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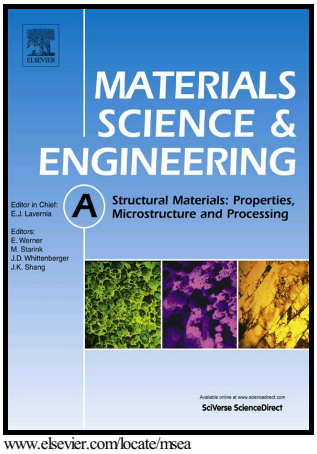

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Deformation mechanisms in nanotwinned copper by molecular dynamics simulation

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Abstract

Nanotwinned materials exhibit simultaneous ultrahigh strength and high ductility which is attributed to the interactions between dislocations and twin boundaries but the specific deformation mechanisms are rarely seen in experiments at the atomic level. Here we use large scale molecular dynamics simulations to explore this intricate interplay during the plastic deformation of nanotwinned Cu. We demonstrate that the dominant deformation mechanism transits dynamically from slip transfer to twin boundary migration to slip-twin interactions as the twin boundary orientation changes from horizontal to slant, and then to a vertical direction. Building on the fundamental physics of dislocation processes from computer simulations and combining the available experimental investigations, we unravel the underlying deformation mechanisms for nanotwinned Cu, incorporating all three distinct dislocation processes. Our results give insights into systematically engineering the nanoscale twins to fabricate nanotwinned metals or alloys that have high strength and considerable ductility.