

The MPB of BNT-xBT from the Titanium NMR Point of View

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The structural features responsible for the enhanced properties at the Morphotropic Phase Boundary (MPB) of $(100-x)(\text{Bi}_{1/2}\text{Na}_{1/2})\text{TiO}_3-x\text{BaTiO}_3$ (BNT-xBT) around ~6BT are still unclear. If this MPB is analogous to that of PZT, rhombohedral and tetragonal displacements of the B-site cation should coexist. Contrastingly, if the chemical modification with barium mainly influences the structure of BNT by changing the tilting of octahedra, the local structure around the titanium nuclei is expected to remain invariant throughout the different regions of the phase diagram. In order to achieve a deeper understanding on this matter, we employed a unique technique sensitive to the local structure, namely, solid-state nuclear magnetic resonance (NMR) spectroscopy.^[1,2,3]

The present contribution reports on how the addition of barium to BNT impacts the local structure of the titanium site.^[3] We analyze $^{47,49}\text{Ti}$ NMR spectra of BNT-xBT with $x=0, 6, 15$, as these compositions are representative of the rhombohedral, MPB and tetragonal regions from the phase diagram of this solid-solution. The comparison between their $^{47,49}\text{Ti}$ NMR spectra demonstrates that the local structure of the B-site does not change significantly as a function of barium content in these perovskites. This result supports the hypothesis that the main structural changes across the MPB in BNT-xBT are constrained to the A-site and are related to the tilting of rigid oxygen octahedra.^[2]

[1] P.B. Groszewicz, et al., *Phys.Rev.B* **90**, 220104 (R)(2014)

[2] P.B. Groszewicz, et al., *Sci. Rep.*, **6**, 31739 (2016)

[3] P.B. Groszewicz, et al., *JAP*, submitted (2017)