Interplay Between Grain Boundary Migration, Grain Rotation and Intra-granular Plasticity in Nanocrystalline Materials

Jakub Mikula[†,a], Shailendra P. Joshi[b], Tong-Earn Tay[a], Rajeev Ahluwalia[†] and Siu Sin Quek[†,*]

[a] Department of Mechanical Engineering
National University of Singapore
9 Engineering Drive 1, Block EA, #07-08, Singapore 117575

[b] Department of Mechanical Engineering
University of Houston, Houston, TX 77204, USA

[†] Institute of High Performance Computing
1 Fusionopolis Way, #16-16 Connexis (North), Singapore 138632
[*]e-mail: quekss@ihpc.a-star.edu.sg

ABSTRACT

Nanocrystalline materials have been engineered in recent decades for the potential to achieve superior mechanical properties such as strength, ductility and toughness. When grain sizes are reduced to < 100nm, these polycrystalline materials exhibit very interesting deformation mechanisms that otherwise contribute little to the macroscopic deformation in their coarser grain counterparts. For example, grain boundary (GB) migration and grain rotation start to play significant roles as the grain boundary to bulk volume fraction increases in nanocrystalline metals [1-3]. In this work, a phase field approach is adapted from the model of Kobayashi, *et al.* [4] to allow for both GB migration and grain rotation while coupled to elasto-plastic mechanics. The basic phase field model in [4] describes the GB network through scalar fields, θ and η. The former describes the grain orientation in 2D, while the latter represents the ordering of the crystal lattice, i.e. $\eta < 1$ in a disordered region like the GB, and $\eta = 1$ in an ordered region like the grain interior . The strain energy of the system is therefore a function of the displacement field and the local grain orientation, θ. Cubic elasticity and a simple Hill yield plasticity theory without hardening are assumed in order to study the effects of both elastic and plastic anisotropy on GB mediated inelastic deformation (migration and grain rotation). The framework is implemented in a bicrystalline gold nano-pillar where the GBs are straight, as well as in an agglomerate of gold nano-sized grains where curvature driven grain growth is also incorporated. The simulations reveal the interplay between the different GB mediated mechanisms considered in the model with elastic and plastic anisotropy, and we elucidate the trends of how varying plastic anisotropies and strain rates affect the overall deformation behavior.

REFERENCES

[1] Farkas,D., Frϕseth, A., and Van Swygenhoven, H., Grain boundary migration during room temeperature deformation of nanocrystalline Ni, *Scripta Materialia* (2006) **55**:695–698.

[2] Rupert,T.J., Gianola, T.S., Gan Y., and Hemker, K.J., Experimental observations of stress-driven grain boundary migration, *Science* (2009) **326**:1686–1690.

[3] Panzarino,J.F., Pan, Z., and Rupert, T.J., Plasticity-induced restructuring of a nanocrystalline grain boundary network, *Acta Materialia* (2016) **120**:1–13.

[4] Kobayashi,R., Warren, J.A., and Carter, C.W., A continuum model of grain boundaries, *Phys. D* (2000) **140**:141–150.