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Microstructural and Atomistic Simulation for Deformation of Nano-grained Metals

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Nano-grain metals deform mainly by neighboring grains sliding pass each other. We adopted a structural evolution algorithm to simulate the process. Actual deformation minimizes the plastic dissipation and stored strain energy for representative steps of grain neighbor switching. Numerical simulations are given for a representing cell composed of 200 non-uniform grains. A theoretical framework concerning the insertion and rotation of 9-grain clusters is proposed that quantifies the experimental data. We also conduct investigation for the rapid stretching of nano-grained metals via molecular dynamics simulation. For nano-grained copper stretched up to 200% at ultra-fast strain rate, the MD simulation indicates a transition from ordered to disordered state.

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