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Growth and investigations of $BaZrO_3$ mesocrystals under different reaction conditions

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Abstract – The influence of template and chloride precursor concentration on the synthesis of barium zirconate powders has been investigated to prepare micro-sized $BaZrO_3$ mesocrystals. Three different templates, polyethylene glycol (PEG), cetyltrimethylammonium bromide (CTAB) and sodium dodecylsulfate (SDS), and two different chloride precursors concentration was used in the experiments. The mesocrystals were synthesized by means hydrothermal microwave process at 140ºC for 40 minutes. Barium zirconate structures were characterized by powder X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), Fourier transform Raman spectroscopy (FT-Raman) and photoluminescence (PL). The formation and growth of decaoctahedron structure is mainly affected under some conditions. A discussion about the morphology and the photoluminescence is proposed.

Barium zirconate was synthesized by a microwave assisted hydrothermal (HTMW) method at 140ºC for 40 minutes. The HTMW method is one of the efficient, most versatile, and highly cost-effective approaches available to obtain crystalline, single-phase micro and/or nano scale materials at lower temperature and shorter reaction times.

In a recent study Moreira, et al[1] have obtained microcrystalline $BaZrO_3$ powders, by a HTMW at 140ºC on a decaoctahedron shape using different times reaction. However for 40 minutes during HTMW process, it renders the existence of intense diffractions peaks marked as BZ phase. In this work, we investigated the preparation of $BaZrO_3$ powders with the same process, but using different chloride precursor concentration and three different templates, polyethylene glycol (PEG), cetyltrimethylammonium bromide (CTAB) and sodium dodecylsulfate (SDS) with intention of control on the particles shape.

Several studies were performed about template-directed approaches and they have been demonstrated to be effective for preparing a lot of materials among various synthesis methods including HTMW heating. Organic additives are also used to produce not only single crystals with complex morphologies but also superstructures made up of nanoparticles.

The XRD of all sample were indexed to a phase-pure cubic perovskite $BaZrO_3$ (JCPDS 06-0399). The room temperature Raman spectra show BZ cubic phase with smallest incrustations of *m*-ZrO_6, *t*-ZrO_6 and $BaCO_3$. Photoluminescence (PL) spectra at room temperature (Fig. 2) of $BaZrO_3$ mesocrystals revealed that the optical proprieties could be modulated trough chloride precursor concentration and presence of templates. The photoluminescence spectra present a continuous band emission profile, due to the contribution of various components. With the excited wavelength at 350.7 nm, the spectra of all samples show that the strong broad blue-green emission peak is at 493 nm, and blue emission peak is at 443 nm. Their intensities change for each synthesis. The FE-SEM micrographs (Fig. 1) show that all the powders consist of well-dispersed particles but with different sizes and morphologies and when the salts concentration is lower, the stability is change. These different synthesis methods used in the $BaZrO_3$ powders preparation, suggest different defects formation, which can be an indicative of different conformations into the cubic structure during the barium zirconate growth.

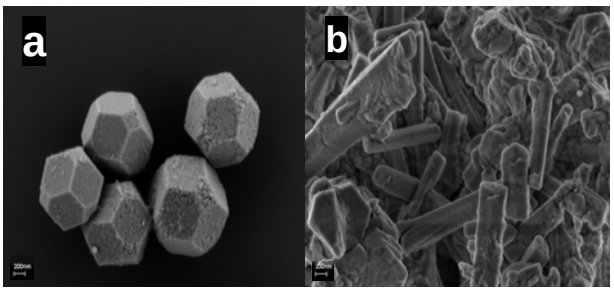

Figure 1: FE-SEM of samples synthesized at 140º for 40 minutes with PEG 400 **a)** using 0.100mol.L^{-1} chloride concentration. **b)** using 0.033mol.L^{-1} chloride concentration.

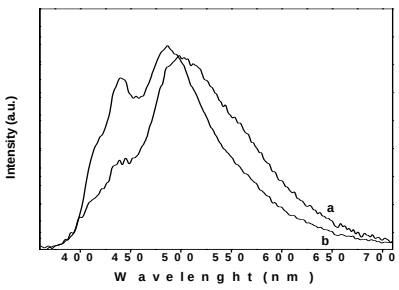

Figure 2: a) Room temperature photoluminescence spectrum of samples synthesized at 140º for 40 minutes with PEG 400 **a)** using 0.100 mol.L^{-1} chloride concentration. **b)** using 0.033 mol.L^{-1} chloride concentration.

References

[1] Moreira, M. L.; Andres, J.; Varela, J. A.; Longo, E. *Cryst. Growth Des.* 2009, 9, 833-839.

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