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Large Scale 3-D Dislocation Dynamics and Atomistic Simulations of Flow and Strain-Hardening Behavior of Metallic Micropillars[1]

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Experimental studies show strong strengthening effects for micrometer-scale FCC as well as two-phase superalloy crystals, even at high initial dislocation densities. This talk shows results from large-scale 3-D discrete dislocation simulations (DDS) used to explicitly model the deformation behavior of FCC Ni (flow stress and strain-hardening) as well as superalloy micro-crystals for diameters ranging from 1 - 20 microns. The work shows that two size-sensitive athermal hardening processes, beyond forest and precipitation hardening, are sufficient to develop the dimensional scaling of the flow stress, stochastic stress variation, flow intermittency and, high initial strain-hardening rates, similar to experimental observations for various materials. In addition, 3D dislocation dynamics simulations are used to investigate strain-hardening characteristics and dislocation microstructure evolution with strain in large 20 micron size Ni microcrystals (bulk-like) under three different loading axes: 111, 001 and 110. Three different multi-slip loading axes, $< 111 >$, $< 001 >$ and $< 110 >$, are explored for shear strains of $\sim$0.03 and final dislocation densities of $\sim$1013/m2. The orientation dependence of initial strain hardening rates and dislocation microstructure evolution with strain are discussed. The simulated strain hardening results are compared with experimental data under similar loading conditions from bulk single-crystal Ni. Finally, atomistic simulation results on the operation of single arm sources in Ni bipillars with a large angle grain boundary is discussed. The atomistic simulation results are compared with experimental mechanical behavior data on Cu bipillars with a similar large angle grain boundary.

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