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STUDY OF THIN FILMS AND NANOMATERIALS AT FACULTY OF MATHEMATICS AND PHYSICS, CHARLES UNIVERSITY IN PRAGUE

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Some details from the X-ray group history can be found in [1]. X-ray analysis was one of the main activities of the Department of Solid State Physics from the very beginning of the Faculty of Mathematics and Physics (founded 1951). The X-ray group was headed by Doc. Josef Šedivý (1951-1985) and then by Prof. Václav Valvoda who was also active in the CSCA as a scientific secretary. In the sixties and seventies, the main focus was given to carbides and nitrides and lattice vibrations studies. Since 1985 intensive studies of nitride thin films, in particular TiN, were performed. Then different streams were followed by individual members - magnetic multilayers, materials deformed by severe plastic deformation, diffusion studied by XRD, quarternary intermetallic compounds, materials with functional gradient of composition, intercalates, high-temperature superconductors, nanocomposites, ferroelectrics etc.

During the last decade, significant update of X-ray instruments was achieved. The laboratory has several new systems - *modern complex diffractometer for investigation of thin films - MRD X'Pert Pro* (Philips) equipped with several optical modules for measurements in different resolution: parabolic Goebel mirror, two four-crystal monochromators, parallel plate collimator, graphite monochromator, triple axis germanium monochromator. The sample holder is placed on the large Eulerian cradle for measurement of stress and texture using also polycapillary optics .

Vertical Panalytical diffractometer X'Pert Pro has several options. For room temperature measurements, the specimen is placed on the *xyz* table with -rotation and inclinations. For conventional symmetric scans, variable slits are used to keep the analyzed specimen area fixed. In the diffracted beam either point detector with monochromator or linear position detector PIXCel can be used. The latter is applied for fast data collection, in particular at non-ambient temperatures and also for line profile analysis requiring low-noise data. Combined parallel-focusing geometry in double-mirror setup is useful for rough surfaces or non-flat specimen. *MRI high-temperature* chamber with both direct and radiant heating can replace the table.

Bruker D8 Avance diffractometer is used for standard powder diffraction and it is equipped with variable slits and Sol-X solid state detector for supression of fluorescent background.

HZG-4 goniometer from Freiberger Präzisionsmechanik is now used for collection of full patterns with Mo radiation.

A new *Rigaku Rapid II system with a cylindrical 2D image plate detector* is designed for collection of single crystal data and structure determination but also for microdi ffraction and very fast collection of Debye-Scherrer patterns. The system is also useful for the analysis of samples containing large grains.

There are several directions of the research nowadays. The X-ray lab participates in an European project on magnetic semiconductors, the investigation of structure of diluted magnetic semiconductors (GaMnAs, GeMn, GaFe N). In the case of GaMnAs in particular we determine the concentration of magnetic Mn ions in various lattice positions (substitutional, interstitial) by anomalous X-ray diffraction and X-ray stading wave method. We study also strain relaxation in laterally patterned magnetic epitaxial layers by high-resolution X-ray diffraction. Another international project deals with in-situ investigation of epitaxial layers of GaN during deposition. Our task is to develop a method for the determination of densities of various types of threading dislocations by X-ray reciprocal space mapping of diffuse scattering. In the field of nanophysics, we study of structure of semiconductor nanoparticles embedded in amorphous matrix by grazing-incidence small angle scattering and diffraction during magnetron deposition and post-growth annealing. We use the DAFS method for the investigation of local chemical composition of semiconductor quantum dots (GeSi, InGaN).

Other directions follow past investigations and methodological development. In collaboration with other departments of the faculty and TU Freiberg, microstructural studies of submicrocrystalline materials obtained by severe plastic deformation are performed by several complementary methods – XRD line profile analysis, TEM, positron annihilation spectroscopy, mechanical testing and EBSD. Anotother stream consists in complex XRD characterization of thin polycrystalline films of different type. The main attention has been given to TiO_2 films, stress analysis, time and thickness dependence of crystallization by in-situ measurements high-temperature studies.

Many studies of different nanocrystalline powders are performed as well. Successful testing of possibility of measurement of pair distribution function of nanocrystalline powders in laboratory conditions was done recently. A new software MStruct for whole pattern fitting suitable for the above analysis (nanomaterials, thin films) was developed by Z. Matěj.

The X-ray lab is frequently used by our colleagues from the group of magnetic properties of the department for several tasks - single crystal quality assesment and orientation, phase analysis and Rietveld analysis of different intermetallic compounds with interesting magnetic properties.

1. V. Valvoda, *Materials Structure*, **8** (2001) 104-105.

full contribution will be published in next issue