Poster

Further insights into the factors influencing the Anatase-Rutile Phase Transition for potential distributed temperature measurements

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High temperature responsive materials have assumed a significant role in advanced technological applications such as microelectronics, cell biology, and diagnostics for their potential use in thermometry. [1] Therefore, investigating the phase transformation process in relation to temperature may be of real importance for developing innovative materials suitable for applications involving, for example, elevated temperatures.

In particular titanium dioxide is widely used in energy and environmental applications (e.g. as gas sensor, photocatalyst, dielectric, and ceramic membrane). [2] It exists in the form of three main polymorphs: anatase and brookite are metastable and can transform in the thermodynamically stable rutile phase. In particular anatase converts to rutile within a temperature range of 400 to 1200°C, depending on various parameters that affect the temperature and the kinetic of the phase transition. [3] The occurrence of this phase shift can significantly impact the properties and efficacy of the final applicative devices. Therefore, the knowledge of the influencing factors, such as the presence of impurities, dopants, morphology and size of the particles, preparation method, heat flow condition, and their control are crucial in managing the anatase-rutile transition for various applications in high-temperature procedures [4,5,6]. Thus, comprehending the effect of such parameters on the stabilities of TiO_2 polymorphs, along with the kinetics of their phase transition and the associated governing mechanism, can be very useful for designing desired single-phase or multiphase microstructures suitable for specific applications. Anatase-rutile transformation is not only strongly dependent on temperature but also time is a parameter to be considered. Indeed, the kinetics of the transformation must be interpreted in terms of all the factors that influence the requisite temperature-time conditions.

We present here the results of systematic PXRD investigations on the anatase-rutile transition phase of a commercial TiO_2 powder. In particular the particle size of the starting powder and the heating duration time were considered as variables to explore their impact on the transformation process aiming to investigate the potential for controlling the temperature range on the anatase-rutile ratio.

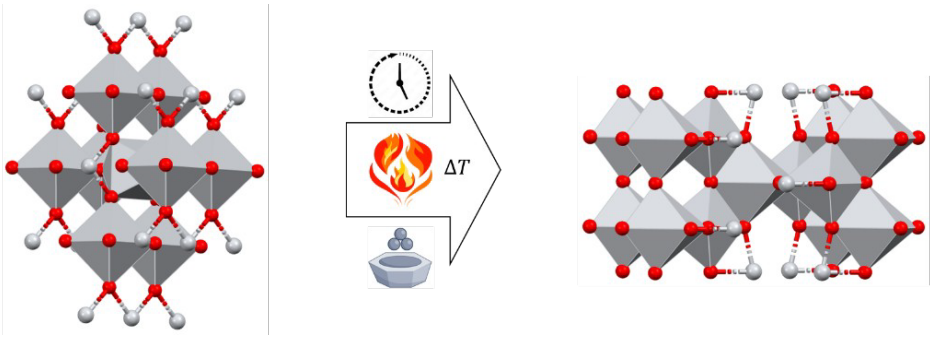

Figure 1. Crystal packing of anatase (left) and rutile (right) forms and the representation of the investigated parameters affecting the phase transition.

[1] M. Zare, K. S. Mikkonnen, *Adv. Funct. Mat.* **2023**, 33, 12, 2213455.

[2] Janus, Magdalena, ed. Application of titanium dioxide. BoD–Books on Demand, **2017**.

[3] Z. Hiroi, *Inorg. Chem*. **2022**, 61, 22, 8393–8401

[4] S. R. Yoganarasimhan, C. N. R. *Rao, Trans. Faraday Soc.* **1962**,58, 1579-1589.

[5] R.D. Shannon, J.A. Pask, *J, Am. Ceram. Soc.* **1965**, 48, 8, 391-398.

[6] H. Albetran, I.M. Low, *Abbreviation: Mater. Today Proc.* **2019**, 16, 25-35.