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A Molecular Dynamics Study on Intermittent Plasticity and Dislocation Avalanche Emissions in FCC and BCC Crystals

Authors : Javier Varillas, Jorge Alcalá

Abstract : We investigate dislocation avalanche phenomena in face-centered cubic (FCC) and body-centered cubic (BCC) crystals using massive, large-scale molecular dynamics (MD) simulations. The analysis is focused on the intermittent development of dense dislocation arrangements subjected to uniaxial tensile straining under displacement control. We employ a novel computational scheme that allows us to inject an entangled dislocation structure in periodic MD domains. We assess the emission of plastic bursts (or dislocation avalanches) in terms of the sharp stress drops detected in the stress-strain curve. The plastic activity corresponds to the sporadic operation of specific dislocation glide processes exhibiting quiescent periods between successive avalanche events. We find that the plastic intermittences in our simulations do not overlap in time under sufficiently low strain rates as dissipation operates faster than driving, where the dense dislocation networks evolve through the emission of dislocation avalanche events whose carried slip adheres to self-organized power-law distributions. These findings enable the extension of the slip distributions obtained from strict displacement-controlled micropillar compression experiments towards smaller values of slip size. Our results furnish further understanding upon the development of entangled dislocation networks in metal plasticity, including specific mechanisms of dislocation propagation and annihilation, along with the evolution of specific dislocation populations through dislocation density analyses.

Keywords : dislocations, intermittent plasticity, molecular dynamics, slip distributions
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