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Atomistic simulation of plastic deformation in metallic nanowires

MIN JI, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — Plastic deformation in metallic nanowires was studied by atomistic simulations using empirical interatomic potentials based on embedded atom method (EAM). Several factors affecting the results of the deformation simulation such as temperature effect and the accuracy of the EAM potentials have been investigated. Deformation structures of Cu, Al and Au 100 nanowires after their yield point were analyzed and compared with each other. We found that metals with different stacking fault (SF) energy behavior differently during the plastic deformation at nanoscale. Furthermore deformation behavior of the nanowires under compression and tension were also compared.

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