Accepted Manuscript

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PII: S0749-6419(17)30460-6

DOI: 10.1016/j.ijplas.2017.10.014

Reference: INTPLA 2267

To appear in: *International Journal of Plasticity*

Received Date: 9 August 2017

Revised Date: 13 October 2017

Accepted Date: 28 October 2017

Please cite this article as: Chandra, S., Samal, M.K., Chavan, V.M., Raghunathan, S., Hierarchical multiscale modeling of plasticity in copper: From single crystals to polycrystalline aggregates, *International Journal of Plasticity* (2017), doi: 10.1016/j.ijplas.2017.10.014.

Hierarchical multiscale modeling of plasticity in Copper: From single crystals to polycrystalline aggregates

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Abstract

Modeling the deformation behavior of polycrystalline materials using the information embedded at grain level is a recent research area of high interest. In view of this, an attempt has been made to imbue the predictions of polycrystalline deformation with the single crystal behavior within the framework of hierarchical multiscale modeling scheme. Face centered cubic Cu has been selected as the model material for demonstration. At the nanoscale, behavior of a single dislocation is quantified in terms of dislocation drag coefficient using atomistic simulations, which is then transferred to dislocation dynamics simulations at the microscale. The collective behavior of a huge dislocation population is then simulated to quantify the necessary hardening parameters to be passed on to crystal plasticity simulations at the mesoscale. Crystal plasticity simulations are performed to simulate the uniaxial tensile behavior of single crystal Cu in multiple crystallographic orientations. The calibrated hardening parameter set for various orientations of single crystal Cu is then refined statistically to introduce a single parameter set, that could adequately capture the uniaxial tensile behavior of polycrystalline Cu. The scheme, therefore, couples atomistics to discrete dislocations to single crystal plasticity to polycrystalline plasticity within the framework of hierarchical multiscale modeling scheme. Experimental data of Takeuchi (1975) and Bronkhorst et al. (1992) has been employed to access the predictive capabilities of our approach. A good agreement has been obtained between these experiments and our simulation results, thereby validating our methodology.

Keywords: Multiscale modeling, Deformation, Molecular dynamics, Dislocation dynamics, Crystal plasticity

1. Introduction

A polycrystalline aggregate comprises of a myriad of randomly oriented single crystals. Modeling the deformation behavior of polycrystalline materials, therefore, starts with describing the elastic and plastic deformation processes occurring at the grain level. However, predicting the mechanical behavior of polycrystals from the response of their

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