Thermal and Non-thermal Effects in Microwaveassisted Hydrothermal: SrTiO₃ the case of study

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Discharges rates, low temperature synthesis associated to improved kinetics of direct crystalline phase formations are usually interrelated with microwave-assisted hydrothermal synthesis. The direct interaction between electromagnetic radiation in the microwave range with the innate dipolar molecular rotation of the water it is the main characteristic of this method, tied to thermodynamics effects. The non-thermal effects correspond to formations of hydrogen bonds (H^{.....}O-H) in the reaction activated state, owing to action of OH⁻ groups over amorphous Sr(OH)₂ and TiO(OH)₂. Instinctively water is formed and uncoupled from hydroxides by dehydratation process, giving place to cubic SrTiO₃ (STO) phase. In addition, OH⁻ groups can be unsystematic incorporated into the oxygen sub-lattice, promoting Ti-O distortions like a non-centrossimetric environment and/or [TiO₆H][•] complex clusters. Thus, the Ti octahedral element introduces the degenerecence loss on the 3d titanium orbital introducing a polarization on STO lattice. Hence, providing the necessary conditions for activation of the first order Raman modes associated to intra gap photoluminescent emission. The samples were characterized thought X-ray diffraction, Raman, infrared and XANES spectroscopy associated to electron microscopy and "ab initio" simulations.



Figure 1: dehydration process of STO nanoparticles.

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