

**MS34-1-2 Nucleation and growth of  $\alpha$ -Ti(HPO<sub>4</sub>)<sub>2</sub>·H<sub>2</sub>O single crystal and its unprecedented structure determination from X-ray single-crystal data**  
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Z. Amghouz<sup>1</sup>, R. Mendoza-Merono<sup>2</sup>, S. García-Granda<sup>2</sup>, A. Adawy<sup>3</sup>

<sup>1</sup>Department of Material Science and Metallurgical Engineering, University of Oviedo - Gijón (Spain), <sup>2</sup>Department of Physical and Analytical Chemistry, University of Oviedo - Oviedo (Spain), <sup>3</sup>Unit of Electron Microscopy and Nanotechnology, Institute for Scientific and Technological Resources, University of Oviedo - Oviedo (Spain)

**Abstract**

$\alpha$ -Titanium phosphate phase  $\alpha$ -Ti(HPO<sub>4</sub>)<sub>2</sub>·H<sub>2</sub>O ( $\alpha$ -TiP) is a tetravalent metal phosphate that has recently gained a special interest in biomedical application owing to its exceptional biocompatibility and ability to be loaded with antimicrobial agents [1-4]. As reported earlier,  $\alpha$ -TiP tends to crystallize into microcrystalline powder that allowed its structural determination using neutron powder diffraction [5]. Here, we report that nucleation and crystallization of single  $\alpha$ -TiP crystals with suitable dimensions (>50 $\mu$ m) for single-crystal X-ray diffraction could be effectuated using a hydrothermal treatment of a metallic titanium (Ti-6Al-4V alloy) in high concentrations of phosphoric acid solutions. Accordingly, the single-crystal X-ray diffraction analysis could be performed and revealed its crystalline structure in a monoclinic space group, P21/c, with  $a=8.6288(5)$  Å,  $b=5.00546(17)$  Å,  $c=19.1468(11)$  Å, and  $\beta=127.555(9)^\circ$ . Although the space group is similar to that previously reported from the neutron powder diffraction [5], the obtained unit cell is considerably larger. A bulk of the obtained crystals were subjected to through analyses using polarization microscopy, scanning electron microscopy combined with energy dispersive X-ray spectroscopy (SEM-EDX), and thermal analysis (TG/SDTA-MS, DSC) and the results confirmed that the obtained crystals bear the general structural properties of the polycrystalline powder.

**References**

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