s8.m28.p4 **Thermal Behaviour of Nanocrystalline SnO_2 Doped with Antimony.** B. Grzeta[a], E. Tkalcec[b], M. Takeda[c], M. Takahashi[c], [a]*Rudjer Boskovic Institute, P.O. Box 180, HR-10002 Zagreb, Croatia;* [b]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulicev trg 20, HR-10000 Zagreb, Croatia;* [c]*Department of Chemistry, Faculty of Science, Toho University, Funabashi, Chiba 274-8510, Japan. E-mail: grzeta@rudjer.irb.hr*

Keywords: Sb-doped tin oxide; X-ray diffraction; Mössbauer spectroscopy

Tin oxide, SnO_2, is a wide-band gap semiconductor. It is widely used in electronic devices. When doped with F, Sb, or Mo it becomes a conductor. In the case of antimony doping it was evidenced that the conductivity was not linearly dependent on the doping level [1]. So, there is an inevitable interest to understand this phenomenon. Recently a structural study of hydrothermally prepared nanocrystalline SnO_2 samples doped with Sb was performed by X-ray diffraction (XRD) and Mössbauer spectroscopy [2]. Samples contained up to 14.0 at% Sb. Diffraction lines were broadened, the line broadening being anisotropic. Both the line broadening and line anisotropy were dependent on the Sb doping level. The samples were tetragonal, with TiO_2 (rutile)-type structure [3], in the space group $P4_2/mnm$. Sb doping of SnO_2 caused an increase of unit-cell parameters. Crystal structure indicated that in the Sb-doped samples both Sb^{3+} and Sb^{5+} ions were substituted on Sn^{4+} sites in the SnO_2 lattice, Sb^{3+} being dominant for the examined samples. Mössbauer spectroscopy confirmed the XRD results. The aim of the present work is to examine the influence of thermal treatment on the Sb-doped SnO_2 samples containing 4 and 8 at% Sb. The samples were thermally treated at 350, 450 and 550 oC for 1 hour, then slowly cooled to RT and examined by XRD and by ^{121}Sb-Mössbauer spectroscopy. Unit-cell parameters of the annealed samples decreased with the increase in thermal treatment temperatures for both Sb contents. This suggested that oxidation of the antimony ion Sb^{3+} took place in the annealing process. Mössbauer spectroscopy showed that Sb^{3+}/Sb^{5+} content ratio in the samples decreased upon annealing. The line broadening in XRD pattern increased up to 350 °C, then decreased upon further heating. On the other hand, the line anisotropy decreased over the whole temperature range. It was noticed that the ratio of full-widths at half-maximum (FWHM) for the diffraction lines 110 and 101 is directly proportional to the Sb^{3+}/Sb^{5+} content ratio in the samples.

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[3] Baur, W. H. (1956). *Acta Cryst.* A**9**, 515-520.

s8.m28.p5 **Microstructure of Severely Deformed Mg(Al) Alloys from X-Ray Diffraction Peak Profile Analysis.** Jenő Gubicza[a] and Nguyen Hoang Nam[a], [a]*Department of Solid State Physics, Eötvös University, Budapest, Hungary. E-mail: gubicza@ludens.elte.hu*

Keywords: Dislocation structure; Crystallite size; Mg(Al) alloy

Severe plastic deformation (SPD) is an effective tool for producing bulk ultrafine grained (submicron grain sized or nanostructured) metals. One of the most common SPD methods is equal channel angular pressing (ECAP) - a technique that results in a homogeneous sub-micron grain structure of the workpiece [1]. The ultrafine grained materials produced by ECAP have an attractive combination of high strength and good ductility due to their low contamination and unique structures. For understanding the mechanical behavior of materials produced by ECAP, it is necessary to characterize their microstructure. In this work the microstructure of Mg(Al) alloy produced by ECAP is studied by X-ray diffraction peak profile analysis. The high resolution X-ray diffraction experiments are performed using a special double-crystal diffractometer (Nonius FR591) with rotating Cu anode [2]. The peak profiles are evaluated by the Multiple Whole Profile (MWP) fitting procedure described in detail in Ref. [3]. In this method, the Fourier coefficients of the experimental profiles are fitted by the theoretical Fourier transforms calculated on the basis of a model of the microstructure [3]. The crystallite size distribution and some characteristic parameters of the dislocation structure (e.g. density and arrangement of dislocations) are obtained from the fitting. Additionally, the procedure enables the determination of the prevailing dislocation slip systems in the sample [4]. The eleven dislocation slip systems in a hexagonal Mg alloy can be classified into three groups based on their Burgers vectors: <a> type, <c> type and <c+a> type [5]. X-ray diffraction peak profile analysis reveals the abundance of <a>-type dislocations besides the <c>- and <c+a>-type dislocations in the ECAP deformed Mg alloy. The correlation between the microstructure and the room and high temperature mechanical behavior is also studied and discussed.

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