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The effect of rare earth element segregation on grain boundary energy and mobility in magnesium and ensuing texture weakening

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ABSTRACT

This paper elucidates a key puzzle related to texture randomization - effect of rare earth on grain boundaries. We use electron back-scatter diffraction and molecular dynamics to compare recrystallization between pure Mg and a Y-containing alloy. The alloy's texture components were initially similar, but the large ⟨*a*⟩ fiber grains in pure Mg overtook all other components. Y segregation homogenized the energies of ⟨*a*⟩ fiber grain boundaries, curtailing conventional recrystallization. Grain boundary mobilities were reduced proportionally to the energy stabilization, reducing the dominance of $\langle 10\bar{1}0 \rangle$ extrusion texture. This allows other grain orientations to stabilize thus producing a more randomized texture.

As the lightest structural metal on earth, magnesium has no equal in the world of structural lightweight metals. When alloyed with small additions of zinc and aluminum, its specific strength can exceed that of steel and even aluminum. However, this increase in strength is correlated with a massive drop of ductility, so much so that forming operations of inner door panels at room temperature become impossible without tearing and fracturing the sheet [1].

The reason for this loss in ductility goes back to the remarkably high values of the critical resolved shear stress of pyramidal ⟨*c* + *a*⟩ $\left(\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle\right)$ slip, the only slip that can provide arbitrary deformation, which exceeds that of twinning. This phenomenon is surprising to the automotive manufacturing engineers, as the most commonly used face-centered cubic metals can only twin under rates approaching the ballistic regime or in materials with sufficiently low levels of the stacking fault energy (e.g. twinning-induced plasticity steels). As pyramidal ⟨*c* + *a*⟩ is the only slip mode that can provide plasticity along the ⟨*c*⟩-axis, grains plastically stretching or extending along their ⟨*c*⟩-axis experience profuse $\{10\bar{1}2\}$ twinning which advances and reorients their lattice. The twinning-induced lattice reorientation, and the concomitant operation of ⟨*a*⟩-slip, including basal ⟨*a*⟩ and prismatic ⟨*a*⟩, lead to the onset of a strain regime with very strong hardening rates, which precipitate the attainment of the ultimate stress at low strain levels, and thus materials failure. $\{10\bar{1}1\}\langle 10\bar{1}2\rangle$ can also appear in grains undergoing contraction or compression along their ⟨*c*⟩-axis. Twins of this mode have a needle-like morphology and stop propagating shortly after their nucleation to develop sharp cracks. These detrimental mechanisms are exacerbated in conventional wrought magnesium alloys, as they tend to exhibit very sharp textures which yields a similar behavior to that of single crystals [2–4]. Hence, in bending conditions, typically occurring in forming operation of inner door panels, a sheet sees the compression fiber deforming and hardening at dramatically different rates than the tension fiber, causing rapid shear failure along the neutral axis.

In an effort to design wrought Mg alloys with a better ductility, extensive studies have been conducted to understand the recrystallization mechanisms responsible for generating strong textures. In general, deformation at high temperature motivates the basal planes of all grains to align themselves with the main loading axis, so ND||[0001] and ED||$\langle 10\bar{1}0\rangle$ fibers develop after rolling and extrusion respectively, where ND is the normal direction to the plate and ED is the extrusion direction [5–9].

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The dominant mechanisms in recrystallization of Mg are grain polygonization entailing formation of sub-grains. This dynamic recovery process has been termed by many authors as continuous dynamic recrystallization (CDRX) [10,11] alluding to the continuous maturity of subgrains. In this mechanism, walls of dislocations build up, initiating the formation of new grains with low misorientation angles. However, as they absorb more dislocations, the walls go on to mature to high angle grain boundaries (GBs), which, depending on their mobility, extend by grain growth phenomena as they consume defects surrounding them. The initial rotations are effected around the Taylor axis associated with the type of dislocations constituting the walls. Barrett et al. [12] demonstrated via a combined study of electron Backscattered diffraction (EBSD) analysis and molecular dynamic (MD) simulations that the rotations settle at specific GBs showing the best combination of low energy and high mobility. Cusps in the energy landscape of the tilt Taylor axis can effectively lock the rotation if the corresponding GB is able to move quickly to absorb the surrounding dislocations. This way, the absorbed dislocations will cease their effect on GB rotation, and they would only be used to accommodating the increase in boundary length associated with grain growth. Because of their low energy and high mobility, 'recrystallization twins' have been frequently observed in Mg, enabling a low-cost transition from polygonization into the grain-growth phase of recrystallization [12].

The addition of rare-earth elements (REEs) to Mg alloys has been shown to noticeably enhance their ductility in deformation conditions close to those imposed in the forming of structural components [13–15]. These improvements have been linked to actions on both texture randomization and enhancement of non-basal slip, which reduced the disparity between critical resolved shear stresses of active deformation modes [16–20]. Hoping to identify design strategies to maximize the beneficial action of REEs on formability, many studies have been conducted to unravel the underlying mechanisms of both effects. It has been suggested that the equalization of hardness of slip system is achieved by dynamic segregation of REEs in the dislocation core which reduces their stacking fault energy. Similarly, segregation into twin boundaries (TBs) reduces their interfacial energy making them more stable and less mobile [21]. Hadorn and Agnew [19] has demonstrated that Y preferencially segregates to interfaces during Mg DRX, in agreement with transmission electron microscopy by Nie et al. [21] which showed a regular segregated structure of REEs in interfacial extension sites. The atomic radius of most RE elements is slightly larger than Mg, making them ideal segregation candidates to retard the movement of defects and reduce their energies. However, the REE effect cannot be explained by size mismatch alone, since non-REEs such as Ca do not behave similarly. In fact, Stanford et al. [22] have shown that Ca additions in pure Mg enhance texture sharpening during DRX, like traditional Mg alloys. The role of RE elements therefore, must be a complex function of their valence electronic structure, which interacts favorably with a Mg matrix to promote texture weakening.

Based on results revealing the cause of texture sharpening in traditional Mg alloys, Barrett et al. [12] hypothesized that REEs randomize texture by leveling out the differences in GB energies encountered in traditional Mg alloys, and thus promote equal growth opportunities as much as equal nucleation opportunities. This hypothesis is in contrast to other explanations based on bolstering of $\langle c+a \rangle$ slip activity, solute drag, particle stimulated nucleation, and shear localization enhancement [14,20,23-26].

In reality, the question of Mg texture randomization by REEs should not be studied independently from the dynamic recovery mechanisms leading to the strong basal texture in conventional Mg alloys. So a well-posed question is how does REEs upset those mechanisms? By comparing relevant properties of pure Mg and MgY using a combined EBSD characterization and MD simulation analysis, this paper reveals key mechanisms governing the way REEs alter GB formation and migration. We use Yttrium as a pilot REE to demonstrate our hypothesis, capitalizing on the vast literature for the effect of this element on texture weakening.

A high Purity Mg (99.999 wt%) and Y-containing Mg alloy with the chemical composition of Mg-2.05 Y-0.40 Zn-0.57 Al-0.29 Mn (wt%) were received in the as cast condition. The nominal compositions were verified employing the atomic emission spectroscopy (ICP-AES) method. The billets were solution heat-treated at 450 °C for 10 h under flowing argon gas atmosphere followed by instantaneous water quenching. Solution treated samples were subject to indirect extrusion at ram speeds of 10 and 40 mm/min with area reduction ratios of 6 and 25 at 450° followed by air cooling. Samples cut along extrusion direction (ED) were grounded exploiting standard metallographic techniques and polished using 0.06 mm colloidal silica (Struers OPS) for 10 min. In preparation for EBSD, Electro-polishing was conducted on polished samples in Struers C1 solution at 25 V for 120 s. EBSD analyses were carried out using a field emission scanning electron microscope (SEM) at the operating voltage of 20 kV.

Simulations were run on a set of optimized $\langle c \rangle$-axis tilt bicrystals. This data set was constructed with pure Mg by minimizing geometrically constructed bicrystals with a conjugate gradient approach, equilibrating for 5 ps, and minimizing the energy again. In some cases, high energy atoms were removed from the resulting structure and the process was repeated. The lowest energy structure was selected for analysis. These structures were previously generated with the Liu et al. [27] potential for a previous work [12]. For this study, we generated the same GBs with the Kim et al. [28] potential and verified that the predicted structures and energies agreed with the Liu et al. [27] potential. The GBs were also verified by comparisons with the potential by Wu et al. [29].

GBs for Mg-Y alloys were developed using the potential by Kim et al. [30]. We compared these results to Pei et al.'s [31] potential, but found Pei et al.'s [31] potential predicted unrealistic GB structures even for pure Mg. All results shown here are obtained from Kim et al.'s [30] potential. We analyzed the pure Mg tilt boundaries and identified GB atomic sites where the atoms had a greater than ideal nearest neighbor distances, like the sites observed by Nie et al. [21] to be filled by REEs. These sites were filled with Y atoms and the resulting energy was then measured. These results are labeled as the idealized segregation energy. We deemed, however, that such highly geometric segregation is not likely to be achieved in a deforming material. Therefore, for comparison, we constructed simulations on the relaxed bicrystals where we replaced random atoms throughout the bicrystal with Y atoms to make a 3 wt% alloy. These simulations were equilibrated at 600 K for 500 ps to encourage segregation and GB mobility. We ran three simulations for each orientation to report a range of energies for random segregation.

All simulations were run using LAMMPS [32] and analyzed with OVITO [33].

Analysis of the experimental results with EBSD (Fig. 1) shows that Y significantly alters the texture, as has been previously reported. Notably however, some small grains in pure Mg are observed which have the characteristic "rare-earth" orientation. These grains are infrequent and do not grow significantly. In contrast, the $\langle 10\bar{1}0 \rangle$ and $\langle 2\bar{1}\bar{1}0 \rangle$ pole textures dominate the microstructure. In the Mg-Y alloy, the grain orientations are distributed much more widely, but grains near the $\langle 2\bar{1}\bar{1}1 \rangle$ pole tend to be larger, creating a high intensity texture component. The characteristic $\langle 10\bar{1}0 \rangle$ pole is still prominent, largely due to unrecrystallized grains. Taken together, it appears that pure Mg and Mg-Y have the same texture components during early DRX, but Y changes the mechanism in a way that growth of the basal grains is curtailed and the non-basal components thrive. Clearly, to change the texture in this way, Y impurities must alter the CDRX mechanism which is prevalent in conventional Mg alloys. Pure Mg's recrystallization texture mainly results from grains falling into