

Targeted Mg–Y–Zn Alloy Design Based on Revised LPSO Phase Compositions and Equilibria

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Keyword

ICME • Magnesium • Thermodynamics • LPSO • HAADF-STEM

Extended Abstract

The properties of Mg alloys may be significantly enhanced due to the formation of long-period stacking ordered (LPSO) phases. The Mg–Y–Zn alloy system is most important since different LPSO structures (14H, 18R, and 10H) together with other intermetallics may be formed in such complex Mg-rich alloys. The precise knowledge of phase equilibria and transformations in MgY–Zn alloys is indispensable for targeted alloy design. The experiments and the first-principle calculations on LPSO phases including 14H and 18R in the Mg–RE–Zn systems by Egusa and Abe [1] have proved that RE and Zn atoms are confined into a cage-like cluster where the ideal stoichiometric atomic ratio of Y/Zn was 4/3 according to the crystallographic lattice sites. This ratio of Y/Zn = 4/3 was confirmed, also for 10H, in a later study by Schmid-Fetzer et al. [2], presenting also a revised thermo-

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dynamic description of the phase diagram, superseding the earlier work by Gröbner et al. [3]. The novel LPSO phase 10H was found in the as-cast samples by Yamasaki et al. [4] while the conditions under which it is thermodynamically stable remained unclear. In all currently available thermodynamic descriptions and calculated ternary phase equilibria, all of the LPSO phases are treated as stoichiometric compounds, including the recent work describing 14H, 18R, and 10H [2].

This work demonstrates that significant solid solubilities should be considered for the LPSO phase compositions and also that 10H is a thermodynamically stable phase at least from 400 to 500 °C. This changes the phase equilibrium relations in the Mg-rich corner significantly. The present experimental work on Mg-rich alloys annealed at 400 and 500 °C comprises dedicated characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM) with energy dispersive spectrometry (EDS), transmission electron microscopy (TEM), and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) for microstructure and phase analyses. Validated phase diagrams at these temperatures are constructed by Ruan et al. [5], where more details can be found. Figure 1a shows the isothermal section in the Mg-rich corner of the Mg-Y-Zn system at 500 °C. The revised composition ranges with significant solid solution of the 18R and 14H phases and corresponding phase equilibria are developed from our critical assessment of the entirety of experimental data including the present work and literature data.

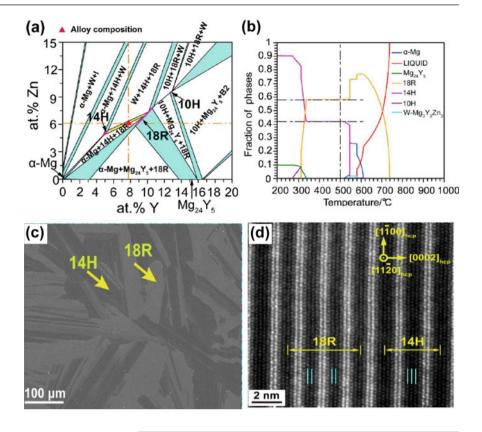
Based on that knowledge and thermodynamic Mg–Y–Zn phase diagram calculations the alloy composition and the heat-treatment temperature of a $Mg_{86}Y_8Zn_6$ (at.%) alloy with sole LPSO structures 18R and 14H were successfully tailored. In earlier studies that was only achieved by directional solidification processing at solidification rates of 30 or 10 mm/h but not by conventional casting technique. That is due to brittle phases such as W-Mg₃Y₂Zn₃ and Mg₂₄Y₅

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Fig. 1 a Isothermal section of the Mg-rich Mg–Y–Zn phase diagram at 500 °C with the Mg₈₆Y₈Zn₆ alloy composition marked; **b** Calculated equilibrium molar phase fractions of this alloy; **c** SEM image with sole LPSO structures 18R and 14H of this alloy; **d** HAADF-STEM image taken from the phase boundary of 18R and 14H in Fig. 1c



which inevitably crystallize during casting. Figure 1b shows the presently calculated variation of equilibrium molar fraction of the constituent phases of this alloy from the liquidus temperature down to 200 °C. It indicates the two-phase equilibrium 18R + 14H for this alloy from somewhat above 500 °C (dashed line) down to at least 400 ° C. Indeed, after annealing at 500 °C for 240 h, the microstructure of the as-cast Mg₈₆Y₈Zn₆ alloy composed of a-Mg, W-Mg₃Y₂Zn₃, 18R and 14H was thoroughly transformed to that solely composed of 18R and 14H. This is demonstrated in Fig. 1c, the SEM image with sole LPSO structures and in detail in Fig. 1d, the HAADF-STEM image taken from the phase boundary of 18R and 14H with the electron beam parallel to [11-20]hcp. A narrow composition and temperature window to avoid adverse phases is indicated by the present work, and more details are given by Ruan et al. [6]. The validated thermodynamic calculations of the phase diagram are key to this targeted MgH-Y-Zn alloy design.

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