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Atomistic Simulations of Deformation of Nanoscale FCC Materials SHIVRAJ KAREWAR, NIRAJ GUPTA, University of North Texas, ALEX STUKOWSKI, Lawrence Livermore National Laboratory, MICHAEL BASKES, Los Alamos National Laboratory, SRINIVASAN SRIVILLIPUTHUR, University of North Texas — We compare the deformation behavior of gold single crystal nanospheres with ∼6-30 nm diameters with gold spherical shells of varying inner to outer diameter ratios. Gold nanospheres are modeled with an EAM potential and the indenter is described by a repulsive potential. Yield strength dependence on sample size, geometry and temperature was studied in these nanospheres. The deformation mechanism is aided by the continuous displacement burst accompanying dislocation escape from the nanospheres. Based on this, a dislocation starvation mechanism has been discussed. Extended dislocations are found to be the prominent defect type in both solid and hollow nanospheres. Flow stresses are lower in hollow nanoshells. Low flow stresses are accounted for the presence of additional surface area for dislocation nucleation and emergence at the inner surface of the hollow shell.

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