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Yield asymmetry design of magnesium alloys by integrated computational materials engineering

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ABSTRACT

Deformation asymmetry of magnesium alloys is an important factor on machine design in the automobile industry. Represented by the ratio of compressive yield stress (CYS) against tensile yield stress (TYS), deformation asymmetry is strongly related to texture and grain size. A polycrystalline viscoplasticity model, modified intermediate ϕ-model, is used to predict the deformation behavior of magnesium alloys with different grain sizes. Validated with experimental results, integrated computational materials engineering is applied to find out the route in achieving desired asymmetry via thermomechanical processing. For example, CYS/TYS in rolled texture is smaller than 1 under different loading directions. In other textures, such as extruded texture, CYS/TYS is large along the normal direction. Starting from rolled texture, asymmetry will increase to close to 1 along the rolling direction after being compressed to a strain of 0.2. Our modified ϕ-model also shows that grain refinement increases CYS/TYS. Along with texture control, grain refinement also can optimize the yield asymmetry. After the grain size decreases to a critical value, CYS/TYS reaches to 1 because CYS increases much faster than TYS. By tailoring the microstructure using texture control and grain refinement, it is achievable to optimize yield asymmetry in wrought magnesium alloys.

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1. Introduction

Due to their unique deformation behavior and excellent strength-to-weight ratio [1], magnesium alloys have long been applied in the automobile industry. Magnesium is the lightest of all the engineering metals with a density of 1.74 g/cm^3, 35% lighter than aluminum and more than four times lighter than steel. It is also abundant as the eighth most common element on earth. To further increase fuel efficiency, improve vehicle performance, and reduce carbon dioxide emissions, more lightweight magnesium alloys will be applied in automobiles to support vehicle weight reduction. Currently, the average usage of magnesium in cars produced in North America is 20 kg. To achieve the goal of increasing magnesium usage to 100 kg by 2020, there still are significant technical hurdles to improved performance, manufacturability, costs, and modeling required for magnesium alloys, as pointed out by Joost [2]. One of the challenges for broader application of magnesium alloys is insufficient strength and stiffness for certain structural applications. The high strengths stated in most studies of magnesium alloys withstand only some specific loading conditions, but not others. Fully understanding the anisotropic behavior and yield asymmetry is important in processing and design. Furthermore, this knowledge will enable materials engineers to design processes that improve the collective behavior of magnesium alloys. Incorporating magnesium alloys' unique deformation behavior into processing and design models will be performed using integrated computational materials engineering.

Magnesium alloys are low-symmetry materials with hexagonal close-packed (HCP) crystal structure, which is different from steels and aluminum alloys with high symmetry structure. Complex deformation mechanisms activated during deformation in magnesium produce tension–compression yield asymmetry, a ratio of compression yield stress (CYS) and tension yield stress (TYS) represented by CYS/TYS. This asymmetry usually is not observed in aluminum or steel but is universal in magnesium alloys. In some cases, CYS is only 1/2 to 1/3 of TYS, leading to restriction of most structural applications subjected to both tension and compression loading simultaneously.

Tension compression yield asymmetry has been studied by Yin et al. on extruded AZ31 [3]. Loading direction and grain size have significant influence on yield asymmetry. When the loading direction moves away from the extrusion direction (ED), CYS/TYS increases to greater than 1. Asymmetry also is reduced when grain size decreases. When the grain size is refined from 28 μm to 9 μm, CYS/TYS increases from 0.75 to 0.85. Similarly, Kleiner and

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Uggowitzer investigated the influence of loading direction on yield asymmetry in extruded AZ61 Mg alloy [4]. They also observed a strong anisotropy of yield strength: high yield strength around 200 MPa only for extension along the ED and much lower strength along the other loading directions or for compression loads.

Adjusting the component content in magnesium alloys will influence the microstructure and yield asymmetry. For indirect extruded Mg–5Sn–*x*Zn alloys, Tang et al. [5] found that increasing Zn content will increase the amount of fine particles of MgZn and lower the degree of yield asymmetry. The decrease of yield asymmetry is not due to the texture because the basal textures are similar for all of the as extruded samples with different Zn content. It is attributed to the grain refinement from increasing the number of dispersion particles.

Changing processing parameters will change the microstructure as well as the mechanical deformation behavior. Park et al. [6] studied the effects of processing conditions on texture, grain size, and mechanical properties of indirect-extruded AZ31. Increasing the Zener–Holloman parameter by adjusting the extrudate exit temperature and ram speed resulted in a finer grain size, weaker texture, and lower yield asymmetry. With Z increased from 0.5×10^{11} to 7.7×10^{11}, the yield asymmetry increased from 0.65 to 0.92. It is possible to use a processing path model [7,8] to identify the processing path toward desired asymmetry by designing the processing sequence, parameters, and metrics. To achieve this goal, a systemic study of yield asymmetry due to texture, loading conditions, and grain size is necessary to build up solid knowledge on the deformation behavior determined by microstructure and loading conditions.

The influence of grain size on mechanical deformation behavior of magnesium alloys has been studied by several groups from different perspectives. Chang et al. studied the effective deformation behavior of hot extruded AZ31 alloy with different grain sizes [9]. The Hall–Petch effect was observed, and the slope for compression is higher than that for tension. A similar phenomenon also has been observed by Wang et al. [10] in AZ31 magnesium alloys with various grain sizes prepared by equal channel angular pressing, conventional extrusion, and annealing. It also was observed that the Hall–Petch slope for compression is higher than the slope for tension. At a large grain size, there is a large gap between the yield strength of CYS and TYS, with CYS/TYS smaller than 1. This ratio increases with the decrease of grain size due to the higher Hall–Petch slope for compression.

Generally, the effect of grain size on the mechanical properties of magnesium alloys are attributed to different deformation mechanisms activated during compression and tension testing. The activities of deformation mechanisms also are determined by grain size, texture, and temperature. A complete study regarding the effect of grain size on the deformation mechanism of tensile properties was performed by Jain et al. [11]. In the range of grain sizes they studied, from 13 to 140 μm, the experimental data did not reveal a strong influence of grain size on the relative activities of deformation mechanism. Strain anisotropy also does not change significantly with grain size in the experimental study. The Hall–Petch effect was observed for tensile flow stress, strengthening with the decrease of grain size when loaded along different direction. To simulate the mechanical behavior of magnesium alloys with different grain sizes, a viscoplastic self-consistent (VPSC) polycrystalline plasticity model was modified by introducing the Hall–Petch response to the critical resolved shear stress (CRSS) of the individual slip and twinning mechanisms. Simulation from the modified VPSC model demonstrated that Hall–Petch dependence of the prismatic slip mechanism has a dominant effect on the effective deformation behavior.

A complete study on compressive deformation behavior of magnesium alloys with different grain sizes was performed by Barnett et al. [12]. The influence of temperature on the deformation behavior and deformation mechanism activated also is investigated. From the grain size point of view, twinning dominated deformation at large grain sizes, and slip dominated the deformation at small grain sizes. In regard of temperature, twinning dominated at low temperature, and slips dominated at high temperature. Samples with grain size varying between 3 and 23 μm are studied. When compared with Jain's study on tensile properties, grain size has no significant influence in the deformation mechanism in tensile. On the other side, Barnett's study demonstrated significant influence of grain size on the deformation mechanism in compression. The transition was observed only at the small grain size. An empirical model was derived for Hall–Petch curves in slip and twinning dominated deformation scenarios. Slope for twinning dominated flow is much higher than the slope for slip dominated flow.

Deformation mechanisms activated by mechanical deformation may be modeled using the polycrystalline plasticity model. From experimental observation, deformation mechanisms activated in magnesium alloys during deformation include the basal, prismatic, and pyramidal slip systems and twinning systems. The first- and the second-order pyramidal $\langle c + a \rangle$ slip systems occur mainly at high temperature and were held responsible for the good elevated temperature ductility of HCP metals, such as magnesium alloys. The $\langle a \rangle$ slip systems comprise only four independent slip systems and, thus, cannot accommodate plastic deformation in the crystallographic c direction of the single crystal. The basal $\langle a \rangle$ and the prismatic $\langle a \rangle$ planes are mutually orthogonal. However, because the $\langle 11\bar{2}0 \rangle$ slip directions are perpendicular to the c-axis and confined to the basal plane, there are only two independent slip systems of each type. As such, basal $\langle a \rangle$ and prismatic $\langle a \rangle$ slips together possess only four independent slip systems. To accommodate more deformation, twinning usually is activated at low temperature. Therefore, HCP metals often are nearly inextensible along their c-axis. If activated, pyramidal $\langle c + a \rangle$ systems will provide the additional fifth independent slip system necessary for the accommodation of an arbitrary plastic deformation. However, the slip resistance of pyramidal $\langle c + a \rangle$ slip systems usually are much higher than those of basal and prismatic systems. Even when five independent slip systems are available, the difference of the CRSS between different deformation mechanisms (basal, prismatic, and $\langle c + a \rangle$ pyramidal) can be large enough to introduce an important plastic anisotropy at the single crystal level. Therefore, the mechanical behavior of HCP metals is controlled by the relative strengths and substantially different hardening responses of the various slip modes [13].

It is well known that in addition to crystallographic slip from dislocation movement, HCP materials exhibit a greater tendency to mechanically twin than cubic materials. In the absence of pyramidal $\langle c + a \rangle$ slip, twinning may supplement the $\langle a \rangle$ slip for full kinematic freedom. Twinning provides additional deformation, which relaxes the requirements for five independents slip modes and may help a material to satisfy the Taylor criterion [14,15]. However, as a polar mechanism [14], twinning depends strongly on temperature, alloying content, stacking fault energy, and crystal lattice structure, which complicates modeling of the interaction between slip and twinning [16]. At low temperature, twinning will compete with slip to accommodate the crystal motion. However, in warmer processing regimes, twinning may become a less favorable deformation mechanism than slip.

In this study, we will first apply validate intermediate ϕ-model in simulation of magnesium alloys then use the ϕ-model to predict the yield asymmetry of magnesium alloys with different texture and grain size under varied loading conditions. The routes to achieve the desired yield asymmetry through thermomechanical processing and grain refinement are identified. This process demonstrates how to use integrated computational materials