

## VARIATIONAL AND COMPUTATIONAL ASPECTS OF PROBLEMS IN SINGLE-CRYSTAL GRADIENT PLASTICITY

\* B. Daya Reddy<sup>1</sup> and Andrew T. McBride<sup>2</sup>

<sup>1</sup> University of Cape Town  
CERECAM  
7701 Rondebosch  
South Africa  
daya.reddy@uct.ac.za

<sup>2</sup> University of Cape Town  
CERECAM  
7701 Rondebosch  
South Africa  
andrew.mcbride@uct.ac.za

**Key Words:** *plasticity, single-crystal, gradient theories, variational formulations, finite element approximations.*

### ABSTRACT

The absence of an inherent length scale in classical theories of plasticity, and the consequential inability to capture size-dependent effects particularly at the mesoscale, have led to various extensions of classical theories which introduce one or more length scales and incorporate non-local effects in the plastic part of the constitutive relations. One key area of investigation has been concerned with the development of constitutive theories for both single and polycrystals which include dependence on plastic strain gradients (see, for example, [5]).

Two relevant theories that have emerged are, first, those in which gradient effects are manifested through the appearance of the laplacian of plastic strain in the yield condition [1]. Other theories are based on the inclusion of the Burgers vector or tensor as a variable that accounts for dislocation densities in single crystals and incompatibilities in polycrystals [6-8].

In recent work [3,4] the model of gradient plasticity presented in [1] is analysed in detail, and an approximate solution procedure using the discontinuous Galerkin method is constructed, analysed, and implemented. Also for polycrystals, a model of gradient plasticity based on the use of plastic strain gradient and Burgers tensor and presented in [7] is analysed in [9], and conditions for well-posedness established.

The purpose of the present contribution is to address a similar set of questions pertaining to problems involving single-crystal plasticity. A unified framework which accounts for gradient effects in the form either of gradients of slip rates or of the Burgers tensor, is adopted. First, the problem is posed as a variational inequality; this variational formulation is then analysed, and the influence of the gradient terms and associated boundary conditions on well-posedness is explored.

The second contribution concerns the development of numerical simulations using finite element approximations. It is well known [2] that the constraints associated with multiple slip planes leads to complications in the rate-independent theory that arise from the linear dependence of these constraints,

a situation that may be circumvented through the introduction of a viscoplastic regularization. The development of robust, convergent algorithms is explored for rate-independent and -dependent systems, with a view to elucidating the mathematical, physical and computational influence of the gradient terms.

## REFERENCES

- [1] E. Aifantis, "The physics of plastic deformations". *Int. J. Plasticity*, Vol. **3**, 211–247, 1987.
- [2] A. M. Cuitño and M. Ortiz, "Computational modelling of single crystals". *Modelling Simul. Mater. Sci. Eng.*, Vol. **1**, 225–263, 1992.
- [3] J. K. Djoko, F. Ebobisse, A. T. McBride and B. D. Reddy, "A discontinuous Galerkin formulation for classical and gradient plasticity. Part 1: Formulation and analysis". *Comp. Meths. Appl. Mech. Engng*, Vol. **196**, 3881–3897, 2007.
- [4] J. K. Djoko, F. Ebobisse, A. T. McBride and B. D. Reddy, "A discontinuous Galerkin formulation for classical and gradient plasticity. Part 2: Algorithms and numerical analysis". *Comp. Meths. Appl. Mech. Engng*, Vol. **197**, 1-212, 2007.
- [5] N. Fleck, G. M. Muller, M. F. Ashby and J. W. Hutchinson, "Strain gradient plasticity: theory and experiments". *Acta Metall.*, Vol. **42**, 475–487, 1994.
- [6] M. E. Gurtin, "A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations". *J. Mech. Phys. Solids*, Vol. **50**, 5–32, 2002.
- [7] M. E. Gurtin and L. Anand, "A theory of strain-gradient plasticity for isotropic, plastically irrotational materials. Part I: Small deformations". *J. Mech. Phys. Solids*, Vol. **53**, 1624–1649, 2005.
- [8] A. Menzel and P. Steinmann, "On the continuum formulation of higher gradient plasticity for single and polycrystals". *J. Mech. Phys. Solids*, Vol. **48**, 1777–1796, 2000.
- [9] B. D. Reddy, F. Ebobisse and A. McBride, "Well-posedness of a model of strain gradient plasticity for plastically irrotational materials". *Int. J. Plasticity*, Vol. **24**, 55–73, 2008.