Scripta Materialia 160 (2019) 39–43

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.elsevier.com/locate/scriptamat

# Effects of Zn on ⟨c + a⟩ slip and grain boundary segregation of Mg alloys

Hyo-Sun Jang, Byeong-Joo Lee *

*Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang 37673, Republic of Korea*

ARTICLE INFO

*Article history:*
Received 23 June 2018
Received in revised form 7 September 2018
Accepted 8 September 2018
Available online xxxx

*Keywords:*
Magnesium alloys
⟨c + a⟩ slip
Grain boundary segregation
Molecular dynamics (MD)
Monte Carlo simulation

ABSTRACT

Using atomistic simulations, we investigated the effects of Zn on Mg alloys to reveal the mechanism underlying the good ductility and strong basal texture of Mg-Zn solid solutions at room temperature. We found that Zn can activate ⟨c + a⟩ slip by reducing critical resolved shear stress anisotropy among slip systems that improves ductility and that Zn has a low grain boundary segregation tendency. Because twinning and recrystallization, which have decisive effects on the texture evolution, will not be affected significantly due to the low segregation of Zn, Mg-Zn alloys are expected to yield a texture similar to that of pure Mg.


Poor formability at room temperature (RT) remains an impediment to the industrial application of magnesium (Mg) products. The poor formability is due to the limited slip systems of Mg. Previous studies have shown that activating ⟨c + a⟩ slip and weakening basal texture play key roles in improving Mg formability [1,2]. To fulfill these two conditions, various elements have been added to Mg [1–4].

Zinc (Zn) is a representative element added to Mg alloys, e.g., AZ31 and ZX31. The effects of Zn on the slip and texture are important for studying the formability of multicomponent Mg alloys containing Zn. However, studies on the addition of Zn have been conducted mainly for comparison with rare earth/Ca-containing alloys [5–9]. Even among studies of Mg-Zn alloys, most have focused on the effects of precipitates [4,10,11]. The Mg-Zn binary system consists of Mg solid solution (containing Zn up to 3.1 at.% [12]) and precipitates. Mg-Y and Mg-Li alloys activate ⟨c + a⟩ slip and weaken basal texture without precipitates [1]. That is, alloying elements can affect the slip or texture even without precipitates. Therefore, the effect of Zn on ⟨c + a⟩ slip and on the texture in solid solutions should be studied further.

Previous studies have reported that Mg-Zn solid solutions show 14–21% tensile elongation after rolling and annealing [3,8,13,14]. Blake and Cáceres contended that activated prismatic slip improves the RT ductility of Mg-Zn solid solutions [15], because Zn causes solute softening of the prismatic slip in single crystals [16]. However, prismatic slip does not satisfy the Taylor criterion [17] requiring at least five independent slip systems for homogeneous deformation. Furthermore, Stanford and Barnett reported that solute softening of prismatic slip occurs in large grains, including single crystals, because large grains can activate cross slip into prismatic planes with minimum stress [13]. However, small grain samples showing solute strengthening of prismatic slip also show good RT ductility [13,14].

Recently, we showed that solute atoms have stronger dislocation binding tendency and solute strengthening on basal slip planes than on non-basal slip planes, which reduces the anisotropy in critical resolved shear stress (CRSS) between slip systems, activates ⟨c + a⟩ slip, and improves the RT ductility of Mg alloys [18]. Solute-dislocation binding originates from the atomic size mismatch between solute and Mg atoms, and thus, any solute element with atomic sizes different from that of Mg can activate ⟨c + a⟩ slip once an adequate amount is added depending on the size of the solute-dislocation binding. Since Zn differs from Mg in atomic size, it would be interesting to determine whether Zn can indeed activate ⟨c + a⟩ slip through the above-mentioned mechanism.

Despite the good RT ductility of Mg-Zn solid solutions, after rolling and annealing, they show strong basal textures similar to that of pure Mg [5,8,9,14,19]. According to Zeng et al., the rapid growth of tension twin (TT) and preferential growth of recrystallized grains oriented similarly to their parent grains, thus leading to a strong basal texture during cold-rolling [6] and annealing [7], respectively. They asserted that both types of growth arise from a weak pinning effect of Zn on the TT boundary (TTB) and a weak solute dragging effect of Zn in matrix [6,7]. Although the pinning effect of Zn on the TTB was reported to be weak [20], it is difficult to accept that the rapid growth of TT yields a strong deformation texture because twinning including TT would weaken the basal texture by re-orientating crystals [21]. Moreover, the pinning and dragging effects of Zn on other grain boundaries (GBs) are unclear yet.

Many studies have been conducted to clarify the texture evolution mechanism in Mg and Mg alloys. Wang and Huang reported that an anisotropic hcp structure and an almost ideal c/a ratio of Mg result in a

* Corresponding author.
*E-mail address:* calphad@postech.ac.kr (B.-J. Lee).

https://doi.org/10.1016/j.scriptamat.2018.09.022

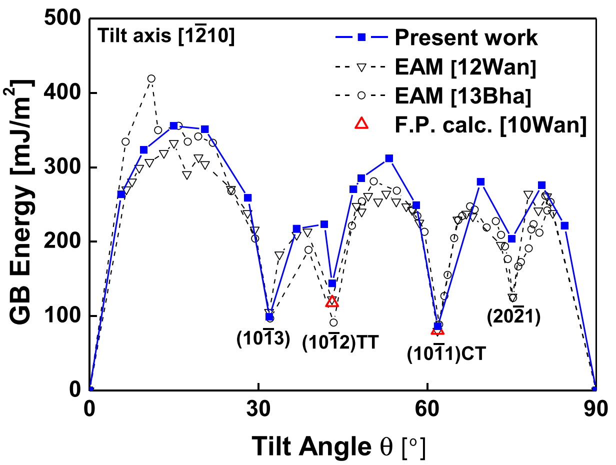


**Fig. 1.** Calculated grain boundary energy of pure Mg as a function of grain boundary misorientation angle for [1$\bar{2}$10] tilt axis in Mg using present 2NN MEAM potentials at 0 K, in comparison with EAM calculations [36,37] and a first-principles calculation results [38].

strong basal texture [22]. Although they showed that a decrease or increase in the c/a ratio could weaken the strong basal texture of hcp materials [22], the change of the c/a ratio in dilute Mg solid solutions is usually too small (<0.01% in the Mg-1.0 at.%Zn alloy [5]) to modify the texture. Instead of focusing on the c/a ratio, studies have been conducted to activate non-basal slip and twins and to modify the recrystallization behaviors in such ways as to weaken the strong basal texture [1,22–24]. Slip behavior in Mg-Zn solid solutions can be investigated through the CRSS anisotropy analysis mentioned above. Twins are reported to nucleate on GBs [5,25,26], and their growth is known to be suppressed by the ordered segregation of solute atoms on TTB [20]. Recrystallization occurs preferentially on GBs and is usually retarded by solute segregation [27]. Therefore, to deduce the evolution mechanism of the strong basal texture in Mg-Zn solid solutions, it is necessary to know the amount of Zn segregated on GBs.

The purpose of the present study is to investigate the effects of Zn on ⟨c + a⟩ slip and GB segregation in Mg-Zn solid solutions. Since both phenomena are in atomic level and rather complex, it is difficult to analyze them by experiment or first-principles methods. To resolve these difficulties, large-scale atomistic simulations were conducted in a framework of semi-empirical interatomic potentials. Using molecular dynamic simulations to calculate the solute-dislocation binding energy and CRSS on slip planes, we investigated whether Zn can activate ⟨c + a⟩ slip. The grand canonical Monte Carlo (GCMC) method [28] was used to simulate Zn segregation on GBs.

The reliability of atomistic simulations depends on the quality of interatomic potentials of the relevant alloy systems. We used the second nearest-neighbor modified embedded-atom method (2NN MEAM) [29] potentials of pure Mg [30] and a Mg-Zn system [31]. The Mg-Zn potential is based on the constituent pure Mg and pure Zn potentials, and the Mg potential parameters used for the Mg-Zn potential are the same as those for pure Mg [30]. The potentials have been reported to accurately reproduce structural, elastic, and thermodynamic properties and generalized stacking fault energy of Mg alloys on basal and non-basal slip planes [31,32]. All simulations were conducted with a radial cutoff distance of 6.0 Å, which is larger than the 2NN distances of Mg and Zn. Because the GCMC code in the LAMMPS package [33] cannot deal with the 2NN MEAM potential, we used an in-house code, KISSMD [34], for the GCMC simulation and LAMMPS for other simulations.

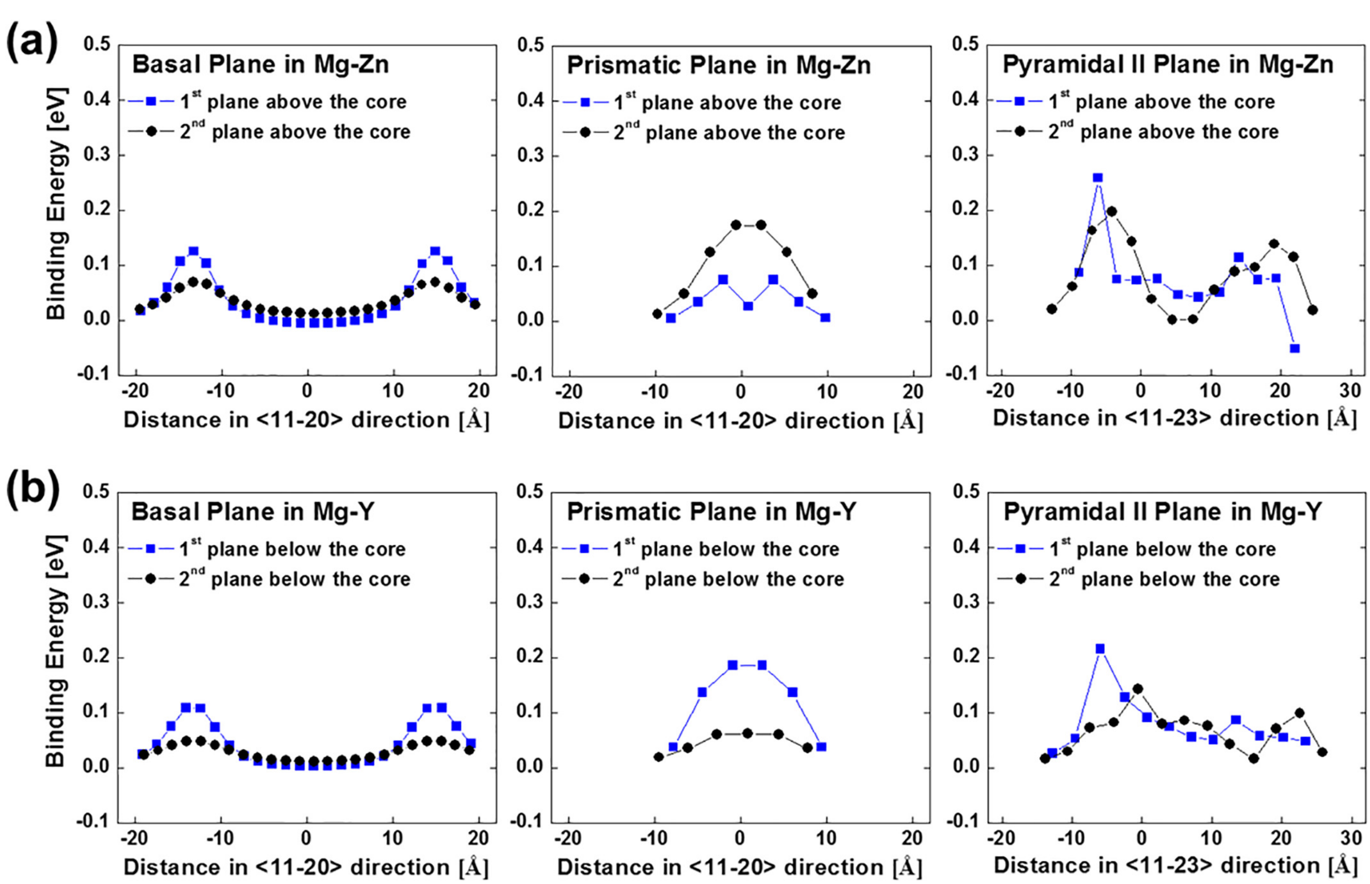


**Fig. 2.** Calculated binding energy between an edge dislocation and a solute atom, (a) Zn, (b) Y [18], on basal, prismatic, and pyramidal II planes at various positions across the dislocation core, obtained using the present 2NN MEAM potential.