An Investigation of the Effect of Change in Crystal Structure on the Mechanical Properties of Nanocrystalline Aluminum Using a Continuum-Atomic Multiscale Bridging Method

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This study aims to investigate the effects of change in crystal structure on the mechanical properties of nanocrystalline aluminum. A continuum-atomic bridging computational algorithm is used to relate the deformation at a continuum scale to the positions of atoms at an atomic scale [1]. The finite element method and the molecular dynamics method are employed for continuum-scale simulations and atomic-scale simulations, respectively. The authors apply this multiscale bridging method to a hexahedral finite element consisting of eight integration points in which nanocrystalline models are embedded. Two loading conditions are considered to discuss the difference of deformation twinning patterns caused by the different macroscopic deformation at each integration point. In addition, the authors also apply several other conditions to study grain-size dependence, grain-orientation dependence, and the effects of different loading conditions. The results confirm that deformation twinning plays a significant role at the stage of plastic deformation in nanocrystalline aluminum. This observation is in good agreement with experimental results [2]. Furthermore, distinct deformation twinning patterns are observed at each integration point in one of the loading cases. These results suggest the possibility of improvement of macroscopic ductility in nanocrystalline metals due to the nucleation and growth of deformation twinning at an atomic scale. These insights help to understand the properties of nanocrystalline metals in more detail.

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