

Influence of the growth process on the photoluminescence behavior of BaWO₄

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Abstract – BaWO₄ powders were prepared by the co-precipitation method in the presence of polyvinylpyrrolidone (PVP) and processed in microwave-hydrothermal system at 140 °C for 30 min. These powders were analyzed by X-ray diffraction (XRD), field emission gun scanning electron microscopy (FEG- SEM) and photoluminescence (PL) measurements. XRD patterns showed that these compounds crystallize in a scheelite-type tetragonal structure. FEG-SEM micrographs indicated that the growth process of the micro-octahedrons is controlled by the oriented-attachment mechanism when the PVP concentration is increased into the aqueous solution. The PL emissions were associated with the intermediary level energy distribution within the band gap.

In the last years, the scientific community has an interest in the development of low-cost synthetic routes with efficient control on the size and shape of the particles as well as environmentally friendly. In principle, microwave-based synthesis techniques can be a good alternative for these purposes. Recently, the microwave technology has been employed to the conventional hydrothermal method to accelerate the formation of molybdates and tungstates with scheelite-type structure [1]. In particular, the BaWO₄ has received special attention because of its photoluminescence, photocatalytic and scintillating properties [2].

In this work, BaWO₄ powders were synthesized by the co-precipitation method in the presence of polyvinylpyrrolidone (PVP) and processed in microwave-hydrothermal system. In the synthesis, tungstic acid (99% purity, Aldrich), barium nitrate (99% purity, Aldrich) and polyvinylpyrrolidone (Aldrich) were used as raw materials. These chemical compounds were dissolved in deionized water at 50 °C under constant stirring. After co-precipitation reaction, this solution was transferred into a Teflon autoclave, which was sealed and placed inside the MH system (2.45 GHz, maximum power of 800 W). Each MH processing was performed at 140 °C for 30 min. After MH processing, the autoclave was naturally cooled to room temperature. The resulting solution was washed with deionized water several times to neutralize the solution pH (≈7). Finally, the white precipitates were collected and dried in a conventional furnace at 50 °C for some hours.

XRD patterns showed that the BaWO₄ powders have a scheelite-type tetragonal structure with space group *I*4₁/*a*, in agreement with the Joint Committee Powder Diffraction Standards (JCPDS) card n° 43-0646 (Figure 1). The particle morphologies were influenced by the PVP concentration into the aqueous solution (Figure 2). In principle, when the PVP content is higher than 2 g, it was observed a growth process of the micro-octahedrons along a common crystallographic orientation (self-assembled structures) via oriented-attachment mechanism. Probably, these morphological modifications were responsible for a reorganization of the intermediary energy levels within the band gap, leading to an increase in the PL intensity as well as a shifting of the maximum emission bands toward the red light visible spectrum (Figure 3).

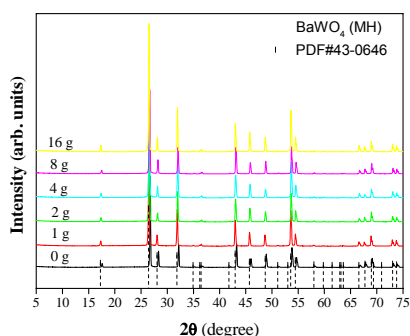


Figure 1: XRD patterns of BaWO₄ powders co-precipitate with different PVP concentrations and processed at 140 °C for 30 min in MH.

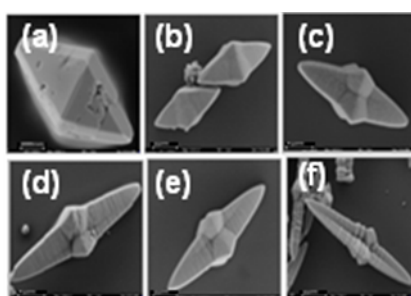


Figure 2: FEG-SEM micrographs of BaWO₄ powders co-precipitate with different PVP concentrations ((a) 0 g, (b) 1 g, (c) 2 g, (d) 4 g, (e) 8 g (f) 16 g) and processed at 140 °C for 30 min in MH.

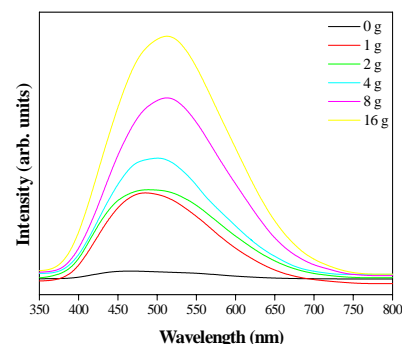


Figure 3: PL spectra of BaWO₄ powders co-precipitate with different PVP concentrations and processed at 140 °C for 30 min in MH.

References:

- [1] L.S. Cavalcante, J.C. Sczancoski, L.F. Lima Jr, J.W.M. Espinosa, P.S. Pizani, J.A. Varela, E. Longo, *Cryst. Growth Des.* 9 (2009) 1002-1012.
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