

**Size Dependent Mechanical Properties and Mechanisms of Single and Nanocrystalline Metals  
from Molecular Dynamics Simulations**

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The size dependent mechanical properties and mechanisms of single and nanocrystalline metals were studied using molecular dynamics simulations. A novel expression of geometrically necessary dislocation density was proposed to predict the nano-indentation size effects with various shape of nanoindenter. The flow stress of nanocrystalline metals with varied grain sizes was studied. In spherical indenters, we found that the calculated hardness and the square root of calculated GND density are inversely proportional to the square root of indenter radius. For the Berkovich indenter, the calculated hardness and the square root of calculated GND density are inversely proportional to the square root of indentation depth. Both size effects and correlation between GND density and hardness agreed with the trend predicted by the theory of strain gradient plasticity. For nanocrystalline metals, solid motion and grain boundary dislocation emission mechanisms were studied to reveal the size-dependent flow stress and the transition from conventional to inverse Hall-Petch relation.

**Keywords:** Nanocrystalline metal, inverse Hall-Petch, strain gradient plasticity, MD