Upscaling microstructural plasticity in metals: emergent aspects in crystal plasticity and grain boundaries

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ABSTRACT

Whereas the basics of coarse scale metal plasticity are well established for several decades, the real challenges ahead are rooted in the multi-scale nature of the fine scale mechanisms and the critical role of microstructures and internal boundaries. With a clear focus on microstructures, homogenization and plasticity, this contribution constitutes a justified and dignified contribution to this Special session in Memory of professor Christian Miehe.

First, the multiscale nature of plasticity in crystalline systems driven by dislocations is analysed. Dislocations are well-known defects in crystals and they have been studied extensively in the literature. At a large scale, various crystal plasticity models exist for many decades aiming to describe the mechanics of crystallographic slip. Whereas the force-velocity relation at the single dislocation scale is adequately approximated by a simple linear relationship, a typical slip law at the continuum level reveals a strongly nonlinear behaviour. We have shown that this yet unexplained mismatch is the result of emergence. The upscaling of this problem is done on the basis of non-equilibrium thermodynamics and statistical mechanics [1-2]. The evolution equation of continuum dislocation densities is derived on the basis of the dynamics of a collection of many dislocations. Both the free energy and the dynamics of the system are systematically derived, whereby the observed nonlinear continuum behaviour naturally emerges at the coarse-grained level.

Dislocation-driven crystal plasticity allows to incorporate the effect of internal boundaries in a microstructure, for which the grain boundary is the prime example. Grain boundaries typically constrain dislocation motion and induce pronounced mechanical effects. A multiscale grain boundary plasticity framework is presented, using a dislocation based gradient enhanced crystal plasticity framework [3]. Driven by the need for a physically based continuum scale description of the grain boundary energy required in continuum modelling frameworks, a multiscale approach is proposed that leads to a continuum representation of the initial grain boundary structure defect content and energy, based on the output of atomistic simulations. A continuum model is developed that incorporates the description of the defect redistribution along the grain boundary into the grain boundary plasticity model. The effect of these mechanisms on the mechanical response will be demonstrated.

Acknowledgment
The research of Marc Geers has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement n° [339392].

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