MS14 Combined approaches for structure characterization of modulated and complex structures

Chairs: Prof. Joke Hadermann, Dr. Phillipe Boullay

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Investigation of the structure of the modulated doubly ordered perovskite $NaLaCoWO_6$ and its reversible phase transition with a colossal temperature hysteresis

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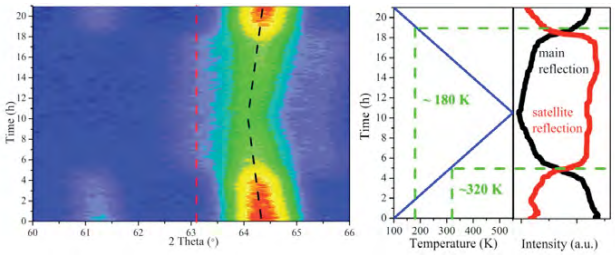
Magneto-electric multiferroics are drawing considerable research interests not only for the variety of attractive fundamental phenomena but also for potential technological applications such as energy efficient memory devices and multiple state memories. To overcome the shortcomings of known multiferroics, a new approach to inducing spontaneous ferroelectric polarization by a combination of two non-polar rotation modes of the oxygen octahedra in magnetic materials was proposed. This so called "Hybrid Improper Ferroelectricity (HIF)"[1] could lead to materials exhibiting high polar fields and a strong coupling with magnetism, making them promising for applications. In the framework of research for more materials displaying HIF experimentally, we have investigated $NaLnCoWO_6$ compounds with Ln= lanthanides.[2] Synchrotron X-ray powder diffraction and neutron powder diffraction have shown that all compounds have layered Na/Ln ordering and rock-salt Co/W ordering, and nine compounds (Ln = Y, Sm-Yb) crystallize in the polar $P2_1$ space group. The structure is indeed the targeted one of a doubly ordered perovskite. The compound $NaLaCoWO_6$ shows however an unusual behavior. At room temperature, transmission electron microscopy evidences a modulated structure that can be attributed to tilt twinning domains of oxygen octahedra. The modulation disappears at a phase transition at low temperature, where the local structure changes symmetry from the $P2_1/m$ to the polar $P2_1$ space group. Neutron powder diffraction reveals, and electron diffraction confirms, an unusually large temperature hysteresis, where the transition takes place at ~180 K on cooling and at ~320 K on heating. The origin of this unusually large hysteresis (140K) will be discussed, in particular the role of the oxygen octahedra tilting modes[3].



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