MS28-05 | Unraveling Local Correlations in Heavily Disordered Ferroelectric $Sr_xBa_{1-x}Nb_2O_6$

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When it comes to structural complexity, $Sr_xBa_{1-x}Nb_2O_6$ has it all. There is occupational disorder of Sr and Ba cations with additional vacant positions in the unfilled tetragonal tungsten bronze structure. Dynamical chains of relative Nb-O_6 displacements are present at high temperatures and gain transverse correlation when going through the ferroelectric phase transition to form domains. Whether the transition is 'normal' or 'diffuse' depends on the Sr content with the latter appearing for $x \geq 0.6$. On the top of that there is an incommensurate modulation which mainly involves rotations of oxygen octahedra; their amplitude being again dependent on the Sr/Ba ratio. This abundance of local disruptions to the long range order is reflected in the reciprocal space being very richly populated with diffuse scattering.

In this work we combine neutron pair distribution function [1] and X-ray diffuse scattering analysis [2] – both for the range of concentrations and temperatures – with multi-scale simulations. First-principles molecular dynamics is used for the understanding of the structure and its dynamics at short distances and provides a basis for atomistic model development. This in turn is instrumental in 3D diffuse scattering analysis. All this information allows us to explore the interrelation between the mentioned local-structure modes and their contribution to the diffuse transition characterized by large dielectric susceptibility over a broad range of temperatures.

[1] M. Paściak et al., *Phys. Rev. B*. **99**, 104102 (2019).
[2] M. Paściak et al., *Phase Transitions* **91**, 969 (2018).