Optical Properties of Domain Walls in Periodically Poled $LiNbO_3$ and $LiTaO_3$ Studied by First-principle Calculation and Raman Spectroscopy

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The Raman spectra of Lithium niobate ($LiNbO_3$) and lithium tantalate ($LiTaO_3$) crystals have been found to be strongly affected by the presence of domain walls. Therefore, spatial mapping of Raman intensity and/or frequency of selected Raman bands can be used to visualize ferroelectric domain structures. Although this technique has been successfully employed in $LiNbO_3$, $LiTaO_3$ and other ferroelectrics, a microscopic understanding of the underlying contrast mechanism is yet missing. In this work, we approach this issue by comparing Confocal Raman spectroscopy data and density functional theory calculations [1]. Thereby we employ a simplified domain wall model, which takes into account that domain walls in $LiNbO_3$ and $LiTaO_3$ are accompanied by large strain and electric fields [2]. Based on this model we calculate Raman shifts, intensities and other properties of domain walls from first principles, and compare them with the experimental data.

[1] S. Sanna, et. al., Phys. Rev. B, **91**, 224302 (2015)
[2] V. Gopalan, et. al., Annu. Rev. Mater. Res., **37**, 449-489 (2007)