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MODELLING OF GRAIN BOUNDARIES IN A STRAIN GRADIENT CRYSTAL PLASTICITY FRAMEWORK

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The grain boundaries, subdividing the grains with different orientations, are natural locations triggering accumulation of the plastic slip and the geometrically necessary dislocations which accommodate the gradients of the inhomogeneous plastic strain. Interactions between the dislocations and grain boundaries plays crucial role in the plastic deformation of metallic materials. The modelling of grain boundaries in plasticity frameworks is essential due to their strong influence on the hardening of the materials. Incorporation of dislocation-grain boundary interaction information at micro level into crystal plasticity frameworks has been a challenge, however a complete understanding of this phenomenon and its macroscopic effects is still not at reach and the necessary input for computational models is still subject of ongoing discussions.

This paper focuses on the continuum scale modeling of dislocation-grain boundary interactions and enriches a particular strain gradient crystal plasticity formulation (convex counter-part of Yalcinkaya et al (2011) and Yalcinkaya et al (2012)) by incorporating explicitly the effect of grain boundaries on the plastic slip evolution. Within the framework of continuum thermodynamics, a consistent extension of the model is presented and a potential type non-dissipative grain boundary description in terms of grain boundary Burgers tensor (see e.g. Gurtin (2008)) is proposed. A fully coupled finite element solution algorithm is built-up in which both the displacement and plastic slips are considered as primary variables. For the treatment of grain boundaries within the solution algorithm, an interface element is formulated. The proposed formulation is capable of capturing the effect of misorientation of neighboring grains and the orientation of the grain boundaries on slip evolution in a natural way, as demonstrated by bi-crystal specimen examples.

REFERENCES

[1] T. Yalcinkaya, W.A.M. Brekelmans, M.G.D. Geers. Deformation patterning driven by rate dependent nonconvex strain gradient plasticity. *Journal of the Mechanics and Physics of Solids.*, Vol. **59**, 1–17, 2011.

[2] T. Yalçinkaya, W.A.M. Brekelmans, M.G.D. Geers. Non-convex rate dependent strain gradient crystal plasticity and deformation patterning. *International Journal of Solids and Structures.*, Vol. **49**, 2625–2636, 2012.

[3] M. E. Gurtin. A theory of grain boundaries that accounts automatically for grain misorientation and grain-boundary orientation. *Journal of the Mechanics and Physics of Solids.*, Vol. **56**, 640–662, 2008.