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Dislocation Engineering in Novel Nanowire Structures

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ABSTRACT

Leveraging defects is a cornerstone of materials science, and has become increasingly important from bulk to nanostructured materials. We use molecular dynamics simulations to explore the limits of defect engineering by harnessing individual dislocations in nanoscale metallic specimens and utilizing their intrinsic behavior for application in mechanical dampening. We study arrow-shaped, single crystal copper nanowires designed to trap and control the dynamics of dislocations under uniaxial loading. We characterize how nanowire cross-section and stacking-fault energy of the material affects the ability to trap partial or full dislocations. Cyclic loading simulations show that the periodic motion of the dislocations leads to mechanical dissipation even at frequencies up to 2x10^10 Hz, orders of magnitude higher than the current state of the art.

KEYWORDS

Nanowires, Mechanical dampening, Stacking fault energy, Dislocation engineering, Molecular dynamics