11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Structural Characterization of $Sr_2NaNb_5O_{15}$ Nanostructured Powders

S. Lanfredi [(1)*], S. A. Dantas[(1)], C. Poline[(1)], A. R. F. Lima[(2)], M. A. L. Nobre[(1)]

(1) FCT, Universidade Estadual Paulista, Campus de Presidente Prudente, SP, Brazil, e-mail: silvania@fct.unesp.br
(2) UEPG, Departamento de Química – Universidade Estadual de Ponta Grossa, PR, Brazil
* Corresponding author.

Abstract – $Sr_2NaNb_5O_{15}$ nanopowders ferroelectric was synthesized by high energy ball milling. Crystalline nanopowders with average size equal to 21 nm were prepared by the precursor calcination at 1150 °C during several hours, in oxygen atmosphere. Structural characterization of $Sr_2NaNb_5O_{15}$ nanopowders was carried out by the X-ray diffraction. The profile of adjusting of the set of diffraction lines and refinement of the structural parameters were performed by the Rietveld method, using the FULLPROF program. From set of crystallographic parameters, graphical representation of the structure of the $Sr_2NaNb_5O_{15}$ was built- up using the CaRIne Crystallography 3.1® software.

Niobates exhibiting tetragonal tungsten bronze structure – TTB type present great interest scientific and technique-industrial as ferroelectric materials. The tetragonal tungsten bronze-type structure (TTB) can be considered as a derivative of the classical perovskite one. It can be described by the chemical formula $(A1)_2(A2)_4C_4Nb_{10}O_{30}$. *A1*, *A2*, and *C* denote different sites in the crystal structure. The *A1* cavities have a cuboctahedral coordination of oxygen atoms, the *A2* cavities a pentacapped pentagonal prismatic, and the *C* cavities a tricapped trigonal prismatic one. The size of these cavities decreases in the order *A2* > *A1*> *C.* Sodium strontium niobate, $Sr_2NaNb_5O_{15}$, was synthesized by high energy ball milling [1]. Crystalline nanopowders were obtained by the precursor calcination at 1150 °C during 10 hours, in oxygen atmosphere. The powder obtained from calcination of the precursor, in oxygen atmosphere, was characterized by X-ray diffraction (XRD). The diffraction pattern was refined, in according to the Rietveld method. The refinement was performed using the program Fullprof. From crystallographic parameters, determined in the refinement, the tridimensional representation of unitary cellule was constructed, using the CaRIne Crystallography 3.1® software [2]. The sites occupancy by the Na^+ and Sr^{2+} cations and the interatomic distances between niobium atoms were determined. Figure 1 shows the Rietveld graphic for the $Sr_2NaNb_5O_{15}$ obtained at 1150 °C for 10 h, in oxygen atmosphere, with the observed and calculated X-ray diffraction as well as their difference. The X-ray diffraction pattern obtained was indexed on the basis of a tetragonal unit cell. From observed reflections, there is only evidence of the rule existence [(*0 k l*) *k* = 2*n*], which is compatible with noncentric space group P4bm. Figure 2 shows the crystallographic structure of the $Sr_2NaNb_5O_{15}$ phase obtained with calcination at 1150 °C during 10 hours. The determination of sites in the structure of the $Sr_2NaNb_5O_{15}$ showed that all pentagonal sites are occupied by equal quantity of Sr^{2+} and Na^+ and all tetragonal sites are occupied only Sr^{2+} atoms. In an other hand, the trigonal sites are empty. It is due to the strontium (Sr^{2+}) and sodium (Na^+) ionic ray values, which are sufficiently large to occupy the trigonal site. The crystallographic structures obtained by $Sr_2NaNb_5O_{15}$ show that the calcination at 1150 °C improves a major structural stability, which can be explained by formation of octahedral arrange of NbO_6.

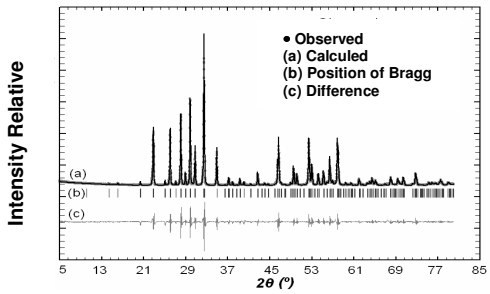

Figure 1: Rietveld graphic for $Sr_2NaNb_5O_{15}$.

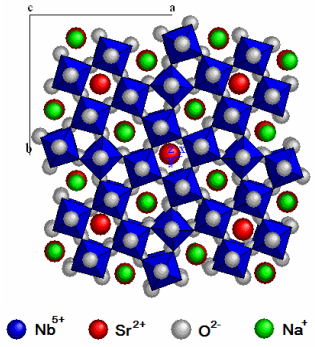

Figure 2: Representation of sites in TTB structure of the $Sr_2NaNb_5O_{15}$.

References

[1] S. Lanfredi, L. R. Trindade, A. R. Barros, N. R. Feitosa, M. A. L. Nobre, Cerâmica 51 (2005) 151.
[2] C.Boudais, D. Monceau, *CaRIne Crystallography 3.1*$^{(R)}$, France, **1998**.