

Continuum model of ultrafine polycrystals with embedded growth nano-twins

* A. Jérusalem¹, M. Dao², S. Suresh³ and R. Radovitzky⁴

Massachusetts Institute of Technology
77 Massachusetts Ave.
Cambridge, MA 02139

¹ Dept. of Aeronautics and
Astronautics
jeru@mit.edu

² Dept. of Materials Science
and Engineering

³ Dept. of Materials Science
and Engineering

⁴ Dept. of Aeronautics and
Astronautics
rapa@mit.edu

Key Words: *Nanocrystalline materials, Nanoscale twins, Crystal plasticity, Copper, Three dimensions, Computational model*

ABSTRACT

It is now well established that nanocrystalline metals can achieve much higher material strength than their microscale counterpart. This has been rationalized by a transfer of deformation mechanism from intragrain plasticity to grain boundary mediated deformation with decreasing grain size. However, because of the higher proportion of grain boundary—more ductile—to grain interior, this increase of strength is accompanied by an overall decrease of ductility. Recent efforts have shown that the embedding of growth nano-twins in ultrafine crystals can lead to the same level of strength as for nanocrystals but without compromising on the ductility [1]. We present here a three-dimensional continuum model of the deformation of nano-twinned ultrafine polycrystal. The associated finite element formulation consider the deformation of each grain explicitly while adopting a homogenized representation of the twins planes in each crystal lattice. The three-dimensional phenomenological model describes the orientation-dependent dislocation blocking and absorption actions of the twins as well as their anisotropic influence on the lattice properties. A fracture criterion based on a maximum slip per unit twin in the twinned slip plane is also implemented. Tensile test simulations capture the increased level of strength with increasing twin densities as well as the failure strain initiation for the largest twin spacings but tend to over-predict its value for the smallest twin spacing. An analysis of this discrepancy as well as a study of the influence of texture on the sample mechanical properties—namely strength and strain-to-fracture—are finally presented.

REFERENCES

- [1] M. Dao, L. Lu, Y.F. Shen and S. Suresh. “Strength, strain-rate sensitivity and ductility of copper with nanoscale twins”. *Acta Materialia*, Vol. **54**, 5421–5432, 2006.