Structure of ferroelectric low temperature phase of yttrium manganate YMn_2O_5 revisited

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The material system YMn_2O_5 has several low temperatures phases, where magnetism and ferroelectricity occur. Especially, the origin of the ferroelectricity (FE) in a phase below T_{FE} = 39 K is an open question. The Literature agrees upon a magnetically driven principal mechanism from changes in the Mn spin configuration, which may be based either on magnetostriction due to symmetric exchange, the antisymmetric inverse Dzyaloshinskii-Moriya interaction or a combination of the two. Both mechanisms are accompanied by specific atomic displacements of ions in the structure. The space group Pbam (55) of the paraelectric phase does not allow the respective polar displacements and a refinement of the charge structure in a lower symmetric phase has not been successful so far, as the applied conventional structure analysis methods lack the required spatial resolution for the expected positional deviations.

We apply the new *Resonantly Suppressed Diffraction* (RSD)[3] method, which is sensitive to minuscule structural changes in the sub-pm range, to shed new light on this controversial discussion. RSD is a structural characterization method in the field of Resonant Elastic X-ray Scattering and tunes the photon energy such that certain reflections approach zero due to destructive interference.

Here, we employ RSD on carefully chosen Bragg reflections below and above T_{fE}. With the data above T_{FE} we refined the static and dynamic displacements of the paraelectric phase, to receive an improved starting model for the structural characterization of the FE phase. With this starting model we were able to characterize the FE phase and consolidating the findings about the origin of ferroelectricity in YMO.

[1] Richter, C., Zschornak, M., Novikov, D. V., Mehner, E., Nentwich, M., Hanzig, J., Gorfman,S. & Meyer, D. C. Nature Communications, 9, 178 (2018).

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