Phase transition in $Ba_2In_2O_5$ studied by *in situ* high temperature X-ray diffraction using synchrotron radiation

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Abstract. The order-disorder phase transition in $Ba_2In_2O_5$ high-temperature ionic conductor was systematically studied by *in situ* high-temperature X-ray diffraction using synchrotron radiation and electrical conductivity. Pure barium indate was prepared by solid state reactions at 1300ºC. The room-temperature structural characterization showed a high degree of phase homogeneity in the prepared material. The reduction of the order-disorder phase transition temperature was verified by electrical conductivity and high-temperature X-ray diffraction. The observed features were explained based on Fourier-transform infrared spectroscopy results that revealed the presence of hydroxyl species in the crystal lattice. The increase of the intensity of few diffraction peaks near the phase transition temperature suggests the formation of a superstructure before the orthorhombic-to-tetragonal phase transition.

Keywords: X ray diffraction, rietveld, barium indate.
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$Ba_2In_2O_5$ mixed oxide has received great attention due to its interesting electrical properties. In the low-temperature range (up to ~ 400ºC) this mixed oxide exhibits proton conduction, and for increasing temperatures, mixed conduction was reported with predominance of ionic conduction above 700ºC[1]. Around 925ºC the magnitude of the electrical conductivity increases abruptly due to an order-disorder phase transition[2]. These changes in the conduction mechanism are in some way related to the crystalline structure of $Ba_2In_2O_5$.

EXPERIMENTAL

Pure $Ba_2In_2O_5$ was prepared by solid state reactions between the cation nitrates. The sintering of pellets was carried out at 1300ºC for 10 h. Phase characterization was done by X-ray diffraction. Phase transition studies were accomplished by *ac* electrical conductivity and *in situ* high-temperature X-ray diffraction using the XPD D10B powder diffraction beamline of the Brazilian Synchrotron Light Laboratory. A special setup was used, which consists of a furnace attached to an automated image plate detection system[3]. All diffraction patterns were fitted through Rietveld refinement using GSAS program.

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RESULTS AND DISCUSSION

Figure 1 shows X-ray diffraction patterns in the 45° to 65° 2θ range collected during heating of the sample up to 950°C. It is worth noting that at a temperature as low as 825°C the order-disorder phase transition has already started and at 882°C it has been finished, in agreement with electrical conductivity results.

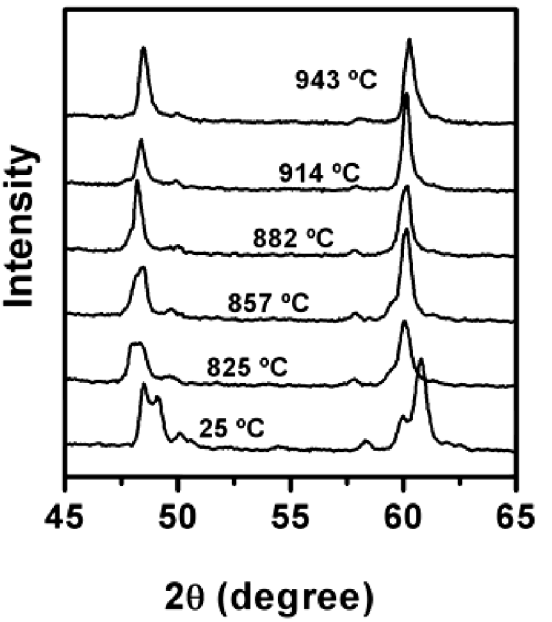

Figure 1 – High-temperature X-ray diffraction patterns of $Ba_2In_2O_5$.

CONCLUSIONS

A reduction of the phase transition temperature by about 50 °C, when compared to materials prepared by the conventional solid state mixture of starting oxides/carbonates was obtained, due to hydroxyls incorporated into the crystal lattice of $Ba_2In_2O_5$.

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