Growth mechanism of octahedron-like BaMoO₄ microcrystals processed in microwave-hydrothermal: Experimental observations and computational modeling

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Article info

Article history:
Received 20 March 2009
Received in revised form 5 May 2009
Accepted 16 May 2009

Keywords:
BaMoO₄
Growth process
Microwave-hydrothermal
Supersaturated solution

Abstract

Octahedron-like BaMoO₄ microcrystals were synthesized by the co-precipitation method at room temperature and processed in microwave-hydrothermal at 413 K for different times (from 30 min to 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 BaMoO₄ microcrystals present an octahedron-like morphology with agglomerate nature and polydisperse particle size distribution. These micrographs also indicated that the microcrystals grow along the [0 0 1] direction. The observed crystallographic planes in these structures were modeled computationally and a crystal growth model was proposed in order to explain the morphological changes as a function of processing time.

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1. Introduction

Currently, ceramic oxides with scheelite-type structure have been employed as scintillators and laser host materials because of its interesting luminescent and structural properties (Bardelli et al., 2008; Hasan, Zaki, Kumari, & Pasupulety, 1988; Minowa, Itakura, Moriyama, & Ootani, 1992; Singh, Dash, Prasad, & Venugopal, 1998a, 1998b; Xiong et al., 2006; Zhu et al., 2007). In particular, the barium molybdate (BaMoO₄) is an important material because of its blue, green and orange luminescence emissions (Chen, Xiao, Yu, Jin, & Yang, 2007; Cui, Bi, Shi, Lai, & Gao, 2007; Hu et al., 2007; Liu, Huang, Li, & Li, 2007; Ryu, Yoon, & Shim, 2005). In the last years, several methods have been used to synthesize this material, such as: solid-state reaction (Postnikov, Gavrilov, & Tarasova, 1988; Minowa, Itakura, Moriyama, & Ootani, 1992; Singh, Dash, Prasad, & Venugopal, 1998a, 1998b; Xiong et al., 2006; Zhu et al., 2007), in particular, the barium molybdate (BaMoO₄) is an important material because of its blue, green and orange luminescence emissions (Chen, Xiao, Yu, Jin, & Yang, 2007; Cui, Bi, Shi, Lai, & Gao, 2007; Hu et al., 2007; Liu, Huang, Li, & Li, 2007; Ryu, Yoon, & Shim, 2005). In the last years, several methods have been used to synthesize this material, such as: solid-state reaction (Postnikov, Gavrilov, & Tarasova, 1988; Minowa, Itakura, Moriyama, & Ootani, 1992; Singh, Dash, Prasad, & Venugopal, 1998a, 1998b; Xiong et al., 2006; Zhu et al., 2007), in particular, the barium molybdate (BaMoO₄) is an important material because of its blue, green and orange luminescence emissions (Chen, Xiao, Yu, Jin, & Yang, 2007; Cui, Bi, Shi, Lai, & Gao, 2007; Hu et al., 2007; Liu, Huang, Li, & Li, 2007; Ryu, Yoon, & Shim, 2005). In the last years, several methods have been used to synthesize this material, such as: solid-state reaction (Postnikov, Gavrilov, & Tarasova, 1988; Minowa, Itakura, Moriyama, & Ootani, 1992; Singh, Dash, Prasad, & Venugopal, 1998a, 1998b; Xiong et al., 2006; Zhu et al., 2007), in particular, the barium molybdate (BaMoO₄) is an important material because of its blue, green and orange luminescence emissions (Chen, Xiao, Yu, Jin, & Yang, 2007; Cui, Bi, Shi, Lai, & Gao, 2007; Hu et al., 2007; Liu, Huang, Li, & Li, 2007; Ryu, Yoon, & Shim, 2005).

In 1980, the solid-state heating promoted by the microwave radiation began to be employed in the sintering of several oxides (Komarneni & Roy, 1986; Komarneni, Li, Stefansson, & Roy, 1993; Ohgushi, Komarneni, & Bhalla, 2001; Roy, Komarneni, & Yang, 1985). In the early 1990s, different ceramic powders were synthesized in liquid phase using this electromagnetic radiation (Abothu, 1967-2001) – see front matter © 2009 Chinese Society of Particuology and Institute of Process Engineering, Chinese Academy of Sciences. Published by Elsevier B.V. All rights reserved. doi:10.1016/j.partic.2009.05.002
 precipitation reaction, Ba²⁺ cations are electron pair acceptor (Lewis acid), while the MoO₄²⁻ anions are electron pair donor (Lewis base). The reaction between these two species (Ba²⁺ + MoO₄²⁻) results in a covalent bond. The covalent bond occurs due to the Lewis acid to occupy the lowest molecular orbital (LUMO), which interacts with the highest molecular orbital (HOMO) of the Lewis base. After co-precipitation reaction, the solution was transferred into a Teflon autoclave, which was sealed and placed inside a MH system (2.45 GHz, maximum power of 800 W). Each MH processing was performed at 413 K for 30 min, 1, 2 and 5 h, respectively. The heating rate in this system was fixed at 298 K/min and the pressure in the autoclave was stabilized at 294 kPa. After MH processing, the autoclave was cooled at RT naturally. 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 353 K for some hours.

2.2. Characterizations

The octahedron-like BaMoO₄ microcrystals were characterized by XRD using a DMax/2500PC diffractometer (Rigaku, Japan) with Cu Kα radiation (λ = 1.5406 Å) in the 2θ range from 5° to 75° and step size of 0.02°/min. The morphologies were verified through a Supra 35-VP FEG-SEM (Carl Zeiss, Germany) operated at 6 keV and with a CM200 TEM (Philips, USA) operated at 200 keV. The growth directions of BaMoO₄ microcrystals were estimated using the selected-area electron diffraction (SAED) and high resolution transmission electron microscopy (HR-TEM).

3. Results and discussion

3.1. X-ray diffraction analyses

Fig. 1(a) shows the XRD patterns of octahedron-like BaMoO₄ microcrystals synthesized by the co-precipitation at RT and processed in MH at 413 K for different times. Fig. 1(b) illustrates the lattice parameter values as a function of processing time.

The XRD patterns revealed that all diffraction peaks of BaMoO₄ microcrystals can be indexed to the scheelite-type tetragonal structure, in agreement with the respective “Joint Committee on Powder Diffraction Standards” (JCPDS) card no. 29-0193 (Fig. 1(a)) (ICDD, 2000). The sharp and well-defined diffraction peaks indicated a high degree of crystallinity, i.e., these materials are structurally ordered at long-range. The obtained data on the position and full width at half height of all diffraction peaks were used in the UNITCELL-97 program (Holland & Redfern, 1997) in order to estimate the lattice parameter values and
Table 1
Comparative results between the lattice parameters and unit cell volume of BaMoO$_4$ obtained in this work with those reported in the literature.

<table>
<thead>
<tr>
<th>Method</th>
<th>T (K)</th>
<th>Time (h)</th>
<th>Average lattice parameters</th>
<th>Unit cell volume (Å$^3$)</th>
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<td>$c$ (Å)</td>
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$T$, temperature; CZ, Czochralski; PP, precursor polymeric; PC, precipitation/calcination; CP, co-precipitation; MH, microwave-hydrothermal.

Fig. 2. FEG-SEM micrographs of octahedron-like BaMoO$_4$ microcrystals synthesized by the co-precipitation at RT and processed in MH at 413 K for different times. (a) and (b) BaMoO$_4$ synthesized by the co-precipitation method at RT; (c) BaMoO$_4$ microcrystals processed in MH system for 30 min; insets in (c) show a microcrystal with well-defined crystallographic planes and its schematic representation obtained through computational modeling; (d) BaMoO$_4$ microcrystals formed after MH processing for 1 h; inset in (d) shows the aggregation process between microparticles; (e) BaMoO$_4$ microcrystals obtained by the MH processing for 2 h; inset in (e) shows the presence of new crystallographic faces; (f) and (g) BaMoO$_4$ microcrystals formed after MH processing for 5 h; insets in (f) show a top view FEG-SEM micrograph of a micro-octahedron with its different crystallographic planes modeled in a computational program; insets in (g) illustrate a micro-octahedron with well-defined faces, where the different planes were modeled computationally.
Fig. 3. (a) and (b) Low magnification TEM micrographs of BaMoO$_4$ processed at 413 K for 30 min; (c) HR-TEM micrograph of a microcrystal, where the inset shows the corresponding SAED pattern; (d) TEM micrographs of agglomerated microcrystals with different sizes; (e) high magnification TEM micrograph of an individual microcrystal selected in (d) (red square); (f) HR-TEM micrograph performed on the edge (red rectangle) of a microcrystal; inset in (f) shows the SAED pattern obtained on this region; (g) low magnification TEM micrographs of BaMoO$_4$ microcrystals processed at 413 K for 2 h; (h) magnified region on the edge of a microcrystal selected in (g); (i) HR-TEM micrograph obtained on the selected region in (h) (red rectangle); inset in (i) illustrates the SAED pattern taken on this region; (j) low magnification TEM micrographs of BaMoO$_4$ microcrystals processed at 413 K for 5 h; (k) top view TEM micrograph of a microcrystal with its respective crystallographic planes modeled computationally; (l) HR-TEM micrograph found on the selected region in (k) (red square); inset in (l) shows the corresponding SAED pattern obtained from the selected region in (l). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)
unit cell volume. The obtained values as a function of processing time are shown in Fig. 1(b) and displayed in Table 1. This table also shows a comparison between the lattice parameter values and unit cell volume data of BaMoO₄ obtained in this work with those reported in the literature (Basiev et al., 2000; Marques et al., 2006; Nassif, Carbonio, & Alonso, 1999; Zhao et al., 2007).

As it can be seen in this table, the synthesis methods influence in the lattice parameters and unit cell volume of BaMoO₄. Based on this observation, we believe that the experimental condi-

![Graphs showing particle height and width distribution](image)

Fig. 4. Average particle height and width distribution of BaMoO₄ micro-octahedrons processed in MH at 413 K for (a) and (b) 30 min, (c) and (d) 1 h, (e) and (f) 2 h, and (g) and (h) 5 h.
tions (heat treatment temperature, heating rate and/or processing time) employed in the synthesis are able to promote the formation of structural defects, residual stresses and/or distortions into the lattice. In the MH system, the small variations observed in our results may arise from distortions into the BaMoO₄ structure, as consequence of the rapid kinetics of formation of the microcrystals by the microwave radiation (Rao, Vaidyanathan, Ganguli, & Ramakrishnan, 1999). The obtained results in this work are in agreement with those reported in the literature (Thongtem, Phuruangrat, & Thongtem, 2008a, 2008b).

3.2. Field-emission gun scanning electron microscopy analyses

Fig. 2(a–g) shows the FEG-SEM micrographs of octahedron-like BaMoO₄ microcrystals synthesized by the co-precipitation at RT and processed in MH at 413 K for different times.

In Fig. 2(a), it was observed that the small BaMoO₄ octahedrons formed at RT by the co-precipitation are agglomerate, presenting a polydisperse nature. As verified in Fig. 2(b), micro-octahedrons exhibited the absence of surface defects on its faces, probably caused by the rapid hydrolysis during the addition of NH₄OH into the solution. Also, this behavior can be related to the formation of a supersaturated solution due to high concentration of the chemical acid/salts dissolved in the aqueous medium (80 ml) (Colfen & Antonietti, 2005). Moreover, these morphological characteristics suggest that the growth rate of each crystal face is usually non-linearly proportional to supersaturation of the solution.

Fig. 2(c) shows that the processing performed at 413 K for 30 min favored the formation of micro-octahedrons with well-defined faces along the different crystallographic planes. However, it was verified that the agglomerate nature still persists in this system. Possibly, the high collision rates and the heating promoted by the microwave radiation during the MH processing intensified the PEG adsorption on the microparticle surfaces. Also, this result demonstrates that the micro-octahedrons were formed by the aggregation of the first small octahedrons in an oriented manner with a subsequent ripening of the aggregates. According to the literature (Colfen & Mann, 2003), the high adsorption rates of this non-ionic or polymeric surfactant on the crystal faces favored the interactions between the tails of surface-adsorbed surfactant molecules, influencing the growth process of the microcrystals. Inset in Fig. 2(c) shows a FEG-SEM micrograph of a BaMoO₄ micro-octahedron, where its crystallographic planes were modeled using the JCrystal-Soft 2006 (Crystal Shape Editor/Viewer 1.05) program (JCRYSTAL, 2006). Gong et al. (2006) observed these same morphologies in BaMoO₄ microcrystals synthesized by the microemulsion method (n-octane/cetyltrimethylammonium bromide/n-butanol systems) assisted by CH system. The MH processing at 413K for 1 h intensified the continuous dissolution/recrystallization process of BaMoO₄ microcrystals (Luo et al., 2008b), inducing the aggregation and subsequent coalescence between the microparticles as well as the formation of surface defects on its faces (Fig. 2(d)) (Ryu & Huh, 2008). The increase in the MH processing for 2 h promoted the formation of micro-octahedrons with new faces (Fig. 2(e)) along the following crystallographic planes: (1 0 0), (0 1 0), (1 0 0) and (0 1 0) (Fig. 2(e) and inset in Fig. 2(e)). After processing performed for 5 h, the presence of large micro-octahedrons was observed because of a considerable increase in the coalescence rate (Fig. 2(f) and (g)). Inset in Fig. 2(f) show a top view FEG-SEM micrograph of a BaMoO₄ micro-octahedron with its respective crystallographic planes modeled through the JCrystalSoft 2006 program (JCRYSTAL, 2006). This program was also employed in the modeling of the other crystallographic planes belonging to an individual BaMoO₄ micro-octahedron (insets in Fig. 2(g)).

3.3. Transmission electron microscopy analyses

Fig. 3(a–l) shows the TEM, high resolution transmission electron microscopy (HR-TEM) micrographs and SAED patterns of octahedron-like BaMoO₄ microcrystals processed in MH at 413 K for different times.

Fig. 3(a) and (b) shows the low magnification TEM micrographs of octahedron-like BaMoO₄ microcrystals processed at 413 K for 30 min. In these micrographs, the presence of bright and dark regions on the morphologies was verified. The bright ones correspond to the individual micro-octahedrons with low atomic density, while the black ones indicate the regions with agglomeration between the particles. Fig. 3(c) illustrates the HR-TEM micrograph performed on the edge of a BaMoO₄ micro-octahedron, where the (0 0 4) planes can be seen (with interplanar spacing of approximately 3.3 Å). The SAED pattern along the [1 1 0] zone axis confirmed that this morphology is well-crystallized, presenting a tetragonal structure (inset in Fig. 3(c)). Microcrystals with different sizes and with agglomerate nature were observed in Fig. 3(d). Fig. 3(e) shows a high magnification TEM micrograph of an individual BaMoO₄ micro-octahedron chosen in Fig. 3(d) (red square). On this selected region, a HR-TEM micrograph as well as the SAED pattern were obtained, as shown in Fig. 3(f). It is well-known that the growth rate of a crystal face is usually related to its surface energy. In this context, the HR-TEM micrograph indicated that the crystal growth occurs preferentially along the [0 0 1] direction. This result is in good agreement with the previously reported by Ryu and Huh (2008). According to these authors, the growth rate in BaMoO₄ microcrystals is faster along the [0 0 1] direction than in the [1 0 0] direction. In principle, we believe that the anisotropic growth in the [0 0 1] direction for the BaMoO₄ micro-octahedrons is caused by differences in the surface energies on each crystal face. Probably, this preferential growth direction has stronger interatomic bonds between the [BaO₈] and [MoO₄] clusters. However, future calculations will be performed in order to understand the influence of the surface energies on the crystal growth process of BaMoO₄ microcrystals.

Fig. 3(g) shows a TEM micrograph of BaMoO₄ microcrystals processed at 413 K for 2 h. As it can be seen in this figure, this processing condition was not able to avoid aggregation process between the particles. The region selected in Fig. 3(h) (red rectangle) was magnified in Fig. 3(i) by HR-TEM. The HR-TEM micrographs found on this region allowed to identify the (1 0 1) and (1 1 2) planes with interplanar spacings of 5.1 and 3.4 Å, respectively (inset in Fig. 3(i)). When the processing time was prolonged for 5 h, large micro-octahedrons were formed because of the crystal growth via coalescence mechanism, as previously described in the text. This affirmation can be confirmed clearly through the TEM micrograph illustrated in Fig. 3(j). Fig. 3(k) shows a top view TEM micrograph of a micro-octahedron, where its crystallographic planes were modeled computationally. In principle, this figure demonstrates that the MH processing performed for long time intervals plays an important role on the morphological changes of BaMoO₄ microcrystals. The HR-TEM micrograph in Fig. 3(l), taken from the selected area by the red rectangle in Fig. 3(k), corresponds to the (2 0 0) plane with interplanar spacing of 2.8 Å. The spots observed in the SAED pattern confirmed the single BaMoO₄ phase with tetragonal structure (inset Fig. 3(l)).

3.4. Particle size distribution (height and width) of BaMoO₄

Fig. 4 shows the average particle height and width distribution of octahedron-like BaMoO₄ microcrystals processed in MH at 413 K for different times.
Both FEG-SEM and TEM micrographs were employed in order to estimate the average particle size distribution of BaMoO$_4$ microcrystals (Fig. 4(a–h)). Fig. 4(a) shows the particle height distribution in the range from 0.25 to 3.25 μm for the BaMoO$_4$ microcrystals processed at 413 K for 30 min. In this figure, it was verified that 86% microparticles with octahedron-like morphology presented an average height from 0.25 to 1.75 μm. Fig. 4(b) shows the particle width distribution in the range from 0.1 to 1.5 μm for the microcrystals processed at 413 K for 30 min. It was evaluated that approximately 84% particles exhibited an average width from 0.3 to 1.1 μm. These results indicate that the initial processing stages of the growth process of micro-octahedrons occurred mainly along the [0 0 1] direction (height) than in the [1 0 0] direction (width). This preferential growth direction in favor of [0 0 1] was due to the driving force in the coalescence process to be related with the reduction of surface energy, aimed at minimizing the area of high-energy faces (Wang, 2000).

The MH processing performed at 413 K for 1 h showed that the aggregation of the microparticles occurred. In the growth process, when two crystals are oriented in the same crystallographic direction and thus coalesce, the adhesion of two crystals can occur with the highest probability. The adhesion with the second highest probability usually occurs when two crystals has a “twin relation” (this case is known as “contact twin”). Moreover, when two crystals have some specific crystallographic relations, called “coincidence site lattice matching”, two crystals adhere strongly. As it can be seen in these figures (Fig. 4(c) and (d)), this behavior promoted the formation of micro-octahedrons with particle height ranging from 0.75 to 3.75 μm and particle width ranging from 0.3 to 1.5 μm. An increase in the growth process was verified for the BaMoO$_4$ microcrystals processed at 413 K for 2 h. In this case, several micro-octahedrons exhibited the new faces along the different crystallographic planes ((1 0 0), (0 1 0), (T 0 0) and (0 T 0)) (inset in Fig. 2(e)). Thus, this growth stage promoted an increase in the particle height distribution from 1.25 to 4.25 μm (Fig. 4(e)) and particle width distribution from 0.7 to 2.1 μm (Fig. 4(f)). After MH processing performed at 413 K for 5 h, large micro-octahedrons with height distributed from 1.25 to 4.25 μm and width from 0.7 to 2.1 μm were noted (Fig. 4(g) and (h)). Probably, the preferential growth is caused by the Ba–O–Mo bonds along the [0 0 1] and/or [0 0 1] directions, which are stronger than the others inside the crystal. This phenomenon is arising from a higher reduction in the surface

Fig. 5. Schematic representation of the synthesis, processing and growth of BaMoO$_4$. (a) Chemical synthesis, (b) co-precipitation reaction, hydrolysis and addition of surfactant (PEG), (c) MH system employed in the processing of BaMoO$_4$ microcrystals, (d) increase of the effective collision rates between the microparticles by the microwave radiation, (e) growth mechanism of microcrystals, (f) morphologic evolution of microcrystals as a function of processing time and (g) different crystallographic planes of micro-octahedrons modeled computationally.
free energy on the (1 0 0), (0 1 0), (0 0 1) and (0 1 0) crystallographic planes. All obtained results clearly indicate that the processing time in a MH system is able to influence the crystal grow processes of BaMoO₄ microcrystals. Therefore, we believe that long processing times imply in a higher exposure of BaMoO₄ microcrystals with the microwave radiation. This interaction accelerates the dissolution/recrystallization mechanism promoted by the microwave heating as well as the effective collision rates between the small microcrystals. Possibly, these effects are key factors on the kinetics of formation, growth process and crystallization rate of these crystals.

3.5. Growth mechanism of octahedron-like BaMoO₄ microcrystals

Fig. 5 shows a schematic representation of all stages involved in the synthesis and growth mechanism of octahedron-like BaMoO₄ microcrystals synthesized by the co-precipitation at RT and processed for different times in MH system.

Fig. 5(a) illustrates the initial formation process of small BaMoO₄ octahedrons by the co-precipitation reaction arising from the solubilization process between molybdic acid and barium nitrate dissolved in deionized water. The hydrolysis rate was increased by the addition of 5 mL of NH₄OH into this solution (Fig. 5(b)). In this case, the interaction between Ba²⁺ and MoO₄²⁻ ions resulted in the formation of the first BaMoO₄ precipitates. This chemical solution was stirred in ultrasound for 60 min to accelerate the co-precipitation rate. A higher interaction between the pre-formed solution was stirred in ultrasound for 60 min to accelerate the co-precipitation rate. A higher interaction between the pre-formed solution was stirred in ultrasound for 60 min to accelerate the co-precipitation rate. A higher interaction between the pre-formed solution was stirred in ultrasound for 60 min to accelerate the co-precipitation rate.

Fig. 5(d) shows a schematic representation of the MH processing of BaMoO₄ microcrystals. Inside this system, the high frequency of the microwave radiation interacts with the permanent dipoles of the liquid phase (H₂O), which initiates a rapid heating resulting from the resultant molecular rotation. Likewise, permanent or induced dipoles in the dispersed phase cause a rapid heating of the particles (Murugan, Samuel, & Ravi, 2006). Thus, the microwave radiation is able to promote the effective collision between the small microparticles (Godinho, Ribeiro, Longo, & Leite, 2008), contributing to the growth of the microcrystals and inducing the formation of new crystallographic faces on them. The adsorption of PEG on the micro-octahedron surfaces favors the aggregation process by means of the interaction between the hydrogen bonds of water with the OH groups of this surfactant (Paria & Khilar, 2004; Somasundaran & Krishnakumar, 1997). Consequently, this mechanism contributes to the coalescence of the micro-octahedrons (Fig. 5(e)). Fig. 5(f) shows the morphological evolution of BaMoO₄ microcrystals as a function of processing time. At RT, these micro-octahedrons are agglomerated with a high concentration of surface defects. After 30 min, it is possible to note the formation of micro-octahedrons with well-defined crystallographic faces. When processed for 1 h, the aggregation process between the small microparticles was induced by the coalescence process, resulting in the growth of micro-octahedrons. The processing performed at 413 K for 2 h induced a fast growth process from BaMoO₄ micro-octahedrons to faceted micro-octahedrons along the different crystallographic planes. This phenomenon is obvious when the surface atoms tend to find new equilibrium positions to balance the free energy, resulting in modifications on the surface and microcrystal morphology (Wang, 2000). The increase in the coalescence rate and the slow kinetics of dissolution/recrystallization during the MH processing performed for 5 h allowed the growth of the micro-octahedrons as well as a considerable reduction of the surface defects. This proposed crystal growth mechanism is in agreement with the reported in the literature (Afanasiev, 2007; Wu et al., 2007). Fig. 5(g) shows the different crystallographic planes of BaMoO₄ micro-octahedrons modeled in the JCrystalSoft 2006 program (JCRYSTAL, 2006). These planes allow an understanding on the growth processes of the micro-octahedrons with the processing time in a MH system. Table 2 shows the lattice parameter values, bond angles between O–Mo–O, distances and Miller indices (h, k, l) employed in the crystal modeling. The verified crystallographic planes for the micro-octahedrons are in agreement with those observed in TEM micrographs (Fig. 3).

<table>
<thead>
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<th>Table 2</th>
<th>Average lattice parameters, bond angles between O–Mo–O, distances and Miller indices (h, k, l) used in the computational modeling of the different crystallographic planes of BaMoO₄ microcrystals.</th>
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4. Conclusions

In summary, octahedron-like BaMoO₄ microcrystals were synthesized by the co-precipitation method at room temperature and processed at 413 K for different times in a microwave-hydrothermal system. XRD patterns revealed that these microcrystals crystallize in a scheelite-type tetragonal structure with space group I₄₁/a. Secondary phases were not verified in this material. FEG-SEM micrographs showed that the processing time conditions in a MH system plays an important role on the growth process of BaMoO₄ micro-octahedrons. The effective collision rates, dissolution/recrystallization mechanism and coalescence process promoted by the microwave radiation were responsible for the morphological changes of the micro-octahedrons. The aggregation process as well as the preferential growth along the [001] direction of the micro-octahedrons are evidences of the influence of PEG adsorption on the different crystallographic faces. A plausible growth mechanism for the morphological evolution of BaMoO₄ micro-octahedrons was discussed in details.

Acknowledgements

The authors thank the financial support of the Brazilian research financing institutions: CAPES, CNPq and FAPESP. Special thanks to Prof. Dr. D. Keyson and Dr. D.P. Volanti by the development of the domestic microwave-hydrothermal system.

References


