Structural phases of nanostructured sodium titanates obtained in different synthesis conditions: a theoretical study

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Nanostructured sodium-based titanates are very promising materials for energy storage and photo-electronic applications. These structures can be obtained by the hydrothermal method developed by Kasuga [1,2]. Hydrothermal synthesis conditions, such as temperature, time and pH, can modify the internal structure and morphology of nanostructures obtaining: nanoparticles, nanotubes and nanorods. As it was presented in [2, 3], temperature, time and pH conditions of hydrothermal treatment influence the morphology, structural, electrical, and optical properties of these compounds. The present work is a theoretical approach based on first principles simulations to understand the structures that are formed and the vibrational and structural properties that are obtained. For the construction of the initial model, we used two paths. First, we assumed phases previously reported in literature linked to the precursors of the synthesized titanates. However, these phases fail to explain the complete behavior of the samples experimentally obtained. In search of new clues about the possible structures that can form the samples (building blocks), we perform X-ray diffraction measurements after the materials have been subjected to a high-temperature thermal process. We found that mostly hexa ($(Na,H)_2Ti_6O_{13}$) and tri ($(Na,H)_2Ti_3O_7$) titanates of hydrogen or sodium are present. Calculations were made on these structures based on first principles in the bulk material and then utilized to build atomistics models on the proposed nanostructures. The results obtained from the theoretical calculations attempt to explain the properties measured as X-ray diffraction, Raman spectroscopy and optical measurements of nanostructures experimentally obtained.

[1] Kasuga, T., Hiramatsu, M., Hoson, A., Sekino, T., & Niihara, K. (1999). Titania nanotubes prepared by chemical processing. Advanced materials, 11(15), 1307-1311.

[2] Amy, L., Favre, S., Gau, D. L., & Faccio, R. (2021). The effect of morphology on the optical and electrical properties of sodium titanate nanostructures. Applied Surface Science, 555, 149610.

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