Structural and optical properties of sol-gel synthesized TiO2 nanocrystals: Effect of Ni and Cr (co)doping

O. Ruzimuradov,

K. Musaev,

S. Mamatkulov,

K. Butanov,

I. Gonzalo-Juan,

L. Khoroshko[1],

N. Turapov,

S. Nurmanov,

J. Razzokov,

V. Borisenko[1],

R. Riedel

2023

[1]Belarusian State University of Informatics and Radioelectronics, 6 P. Brovki Street, Minsk 220013 Belarus

Keywords: TiO_2, metal doping, co-doping, band-gap energy, photoluminescence.

Abstract: Nickel and chromium metal ions have been utilized to dope and co-dope titanium dioxide nanocrystals, thereby broadening the light absorption range of titania into the visible light spectrum. The doped and

co-doped TiO_2 nanocrystals were prepared using sol-gel techniques, with a varied doping concentration that extended from 0.25 to 10.0 wt%.These modified materials underwent comprehensive analysis using standard analytical tools such as X-ray diffraction, Raman spectroscopy, BET surface area measurement, Fourier transform infrared spectroscopy, UV–vis diffuse reflectance spectroscopy, and fluorescence spectroscopy. Powder XRD technique reveals that the modified catalyst majorly contains the anatase polymorph with the transition metal ion either substituting Ti or located as interstitials in the lattice of TiO_2. Raman and UV–Vis absorption spectra of the doped and codoped catalyst a show λmax shift towards longer wavelength when in the metal ion concentration is increased from 0.25 to 10 wt%. FTIR patterns show the stretching and vibration patterns of hydroxyl radicals present in the nanocrystals. The BET surface areas of the doped and codoped TiO_2 nanocrystals have substantially higher surface areas compared with that of the undoped TiO_2. Electronic structural studies of the TiO_2, $(Ti,Cr)O_2$, $(Ti,Ni)O_2$, and $(Ti,Ni,Cr)O_2$ crystals using density functional theory indicated a reduction in the band gap width (E_g) of pure TiO_2 when doped with transition metals. Specifically, the indirect bandgap values for Ni(10%), Cr(10%) and NiCr(5% + 5%) doping were 2.96, 2.83, and 2.7 eV, respectively. Furthermore, the photoluminescence intensity substantially decreased with the incorporation of transition metal ions in the TiO_2 nanocrystals.

Structural and optical properties of sol-gel synthesized TiO2 nanocrystals: Effect of Ni and Cr (co)doping / O. Ruzimuradov [et al.] // Optical Materials. – 2023. – Vol. 143. – P. 114203.