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Molecular dynamics simulations of shock induced deformation twining of FCC single crystal copper ANUPAM NEOGI, SUNIL RAWAT, NILANJAN MITRA, Indian Institute of Technology Kharagpur — Multi-million atom non-equilibrium molecular dynamics simulations has been carried out to demonstrate shock induced deformation pathway of FCC single crystal Cu loaded along <100>, <110> and <111> directions for a varying range of shock intensities. For the shock traveling along <100> crystal direction, slippage based plasticity has been observed to occur up to the shock pressure of ∼58 GPa i.e piston velocity of 1.1 km/s. For higher intensity of shock i.e. shock pressure above ∼60 GPa (piston velocity of 1.2 km/s), predominating nature of twining mechanism has been identified during post-shock relaxation. The underlying atomistic mechanism of this conversion of slip-based to twin-based plasticity has been studied along with distribution of shock induced strain in the deformed matrix and its associated post-shock relaxation. Post-shock relaxation upon unloading has been identified to play a crucial role over the resultant texturing in the target sample. The activation and temporal evolution of different twin systems has been studied. Moreover, a complete atomistic mechanism of this slip-to-twin transition in FCC shocked metal will be discussed.

Anupam Neogi
Indian Institute of Technology Kharagpur

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