11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

A COMPARATIVE STUDY OF THE NUMERICAL TREATMENT OF DISLOCATION TRANSPORT EQUATIONS IN CRYSTAL PLASTICITY

H. Hernández[1]*, T.J. Massart[1], R.H.J. Peerlings[2] and M.G.D. Geers[2]

[1] Building, Architecture Town Planning; Université Libre de Bruxelles (ULB), Avenue F.D. Roosevelt 50, 1050 Brussels, Belgium. hhernand@ulb.ac.be, thmassar@ulb.ac.be

[2] Department of Mechanical Engineering, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands. R.H.J.Peerlings@tue.nl, M.G.D.geers@tue.nl

Key words: *Crystal plasticity, Geometrically necessary dislocations, Statistically stored dislocations, Dislocation transport, Stabilized finite element method.*

Recently advanced plasticity models based on dislocations transport equations have been developed. A key aspect is the fact that plastic slip, hardening and size effects are thereby modelled through the presence, motion and interactions of dislocations, accounting for interactions between geometrically necessary dislocations and statistically stored dislocations densities [3, 4].

The macroscopic continuum description of the interactions of these dislocation densities can be expressed by partial differential equations as illustrated in [2, 5]. However different equation systems are found in the literature in order to model the same physical process using different assumptions. Moreover it has been observed in practical implementations that these different models do not possess the same numerical behaviour.

In this study, a family of such models expressing the transport of dislocations is first selected, resulting in two different approaches. Both rely on the geometrical relation between the plastic slip and the density of geometrically necessary dislocations. In the first approach the geometrical relation serves as a balance equation while an evolution equation for the statistically stored dislocations completes the system of equations. In the second approach, a conservation equation for the total number of dislocations is used instead. The second family of models assessed is the one relying directly on the definition of densities of positive and negative dislocations. More precisely, the evolution of dislocations densities is modelled by two hyperbolic partial differential equations.

This hyperbolic character of the models used to describe the transport of dislocations in addition to the non-linear nature of these systems of equations introduce several numerical difficulties compromising the successful use of these models. We study several stabilization techniques used to overcome the appearance of spurious oscillations [1, 6]. These techniques are implemented in the context of the finite element method and are compared in terms of their numerical performance.

We are focused in the one dimensional case in order to address the mentioned difficulties in detail. Different time integration schemes will also be studied and compared both from the point of view of the numerical properties and computational cost.

REFERENCES

[1] Codina R. 1998. *Comparison of some finite element methods for solving the diffusion-convection-reaction equation*, Computer Methods in Applied Mechanics and Engineering, **156** 185-210.

[2] Dogge M., Peerlings R. and Geers M. 2013. *Continuum modeling of dislocations transport in single slip: Beyond GND interactions*, Submitted.

[3] Groma I. 1997. *Link between the microscopic and mesoscopic length-scale description of the collective behavior of dislocations*, Physical Review B, **56** 5807-5813.

[4] Groma I., Csikor F.F. and Zaiser M. 2003. *Spatial correlations and higher-gradient terms in a continuum description of dislocation dynamics*, Acta Materialia, **51** 1271-1281.

[5] Hirschberger C., Peerlings R., Brekelmans W. and Geers M. 2011. *On the role of dislocation conservation in single-slip crystal plasticity*, Modelling and simulation in Materials Science and Engineering, **19** 085002.

[6] John V. and Schmeyer E. 2008. *Finite element methods for time-dependent convectiondiffusionreaction equations with small diffusion*, Computer Methods in Applied Mechanics and Engineering, **198** 475-494.