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PROCEEDINGS

Atomistic Migration Mechanisms of $[1\bar{2}10]$ Symmetric Tilt Grain Boundaries in Magnesium

Chuanlong Xu[1] and Haidong Fan[1,*]

[1]Department of Mechanics, Sichuan University, Chengdu, 610065, China
[*]Corresponding Author: Haidong Fan. Email: hfan85@scu.edu.cn

ABSTRACT

Grain boundary (GB) is an important microstructure and plays a vital role in the mechanical properties of polycrystalline materials by GB migration and sliding. In this work, molecular dynamic (MD) simulations were performed to investigate the migration mechanisms of $[1\bar{2}10]$ symmetric tilt grain boundaries (STGBs) in magnesium. A total of 15 STGBs with the rotation angle θ from 0° to 90° were studied under a pure shear loading. The results show that the GB migration mechanisms are significantly influenced by the GB structure. For small angle STGBs (θ<28°), the GB migration is mediated by twin nucleation from GB and subsequent twin growth. For large angle STGBs (θ>83°), the GB migration is achieved by the glide of GB dislocations. The medium angle STGBs (28°<θ<83°), which are the majority of studied STGBs, were observed to be transformed into twin boundary (TB) by emitting lattice dislocations/stacking faults (SFs) during migration. The migration mechanisms for medium angle STGBs can be explained by two rules: GB decomposition and emission of lattice dislocations/SFs. This work provides atomic mechanisms on the GB migration, which are important for understanding the GB behaviors and mechanical properties in magnesium.

KEYWORDS

Molecular dynamics simulations; grain boundary migration; magnesium

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