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Effects of elasticity and dislocation core structure on the interaction of dislocations with embedded CNTs in aluminium: An atomistic simulation study

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Dislocation motion is the basic feature of plastic deformation of ductile metals. Anything that interferes with dislocation motion, such as grain boundaries, precipitates, or reinforcement particles, impedes dislocation slip and increases metals' strength. Using molecular dynamics simulation, we studied the interaction of pristine or Ni-coated carbon nanotubes (CNT) with lattice dislocations moving under stress in an aluminum matrix. It was shown that the embedded CNTs increase the stress needed to move dislocations (the yield stress) in a manner that is similar to an array of non-shearable precipitates that are by-passed via the so-called Orowan mechanism. However, the strain hardening mechanism associated with multiple dislocations intersecting CNTs on the same slip-plane was found to differ from the classical picture of Orwan hardening. The strengthening mechanisms observed in these simulations are much more complex and involve crystallographic and non-crystallographic cross-slip of near-screw segments on the CNT-metal interface, dislocation lock formation and annihilation, jog formation, and shedding of prismatic dislocation loops.