

EFFECT OF SUBSTITUTED ALUMINUM IN MAGNESIUM TENSION TWIN

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Abstract

Atomistic simulations are performed in order to study the Aluminum substitution effect on Magnesium twinning mechanism. Multiple twin boundaries are found in pure Mg single crystal under tensile loading condition along $(\bar{1}012)$ crystallographic direction. However, no twinning has occurred under compression loading. Al substitution has been done for 2, 5, 7, and 10% doping. For 2 and 5% Al substitution, number of twins increase when the system is monitored under tensile loading. On the other hand, for 7 and 10% Al doping under tensile loading, no twin has been found. We found that dislocation-twin and dislocation-dislocation interaction are majorly responsible for this behavior and it is important that which one is prevalent.

Introduction

Alloyed magnesium is the lightest metal with specific strength in practical use today. There are many practical application products such as vehicular industries. However its wide-spread use is greatly hampered by its anisotropic plastic response which limits its formability at room temperature [1]. This comes partly from the hexagonal-closed packed crystal structure, where slip in the basal plane is nearly one-hundred times easier than in perpendicular planes. Slip system of Mg is composed of three slips, which are parallel to basal, prismatic and pyramidal slips. Since the (critically resolved shear stress) CRSS of pyramidal slip is much larger than that of the other slips, it is difficult to activate pyramidal slip at room temperature. Although several slip systems have been reported, the slip is commonly in the closed packing basal direction, and does not produce strains parallel to the c axis. It is known that hcp Mg shows much poor ductility compared with fcc Al due to its crystal anisotropy. Magnesium also twins (a deformation mechanism involving extended stacking changes) at fairly low strains. However, because the wrought magnesium alloy is expensive and is poor in formability, the reduction of manufacturing costs and the improvement of formability are required.

Mechanistic explanation of the plastic behavior of material is based upon the dislocation and twin nucleation. This plastic behavior of the material influences on the formability of the material. Formability of elements and their alloys are affected by strain hardening rate, strain rate sensitivity, degree of anisotropy, stress-state at fracture etc. It is well known that traditional magnesium sheet alloys exhibit poor formability via conventional forming operations at ambient temperatures. However, it is also known that at high temperatures and moderate strain rates, magnesium alloys can be extremely ductile and readily formable. Traditional explanations for these phenomena

relate to the behavior of the hexagonal close packed (hcp) magnesium single crystals. The plastic properties of magnesium single crystals were studied in detail during the 1950s and 60s with extensive application of slip trace analyses and constrained deformation experiments [2, 3]. A major conclusion of these studies was that magnesium crystals only possess two independent easy slip systems within the (0001) or basal plane. Thus, it appeared that magnesium, with its hcp crystal structure fails to satisfy the Taylor criterion [4] requiring five independent easy slip systems for homogeneous, generalized ductility of a polycrystalline aggregate. Other slip mechanisms observed [5, 6, 7, 8] during the early studies include the slips in prismatic and pyramidal planes. With reference to the Taylor criterion, it is noted that prismatic slip would offer two independent slip modes beyond the original two of basal slip for a total of four (still short of the required five for uniform plasticity). Pyramidal slip would offer four independent slip modes on its own (the same as basal and prismatic together). Although many investigators [9] performed c-axis compression experiments on single crystals designed to activate dislocations with non-basal Burgers vectors, no evidence of their activity was observed through slip trace analysis. Instead, some twinning mechanism was observed to barely precede fracture [8, 9]. Only after transmission electron microscopy (TEM) was applied to the problem during the early 1970s [10], non-basal dislocations were confirmed to be active within magnesium. In addition to dislocation slip, magnesium exhibits a strong propensity for mechanical twinning, especially the $\{10\bar{1}2\}$ $\langle 10\bar{1}\bar{1}\rangle$ tension twin [2]. Twinning may help a material to satisfy the Taylor criterion [11], however, it must be recognized that twinning is a polar mechanism (only allowing simple shear in one direction, rather than both forward and backward directions like dislocation slip). Furthermore, the amount of strain that twinning can accommodate is directly proportional to the volume fraction of crystal which has twinned. Thus there is a finite amount of strain that may be accommodated by twinning, even under ideal circumstances. Deformation twinning results in a sudden reorientation of the volume fraction of the crystal that is being twinned rather than the gradual reorientation that characterizes slip. Finally, although twinning mechanisms offer more options for plastic accommodation, they generally require an accommodation mechanism of their own in order to avoid large internal stresses leading to failure. Wang et al. recently studied [12] in detail the mechanism of $(10\bar{1}2)$ twin nucleation, however the postulated mechanisms for twin nucleation in models have not been validated so far.

Molecular dynamics (MD) simulations have been successful and powerful tool in revealing the deformation mechanisms in materials. Studies related to the deformation process speculate the major role of deformation twinning

for magnesium. New alloy development involves new solute additions and deformation to affect mechanical properties. In present paper, we observe the Al substitution effect on the Mg twinning for four different amount of Al substitution.

Method

For the purpose of present study, single crystal magnesium samples were created of $20 \times 20 \times 5.5 \text{ nm}^3$ dimension. The samples were first relaxed using an NVT ensemble for 10 nS, and then they were relaxed independently in three directions with NPT ensemble for another 10 nS. Atomistic simulations were carried out using an MD time step of 1 fS. A periodic boundary condition was adopted in all directions. A tensile deformation along the Y ($10\bar{1}2$) direction is performed at a strain rate of 10^8 S^{-1} , whereas deformation in X and Z directions that are on the ($10\bar{1}2$) plane, are carried out by maintaining a zero pressure by Parrinello-Rahman method [13]. Throughout our simulations the temperature was maintained at 300 K. At a particular interval of time we collect the snapshots of the atomic structure to analyze the microstructure.

It has been already found [14] that the interstitial Al atoms in Mg crystal raise the internal energy prohibitively large via density functional theory calculations. However it is easier for the Al atoms to substitute the Mg atoms, and occupy their positions. Accordingly, we randomly doped different amount of Al atoms in Mg single crystal by substitution. The size of the simulation cell, strain rate, and temperature were kept same as for the case of single crystal Mg simulations and Mg with Al substitution. The molecular dynamics simulations in this work employed the embedded atom method (EAM) potential of Sun [15]. This potential has a better agreement on vacancy formation energy than the Liu's [16] potential, and apart from that, the potential is developed by fitting also the vacancy migration energy. It is important to note here that a recent study [17] while investigating the effect of precipitate in aluminum alloys, proposed that thermally activated vacancy movement plays a central role in grain growth mechanism.

Results and Discussion

Stress strain curves for tensile loading with several % of Al substitution are shown in Figure 1. For pure Mg sample, two distinctive peak stress can be observed, where the first peak represent the dislocation nucleation, the second peak correspond to the twin nucleation. A substitutional atom solution relieves hydrostatic stresses and interacts with nearby dislocations. Dislocations surrounded by atmospheres can produce plastic flow in two ways: at low stress dislocations cannot escape from the atmosphere, and solute atoms migrate with the dislocations, however at large stress those dislocations can tear apart and become highly mobile and able to produce rapid flow under small stress. Interstitial Al atoms locally distort the Mg lattice and produce a strain field locally. For 2% Al substitution, the dislocation nucleation peak is increased, however the twin nucleation peak is decreased compared to the pure Mg

sample. With increased Al substitution (more than 2%) these two peaks converged to one peak, such that it is indistinguishable to identify the dislocation or twin nucleation from the stress-strain curve. Applied stress generates the dislocations (and hence the yielding) easily for the samples where Al exists more as substitutional atoms.

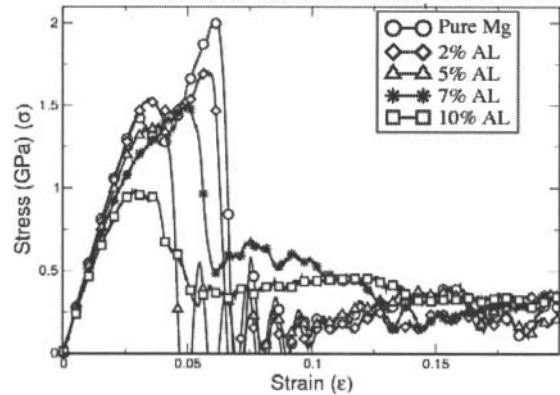


Figure 1: Stress strain curves for the pure Mg, and Mg with several % of Al substituted, under tensile loading.

We found that under tensile loading a twinning occurs, however even at quite larger strain no twinning occurs for the same direction if compressive load is provided. That confirms the fact that twinning is a polar mechanism, unlike dislocations that occurs for applied load in both directions. Figure 2 shows the structures of the sample with pure Mg for compressive loading in a) and tensile loading in b). We found that the twin formation occurs at 6.8 % of strain for pure Mg in tension. Also, we found that the initial twin volume grows with strain and secondary twins nucleate within the primary twin.

Figure 3 shows the microstructure of the samples with different amount of Al substitution. We found that in Figure 3a at 2% of Al substitution number of twins are four at 6.8% of strain. At Figure 3b with 5% Al substitution number of twins are four at 5.8% strain. In Figures 3c and 3d at 7% and 10% Al substitution, respectively we found no twinning occurs even at large strain. It has been also found that strain at which twin nucleates, decreases with increasing amount of Al doping up to 5% of substitution.

Figure 4 shows the evolution of twin-volume with strain for our models. It can clearly be seen that the twin nucleation occurs at higher strain for pure Mg model compared to the models where up to 5% Al is substituted. We can also find that the twin volume increases faster for the cases where Al is substituted compared to the pure Mg case. In our calculations, we have found that the angular rotation of twinned volume have increased up to 87° that in a very good agreement with the previous results. Since for 7 and 10% Al substitution, we do not find any twinning formation, the figure does not contain any data for that higher % s of Al substitution.

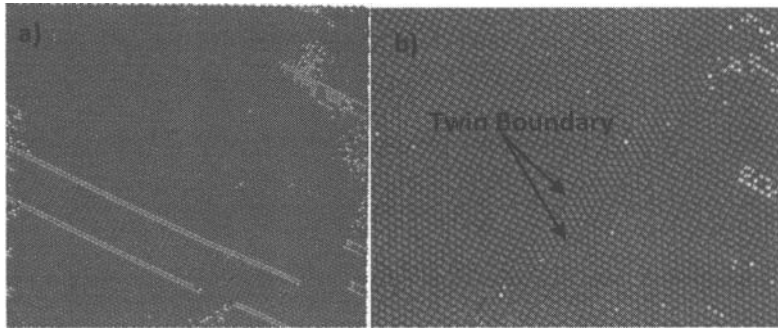


Figure 2: Sample at 6.8% of strain for a) compressive loading and b) tensile loading. Note that b) has a twin formation, while a) does not.

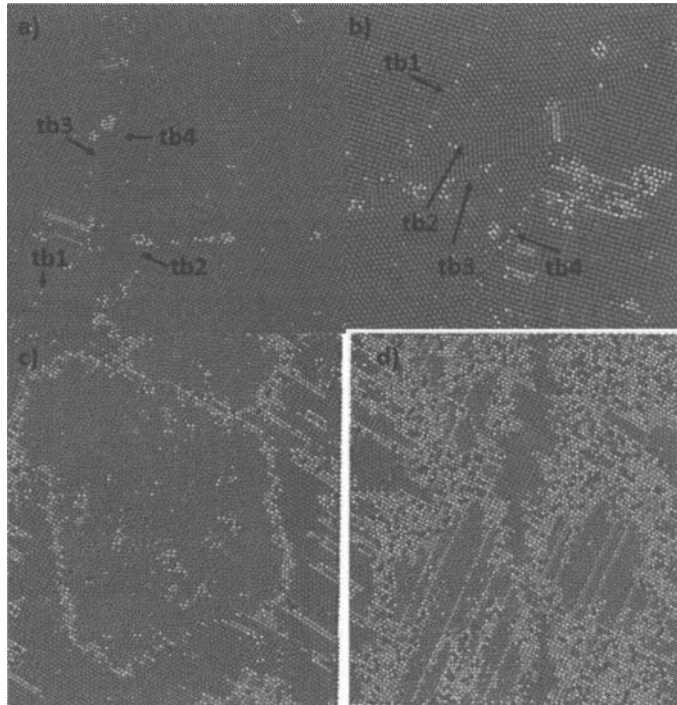


Figure 3: Mg samples with different amount of Al substitution in tensile loading. a): At 6.8% strain for 2% Al substitution, b): At 5.8% strain with 5% Al substitution, c) At 7% strain with 7% Al, and d) At 10% strain with 10% Al substitution. Note that you may find 2 more twins in b), but due to periodic boundary condition, they represent the same twins. Also note that c) and d) has no twins.

We further analyze the microstructure and revealed an interesting interaction of twin boundary with dislocation loop. Figure 5 shows a twin emission and the tip of twin is marked as 'Tip'. Figures 5a and 5b are for a pure Mg tensile deformation at 4.6% and at 9% strain. Figure 5b shows that at larger strain how the number of twins increases and how the secondary twin forms from the primary twin boundary. We have observed that secondary twin always forms from the primary twin boundary plane. Twin boundaries are marked by numbers in Figure 5b.

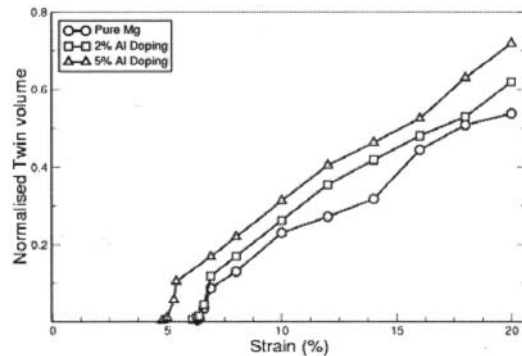


Figure 4: Evolution of normalized Twin volume.

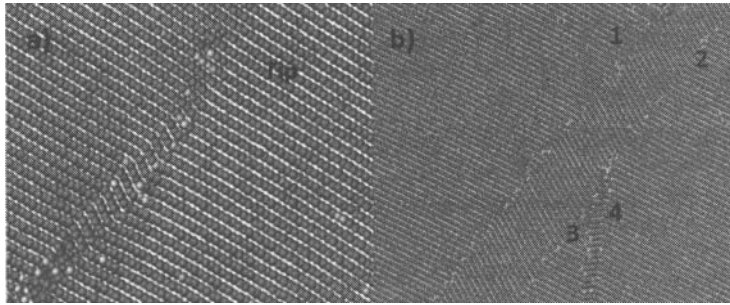


Figure 5: Emission of a twin at a), and development of multiple twins along the primary twin in b). Twin tip is marked by tip.

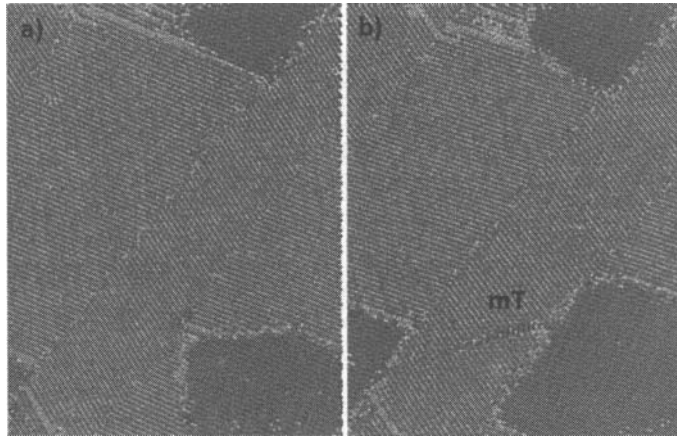


Figure 6: Interaction of dislocation with twin. In a) a dislocation loop emission toward the twin boundary is shown. In b) dislocation growth along the twin boundary is shown. Note a secondary twin formation in b) marked by mT.

In Figures 6a and 6b, we show that the twin boundary interaction with a dislocation loop. It is found that the twin boundary is very rigid and the dislocation loop cannot pass through the twin boundary. In Figure 6a, we show the initial emission of dislocation towards an existing twin boundary at 5% strain. Figure 6b shows the same dislocation-twin interaction at 9.6% strain. We found that even at large strain the dislocation loop grows along the twin boundary plane. This behavior of dislocation-twin interaction certainly due to the fact that twin boundary is very rigid, such that a dislocation cannot penetrate through the twin boundary; instead the dislocation grows along the twin boundary plane. In Figure 6b, however a micro-twin is observed inside the primary twin, marked as mT in the figure. At a later strain (not shown here) this micro-twin also grows. Thus, the interaction compels us in believing the fact that twin- dislocation interaction gives rise to more twins. When there are substituted Al atoms in the Mg system, dislocations occur at less stress state (See Figure 1); these dislocations enhance the twin-dislocation interaction that finally produces more twins. However, when the amount of Al substitution reaches to 7% atomic percentage, enormous number of dislocations are generated. These dislocations then interact mutually. As such, the twin-dislocation interaction ceases and dislocation-dislocation interaction becomes prevalent. When these dislocation-dislocation interactions become predominant, twin formation becomes sluggish. The interaction between two dislocations or a dislocation with a

twin is inherently a dynamic nature of interaction of two defected lines. The atoms inside those defected-lines although possess a symmetrical nature of crystal structure (hcp for this case). These atoms being intelligent being at a given time knowing all the forces that causes them to move, try to dissipate the stress in such a fashion that the interaction energy of those two defected-lines minimized. Typically for two dislocation loops interaction, the atoms inside them are trying to reorient themselves to minimize the interaction energy, and hence no effort is being taken to penetrate the twin boundary. Naturally, when the dislocation-dislocation interaction becomes prevalent than the dislocations-twin interaction (which is 7% or higher for the present study), new twin formation does not take place.

In order to increase the formability of Mg we need to get the homogeneous and generalized ductile behavior for Mg. Since the slip systems are limited, and Mg fails to satisfy Taylor criterion, twinning is the alternative to increase the formability of Mg. We found in the present paper that how the evolution of twinning changes with the Al substitution. It should be kept in mind that the present calculation deals a tensile loading condition only for a particular orientation of single crystal Mg. In reality, there are several grains oriented in different directions with multiple grain boundary and different amount of multi-dimensional defects in it. Nevertheless, the nature of the dislocation-dislocation interaction or the dislocation-twin interactions discussed in the paper remains the same for polycrystalline

aggregate. Perhaps it could be a nice future study to see the dislocation-twin interactions for a polycrystalline Mg sample with low angular misorientation.

Conclusion

Atomistic simulations are performed in order to study the Aluminum substitution effect on Magnesium twinning mechanism. Deformation twinning are found in pure Mg under tensile loading condition, however no twinning has occurred under compressive loading. It has been found that for 2 and 5% of Al substitution, twinning occurs at low strain compared to pure Mg case, but for 7 and 10% Al substitution, no twinning has been found. The interaction of dislocations with other dislocations and twin are held responsible for this behavior particularly for this orientation. For small (2 and 5%) amount of Al substitution the dislocation interacts with twin and their interaction gives rise to more twins, however for 7% or more Al substitution, dislocation-dislocation interaction becomes prevalent and no twins occur.

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