Molecular dynamics study of Al solute-dislocation interactions in Mg alloys

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Abstract. In this study, atomistic simulations are performed to study the effect of Al solute on the behaviour of edge dislocation in Mg alloys. After the dissociation of an Mg basal edge dislocation into two Shockley partials using molecular mechanics, the interaction between the dislocation and Al solute at different temperatures is studied using molecular dynamics. It appears from the simulations that the critical shear stress increases with the Al solute concentration. Comparing with the solute effect at $T = 0$ K, however, the critical shear stress at a finite temperature is lower since the kinetic energy of the atoms can help the dislocation conquer the energy barriers created by the Al atoms. The velocity of the edge dislocation decreases as the Al concentration increases when the external shear stress is relatively small regardless of temperature. The Al concentration effect on the dislocation velocity is not significant at very high shear stress level when the solute concentration is below 4.0 at%. Drag coefficient B increases with the Al concentration when the stress to temperature ratio is below 0.3 MPa/K, although the effect is more significant at low temperatures.

Keywords: Mg alloys; molecular dynamics; solute effect; edge dislocation; drag coefficient; critical shear stress

1. Introduction

Magnesium (Mg) alloys have been constantly developed for various structural applications because of their light weight and high specific strength (Kainer 2000). However, due to the hexagonal close packed (HCP) structure their limited formability and mechanical anisotropy are the main obstacles for their wider applications. Since the mechanical properties of metals including strength and ductility can be influenced by alloysolute, a thorough understanding of the role of the solid solute in the microstructure-property relations is essential to the improvement of these mechanical properties of Mg alloys. In particular, studies at the atomistic level can help elucidate important aspects of solute-dislocation interaction and dislocation motion under different temperatures.

Dislocations in the alloys are pinned through interactions with the solute atoms. Compared with dislocation motion in pure crystal, higher shear stresses are therefore required for dislocation moving through a solute field. Solute strengthening is typically divided into two categories: strong

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