Determination of a Unique Long-period Ordered Structure in a Mg$_{97}$Zn$_1$Er$_2$ Alloy by Aberration-corrected STEM

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Mg alloys containing a small amount of Zn and Y, e.g., Mg-1at.%Zn-2at.%Y (denoted as Mg$_{97}$Zn$_1$Y$_2$ hereafter), reveal excellent mechanical properties with high yield strength ~600Mpa and elongation ~5% at room temperature. One of the remarkable microstructural features is formation of a novel type of long-period ordered (LPO) structures [1]. They are unique structures, as being long-period chemical-ordered as well as stacking-ordered; their long-period stacking polytypes are denoted as 18R, 14H, 10H, 24R, all of which are composed of a common structural unit represented by local ABCA stacking where B- and C-layers are significantly enriched by Zn and Y (these particular layers are denoted as B’- and C’-layers hereafter). These long-period ordered (LPO) structures were firstly identified in Mg-Zn-Y alloys, but at present the LPO phases have been found in several Mg-Zn-RE (RE: Rare Earth = Dy, Ho, Er, Tm, Gd, Tb) alloys [2]. Looking carefully the electron diffraction patterns taken along the stacking direction (c-axis), we find many weak satellite spots that suggest a further ordering within the B’- and C’-layers. In the present work, we investigate the detailed chemical order in the LPO Mg-Zn-RE phases, using aberration-corrected ultrahigh-resolution STEM. We have chosen a 14H-type LPO phase in the Mg$_{97}$Zn$_1$Er$_2$ alloy [3] because of two major reasons; i) the atomic arrangement of the close-packed planes can be successfully imaged for the H-types structure (note that an electron incidence along [0001] cannot be a zone-axis illumination for the R-type (rhombohedral) lattice), and ii) Er is a large Z element (Z=68) so that individual Er atoms can be detected by Z-contrast, even they are embedded in the complicated structure.

Cs-correction effects appear to be quite significant for direct imaging of the close-packed atomic structures, as clearly demonstrated in Fig. 1. After Cs-correction, T$_2$T$_0$ reflections can be reproduced in the FFT pattern. Extra weak spots are also reproduced, which indicate the six-times long-period modulation along $<T_2T_0>_{\alpha}$, within the close-packed B’- and C’-layers. Since the Z-contrast provides enhanced chemical potentials, it can be directly deduced that the long-range modulation is predominantly due to a concentration modulation along $<T_2T_0>_{\alpha}$. To investigate its average features, we construct auto-correlation map from the Cs-corrected image, and the result is shown in Fig. 2. Average modulated structure can be derived from the map, including the short-range Er configurations that should be related to the most intense site in the auto-correlation map. Accordingly, Er-Er distance is found to be at the second-nearest sites, which are attributed to a D0$_{19}$-type short-range configuration and in fact frequently observed in the Z-contrast image. By referring further details of the intensity distributions, we constructed an average model of the complex long-range modulated structure, as shown in Fig. 3.
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References

Fig. 1 Atomic-resolution Z-contrast images taken along [0001] axis of the 14H-Mg$_9$Zn$_1$Er$_2$, obtained with non-Cs-corrected (left; JEOL-2010F, Cs=0.5mm) and Cs-corrected (right; JEOL-ARM200) STEM.

Fig. 2 Auto-correlation map reconstructed from the Cs-corrected Z-contrast STEM image in Fig. 1.

Fig. 3 Average model of the modulated structure, where the composition equivalent sites are represented by $\alpha$, $\beta$ and $\gamma$. 