

Structural evolution and electrical properties in the $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ - $\text{Na}_{0.5}\text{Bi}_{0.5}\text{ZrO}_3$ (NBT - NBZ) and $\text{K}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ - $\text{K}_{0.5}\text{Bi}_{0.5}\text{ZrO}_3$ (KBT - KBZ) solid solutions

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The perovskite compounds ABO_3 are one of the most common oxide structures and thus have been extensively studied. Indeed, they present a very large panel of interesting physical properties (ferroelectricity, piezoelectricity, superconductivity ...). Concerning piezoelectric properties, the industrially-used compounds mainly belongs to the PZT family ($\text{PbZr}_{(1-x)}\text{Ti}_x\text{O}_3$), because of their unequalled properties. Considering the restrictions on the use of hazardous substances, lead-based materials are now only tolerated for piezoelectric devices. Among the available ferroelectric lead-free materials, Bi-based compounds such as $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT, space group R3c) and $\text{K}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (KBT, space group P4mm) present interesting dielectric and ferroelectric - piezoelectric properties. As for PZT, such properties can be modulated by binary or ternary solid-solution formation (NBT-KBT, NBT-BaTiO₃, NBT-PbZrO₃, NBT-BiScO₃, NBT-BiFeO₃ ...). Some of them improve the piezoelectric properties, while other one suppresses the ferroelectricity, inducing sometimes interesting dielectric properties and relaxor behavior. Thus, as for the PZT, the understanding of the relationships between structure and electrical properties is necessary, in order to be able to modulate and control the properties of these compounds.

Nowadays, most of the published studies devoted to KBT and NBT concern substitutions in the A-site of the perovskite lattice. But up to date, very few studies devoted to substitutions in B-site alone are available. Like for PZT, Zr^{4+} ion would logically replace Ti^{4+} in B-site. In order to test for this hypothesis, we selected the solid solutions: $\text{Na}_{0.5}\text{Bi}_{0.5}\text{Ti}_{1-x}\text{Zr}_x\text{O}_3$ and $\text{K}_{0.5}\text{Bi}_{0.5}\text{Ti}_{1-x}\text{Zr}_x\text{O}_3$. X-ray diffraction patterns revealed that these solid solutions are obtained, thus leading to the new perovskite compounds $\text{Na}_{0.5}\text{Bi}_{0.5}\text{ZrO}_3$ (NBZ) and $\text{K}_{0.5}\text{Bi}_{0.5}\text{ZrO}_3$ (KBZ), with pseudo-cubic symmetry. Their crystalline structure is presently under investigation. However, the mean pseudo-cubic lattice parameter increase with Zr^{4+} content, according to the ionic radii, and follows Vegard's law, confirming the formation of a solid solution. The structural distortion of NBT (rhombohedral) and KBT (tetragonal) decreases, in agreement with the tolerance factor. According to these results, piezoelectric properties were detected only close to NBT and KBT: thus the ferroelectric order is suppressed by this substitution. Finally, the dielectric properties were also studied. Close to NBT and KBT, the dielectric behaviour globally corresponds to the one of these compounds. For higher values of x, a relaxor behaviour is observed together with a decrease of the relative permittivity at the maximum of the curves, and with a flattening of these curves. These solid - solutions appear thus as very interesting in order to improve the understanding of the structure / properties relationships for the Bi-based perovskite compounds [1].

[1] M. Bengagi, F. Morini, M. El Maaoui and P. Marchet, *Phys. Status Solidi A* **209**, 2063 (2012).