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ABSTRACT:

Stress-Assisted Structural Transformation and Plastic Deformation in Mo/Cu Bicontinuous Intertwined Composites

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Structural transition in Molybdenum has been reported to occur under large stresses in thin nanowires and tip of a crack. Here, we use Molecular Dynamics (MD) simulations to demonstrate that a uniform 3-step structural transformation of Molybdenum atoms can occur in Mo/Cu bicontinuous intertwined materials during tensile loading. The Mo atoms first transit from a <001>-oriented bcc structure to a <001>-oriented fcc structure via Bain transformation. The <001>-oriented fcc phase then transforms to a <110>-oriented bcc via Pitsh transformation. This novel homogenous transformation results into a stress-strain curve containing two elastic and two plastic regimes as well as enhanced plasticity with few dislocation slips and twinning. Our results reveal that the driving force for such phase transformation is the high interfacial stress in the bicontinuous intertwined struc-ture. This study suggests new strategies for improving the ductility of ultra-strong nanocomposite metals