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Growth mechanism of $BaMoO_4$ microcrystals processed in microwave-hydrothermal: Experimental observations and computational modeling

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Abstract – $BaMoO_4$ microcrystals were synthesized at room temperature by the co-precipitation method and processed in a microwave-hydrothermal (MH) at 413K for different times (30 min - 5 h). These microcrystals were analyzed by X-ray diffraction (XRD), Field emission gun-scanning electron microscopy (FEG-SEM) and transmission electron microscopy (TEM).

Currently, materials with scheelite-type structure have been employed as scintillator and laser host materials due to its interesting luminescent and structural properties [1]. In particular,($BaMoO_4$) is an important material because of its blue, green and orange luminescence emissions [2-3].

$BaMoO_4$ microcrystals were synthesized at room temperature by the co-precipitation method and processed in a microwave-hydrothermal (MH) at 413K for different times (30 min - 5 h). These microcrystals were analyzed by X-ray diffraction (XRD), Field emission gun-scanning electron microscopy (FEG-SEM) and transmission electron microscopy (TEM). XRD patterns showed that this material presents a tetragonal structure without the presence of deleterious phases. FEG-SEM and TEM micrographs revealed that the $BaMoO_4$ microcrystals present an octahedron-like morphology with agglomerated nature and polydisperse particle size distribution. These micrographs also indicated that the microcrystals growth along the [001] direction. The observed crystallographic planes in these structures were simulated computationally and a crystal growth model was proposed in order to explain the morphological changes as a function of processing time.

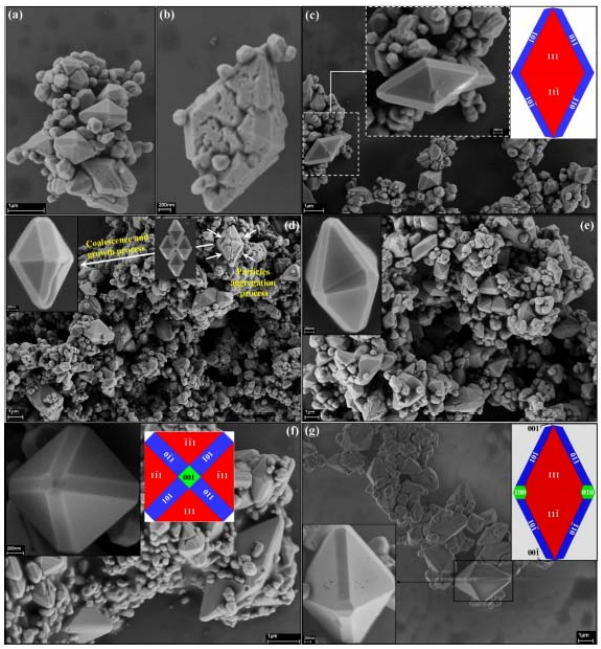

Fig. 1: FEG-SEM micrographs of $BaMoO_4$ microcrystals processed in MH system at 413K for different times. (a,b) $BaMoO_4$ microcrystals formed at room temperature by the co-precipitation method; (c) 30 min; with well-defined crystallographic planes; (d) inset shows the aggregation process between the microparticles (e) $BaMoO_4$ after 2 h; (f,g) $BaMoO_4$ after 5 h; insets in (f) show a top view FEG-SEM micrograph of a micro-octahedron with its different crystallographic planes simulated by computational modeling; insets in (g) illustrate a micro-octahedron with well-defined faces, where the different planes were modeled computationally.

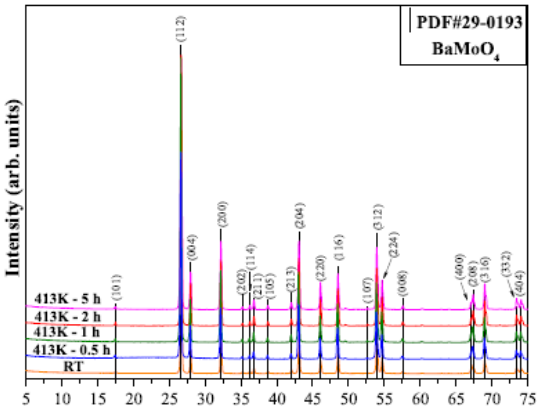

Fig. 2: XRD patterns of BaMoO4 microcrystals processed in MH system at 413K for different times. The vertical lines show the position and relative intensity of JCPDS card no 29-0193 card.

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