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Strain-gradient regularization of deformation bands and dislocation structures in finite strain crystal viscoplasticity

Jean-Michel Scherer[1]

[1] Mines Paris, Université PSL, Centre des Matériaux (MAT), UMR7633 CNRS, 91003 Evry, France, France.
jean-michel.scherer@minesparis.psl.eu

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Abstract

The interaction between slip systems in crystals with strong latent hardening can lead to the segregation of plastic deformation into single-slip regions, a phenomenon commonly referred to as patchy slip [1]. This behavior has been documented experimentally and reproduced in both rate-dependent and rate-independent crystal plasticity simulations [2,3]. Despite these advances, the mechanisms governing the selection of the characteristic size of single-slip regions and associated dislocation structures remain poorly understood. In classical crystal plasticity formulations, the absence of an intrinsic material length scale results in deformation patterns whose size depends on numerical discretization, domain size, and boundary conditions, thereby limiting the predictive capability of such models and complicating comparisons with experimental observations. In this work, we revisit deformation band formation within a finite-strain framework using a dislocation-density-based crystal viscoplasticity model. Strong latent hardening is introduced through an interaction matrix describing dislocation interactions across multiple slip systems, while weak rate sensitivity promotes an almost rate-independent response. Both finite element (FE) and fast Fourier transform (FFT) solvers are employed and systematically compared in order to assess the robustness of the predicted deformation patterns and their sensitivity to numerical implementation. In the absence of any regularization, both solvers predict the spontaneous emergence of laminate-type microstructures composed of single-slip regions separated by dislocation walls. Two-dimensional plane strain simulations reveal that the characteristic thickness of single-slip bands and dislocation walls depends strongly on mesh resolution and element type, but also on the choice of periodic or non-periodic boundary conditions. While the qualitative morphology of the patterns is preserved across numerical settings, their characteristic length scales are not, highlighting the fundamentally ill-posed nature of size selection in classical crystal plasticity. Similar behavior is observed in three-dimensional single-crystal simulations, where dislocation cell sizes are likewise governed by a numerical length scale rather than material parameters. To overcome this limitation, the constitutive framework is extended to strain-gradient crystal plasticity by incorporating gradients of plastic slip, thereby introducing a physically motivated material length scale. This regularization leads to a well-defined selection of deformation microstructure size. The resulting single-slip band thickness and dislocation wall width become independent of discretization and follow a power-law relationship with the material length scale, indicating a transition from numerically controlled to physically controlled pattern formation. Finally, simulations of two- and three-dimensional polycrystals demonstrate that deformation patterning persists at the grain scale under multiaxial loading conditions. Despite the additional complexity introduced by grain interactions and heterogeneous stress states, strong latent hardening continues to promote the formation of localized single-slip regions. These results highlight the relevance of strain-gradient regularization beyond idealized single-crystal configurations and provide a framework for linking deformation patterning, dislocation structures, and intrinsic material length scales.

Keywords:

Crystal plasticity Finite strain viscoplasticity Deformation patterning Dislocation structures Latent hardening Lamination Strain gradient plasticity Finite element method Fast Fourier Transform

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