X-ray Diffraction Study of Thermal Properties of Titanium Oxide

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Temperature dependence of microstructure of titanium oxide, TiO_2, and the phase transition of anatase (**A**) to rutile (**R**) were studied by *in situ* X-ray powder diffraction and Raman spectroscopy, as well as by TEM and SAED techniques. The as-synthesized TiO_2 p.a. showed a gradual transition **A** $\rightarrow$ **R** during the temperature increase from ≈1200 K to ≈1570 K and during the temperature decrease to ≈600 K. High-energy ball-milling at room temperature induced a partial transition **A**$\rightarrow$**R**. The transition continued during the temperature increase to ≈1370 K and during the temperature decrease, and is accompanied by sharpening of diffraction lines. Anisotropy of thermal expansion was noticed for both **A** and **R**. In the transition **A**$\rightarrow$**R**, the nuclei of **R** are formed either throughout the **A** crystallites (in case of as-synthesized TiO_2 p.a.) or mainly in the interior of the **A** crystallites (in case of milled TiO_2 p.a.). These nuclei grow in number and size with a prolonged time of thermal agitation.

Keywords: titanium oxide, phase transition, thermal expansion