

Effect of Li on the deformation mechanisms of nanocrystalline hexagonal close packed magnesium



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ABSTRACT

Addition of solutes such as lithium enhances ductility of hexagonal-close-packed (hcp) magnesium (Mg). However, the atomistic underpinning of Li addition on individual deformation mechanisms remain unclear and is the focus of the present work. We compared the deformation mechanisms in nanocrystalline (NC) and single crystal simulation systems of pure Mg and Mg-Li hcp alloys. Five deformation modes are observed in the pure NC Mg with randomly oriented grains – one basal $\{0001\} \langle 11\bar{2}0 \rangle$, one pyramidal type-I $\{10\bar{1}1\} \langle 11\bar{2}3 \rangle$, and three twinning slip systems $\{10\bar{1}2\} \langle 10\bar{1}1 \rangle$, $\{10\bar{1}3\} \langle 30\bar{3}2 \rangle$, and $\{10\bar{1}1\} \langle 10\bar{1}2 \rangle$. Distributing 10 at.% Li randomly to this NC Mg decreased its compressive yield strength by 14.5%. This also increases the ductility by activating non-basal deformation modes and by reducing the plastic anisotropy. We benchmarked these results by comparing the effect of Li addition on these deformation modes in Mg single crystals. Finally, we present a formability parameter (F_p) model based on unstable stacking fault energy, twin fault energy, and nucleation stress for dislocations (τ_{NS}). Quantifying the changes in F_p values for the Mg-Li alloys with respect to pure Mg in single crystal simulations explain the decrease in compressive yield strength and change in deformation mechanisms with Li additions. A sensitivity analysis study, comparing our CD-EAM results with a MEAM potential, shows that the effects of Li on the single deformation mechanisms are potential independent. Lastly, while results for Mg-10 at.% Li random alloy are presented here, similar conclusions can be drawn for other compositions of this hcp Mg-Li alloy.

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1. Introduction

Multicomponent Mg-Li-X-X-X alloys, where X = Al, Zn or Zr, are receiving renewed interest in many aerospace, automobile, and structural applications because of their ultra-light weight and high specific strength [1]. In addition, they have good machinability, castability, thermal conductivity, and recyclability. In comparison, the density of most commonly used Al alloys and steels is about 1.5 and 5 times larger. The hcp Mg, however, has low formability at room temperature because it has less than five independent slip systems required by the Von Mises criterion [2]. Only Basal $\langle a \rangle$ slip is activated for pure Mg at room temperature, which cannot accommodate deformation along $\langle c \rangle$ direction. A high plastic anisotropy between basal and non-basal deformation modes also impedes homogeneous deformation. Room temperature ductility

and formability of Mg can be enhanced by [3]: (i) refining grain sizes by severe plastic deformation or dynamic recrystallization, (ii) modifying texture of sheet material, and (iii) adding solutes such as Li. A fundamental understanding of deformation mechanisms in simple binary NC Mg-Li alloys, which are still largely unknown, can guide us in developing stable and strong Mg-Li-X-X-X multicomponent alloys.

Fig. 1 shows the large plastic anisotropy between the nucleation stresses for basal and non-basal slip modes for bulk hcp systems. Basal slip is dominant in coarse grains and a high plastic anisotropy is observed because the nucleation stress for non-basal slip is about *hundred times* higher than the basal slip. This large plastic anisotropy cannot satisfy the homogeneous deformation condition required by the Von Mises criterion, which gives rise to poor ductility and formability in bulk Mg alloys. Nanometer grain sizes [4] and alloying reduce this plastic anisotropy factor to about two, and triggers all the slip systems. In the present work, we will focus on the deformation mechanisms of Li alloying effects at the nanometer grain size in Mg.

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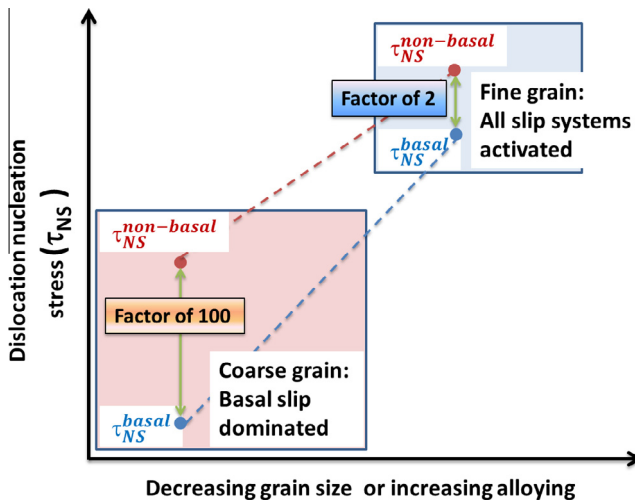


Fig. 1. A schematic diagram showing the magnitude of anisotropy in nucleation stresses of basal and non-basal slip systems (τ_{NS}) in hcp systems (adapted from [4]). The anisotropy reduces when grain size is reduced to nanoscale and/or via alloying element additions.

Recently molecular dynamics (MD) was employed to reveal the deformation mechanisms in Mg NC materials [5–12]. Kim et al. [5,6] discuss the existence of basal and non-basal slip systems and twinning systems in the preferentially oriented columnar grains in the NC Mg during creep. They also studied the effect of grain size on deformation in randomly oriented 3-D NC Mg [7]. The recent paper by Moitra [8] also discusses the effect of grain size on the microstructural properties of pure Mg. Pozuelo et al. [12] investigated how twins influence deformation in Mg–Al alloys. Bhatia et al. discussed the creep behavior in Mg–Y alloys [9]. Miyazawa et al. showed the effects of segregated Al on twinning mechanisms in Mg [10]. In addition, Reddy and Groh [11] analyzed the effect of segregated Ca on the yield surfaces of NC magnesium using a MgCa–MEAM potential [13].

Our present work aims to study the strength and deformation mechanisms in randomly oriented hcp NC and single crystal Mg–Li alloys using MD simulations. It focuses on the qualitative and quantitative effects of Li addition in NC hcp Mg. The qualitative effects such as nucleation of deformation modes, and quantitative effects such as yield strength and formability changes are analyzed. We develop a two-parameter model that quantifies how the Li addition influences the relative ease of activating each slip system in a single crystal Mg. Nucleation stress for dislocations (τ_{NS}) and fault energy (FE) of the dislocations or twins obtained from our MD simulations are used to determine the two parameters in our model. The knowledge of the deformation processes in the single crystal Mg–Li system is then used to explain the effect of the Li addition in NC Mg.

The paper is organized as follows. Section 2 presents the simulation methodology. Section 3 reviews the slip and twin systems in hcp structure, and provides their signature in the framework of the empirical potential used in this study. Section 4 discusses the results on the mechanical behavior and deformation mechanisms in NC Mg and Mg–Li alloys. Finally, Section 5 summarizes how Li addition affects individual slip systems and correlates them with deformation processes in the NC Mg–Li alloy.

2. Simulation methodology

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), a classical MD code, is used for simulations [14]. Common neighbor analysis (CNA) is used to identify the local crystal

structure of atoms as face centered cubic (fcc), hcp, and to locate non-basal slip system or grain boundary atoms [15]. OVITO software is used for visualizing our simulations by highlighting crystal defects after removing thermal noise via a short minimization run [16].

A recently developed Mg–Li interatomic potential [17], based on the concentration dependent embedded atom method (CD-EAM) formalism [18], was used in this study. This potential was created from pure elemental interatomic potentials for Li and Mg [19,20], respectively. For pure Li EAM potential, predicted values of lattice constants, cohesive energy, vacancy formation energy, melting point, and elastic constants are in good agreement with literature. The pure Mg EAM potential also reproduces the literature values of lattice constants, cohesive energy, melting points, and elastic constants [20]. Yasi et al. and Groh et al. [21,22] found this potential in good agreement with first principles calculations for stacking fault energies (SFE) of basal and prismatic slip systems. Nogaret et al. and Ghazisaeidi et al. [23,24] showed that this potential reproduces the stacking fault energy for pyramidal type I slip system but the core structure differs from density functional theory (DFT) results. They also discussed that Mg potential does not possess a stable stacking fault for the pyramidal type II slip system while *ab initio* and another Mg EAM potential [25] do. Although it was accepted that dislocation activity on the pyramidal II slip system was the main deformation mode to accommodate deformation along the $\langle c \rangle$ axis [26,27], recent experimental analysis revealed pyramidal I as the dominant slip mode in Mg single crystal under compression along the $\langle c \rangle$ axis. The pure Mg potential used in this study describes five independent slip systems, satisfying the Von Mises criterion. Therefore, we believe that this potential can be used to model the deformation of NC magnesium. However, to validate the reliability of our CD-EAM Mg–Li potentials results, we compare the results of nucleation stresses (τ_{NS}) for different deformation modes in single crystals with recently published modified embedded atom method (MEAM) Mg–Li potential [28]. In addition, and unlike in the crystal plasticity work of Agnew et al. [29,30], non-basal deformations resulting from Li addition can be characterized in our atomistic simulations without making prior assumptions.

The Mg–Li CD-EAM cross-potential was fitted to experimental variation of lattice constants and heat of mixing. It reproduces *composition dependent* lattice and elastic constants, heat of mixing, basal SFE, and the experimental Mg–Li phase diagram. These properties are perhaps the most relevant ones for our deformation studies. In the present paper we show an increase in the pyramidal type I SFE with Li addition, in agreement with a recent first principles study [31].

Fig. 2 schematically shows the NC Mg system, containing eleven randomly oriented grains and general grain boundaries, used in our simulations. The grains are generated randomly inside the nanocrystalline (NC) simulation system. The grains are grown from randomly chosen nucleation points inside the dimensions of the NC system in random crystallographic orientations. The grains grow until they reach within a cutoff distance of 0.5 Å from each other. This construction methodology of NC system gives randomly oriented grains with general grain boundaries, which has been observed experimentally. The average diameter of each grain, calculated by multiplying the number of atoms in a grain by atomic volume, is ~ 13 nm. We chose this grain size to compare our results with the recent work of Moitra et al., which uses the same pure Mg potential as here [8]. They showed that nanocrystalline grains greater than 10 nm diameter deform primarily via dislocation glide, whereas samples with smaller grains primarily exhibit grain boundary sliding and cracking. The grain size in the present work is therefore large enough to deform mainly by dislocation nucleation. The NC simulation cell is $231 \times 248 \times 234 \text{ \AA}^3$ and has 580,964 atoms. Periodic boundary conditions are used in all directions.

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