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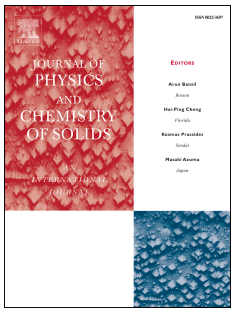

Atomistic modeling of grain boundary behavior under shear conditions in magnesium and magnesium-based binary alloys

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Atomistic modeling of grain boundary behavior under shear conditions in magnesium and magnesium-based binary alloys

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Abstract In this study, the structure, the energetic, and the strength of a $\{10\bar{1}1\}\langle 11\bar{2}0\rangle$ symmetric tilt grain boundary in magnesium and magnesium binary alloys were analyzed in the framework of (semi-)empirical potentials. Following a systematic investigation of the transferability and accuracy of the interatomic potentials, atomistic calculations of the grain boundary energy, the grain boundary sliding energy, and the grain boundary strength were performed in pure magnesium and in binary MgX alloys (X = Al, Ca, Gd, Li, Sn, Y, Ag, Nd, and Pb). The data gained in this study were analyzed to identify the most critical material parameters controlling the strength of the grain boundary, and their consequence on atomic shuffling motions occurring at the grain boundary. From the methodology perspective, the role of in-plane and out-of plane relaxation on the grain boundary sliding energy curves was investigated. In pure magnesium, the results showed that in-plane relaxation is critical in activating $b_2^{\{10\bar{1}1\}}$ twinning dislocation resulting in grain boundary migration. In the alloy systems, however, grain boundary migration was disabled as a consequence of the pinning of the grain boundary by segregated elements. Finally, while the grain boundary energy, the shape of the grain boundary sliding energy curves, and the grain boundary sliding energy are critical parameters controlling the grain boundary strength in pure magnesium, only the grain boundary energy and the segregation energy of the alloying elements at the grain boundary were identified as critical material parameters in the alloys system.

Keywords: magnesium binary alloys; grain boundaries; molecular statics; segregation energies; defects; anelasticity; mechanical properties; metals

1. Introduction

As a consequence of the high plastic anisotropy at low and room temperature between basal and non-basal slip in magnesium, additional deformation modes to dislocation-based plasticity have to be taken into consideration when modeling the inelastic behavior of magnesium. While several deformation modes could be listed, this study focuses on (i) the properties of symmetrical tilt grain boundary, and (ii) on the mechanism of grain boundary sliding. Since grain boundary sliding is a major deformation mode in fine-grained magnesium, the control of such deformation mode in magnesium and its alloys would offer a solution to improve the formability of magnesium and its alloys.

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