

The use of photoluminescence as a tool to investigate the nature of disorder degree at CaTiO_3 compounds.

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Abstract: CaTiO_3 (CT) powders were synthesized by hydrothermal microwave (HTMW) method using two types titanium precursors (titanium (IV) isopropoxide $[\text{Ti}(\text{OC}_3\text{H}_7)_4]$ and TiCl_4). The X-ray diffraction (XRD) for both materials analyzed present a single phase indexed as $Pbnm$ space group in a typical orthorhombic CaTiO_3 structure (Fig.1). FT-Raman spectra indicated a great arrangement in a short range. UV-vis (ultra-violet visible) measurements did not show any substantial changes in the optical absorbance. Both Photoluminescence (PL) emission spectra present a broad different profile bands. The FE-SEM micrographs images reveal micro-cubes-like (Fig.2).

The ATiO_3 (A = Pb, Ca, Sr, and Ba) perovskites have attracted considerable attention and constitute one of the most important classes of mixed oxides, suitable for various applications owing to their physical properties, and have been extensively studied as candidates for electro-optical devices. CaTiO_3 belongs to the important group of compounds with perovskite-type structure and are attractive candidates for use as dielectric resonators in wireless communication system and as potential material for biological applications¹. In the literature, the synthesis of crystalline CT perovskite powders was reported at temperatures below 550°C from polymeric precursor method and for temperatures larger than 1200°C from solid state reaction². Recently, an alternative microwave assisted hydrothermal (HTMW) method has been developed^{3,4}. Its is a genuine low temperature method, which allows high heating rates and short annealing times by reason of direct interaction from microwave radiation with the matter. In this way, the HTMW process allows a rapid and homogeneous microwave heating during the hydrothermal method, accelerating like this the crystallization process of the synthesized products by the increase of the nucleation rate³.

The experimental procedure was performed as following. Two different solutions (*solution 1 and solution 2*) are prepared using in the first one 0.05 mol of the Ti precursors (*solution 1*: titanium (IV) isopropoxide $[\text{Ti}(\text{OC}_3\text{H}_7)_4]$ and *solution 2*: TiCl_4) was slowly added, separately, in 30 mL of deionized water at 0°C , after that it is added $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$. The two precursor solutions (*1 and 2*) were mixed under constant stirring with 50ml of the KOH solution (6.0M) to act as a mineralizer. These reaction al two mixtures was loaded in a 110 mL Teflon autoclave. The autoclave was sealed and placed in the Microwave-Hydrothermal system at 413 K for 2, 4, 8, 16 minutes. The X-ray diffraction (XRD) (Fig.1) for both materials analysed present the some type of diffraction patterns like a single phase indexed as orthorhombic CaTiO_3 structure with $Pbnm$ space group, than a more sensitive analyze became important. Hence typical FT-Raman spectra indicated a great arrangement in a long and short range. Therefore, it was observed an upward peak around 537 cm^{-1} assigned to Ti-O torsional modes, implying on the structural distortion in two CT compounds. The room temperature photoluminescence (PL) were used as a tool to investigate the nature of disorder degree at different synthesized compounds. Both PL spectra present a broad different profile bands, indicating two different mechanisms for the PL emission. The FE-SEM micrographs (Fig.2) images reveal micro-cubes-like cages by face-sharing growth with similar morphology of the calcite crystals⁵.

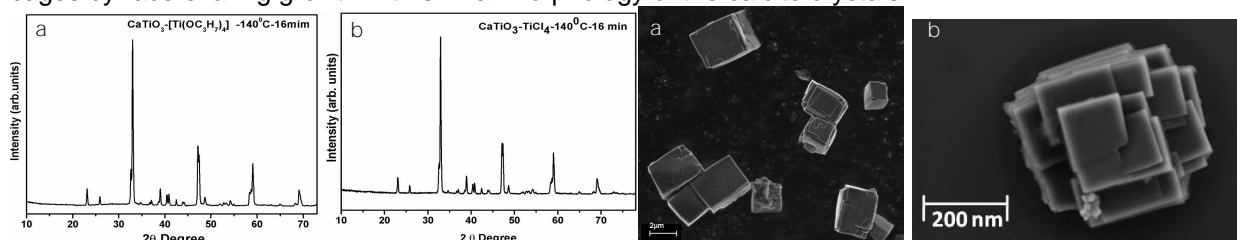


Figure 1: XRD Ray-X patterns of a) $\text{CT}[\text{Ti}(\text{OC}_3\text{H}_7)_4]$ and b) $\text{CT}-\text{TiCl}_4$.

Figure 2: FE-SEM micrograph of a) $\text{CT}[\text{Ti}(\text{OC}_3\text{H}_7)_4]$ and b) $\text{CT}-\text{TiCl}_4$.

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