11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Energy Gap Evolution in a ferroelectric oxide belonging to the tetragonal tungsten bronze family

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Abstract – Materials oxides belonging to the tetragonal tungsten bronze family (TTB) have show growing applications of high technology. The distribution of cations in the niobates with TTB structures has strong influence on their electrical and optical properties. The semiconductor character of the oxide niobate potassium and strontium was investigated by determining the energy gap. The nanopowders of ultra $KSr_2Nb_5O_{15}$, single-crystalline were prepared by modified polyol method. The powders were characterized by absorption spectroscopy in the ultraviolet region. Increasing the calcination temperature causes a decrease of energy gap by reducing the character of the insulating.

Ferroelectric oxides, in particular some oxides with tetragonal tungsten bronze structure (TTB), lead free, are natural candidates to replace materials based on solid solutions of lead zirconate titanate (PZT). Niobates materials have attracted interest from various sectors of science and high technology. This material has a wide range of properties. In addition, Brazil has a large reserve of niobium (CBMM Araxa-MG) and now knows or expertise in the preparation of products based on niobium.

The ferroelectric phase ceramic oxide niobate potassium and strontium, $KSr_2Nb_5O_{15}$ (KSN), were synthesized by modified polyol method (MPM) from the initials reagents: strontium nitrate $Sr(NO_3)_2$, potassium nitrate KNO_3, salt complex Niobium $NH_4H_2[NbO(C_2O_4)3].3H_2O$. The final temperature of calcination is between 350°C and 1100°C for phase KSN. For X-ray diffraction (XRD) was determined the average size of crystallites of the samples with values between 2 and 42 nm. For the structural characterization of samples were realized measurements of absorbance spectroscopy in the ultraviolet and visible region of electromagnetic spectrum (UV-Vis), with spectrometer Cary 50 Conc model, using the dispersion of ceramic powders in phosphoric acid (H_3PO_4) with concentration of 10^{-5} molar and wavelength between 200 and 700 (nm). α is the absorbance coefficient, the representation of $[(E_f.\alpha)^2]$ in Y-axis and the photon energy (E_f) in X-axis, is that the extrapolation of the curve point to $[(E_f.\alpha)^2]$ equal to zero is obtained the energy gap (E_g).

Figure 1 shows the estimate of energy gap (difference between the conduction and valence bands) to KSN_{350} in electron-volts (eV). This sample can be classified as semiconductor just to present values of energy gap (between 1 and 5 eV). The determination of the energy gap for other samples was obtained using the same methodology. According to Figure 2, the energy gap of the ceramic phase has non-linear decreases with increasing temperature. In general, this result can be associated with the increase of calcination temperature and the increase of the crystalline of the sample.

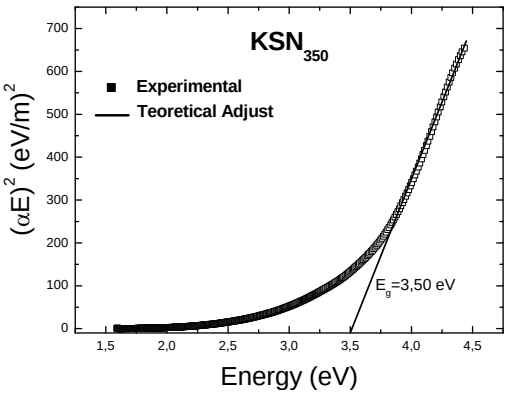

Figure 1: FTIR for phase BaTiO3 ceramics with the identification number of wavelength for each band.

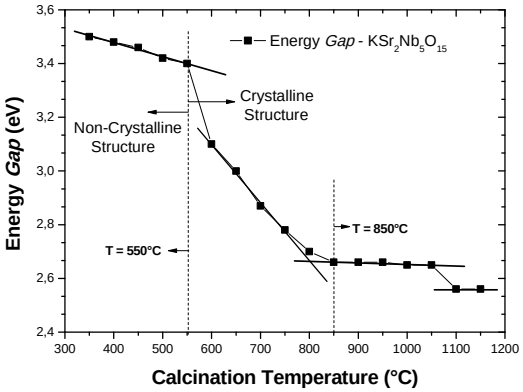

Figure 2: Diagram of impedance for nanofluido with 1 wt% BaTiO3 suspended in butoxyethanol.

[1] A. Milutinovic, D. Popovic, D. Vasiljesevic-Radovic, Z. V. Popovic and Z. D. Dohcevic-Mitrovic. Appl. Phys. A. 84, (2006), 197-202.