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Editors
Jelena **MILOVANOVIĆ**
Vuk **FILIPOVIĆ**
Života **SELAKOVIĆ**
Snežana **PAPOVIĆ**
Branko **KORDIĆ**
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

Page Layout and Design
Jelena **KESIĆ**
Mila **LAZOVIĆ**
Mihajlo **JAKANOVSKI**

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Development and Research Centre of Graphic Engineering
Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

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ИНОВАЦИЈА

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Contents

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The influence of dopants on anatase-rutile phase transition

Natalija D. Milojković[1], Bojana M. Simović[2], Milan M. Žunić[2], Aleksandra H. Dapčević[1]

[1] *University of Belgrade - Faculty of Technology and Metallurgy, Belgrade, Serbia*
[2] *University of Belgrade - Institute for Multidisciplinary Research, Belgrade, Serbia*

Titanium dioxide exists in three different crystalline forms: anatase, rutile, and brookite. It is well known that on heating, anatase and brookite can be easily transformed to rutile which is considered as the most stable phase [1]. The aim of this study was to investigate the influence of different dopants on anatase-rutile phase transition. Doped TiO_2 samples (TiO_2-*M*, *M* = V, Mn, and Cu) containing 5 at% of the dopant were prepared by mixing anatase and appropriate oxide (V_2O_5, MnO_2, and CuO) in agate mortar for 30 min. In order to determine the heat treatment conditions, TG/DTA analysis of the samples was performed. Finally, mixed powders as well as the pure anatase phase (TiO_2) were heat treated at 700 ˚C for 3 h. XRD analysis was performed to estimate the phase composition, unit cell parameters, and crystallite sizes. Rutile was formed in all samples: 2.8 wt% in TiO_2, 25.5 wt% in TiO_2-Mn, 75.8 wt% in TiO_2-V, and 95.2 wt% in TiO_2-Cu. In TiO_2-Mn, TiO_2-V, and TiO_2, anatase was present beside rutile, while in the case of TiO_2-Cu 4.8 wt% of the unreacted CuO was found. Obtained results revealed that all the dopants accelerated anatase-rutile phase transition in the following order: $Cu^{2+} > V^{5+} > Mn^{4+}$. It is well known that defects are the driving force for the anatase-rutile phase transition and since Ti^{4+} and Mn^{4+} are isovalent, no new defects were formed by incorporating Mn^{4+} ions into TiO_2 lattice. This resulted in the least amount of rutile in TiO_2-Mn comparing to TiO_2-V and TiO_2-Cu where new defects were probably formed. As no initial oxides were found in TiO_2-Mn and TiO_2-V, it can be concluded that Mn^{4+} and V^{5+} ions were incorporated into the anatase lattice. On the other hand, in the case of TiO_2-Cu, even 4.8 wt% of initial CuO was found. The detected residue of CuO can be explained by the fact that the ionic radius of Cu^{2+} for an octahedral environment (0.870 Å) is much larger than that of Ti^{4+} (0.745 Å), unlike those for Mn^{4+} (0.670 Å) and V^{5+} (0.680 Å). Although almost all introduced quantity of CuO, i.e. 96 %, was found in TiO_2-Cu, a small amount was surely necessary to cause the anatase-rutile phase transition. According to calculated crystallite sizes which were in the range of 55 – 90 nm, nanocrystalline samples were prepared.

References

1. P. I. Gouma, M. J. Mills *J. Am. Ceram. Soc.* **2001**, *84* (3) 619–622.