



Figure 1. XRD Refinement for a) $\text{Ba}_2\text{CoTeO}_6$ and b) $\text{Ba}_2\text{NiTeO}_6$ made by FULLPROF program. Inset is 3D visualization program for structural models made by Vesta software.

Keywords: double perovskite, sol-gel synthesis, XRD refinement

MS16-P4 Phase transitions in relaxor ferroelectric materials with tungsten bronze type structures

Siegbert Schmid¹, Thomas A. Whittle¹

1. School of Chemistry, The University of Sydney, Sydney NSW 2006, Australia

email: siegbert.schmid@sydney.edu.au

Ferroelectric materials are essential for modern electronic applications, from consumer electronics to sophisticated technical instruments. Relaxor ferroelectric materials provide the advantage of high dielectric constants over broad temperature ranges not seen in traditional ferroelectrics. Tungsten bronze type compounds have been shown to display a variety of industrially relevant optical and electronic properties amongst others. There is a fundamental relationship between the physical properties displayed by ferroelectrics and the crystal structures in which they form. Of particular interest are compositions and temperatures near phase transition. These are important because near phase transitions, particularly morphotropic phase transitions, physical properties are often dramatically enhanced.^{1,2} This work focuses on the structural investigation of tungsten bronze type relaxor ferroelectric materials in the system $\text{Ba}_x\text{Sr}_{3-x}\text{Ti}_{1-y}\text{Zr}_y\text{Nb}_4\text{O}_{15}$ ($0 \leq x \leq 3$; $0 \leq y \leq 1$). A combination of X-ray, neutron (ToF and constant wavelength) and electron diffraction were employed to map the room temperature phase diagram. In addition, morphotropic phase boundary compositions were determined accurately. Variable temperature synchrotron X-ray diffraction studies were utilised to further explore the phase diagram for non-ambient conditions. Temperature dependent phase transitions were determined and the relationship between composition and transition temperature analysed. Structural models used in this work resulted from Rietveld refinements against powder diffraction data. This work will shed light on new lead free relaxor ferroelectric materials.

1. Ahart, M.; Somayazulu, M.; Cohen, R. E.; Ganesh, P.; Dera, P.; Mao, H.-k.; Hemley, R. J.; Ren, Y.; Liermann, P.; Wu, Z. *Nature* **2008**, *451*, 545.

2. Pandey, D.; Singh, A. K.; Baik, S. *Acta Crystallogr A* **2008**, *64*, 192.

Keywords: tungsten bronze type structures, phase transitions, relaxor ferroelectrics