Accepted Manuscript

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PII: \$1359-6454(18)30055-7

DOI: 10.1016/j.actamat.2018.01.024

Reference: AM 14318

To appear in: Acta Materialia

Received Date: 28 September 2017
Revised Date: 28 December 2017
Accepted Date: 16 January 2018

Please cite this article as: S. Haouala, J. Segurado, J. LLorca, An analysis of the influence of grain size on the strength of FCC polycrystals by means of computational homogenization, *Acta Materialia* (2018), doi: 10.1016/j.actamat.2018.01.024.

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An analysis of the influence of grain size on the strength of FCC polycrystals by means of computational homogenization

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Abstract

The effect of grain size on the flow stress of FCC polycrystals is analyzed by means of a multiscale strategy based on computational homogenization of the polycrystal aggregate. The mechanical behavior of each crystal is given by a dislocation-based crystal plasticity model in which the critical resolved shear stress follows the Taylor model. The generation and annihilation of dislocations in each slip system during deformation is given by the Kocks-Mecking model, which was modified to account for the dislocation storage at the grain boundaries. Polycrystalline Cu is selected to validate the simulation strategy and all the model parameters are obtained from dislocation dynamics simulations or experiments at lower length scales and the simulation results were in good agreement with experimental data in the literature. The model is applied to explore the influence of different microstructural factors (initial dislocation density, width of the grain size distribution, texture) on the grain size effect. It is found that the initial dislocation density, ρ_i , plays a dominant role in the magnitude of the grain size effect and that dependence of flow stress with an inverse power of grain size $(\sigma_y - \sigma_\infty \propto d_g^{-x})$ breaks down for large initial dislocation densities ($> 10^{14} \,\mathrm{m}^{-2}$) and grain sizes $d_q > 40 \ \mu \text{m}$ in FCC metals. However, it was found that the grain size con-

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