Molecular Dynamics Studies of Crystalline Metals Under Hydrostatic Loading

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Metallic materials in the single-crystalline or polycrystalline form are the essential model system for the development of the dislocation theory. By using molecular dynamics simulations with suitable interatomic potentials, the mechanical behavior of the crystalline metals under the hydrostatic stress, as well as other stress states, is simulated, and results are compared with the dislocation theory. In addition to impose the periodic boundary conditions to simulate bulk behavior, metals in the form of nanoparticles are also considered. Comparisons among various stress states were made to delineate different deformation mechanisms governed by dislocations in confined geometry, bounded by grain boundaries or free surfaces. Furthermore, interactions between dislocations and other defects, such as vacancies or other dislocations, are studied to shed light on strengthening mechanisms in metals with nanoscale grains.

Keywords: Molecular dynamics simulation, Crystalline metal, Dislocation, Mechanical properties, Hydrostatic stress