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Oligomers of the left-handed Z-DNA diffract X-rays to the highest resolution among all crystal forms of DNA. We present the crystal structure of a Z-DNA hexamer duplex d(CGCGCG)₂ determined at ultrahigh resolution of 0.55 Å. The structure has been refined to R = 6.77% in the full-matrix anisotropic mode with total absence of stereochemical restraints for DNA, according to the practice of small-molecule crystallography. This way led to very accurate, unbiased values of atomic coordinates and displacement parameters, accompanied by reliable estimates of their standard uncertainties. In consequence, we are able to present a detailed analysis of very fine features of the Z-DNA stereochemistry, not available in the existing literature. Detailed comparisons of the stereochemical library values with the present accurate Z-DNA parameters, shows in general a good agreement, but also reveals significant discrepancies in the description of guanine-sugar valence angles and in the geometry of the phosphate groups.

It should be noted that the crystal structure presented here has a nearly record-breaking resolution in the PDB, where it is surpassed only by crambin (1EJG and 3NIR) determined at 0.54 and 0.48 Å resolution. In the area of nucleic acids, it is currently the highest-resolution model.

Keywords: Z-DNA, ultra-high resolution

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Direct Determination of Long-period Stacking/Ordered Structures in Mg₈₁Zn₈RE₁₁

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Mg alloys containing a small amount of Zn and Y, e.g., Mg-1at.%Zn-2at.%Y alloy, 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 stacking/ordered (LPSO) structure [1], which is long-period chemical-ordered as well as stacking-ordered. There are long-period stacking polytypes denoted as 18R, 14H, 10H, 24R, (Fig.1) 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 LPSO structures were firstly identified in Mg-Zn-Y alloys, but at present the LPSO 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 LPSO Mg-Zn-RE phases, using aberration-corrected scanning transmission electron microscopy (STEM). Since the reported compositions of the LPSO phases were different by the nominal compositions of the alloys, we considered that the chemical order in the LPSO phases also changes by them. Therefore we have chosen LPSO phases in the Mg₉₇Zn₁Y₂ alloy, the Mg₉₇Zn₁Er₂ alloy and the Mg₈₅Zn₆Y₉ alloy.

Using the technique of electron diffraction and direct observation by STEM, we determined the chemical order in the LPSO phases. The chemical order was formed by 6-times periodic structures within the

basal planes. From the results of direct observations, we found that there were clusters of additional elements which have ordered configurations similar to a L₁2-type structure. 6-times periodic structures within basal planes were composed by the periodic arrangements of these clusters. The difference of the nominal compositions of the alloys did not affect the configuration of the cluster, however the densities of clusters in the basal planes were seem to be changed by the nominal compositions. Finally, we constructed averaged models of the LPSO phases from the experimental results. The validity of the model was confirmed by simulations of electron diffraction and STEM image.

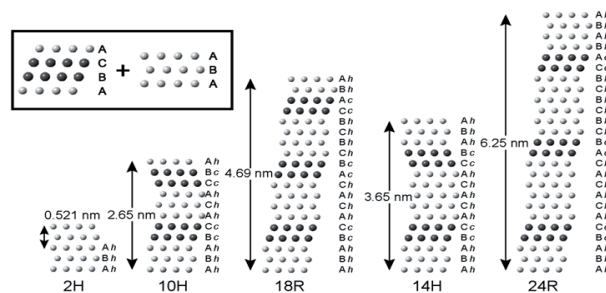


Fig. 1 Stacking polytypes of LPSO phases

[1] E. Abe, Y. Kawamura, K. Hayashi, A. Inoue, *Acta Materialia* **2002**, *50*, 3845-3857. [2] Y. Kawamura, M. Yamasaki *Materials Transactions* **2007**, *48*, 2986-2992.

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A Method to Determine the 3D Morphology and Crystallography of Nanoparticles

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Nanocrystals have unique properties which are different from the bulk material and strongly dependent on their morphology and crystallography. Characterising the morphology and crystallography is important for understanding the relationship between shape and properties and for determining the mechanism controlling nanocrystal growth.

In this paper we describe a rapid method to measure the thickness profile of a nanoparticle from a single annular dark field scanning transmission electron microscope (ADF-STEM) image [1]. This method deliberately uses ADF-STEM images just below lattice resolution, to enable relatively fast image quantification and measurement but at the expense of spatial resolution. Our focus here is on speed, to provide scientists working on nanocrystals a route to make a meaningful statistical comparison of the shape and properties of a large number of particles in a practical timeframe.

We have applied this

