Poster

Long period stacking ordered (LPSO) Y-Ni-Mg phases studied by 3D electron diffraction

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Long period stacking ordered (LPSO) phases represent a hot topic in the Mg-based alloys research. Despite numerous efforts[1,2], the structural characterization of these intermetallics cannot be yet considered fully satisfactory due both to their intrinsic structural complexity and to several unavoidable experimental difficulties. In this work we present the results of a combined 3D-ED/XRD study, by which the complete crystal structures of three Y-Ni-Mg LPSO phases were obtained and elucidated for the first time: $(Mg@Y_8Ni_6)Mg_{18}$, *tI*66-$Nd_{8+x}Ru_6Mg_{19-x}$, $(Mg@Y_8Ni_6)_{16}Mg_{505}$ and $(Mg@Y_8Ni_6)_3Mg_{154}$. Two thin (<100 nm) lamellae of the latter two phases were extracted by FIB-SEM, and further characterized by a TEM equipped with a single electron ASITIMEPIX detector: 3D-ED data were collected with a parallel beam, either in continuous or precession-assisted stepwise mode[3]. Both phases are modulated structures described in 6D and 5D superspaces, respectively. In the commensurate approximation, the average models are *oF*2980-$(Mg@Y_8Ni_6)_{16}Mg_{505}$ (SG *Fmm*2) and *hR*1194-$(Mg@Y_8Ni_6)_3Mg_{154}$ (SG *R*-3*c*), characterized by giant unit cells.
The structural analysis of these compounds resulted in a generalized description of Y-Ni-Mg LPSO phases in terms of $Mg@Y_8Ni_6$ clusters more or less densely distributed in a Mg matrix, justifying the proposed formulas. An LPSO classification based on the layers stacking modes is proposed, leading to *fcc* (*c*-type) and hybrid *fcc/hcp* ($(h)_ncc$-type) subfamilies, the former being identified in this work (see figure).

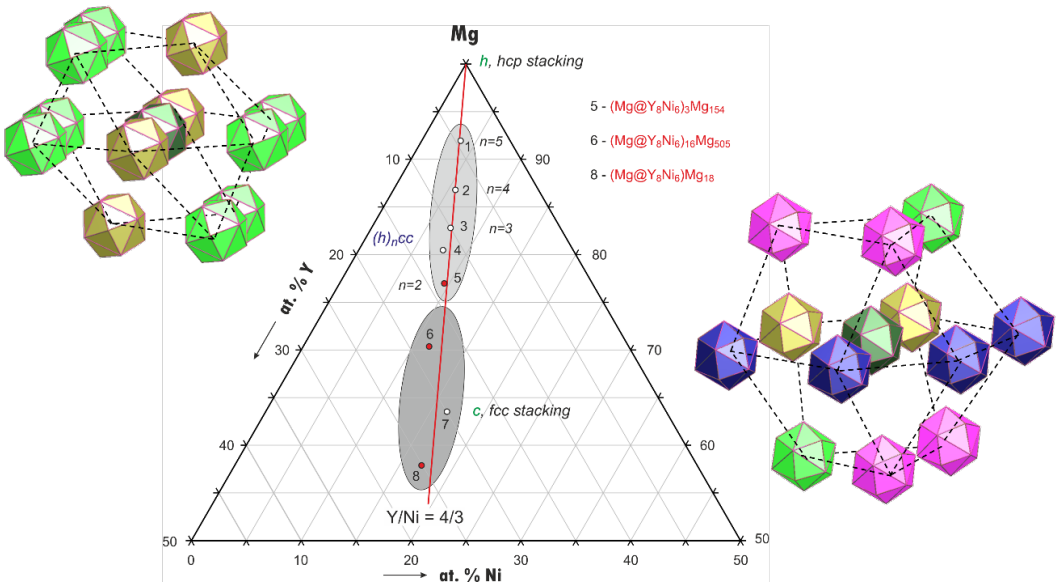

Figure. Gibbs triangle showing the Y-Ni-Mg LPSO phases distributed between two sub-families according to the topology of the layer stacking. First sphere coordination of clusters in LPSO-8 and LPSO-5 deriving from their fcc and hcp packing are shown as well.

The inter-clusters coordination in form of distorted anticuboctahedra or cuboctahedra is characteristic of members of the two families. Increasing the magnesium content, the ratio between Mg and the Mg@Y8Ni6 units increases: despite the general dilution, clusters are positioned in form of aggregates at similar inter-cluster distances (around 9, 12 and 13 Å), the distribution of which is at the origin of structural modulation.

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[3] Gemmi, M., Mugnaioli, E., Gorelik, T., Kolb, U., Palatinus, L., Boullay, P., Hovmöller, S., Abrahams, J.P. (2019) ACS Cent. Sci. 5, 1315.