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Understanding Ferroelectricity in Nanometric Sodium Niobate by Differential Phase Contrast

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The polarization present in ferroelectric nanostructured materials can be identified and measured using the technique of Differential Phase Contrast (DPC) [1–3]. Although a direct correlation between the produced DPC contrast and the ferroelectric field has been shown for thin samples, the analysis of the results is hindered for thick samples (> 5 nm) due to dynamical effects. The optimal conditions for the materials analysis depend on several parameters, including the sample structure, thickness, and tilt angle [4], and some studies suggest large sample tilts, as reported by Nakamura et al. [5] and Haas et al. [6]. As a result, in this study, we explore a perovskite material, NaNbO3 (NN), by DPC simulation to identify the optimal tilt angle of the sample from the zone axis, to reduce dynamical effects, and allow the direct correlation between the deflection of the beam and the inherent electromagnetic field of the sample.

DPC images were simulated by a multislice method using Dr. Probe software [7], using NN orthorhombic structure model (s.g.: P21ma) (ICSD code 39624), an acceleration voltage of 200kV, and the microscope parameters reported by Haas et al. (2019) [6]. The images were simulated along the most common zone axes found experimentally for this material, namely [100], [010], [001], for tilt angles between 0° and 9°, and maximum sample thickness of 200 nm. A four-quadrant annular segmented detector was used to calculate the DPC signal, which was used to determine the deflection of the electrons based on Lazić et al.[8].

The best conditions, to mitigate dynamical diffraction and analyze the ferroelectric field of NN, were selected based on the smallest fluctuations of the electron deflection and its magnitude. The NN structure showed optimal conditions for tilts of 6° in the x-direction and 9° in y-direction for the zone axes [100] and [001], and 9° (x-direction), and 3° (y-direction) were found for the zone axis [010] (Figure 1). Comparing the results for each zone axis is possible to observe that variations in thickness and crystal orientation within the nanostructure can promote variations in contrast (Figure 2), but under the optimal tilt condition, changes in thickness do not interfere significantly in the average modulus of electron deflection image contrast, which means a good correlation between contrast and the atomic electric field. These conditions could favor the observation of the ferroelectric field present in thick samples. In summary, the optimal conditions encountered in this study are dependent on the zone axis of the sodium niobate, while the simulations show DPC as a promising tool to help analyze ferroelectric fields in thicker nanomaterials.

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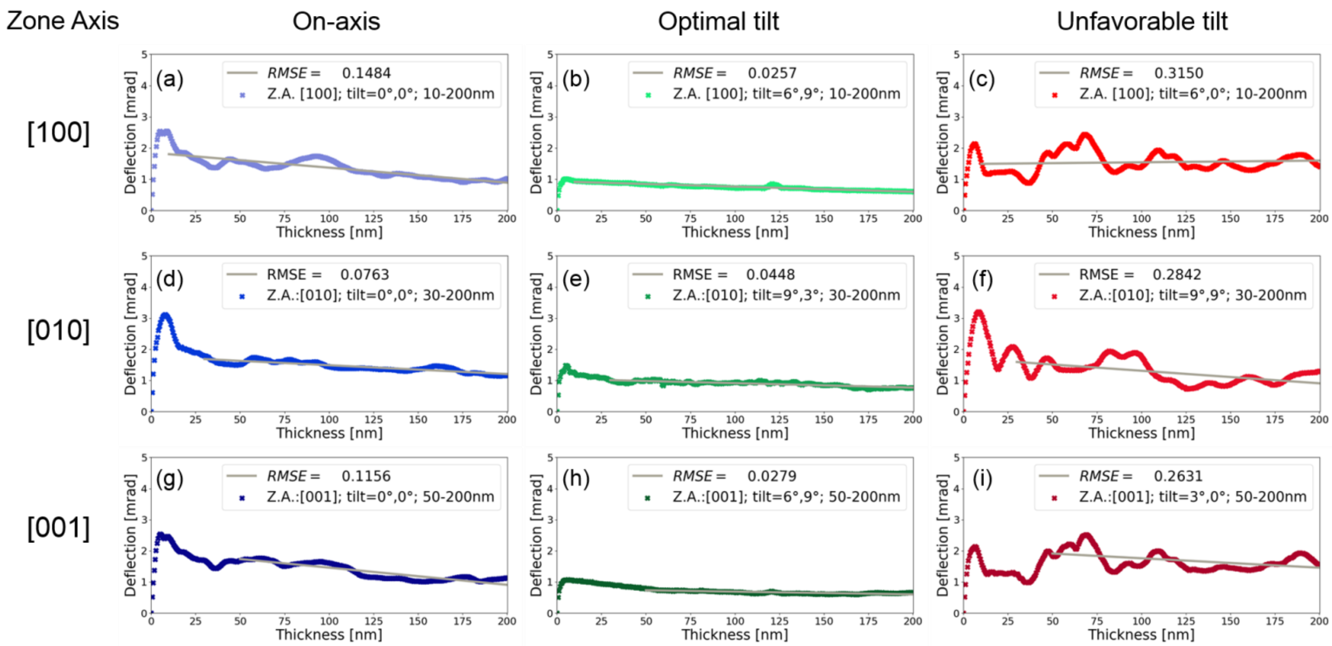

Figure 1. Graphs relating the average modulus of electron deflection per unit cell and NaNbO3 thickness, for each zone axis [100] (a-c), [010] (d-f), and [001] (g-i) for the conditions on-axis, optimal tilt result, and unfavorable tilt result.

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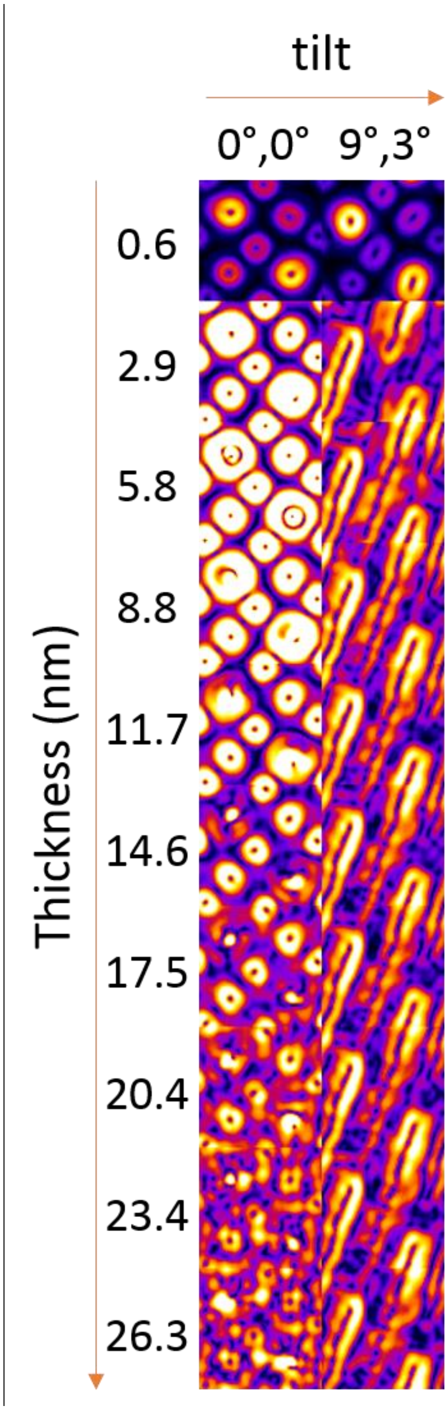

Figure 2. Images of the modulus of electron deflection with the increase of thickness, for two different tilt conditions at [010] zone axis of NaNbO3 (a) on-axis, (b) the optimal tilt condition 9° in the x-direction and 3° in the y-direction.

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