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$NaNbO_3$ synthesis by combined EDTA/Citrate complexation

Ila Gabriele Diniz Dias de Azevedo [1,2], Camila Pacelly Brandão de Araújo [1,3], Carlson Pereira de Souza [1,4], Christian Turquat [2], Madjid Arab [2], André Luis Lopes Moriyama [1,4]

1 Graduate Program in Chemical Engineering, Technology Center, Federal University of Rio Grande do Norte, Campus Universitário, Lagoa Nova, 59078-970, Natal, Rio Grande do Norte, Brazil
2 Institute of Materials, Microelectronics and Nanosciences of Provence, Nano-Structure, Reactivity & Environment Team, University of Toulon, Bât. R - Campus La Garde, Av. de l'Université, 83130, La Garde, France
3 School of Science and Technology, Anel Viário Contorno do Campus s/n - Capim Macio, 59078-970, Natal, Natal, Rio Grande do Norte, Brazil
4 Department of Chemical Engineering, Technology Center, Federal University of Rio Grande do Norte, Campus Universitário, Lagoa Nova, 59078-970, Natal, Rio Grande do Norte, Brazil

INTRODUCTION & AIM

Sodium niobate ($NaNbO_3$) is a n-type perovskite-structured semiconductor that exhibits polymorphism across a wide temperature range, granting it exceptional physical and chemical properties. This material is researched for various applications, including photocatalysis, electrocatalysis, sensors, and electronic devices (1).

The functional properties of the materials are controlled by morphology, particle size, and crystalline structure. For sodium niobate, traditional synthesis routes often produce large particles and a wide bandgap (~3.4–3.5 eV), limiting its optical absorption. Therefore, adopting a low-temperature chemical route capable of refining particle size, engineering defects, and tuning the bandgap is crucial to expanding its technological performance (2).

Among chemistry methods (such as sol-gel, coprecipitation, and polymeric precursor routes), the combined EDTA-citrate complexation method stands out as a highly promising alternative. This approach utilizes ethylenediaminetetraacetic acid (EDTA) and citric acid as co-chelating agents to form stable metal-chelate complexes (3).

This work reports the synthesis and structural characterization of $NaNbO_3$ via the combined EDTA/citrate route. The material was prepared using a 1:1:3 molar ratio of metal ions: EDTA: citric acid, followed by a pre-treatment at 230 °C and final calcination at 700 °C.

METHOD

The molar proportion between metal ions: EDTA:citric acid was 1:1:3, according to (4). The calcination temperature was set at 700°C.

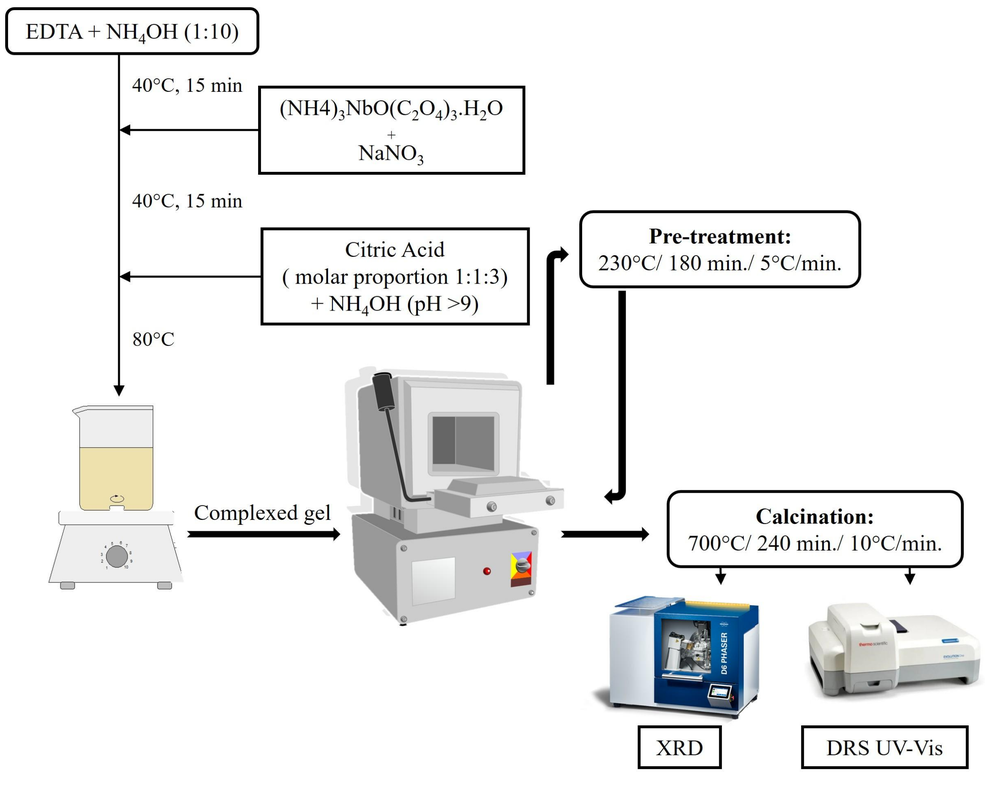

Figure 1: Synthesis methodology of $NaNbO_3$ by the combined EDTA-Citrate complexation method.

RESULTS & DISCUSSION

$NaNbO_3$ exhibited an orthorhombic crystalline structure containing only sodium niobate without any residual peaks, figure 2. Sodium niobate can exist in different polymorphic forms, mainly associated with two space groups: Pbcm and $P2_1ma$. The Rietveld refinement revealed that the material has a $P2_1ma$ space group identified by the CIF 9014103. Based on the atomic positions, it is observed that sample maintains the basic the perovskite network, particularly the BO_6 polyedra centered on niobium cation site, with lattice parameters a = 5.565Å, b = 7.774 Å and c = 5.521 Å. The crystallite size of sodium niobate was obtained using a Scherrer-type relationship, with values 169.91 nm.

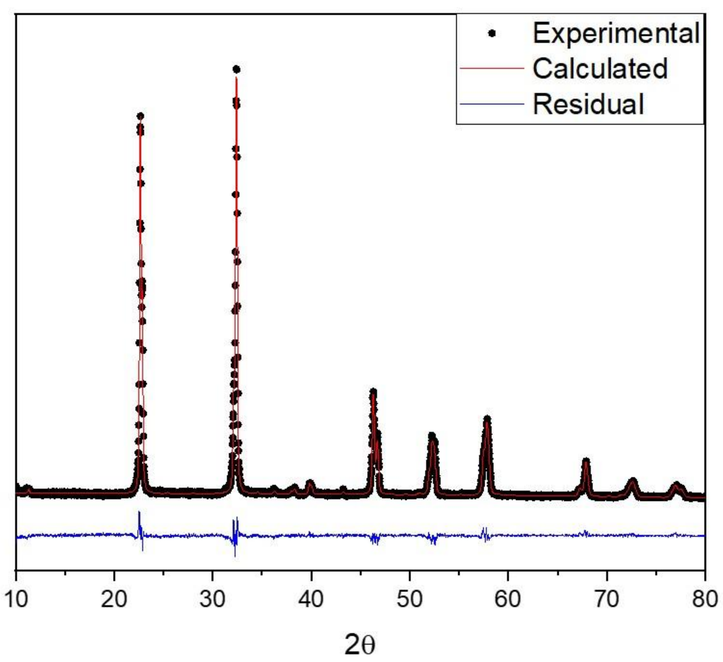

Figure 2: Rietveld refinement plot of $NaNbO_3$ with $P2_1ma$ space group.

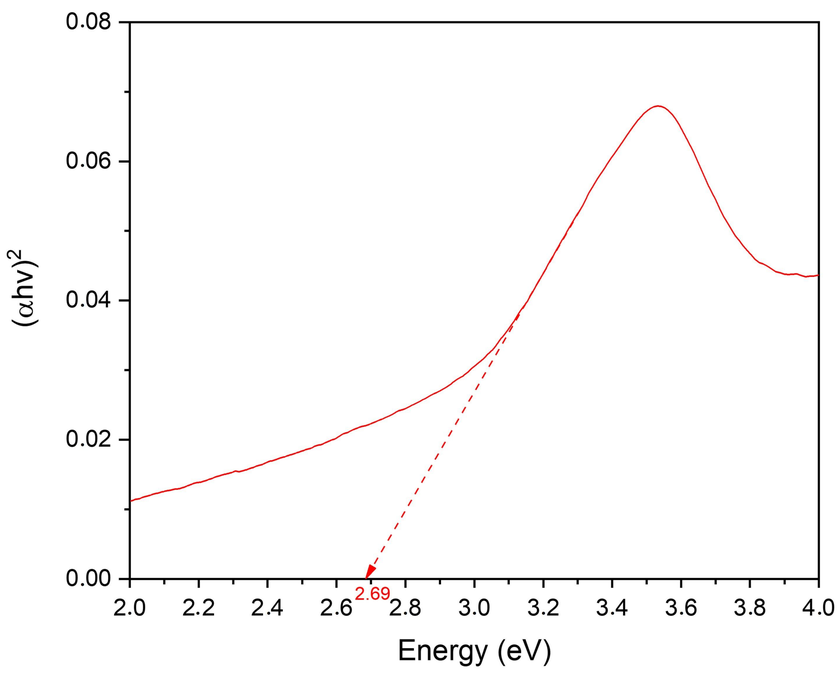

Figure 3: Tauc plots of the samples.

The bandgap energie of the $NaNbO_3$ sample was determined according to the Kubelka-Munk and Wood and Tauc equations, and the values were obtained by extrapolating the linear region with the steepest curve of the profile obtained. Density functional theory (DFT) calculations of the electronic properties of orthorhombic $NaNbO_3$ with space group $P2_1ma$ have shown that the material exhibits a direct band transition (5). The bandgap value obtained is 2.69 eV, which are lower than those reported in the literature (~3.4 eV). Structural ordering and local distortions on NbO_6 octahedra, caused by the clumping of particles with increasing temperature, can lead to significant changes in the optical bandgap. In particular, the oxygen vacancies that introduce intermediate electronic states within the bandgap.

CONCLUSIONS

The synthesis of sodium niobate ($NaNbO_3$) using the combined EDTA-citrate complexation method proved efficient with calcination at 700 °C, forming a pure orthorhombic crystalline phase with a $p2_1ma$ space group. The method used provided adjustable structure and optical properties, expanding its potential for various technological applications such as hydrogen production and storage, which will be addressed in future work.

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