



Toetab TÜ ja TTÜ doktorikool “Funktsionaalsed materjalid ja tehnoloogiad”(FMTDK)

*ESF projekt 1.2.0401.09-0079*

# Investigation of nickel-doped titania thin films deposited on native oxide covered Si(100) substrate by the sol-gel method

U. Joost[1,2], R. Pärna[1], E. Nõmmiste[1], T. Käämbre[1], A. Kikas[1], I. Kuusik[1], M. Hirsimäki[3], I. Kink[1,2] and V. Kisand[1]

[1]Institute of Physics, University of Tartu, Riia 142, 51014 Tartu, Estonia
[2]Estonian Nanotechnology Competence Center, Riia 142, 51014 Tartu, Estonia
[3]Surface Science Laboratory, Tampere University of Technology, P.O. Box 692, FIN- 33101, Tampere, Finland

Titania ($TiO_2$) is a material that has attracted great attention for many advanced applications using the sunlight. It has been studied extensively as a promising photocatalyst [1], solar energy cell material [2], antifogging and self-cleaning coating [3,4]. Unfortunately, it absorbs only a fraction of sunlight, which restricts the use of titania. One effective method proposed to enhance the absorption properties of titania is to dope it with anions or cations [5-8]. The key idea here is that the doping modifies the electronic structure, which would effectively shrink the band gap. A narrower band gap offers more effective electron-hole pair generation and it might extend the lifetime of electron-hole pairs, which is especially important for the applications using sunlight [9]. One promising dopant is nickel - nickel doping has effectively increased the photocatalytic activity of a titania film [10].

Nickel-doped titania thin films have been prepared on methanol-cleaned $SiO_2$/Si(100) substrate by using the sol-gel deposition and annealing in the air at 450 to 1150 °C. Several experimental techniques (Atomic Force Microscopy, X-ray Diffraction, X-ray Reflection, Raman spectroscopy, Energy Dispersive X-ray Analysis, X-ray Photoelectron Spectroscopy, X-ray Absorption Spectroscopy, UV-VIS Spectroscopy and Hydrophilicity measurements) have been applied to characterize these films. Further, the results of this study were compared to previous investigated nickel-doped titania on HF-etched Si(100). The morphological and structural properties of nickeldoped titania were found to be dependent on the kind of the substrate on which the films were prepared. The thin films deposited on $SiO_2$/Si(100) were more uniform, had smaller RMS roughness, better crystalline and an anatase transformation to rutile phase occurred at 150 °C lower temperature compared to films on HF-etched Si(100). Nickel in the films appeared to be in the 2+ oxidation state, mainly in the $NiTiO_3$ phase. Its compounds segregated to the surface of the film, forming islands. Nickel doping red-shifted the titania fundamental absorption edge further into the visible range. We demonstrated that a well-crystallined anatase was crucial for obtaining a good light-induced hydrophilic nickel-doped titania surface.