MS14-P04

Atomic displacements in yttrium-manganese-oxide with and without fe-substitution, revealed by resonant X-ray diffraction

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Yttrium-Manganese-Oxide YMn_2O_5 (YMO) is studied since 1973 due to its remarkable magnetic properties, e. g. different modulation phenomena and several respective phase transitions. The ambient temperature phase of YMO is paraelectric and paramagnetic. The lattice has the orthorhombic space group *Pbam* (55) and its building units are $[MnO_5]$ pyramides and $[MnO_6]$ octahedra, the latter forming chains along the *c* direction. At 45 K, 40 K, 39 K and 19 K, the structure changes between several magnetic modulations [1]. Here, we are interested in the commensurate modulated phase between 39 K and 19 K. Presumably within space group $Pb2_1m$ (26), the respective lattice modulation vector is 0 0 ½, whereas the polarization points along *b*. However, crystal structure refinements in a non-centrosymmetric space group showing polar displacements have not yet been successful. Moreover, there is still disagreement about the interplay of magnetic superstructure and a polar displacement pattern. To analyze possible displacements of the commensurate phase in detail, we apply the newly developed and highly sensitive Resonant X-ray Diffraction (RXD) Method *REXSuppress* that uses destructive interference of the intensity at carefully chosen Bragg reflections [2]. For this structure analysis, we determined atomic displacement parameters (ADP) of the high and low temperature phase with the same method and surveyed the appearance of superstructure reflections that would accompany the transition to space group $Pb2_1m$ (26).

Additionally, we examined the distribution of Fe in Yttrium-Manganese-Iron-Oxide ($YMnFeO_5$), which results from the substitution of 50% Mn. The element- and site-selectivity of RXD is capable of separating the two distinct Mn Wyckoff sites (pyramide and octahedron), in particular with the octahedral site possessing forbidden reflections (reflection condition hkl with $h + k = 2n$). Thus, the question of occupation is easily accessible and will be treated similar as by [3].

References:

[1] Y. Noda et al., J. Phys.: Condens. Mat. 20 434206 (2008).
[2] C. Richter et al., Nat. Commun. 9(1) 178 (2018).
[3] F. Winderlich et al., Phys. Rev. B 82(1) 014409 (2010).

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MS15- Crystallography in Earth and space

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MS15-P01

Evidence of screw dislocation on gypsum crystals as principal mechanism of growth at low supersaturation

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Gypsum mineral mainly occurs on evaporitic environment around the world [1, 2]. It has also been reported as a relevant phase in Mars [3-5]. The growth conditions during the growth of gypsum crystals influences the surface growth mechanisms and the habit. Many authors suggest that the growth mechanisms of gypsum crystals at low supersaturation is due to dislocation growth, these studies are based on kinetic data fitted to theoretical equations[6, 7]. However, the observation of hillocks on the surface gypsum crystals has been challenging. A couple of studies on the cleavage face (010) of gypsum by Atomic Force Microscopy (AFM) and Differential Interface Contrast Microscopy (DICM) shown some hillock but only one of them could be clearly identified as a screw dislocation, so the authors conclude that the main growth mechanism at low supersturation on this face is by 2D nucleation[8, 9]. Equivalent studies on the (120) face are missing, mainly due to the roughness of these faces. In a preliminary study of the gypsum (120) face using crystals growing by evaporation, we observed that hillocks spread on (120) at low supersaturation. Those hillocks are made by monolayers with a height of 4.30 Å corresponding to the d-spacing. These hillocks show an asymmetric morphology (figure 1).