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Atomistic study of Size Effect in Torsion Tests of Nanowire

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Existing theories have had to be modified as a result of trends in miniaturization. For smaller nanostructures and nanostructured materials, the continuum theory must be reconsidered. In this paper, the torsion deformation of the atomistic model of single crystal and polycrystalline nanowire is studied using molecular dynamics. Torsion deformation is incorporated using a twisted periodic boundary condition (TPBC). We focus on grain refinement and size effect as they are affected by the combination of two length scales, i.e., radius of specimen and grain size. The result is compared with that from continuum strain-gradient plasticity. The efficiency of TPBC is confirmed in the analysis. Polycrystallization is observed in single crystal cases. The torque-twist curves show a tendency for smaller to be softer. A discrepancy exists with continuum predictions from dislocation theory. An important result is that deformation at the grain boundary is significant in nano-scale deformation rather than dislocation movement.

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