

Defects Interaction between Twin Boundary and Dislocations emitted from a Crack of Magnesium by Molecular Dynamics Simulations

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Abstract

Atomistic defects interaction between a twin boundary of $(10\bar{1}1)$ and the dislocations emitted from a crack introduced near the twin boundary of pure magnesium (Mg) was examined using molecular dynamics simulations. The interatomic potential employed is the embedded-atom method (EAM) type many-body potential by which surface energy tends to be relatively lower than that by ab-initio calculation. The position of the crack, which was modeled by the removal of a few layer atoms, was changed from on the twin boundary to sufficiently far from the boundary. This problem intrinsically involves the energetically competitive events among dislocation nucleation from the crack tip, crack propagation, reaction between the piled-up dislocation and the twin boundary, and twin boundary opening. The preferential event is strongly dependent to the position of the crack. The crack placed within almost 20nm from the twin boundary show the unstable crack opening after emission of the basal dislocations. However, the crack far from the boundary happens to nucleate the basal dislocations which are piled up in front of the twin boundary. The back stress of these dislocations might reduce the stress concentration around the crack tip and then the crystallographic reaction between the piled-up dislocations and the twin boundary finally yields the void nucleation on the boundary. These competitive atomistic behaviors suggest the improvement of the fracture toughness of Mg.

Keywords: Magnesium, Defect interaction, twin boundary, crack, dislocation nucleation, Molecular dynamics