Competing grain-boundary- and dislocation-mediated mechanisms in plastic strain recovery in nanocrystalline Aluminum

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Recent experiments (Rajagopalan et al., 2007, *Science*, 315:1831) have demonstrated that plastic strains in nanocrystalline Al and Au films with grain sizes on the order of 50 nm are partially recoverable. To reveal the mechanisms behind such strain recovery, large-scale molecular dynamics simulations were performed for plastic deformation in nanocrystalline Al with mean grain sizes of 10, 20 and 30 nm. The results indicate that the inhomogeneous deformation in a polycrystalline environment results in significant residual stresses (see top right figures) in the nanocrystals. Upon unloading, these internal residual stresses cause strain recovery via competitive deformation mechanisms including dislocation reverse motion/annihilation (see middle figures) and grain-boundary (GB) sliding/diffusion (see bottom right figures) By tracking the evolution of each individual deformation mechanism during strain recovery, the fractional contributions (see bottom right figures) by GB and dislocation deformation mechanisms to the overall recovered strain were quantified. The current study indicates that, even under strain rates as high as those in molecular dynamics simulations, GB-mediated processes play important roles in the deformation of nanocrystalline metals.

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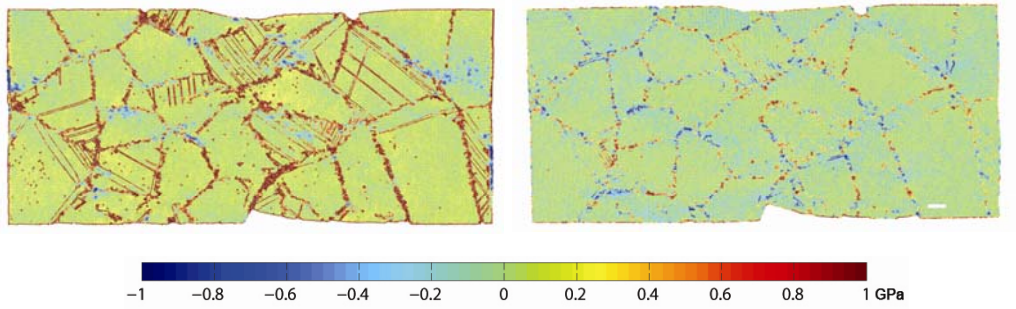
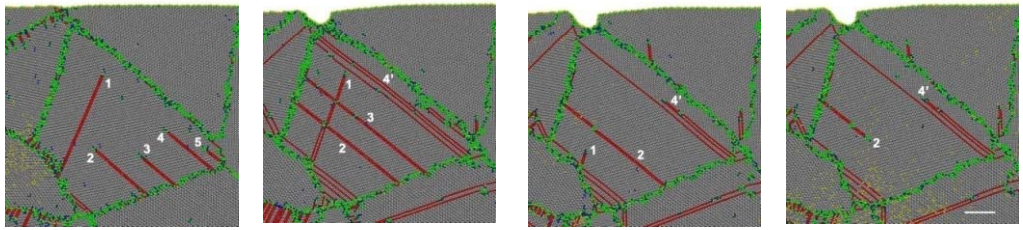
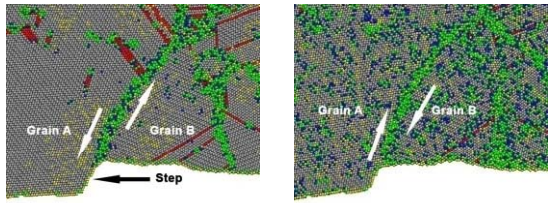
Residual stress caused by inhomogeneous deformation



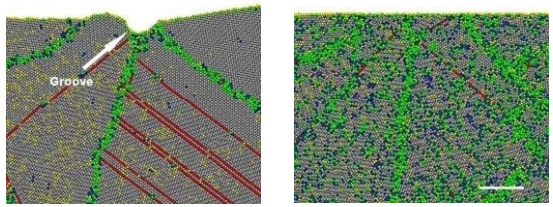
Reverse motion of dislocations



GB sliding



GB diffusion



Fraction