Structural and microstructural study of brookite based TiO2 nanocomposites with carbon black (C)

**Aleksandar Kremenović** 1, Mirjana Grujić-Brojčin 2, Nataša Tomić 2, Maja Šćepanović 2

*1 Faculty of Mining and Geology, University of Belgrade, Belgrade, Serbia
2 Institute of Physics, University of Belgrade, Belgrade, Serbia*

Structural and microstructural properties of TiO2-based nanocomposites with carbon black (C), synthesized by sol-gel-hydrothermal method, have been studied by XRPD and Raman scattering. Detailed size-strain analyses of XRPD and Raman scattering results are presented in order to investigate the influence of C content on brokite and anatase phase formation. The XRPD size-strain analyses have resulted in reliable structure and microstructure results for both anatase and brookite and their relative abundance ratio has been refined by Rietveld method. The brookite and anatase crystallite sizes are estimated by XRPD at ~ 27–29 and 14–17 nm, respectively. The Raman spectra of all samples are dominated by the most intensive modes of anatase (*Eg*) and brookite (*A*1*g*). The analysis of anatase *Eg* mode by PCM (Phonon Confinement model) has revealed partial compensation of phonon confinement due to anatase nanocrystallite size and tensile deformation of anatase lattice. The refined unit cell parameters obtained from XRPD have shown that C atoms did not enter in the significant amounts into brookite and anatase crystal structures. On the other side, the Raman spectra have revealed features assigned to carbon. The results of both analyses imply that the presence of carbon could influence the formation of brookite and anatase phase in the TiO2-based nanocomposites synthesized by the hydrothermal method [1].

[1] A. Kremenović, M. Grujić-Brojčin, N. Tomić, V. Lazović, D. Bajuk-Bogdanović, J. Krstić, M. Šćepanović, Size-strain line broadening analysis of anatase/brookite (TiO2) based nanocomposites with carbon (C) – XRPD and Raman spectroscopy, *Acta Crystallographica* ***B***, in press.

**Keywords: size-strainline broadening; XRPD; Raman spectra; phonon confinement model**