

Abstract Submitted
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Grain Rotation and Growth in Nanocrystalline Silver and Silver/Copper Alloys MICHAEL CHANDROSS, SHENGFENG CHENG, Sandia National Laboratories — Grain rotation and growth play important roles in nanotribology and the plastic deformation of nanocrystalline metals and alloys. It is difficult, however, to study these processes with full atomistic detail experimentally. We used molecular dynamics simulations to investigate the grain rotation, coalescence, and growth in pure silver and silver/copper alloys after imposing various modes of deformation, including stretch, compression, and shear. Our results show that the degree of grain rotation and growth in pure silver depends on the state of stress in the sample and is most significant under shear deformation, where very large grains are observed after substantial shear. However, in silver/copper alloys, almost no grain growth was found even under strong shear. The presence of atoms with different lattice constants in alloys stabilizes the grain boundaries and makes grain coalescence less energetically favorable. The implications of these results on nanotribology of pure metals and alloys are discussed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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