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

Quantifying the effect of deformation mechanisms in nanocrystalline metals

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Key Words: *Uncertainty quantification, nanocrystalline metals.*

Dislocation dynamics simulations have advanced the understanding of the mechanical behavior of polycrystalline materials. However, the predictability of these simulations is limited specially by the incorporation of complex mechanisms such as grain boundary deformation and dissociation into partial dislocations as well as realistic representations of texture and grain structure. Quantifying the effect of these mechanisms is needed to understand the limitations of dislocation dynamics predictions.

We investigate deformation of ultra fine and nanocrystalline metals using a phase-field approach to dislocation dynamics. We include grain-boundary mediated deformation constitutive equations and the gamma surface directly from atomistic results. As a result, our simulations include dissociation into partial dislocations that are of key importance in simulations of nanocrystalline materials. We quantify the importance of the different mechanisms, including grain boundary deformation, dissociation into partial dislocations, gliding and climbing on the mechanical response for different microstructures and strain rates.