

STUDY OF CRYSTAL STRUCTURE, MORPHOLOGY AND COMPOSITION OF THE  $\alpha$ -MoO<sub>3</sub> DOPED WITH NEODYMIUM, OBTAINED BY THERMAL PRECIPITATION.

R. E. Garzón<sup>(1)</sup>, J. E. Alfonso<sup>(2)</sup>, J. Torres<sup>(2)</sup> and L. C. Moreno<sup>(3)</sup>

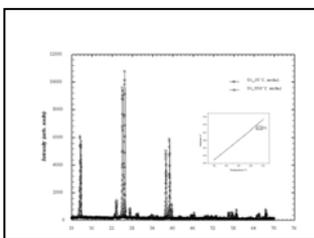
- (1) Universidad Distrital Francisco José de Caldas. Carrera 7 No 40 53, Bogotá-Colombia. regarzonv@unal.edu.co.  
 (2) Departamento de Física. Universidad Nacional de Colombia, Carrera 30 Calle 45 ciudad Universitaria. jealfonsoo@unal.edu.co.  
 (3) Departamento de Química. Universidad Nacional de Colombia, Carrera 30 Calle 45 ciudad Universitaria Bogotá-Colombia. lmorenoa@unal.edu.co

**Abstract**

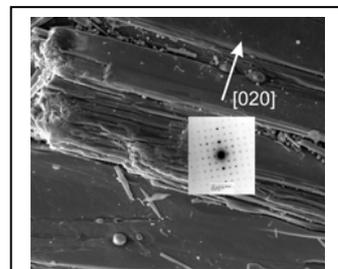
Molybdenum trioxide is a material with chromogenic properties, i.e. its optical properties change in accordance with the impinging radiation, which has led to technological applications such as optical units for massive storage of information, thank mainly to its capability to switch between two optical states [1]; furthermore, the development of thin film devices based on MoO<sub>3</sub> has allowed its application as gas sensors [2], smart windows [3], moreover, the scientific community's attention has been aimed as well on the development of solid state micro batteries in which the MoO<sub>3</sub> is used as cathode material and Li ions move through channels in the  $\alpha$ -MoO<sub>3</sub> structure.

Compounds of  $\alpha$ -MoO<sub>3</sub> Nd doped from powder samples at concentrations of (0.2%, 1.0%, 5.0%, 10.0% and 20% %at) were developed by thermal precipitation in order to fabricate materials with optoelectronic properties such as photoluminescence emission in the visible and infrared spectrum. Sample preparation was carried out from a solid phase reaction of  $\alpha$ -MoO<sub>3</sub> and Nd<sub>2</sub>O<sub>3</sub> in an isopropanol solution, stirred permanently for 8 hours at 298°K and then dried up for 8 hours at 353°K; the final stage to obtain the compounds was performed through a calcination process at 823°K for 20 hours.

The behavior of the lattice parameters as a function of temperature as well as the evaluation of thermal dilation coefficients were studied through X-Ray Diffraction as a function of temperature in steps of 323°K up to the final 823°K; growth directions and crystallographic orientations of doped and non doped materials were evaluated by (TEM). The study of the morphology and particle size was performed through (SEM); the chemical composition of the oxides obtained was carried out by scattered electron spectroscopy (EDX). XRD results allowed establishing the behavior of the thermal dilation coefficients ( $\alpha_c$ ),  $\alpha$ -MoO<sub>3</sub> and obtained oxides lattice parameters, which showed a 2% variation; it is important to point out that the  $\alpha_c$  variation of the c lattice parameter presents a negative value. TEM studies (fig. 2) have helped establishing that both growth directions and plane families, found through XRD, agree with each other. On the other hand, SEM study has shown that the doped and non doped materials' morphologies are not markedly different. Finally, EDS studies have shown that the Nd composition (%at) in the doped  $\alpha$ -MoO<sub>3</sub> do not present a tendency with the rising Nd concentration.



**Figure 1:** XRD pattern for samples with 5% of Neodymium at 323 K and 823 K. The inset square shows the curve fitting for the b lattice parameter.



**Figure 2:** Electron pattern diffraction and micrograph SEM for the  $\alpha$ -MoO<sub>3</sub> doped with 5% neodymium.

**References**

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