

SrTiO₃ with cubic and tetragonal phases at room temperature

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Abstract – Strontium titanate has an ideal cubic perovskite structure at room temperature, but a recent paper reported the observation of room temperature ferroelectricity in tetragonal SrTiO₃ thin films. The present work reports the coexistence of the cubic and tetragonal phases at room temperature for the SrTiO₃ powders synthesized by polymeric precursor method. The presence of the two phases was confirmed by micro-Raman spectroscopy and Rietveld refinement of the XRD patterns of the samples heat treated between 550 and 700 °C. Acknowledgements: The authors acknowledge the financial support of CNPq/MCT and FINEP.

Strontium titanate has an ideal cubic perovskite structure at room temperature. Sr atoms are located at the vertex of the cubic unit cell, Ti atoms are located in the center and O atoms are located in the face center positions. This structure can also be described as a TiO₆ regular octahedron surrounding a Ti atom. It is well known that SrTiO₃ shows a displacive phase transition at 110 K. Below this temperature it adopts a tetragonal structure, becoming cubic at higher temperatures. A recent paper reported the presence of ferroelectricity in tetragonal SrTiO₃ thin films, at room temperature [1]. Tetragonal structure is characterized by the tilting of the corner-linked TiO₆ octahedra about their four-fold axes, the octahedra in successive layers being tilted in opposite senses [2].

In this work, SrTiO₃ was synthesized by polymeric precursor method [3]. The polymeric resin was calcined at 300 °C for 1 h. After this first calcination, the powder precursor was submitted to a milling process in an alcoholic medium using an attritor mill. A second calcination was performed in an oxygen atmosphere at 300 °C for 12 h. This powder precursor was heat treated in air between 400 and 700 °C for 2 h. The structural transformation was evaluated by micro-Raman spectroscopy, infrared spectroscopy (IR) and X-ray diffraction (XRD). The samples heat treated at 550, 600 e 700 °C were characterized by means of the Rietveld refinement of the XRD patterns.

Short range ordering started at 550 °C when a higher definition of the Me-O band was observed in IR spectrum, besides the long range ordering, indicated by perovskite peaks in XRD patterns. Rietveld refinement data showed two phases (cubic and tetragonal) for the SrTiO₃ and a small amount of SrCO₃ (Table1). The coexistence of the cubic and tetragonal phases was confirmed by micro-Raman spectroscopy. Two peaks were observed (Fig.1), after calcination at 550 °C, being assigned to TO₄ (545 cm⁻¹) e LO₄ (793 cm⁻¹) phonon modes of the tetragonal phase, besides two broad bands centered in the 200-400 and 600-750 cm⁻¹ regions assigned to the cubic phase [4].

Table 1: Result of Rietveld analysis in relation to phase composition

Temperature (°C)	SrTiO ₃ (Pm3m) (%)	SrTiO ₃ (I4/mcm) (%)	SrCO ₃ (%)
550	20.94	72.15	6.91
600	28.56	60.97	10.47
700	22.66	74.44	2.90

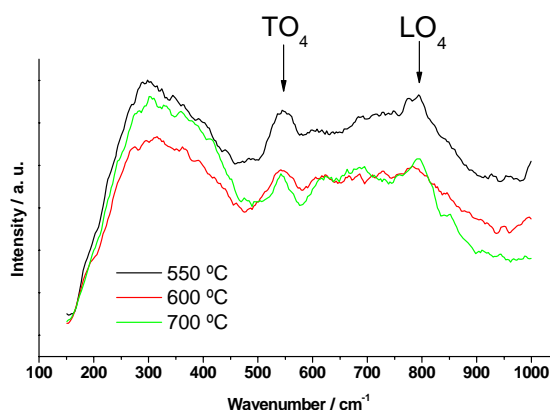


Figure 1: Micro-Raman spectra of the SrTiO₃ powders calcined at different temperatures.

References

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