Modeling of microstructural pattern formation in finite-deformation crystal plasticity

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ABSTRACT

The relation between microstructure and macroscopic constitutive response is crucial in the design and modelling of materials. To interpret and model the material behaviour, enabling us to design challenging structural properties, it is essential to better analyse and understand the interactions of different, even competing strain hardening and defect pattering mechanisms at different length scales. In this regard, material instabilities related to different microstructural mechanisms represent a key to the modelling of a number of phenomena. Experiments indicate that materials often do not deform homogeneously under an imposed deformation but rather by forming microstructural patterns, where spatial lamination of different domains represents a representative example. A particular example is the non-quasiconvex free energy density in multiplicative single-slip crystal plasticity which leads to a fine-scale microstructure. Two prominent approaches handling this type of free energy density are generally used. The first approach is based on the approximation of the quasiconvex hull by lamination, i.e. by constructing an energy-minimizing first-order laminate microstructure [1,2]. The second approach is based on strain-gradient plasticity applied to representative unit cells whose effective properties are obtained from homogenization [3-5]. This contribution deals with a comparison of these two approaches for finite-deformation single-slip crystal plasticity [6]. The non-quasiconvex energy, arising naturally from the finite-deformation formulation, serves as the driving force for the emergent microstructure. The competition between the kinetics and the relaxation of the free energy is an essential feature, in particular of the gradient-based model. Results of the gradient-based model are compared to those of an effective laminate model based on energy relaxation and accounting for domain wall energy. As will be shown, both models predict the formation of first-order laminates but show significant differences in the stress-strain response. Algorithmic and numerical aspects will be discussed and compared which clearly explain these differences that can be minimized by the introduction of the domain wall energy.

REFERENCES

[1] C. Carstensen, K. Hackl, A. Mielke, Non-convex potentials and microstructures in finite-strain plasticity, Proc. R. Soc. Lond. Ser. A 458(2018) (2002) 299–317.
[2] D.M. Kochmann, K. Hackl, The evolution of laminates in finite crystal plasticity: a variational approach, Contin. Mech.Thermodyn. 23 (1) (2011) 63–85.
[3] T. Yalcinkaya, W.A.M. Brekelmans, M.G.D. Geers, Deformation patterning driven by rate dependent nonconvex strain gradient plasticity, J. Mech. Phys. Solids 59 (2011) 1–17.
[4] B. Klusemann, T. Yalcinkaya, Plastic deformation induced microstructure evolution through gradient enhanced crystal plasticity based on a non-convex Helmholtz energy, Int. J. Plast. 48 (2013) 168–188.
[5] B. Klusemann, T. Yalcinkaya, M. Geers, B. Svendsen, Application of non-convex rate dependent gradient plasticity to the modeling and simulation of inelastic microstructure development and inhomogeneous material behavior, Computational Materials Science 80 (2013) 51–60.
[6] B. Klusemann, D.M. Kochmann, Microstructural pattern formation in finite-deformation single-slip crystal plasticity under cyclic loading: Relaxation vs. gradient plasticity, Comput. Methods Appl. Mech. Engrg. 278 (2014) 765–793