Neutron Powder Diffraction Experiments on multiferroic $DyMnO_3$

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Multiferroic materials of particular interest are the frustrated magnetic compounds that exhibit a strongly coupled electric polarization (EP) [1]. One such compound is $DyMnO_3$ which exists in an orthorhombic (o-DMO) and hexagonal modification depending on the synthesis conditions [2]. In the present work the o-DMO is investigated by means of neutron powder diffraction focusing on the magnetic phase transitions and the behavior of the structural parameters in different magnetic and multiferroic phases. Below $T_{N,Mn}$ =39 K, the Mn moments order sinusoidally with no EP. Then T_l=16 K the Mn moments order in a spin spiral structure with an induced Dy moment and EP and finally below $T_{N,Dy}$=9 K a collinear ordering of the Dy moments takes place that reduces the EP significantly [2]. Single phase samples are prepared via the solid state route and neutron diffraction (ND) experiments are carried out at the high flux ND beamline Wombat and at the high resolution ND beamline Echidna at OPAL. O-DMO crystallizes in the space group *Pbnm*. All three magnetic phase transitions are identified and are in good agreement with [2]. Below $T_{N,Mn}$ an increased rotation of the rigid MnO6 octahedra in the ab plane, likely due to the competition between nearest neighbour and next nearest neighbour superexchange interactions takes place. However below T_l the MnO_6 octahedra are significantly distorted along the c axis, the direction of the EP. Therefore the correlation between significant changes in the Mn-O bonds and the spontaneous EP are evident below T_l. The reduction of EP below $T_{N,Dy}$ on the other hand correlates with the rapid increase in the orbital ordering angle towards the 120° corresponding to the $3x^2-r^2/\ 3y^2-r^2$ character of the orbitals.

[1] Y. Tokura and S. Seki, Adv. Mater. 22, 1554 (2010).
[2] S. Harikrishnan et al., J. Phys: Condens. Mater 21, 096002 (2009).