation evolution as well as the evolution of dislocation content during viscoplastic deformation. In a previous work by Abrivard et al. [2], the KWC model was amended to include stored energy due to dislocation content as a driving force for grain boundary migration. Coupled with a single crystal plasticity model in a sequential scheme, the phase field approach could be successfully used to model grain growth following viscoplastic deformations.

The aim of the current work is to treat the mechanical and phase field equations in a unified thermodynamically consistent framework. In addition to including elastoplastic stored energy as a driving force for grain boundary motion, the possibility of reorientation both due to deformation and to grain growth is taken into account. The crystal plasticity approach provides a mean of calculating the elastic rotation during deformation while the change in orientation due to grain growth is handled by the phase field model. To have strong coupling between the models it is necessary to reconcile the evolution laws provided by the two approaches while at the same time keeping the distinction between mechanically and chemically driven processes when formulating balance laws and constitutive equations. Using the proposed approach, numerical calculations are performed on a bicrystal of different orientation and dislocation content exposed to thermo-mechanical loading inducing concurrent viscoplastic deformation and grain boundary motion.

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REFERENCES

[1] Kobayashi, R. and Warren, J.A. and Carter, W.C. A continuum model of grain boundaries. *Physica D*, **140**, 141–150, (2000).

[2] Abrivard, G. and Busso, E.P. and Forest, S. and Appolaire, B. Phase field modelling of grain boundary motion driven by curvature and stored energy gradients. *Philosophical Magazine*, **92** (28–30), 3618–3664, (2012).