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Twin boundary sliding in single crystalline Cu and Al nanowires

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A B S T R A C T

Twin boundary sliding (TBS) is a deformation mode that is typically observed in nanocrystalline metals and usually occurs at multiple locations in the twinned region, including twin boundaries, of a crystal in a situation in which additional deformation *via* twinning is limited. Unlike the well-established dislocation slip and necking deformation process that occurs in large crystals, recent theories that explain TBS are often controversial, and much remains unsettled. Herein, we develop a factor that enables the prediction of deformation pathways by quantitatively analyzing the relative tendency for the formation of partial dislocations based on the dislocation and fault energy theories. The developed factor considers the effects of static/extrinsic features, such as the stacking fault energy (SFE) as well as the crystal size and orientation, and dynamic structural states characterized by the various fault energies of a material. The factor is initially validated using a Cu crystal exhibiting low SFE for various orientations and sizes. To determine whether the proposed factor can be generically extended to crystals with high SFE, we perform micro-mechanical tensile tests and molecular dynamics simulations on Al nanowires. The developed factor produces self-consistent results even for metals exhibiting different SFE values. The observations can be used as a guideline to design nanoscale structures for load-carrying applications.

1. Introduction

Twinning is the fundamental mode of plastic deformation activated by successive slips of the twinning partial dislocation on adjacent slip planes and has attracted considerable attention for improving the strength while maintaining a large plastic strain [1–9]. However, under a certain condition, twin migration is impeded by the large-scale sliding of a twin boundary, resulting in a large offset on the crystal surface [10, 11]. This irreversible deformation, which is referred to as twin boundary sliding (TBS), is usually observed at multiple locations in the twinned region, including twin boundaries, of a crystal in a situation in which additional deformation *via* twinning is limited [10, 11]. Despite the importance of TBS in determining plastic deformation and the fracture of nanocrystalline materials, little is known about the TBS generation conditions and formation mechanism.

Although TBS is typically observed during high-temperature deformation [12], recent atomic simulations suggest the possibility of TBS at low temperatures [13, 14]. The subsequent experimental studies have denoted that TBS can occur during the deformation of face-centered cubic (fcc) metal nanowires (NWs) at room temperature. Yue et al. performed tensile tests on Cu NWs along various orientations and claimed that TBS is independent of the crystal orientation and occurs when the NW diameter reaches a critical size [10]. Subsequently, Wang et al. performed compression tests with respect to the Cu nanopillars and observed that TBS occurs only along specific orientations, regardless of the crystal size and species of crystals. Based on the experimental observations, Wang et al. claimed that TBS occurs when the Schmid factors evaluated along the leading and trailing partial dislocations with respect to the loading direction are similar or comparable [11]. These two conflicting results imply that the existing theories, which only consider either the crystal size or orientation, are insufficient to explain the TBS phenomenon; thus, advanced experiments and theoretical analyses are required.

TBS is a deformation process resulting from the alternate generation of both the twinning and trailing partial dislocations at the twinned region or on a coherent twin boundary and occurs when the generation of partial dislocations on successive slip planes is hampered. When viewed from the perspective of the stresses that activate partial dislocations, this peculiar deformation corresponds to a situation in which the stresses responsible for the formation

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