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Diffuse scattering and local polar correlations in ferroelectric materials

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Modern ferroelectric materials (e.g. PbMg1/3Nb2/3O3 - PbTiO3) are often based on ternary and quaternary oxides where disorder constitutes a groundwork for exceptional electromechanical properties. While the basic role of the inhomogeneity (strain and/or local electric field generated by occupational disorder locks and enhances the 'transition state' and thus electromechanical coupling) is widely accepted, precise description of mechanisms governing polar correlations is still lacking. In particular, indicating the role of ferroelectric soft phonon modes, their 'interaction' with inhomogeneous medium and relation to (quasi) static polar state at low temperatures constitutes an intriguing and fundamental problem [1,2]. Diffuse scattering analysis providing information about atomic to mesoscale correlations is a method of choice for studying of these phenomena; the fact that has been proven by an abundance of X-ray, neutron and electron diffraction results for ferroelectric materials in the recent years. At the same time, interpretation has been very often ambiguous, calling for better understanding of how the experimental data should be approached. We address some principal questions related to the diffuse scattering analysis of ferroelectric and related compounds. Can we gain some insight into the local structure treating data 'ab-initio', without assuming any model of polar correlations [3]? Can we separate static and dynamic contributions to the diffuse scattering (e.g. by calculating theoretical phonon-related thermal diffuse scattering)? The study is carried out using atomistic computational methods including reverse Monte Carlo, molecular dynamics and density functional theory based calculations.

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