MS46-P2 Highly-Oriented and Stressed Nanocrystalline ZnO Films Prepared by Pulsed Laser Deposition. Radomír Kužel,[a] Jakub Čížek,[b] Michal Novotný,[b] [a]*Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic* , [b]*Institute of Physics, Academy of Sciences of the Czech Republic*
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ZnO thin films were grown by pulsed laser deposition (PLD) on three different substrates: sapphire (0001), MgO (100) and fused silica (FS). The structure and morphology of the films were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) and defect studies were made using slow positron implantation spectroscopy (SPIS) [1]. SEM pictures showed the films to be nanocrystalline with lateral size of the grains within the range of 20-70 nm. The thickness of films determined by optical reflectance, X-ray reflectivity and SPIS were about 80 nm on MgO and FS substrates. The film deposited on sapphire was thinner (40 nm). All the films exhibited wurtzite ZnO structure but their microstructure was very different. Standard glancing-angle parallel beam diffraction used routinely for analysis of nanocrystalline thin films nor symmetric Bragg-Brentano diffraction were sufficient for characterization of the films. A combination of different XRD scans with the use of the Eulerian cradle was required for revealing of main structural features. The film deposited on FS showed fiber (000l) texture characterized by the FWHM of rocking curve of about 10°. The film grown on MgO indicated even stronger (000l) texture (FWHM below 1°) and phi-scans of asymmetric diffraction planes detected local epitaxy in a form of domains with two different orientations. Surprisingly, 40nm thick film on sapphire didn't show this expected (000l) texture but more complicated orientation of several domains epitaxially grown on the substrate, probably due to very small thickness. Extremely high compressive in-plane stress in the film on MgO was detected (more than 10 GPa) by mapping of diffraction spots. The films on sapphire and FS were stress-free and in tensile stress (1 GPa), respectively. XRD line broadening was analyzed by combination of different asymmetric scans and crystallite size and microstrain were estimated from the Williamson-Hall plots constructed for the combination of these diffraction planes inclined differently with respect to the surface. SPIS revealed high density of open-volume defects in films on MgO and sapphire. Some methodological aspects of XRD studies of thin nanocrystalline films with strong preferred orientation were discussed.

[1] M. Novotný et al. (2012). *Journal of Physics D.* **45**, no. 22 in press.

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MS46-P3 Simulation of X-ray diffraction line broadening caused by stress gradients and determination of surface stress distribution by Fourier analysis. V.I. Monin[1], J. T. Assis[1], S.M.Iglesias[2], [1] *Politechnic Institute of Rio de Janeiro State University, Nova Friburgo-RJ, Brazil,* [2] *State University de Santa Cruz, Ilhéus, Brazil.*
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Different physical, mechanical and chemical processes like ion implantation, oxidation and others create on the surface of materials residual stress state characterized by high level and strong gradient. X-ray diffraction method widely used for stress measurements has some difficulties in interpretation of experimental data when the depth of X-ray penetration is compared with thickness of surface layer where inhomogeneous stress distribution is localized. Early it has been shown [1] that diffraction line broadening occurs when analyzed surface is characterized by strong gradient. The interest to study the diffraction line broadening is connected with possibility to obtain information about parameters of surface stress distribution. In the present paper the convolution and deconvolution concepts of Fourier analysis were applied to study X ray diffraction line broadening caused by surface stress gradients. Developed methodology allows determining of stress distribution when the surface stresses characterized with strong gradient.

[1] Monin, V.I., Assis, J.T. & Philippov, S. A. (2004). *SPIE* v. 5400, 196-199.

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