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Structural and optical properties of $MgTiO_3$ powders based on the vacancy/distorted clusters and octahedral tilting

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Abstract – $MgTiO_3$ powders were synthesized by the complex polymerization method and heat treated at different temperatures for 2 h. X-ray diffraction patterns and Micro-Raman spectra showed that the crystalline powders have a rhombohedral structure. X-ray absorption near-edge structure analyses spectra indicated that the local structure of crystalline $MgTiO_3$ powders is composed only by [TiO_6] clusters, while the disordered powders exhibit the presence of both [TiO_5] and [TiO_6] complex clusters into the lattice. Ultraviolet-visible spectra revealed different optical band gap values with the heat treatment temperatures. Photoluminescence behavior was attributed to the structural order-disorder and/or distortions on the [TiO_6]–[TiO_6] complex clusters.

$MgTiO_3$ is a ceramic oxide characterized by an ilmenite structure with space group *R*3 [1]. In the last years, this material has been investigated and employed as ceramic capacitors and resonators due to its low dielectric loss and high thermal stability at high frequencies [2]. $MgTiO_3$ powders were synthesized by the polymeric precursor method using magnesium acetate (98% Aldrich), titanium butoxide (99% Aldrich), ethylene glycol (99.5% Synth) and citric acid (99.5% Synth) as raw materials. Initially, titanium citrate solution was prepared, employing the gravimetric procedure in order to estimate the stoichiometric value correspondent to the mass of titanium oxide. Then, stoichiometric quantities of magnesium acetate were dissolved into this solution. Afterwards, ethylene glycol was added into this solution at 120°C to promote the citrate polymerization by the polyesterification reaction. The obtained precursors were heat treated at 450°C, 500°C, 550°C and 700°C for 2 h under air atmosphere. XRD patterns and MR spectra showed that the powders heat treated from 450°C to 550°C present a high degree of structural order-disorder at long and short-range. XANES spectra indicated that the increase of heat treatment temperature favors a transformation of [TiO_5]–[TiO_6] to [TiO_6]–[TiO_6] complex clusters into the structure. UV-vis absorption spectra showed that the increase of optical band gap values is caused by a reduction of intermediary energy levels within the band gap. PL spectra indicated that the $MgTiO_3$ powders heat treated at 450°C for 2 h exhibited the highest intensity, which was mainly attributed to the high degree of structural order-disorder into the lattice. The reduction of PL emission with the increase of heat treatment temperature was related with the decrease of intermediary energy levels within the band gap, as consequence of a high formation of [TiO_6]–[TiO_6] clusters into the lattice [3].

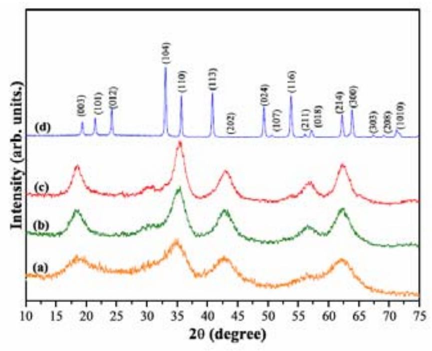

Figure 1: XRD patterns of $MgTiO_3$ powders heat treated at (a) 450°C, (b) 500°C, (c) 550°C and (d) 700°C for 2h.

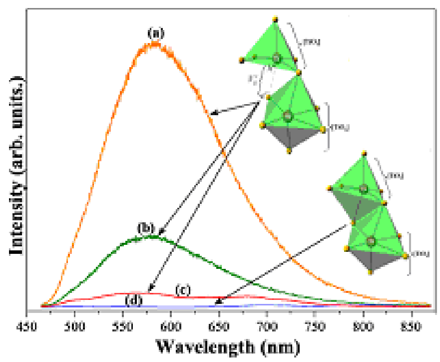

Figure 2: PL spectra of $MgTiO_3$ powders heat treated at (a) 450°C, (b) 500°C, (c) 550°C and (d) 700°C for 2h. Inset shows the [TiO_5]–[TiO_6] and [TiO_6]–[TiO_6] complex clusters.

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