they could use a portfolio of all symbols and it was then sufficient to move specific symbols to relevant positions. A similar way was used for space groups (complete diagrams of general positions with symmetry elements or vice versa complete diagrams of symmetry elements with general positions, determination or estimation of the space group)

A little more complicated was preparation of *online practical course*. This is the basic problem of powder diffraction – determination of lattice parameter of unknown cubic phase and then also phase analysis of mixture of 3-6 phases. Since, the task consists mainly in evaluation, it was decided to adopt this also to online form. This practical part always begins with a short excursion in X-ray laboratory showing them a few instruments, description of powder diffractometer, preparation of different samples, specimen alignment and automatic measurement in symmetrical scan. So, everything was recorded to video and what was only missing for students was their own specimen preparation. This is followed by demonstration of fast evaluation of powder pattern and generation of a file with peak parameters. Students used this output (each with different parameters) to index peaks according to procedure described on web link and determined the lattice parameter considering the instrumental aberrations. The first part is closed by looking into the Powder Diffraction File in order to find the phase. However, usually it is not found because the lattice parameter deviates from the database value from some reason. This reason is discussed.

In the second part, the pattern was evaluated in different software, the list of peaks was generated (2 , d, I) and the students obtained scanned education edition of Hanawalt index and made the search. Finally, for homework, the students should download 30-days trial of program Match and use it for the phase analysis of the mixture. Each of the students received different dataset.

Finally, I think that such tools can be well used for teaching even if, hopefully, we will come back to more or less normal time.

Session V, Friday, November 27

L16

BASHELIXIR HAS NEW FEATURES AND NEW GUI

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Many computational tools to perform experimental phasing have been developed. Most of them are concentrated in the *CCP4* [1] and *PHENIX* [2] program packages. Recently, the command-line tool *baSHELiXir* [3] has been published to provide fast and efficient phasing protocols linked to the application of the *SHELX C/D/E* [4,5] program package. The program independently enables searches for the correct space group, screening of the solvent content parameter and high- and low-resolution diffraction limits. In *baSHELiXir*, *SHELXE* processes are parallelized to reduce the computational time and provide a thorough analysis of the computational results based on provided data.

Several cases have been selected to demonstrate the full applicability and capacity of *baSHELiXir*. They cover single-wavelength anomalous dispersion, multiple-wavelength anomalous dispersion with two to five datasets collected at different wavelengths, single isomorphous replacement with anomalous scattering and radiation-damage-induced phasing protocols.

baSHELiXir is a powerful tool for a thorough analysis of experimental phasing information contained in crystallographic data. It is simple to use from the command line. Moreover, a graphical user interface has been developed for easier launching of the analysis.

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L17

THE CRYSTAL STRUCTURE OF THE FIRST HALOALKANE DEHALOGENASE TETRAMER

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Haloalkane dehalogenases (EC 3.8.1.5) are microbial enzymes that catalyze the breakdown of halogenated compounds resulting in a halide ion, proton and alcohol. These enzymes are applied in industrial catalysis, bioremediation and biosensing of environmental pollutants. Novel haloalkane dehalogenase DpaA that belongs to the superfamily of / hydrolases was isolated from a psychrophilic and halophilic bacterium *Paraglaciecola agarilytica* NO2 found in marine sediment collected from the East Sea, Korea. Here, we report its crystallization and X-ray diffraction data analysis. DpaA was crystallized using the sitting drop vapor diffusion method. Two independent crystallization and data collection experiments resulted in several data sets with the resolution ranging from 2.2 to 3.0 Å and from 2.5 to 3.17 Å, respectively. During structure solution DpaA shows interesting structural properties of its tetramer conformation and its interactions between individual chains. The difficulties during initial data processing and the right space group determination reveal the presence of pseudotranslation at every collected data set, which required further investigation and improvements of the existing model. Finally, merohedral twinning and subsequent structure modeling and refinement resulted in a tetrameric model of DpaA, highlighting an uncommon multimeric nature for a protein belonging to the HLD-I subfamily.

This research is supported by the Grant Agency of the Czech Republic (grant No. 17-24321S); DAAD mobility grant (grant No. DAAD-16-09); European Regional Development Fund-Project (grant No. CZ.02.1.01/0.0/0.0/15_003/0000441; grant No. CZ.02.1.01/0.0/0.0/16_019/0000778; grant No. LM2015047; grant No. LM2018121); GAJU (grant No. 017/2019/P); Czech Ministry of Education (grant No. CZ.02.1.01/0.0/0.0/16_026/0008451).

L18

ADVANCED BIOLOGICAL APPLICATIONS OF SAXS IN-HOUSE

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Small angle X-ray scattering (SAXS) serves as one of the complementary methods of structural biology. SAXS allows both characterization and low resolution structural studies of macromolecules, with advantage of liquid samples. Several such complementary methods can be directly coupled with SAXS. Thanks to the high flux X-ray sources like MetalJet (Excillum), these applications are now possible not only at sunchrotrons, but also in-house. Here, in situ UV-Vis absorbtion spectroscopy and size exclusion liquid chromatography coupled with SAXS, as available in Centre of Molecular Structure, will be presented.

Centre of Molecular Structure is equipped with SAXSPoint 2.0 (Anton Paar) instrument with MetalJet C2+ X-ray source and Eiger 2M detector. Samples can be loaded to variety of the capillaries using an autosampler. The set of temperature controlled sample stages include low noise cell and capillary capable of in situ UV/Vis absorption spectrometry. Recently, a dedicated liquid chromatography system AktaGo (GE Healthcare) was introduced.

The Centre of Molecular Structure is supported by: MEYS CR (LM2018127); project Czech Infrastructure for Integrative Structural Biology for Human Health (CZ.02.1.01/0.0/0.0/16_013/0001776) from the ERDF; UP CIISB (CZ.02.1.01/0.0/0.0/18_046/0015974), a ELIBIO (CZ.02.1.01/0.0/0.0/15_003/0000447).

Session V, Friday, November 27

L19

INTRODUCTION TO NANOTOXICOLOGY

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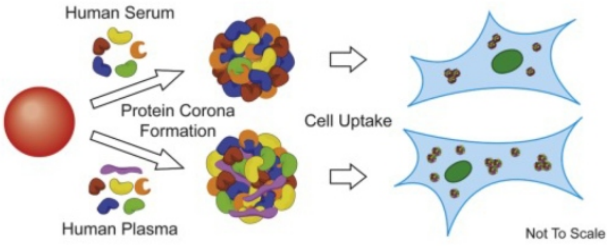
The nanoparticles are widely used not only in laboratories but also in our households. They are just everywhere we look. We add them to the food, medical products, cosmetics etc. We are actually making so much nanoparticles that they become significant pollutant of our natural environment. This stands in contrast with nature made nanoparticles - their quantity is 9x higher but they are natural part of environment and are not causing significant problems.

In this talk I would like to concentrate on the tools and methods of studying the nanotoxicity of nanomaterials and interaction of nanomaterials with the biological environment. Especially I would like to speak about protein corona formation and its influence on the nanoparticle destiny in the biological environment. I would like to address the key properties of nanoparticles which are influencing their toxicity. For example: size, shape, surface charge, surface groups and composition.



L20

STRUCTURE AND MICROSTRUCTURE OF ROTARY-SWAGED W-Ni-Co PSEUDOALLOY STUDIED BY NEUTRON DIFFRACTION

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Tungsten heavy alloys (THAs) are two-phase composites consisting of tungsten particles/agglomerates surrounded by a ductile matrix [1]. Due to their superb mechanical properties and high specific mass, tungsten heavy alloys are used in demanding applications, such as kinetic penetrators, gyroscope rotors, or radiation shielding. Effective structure refinement can be introduced via methods of severe plastic deformation. However, their structure, consisting of hard tungsten particles embedded in a soft matrix, makes the deformation processing a challenging task.

This study focused on the characterization of deformation behaviour during thermomechanical processing of a W-Ni-Co tungsten heavy alloy (THA) via the method of rotary swaging at various temperatures. Rotary swaging is an intensive plastic deformation method advantageously used in the industry to gradually reduce cross-sections and increase lengths of axisymmetric workpieces [2].

The primary aim was to determine microstrain and characterize the dislocations and active slip system in the original sintered THA as well as in the rotary swaged bars, in order to characterize the effects of thermomechanical treatment on the microstructure. Emphasis was given on the investigation by neutron diffraction. Characterization of advanced materials by neutron powder diffraction provides information not accessible by other techniques. Thanks to the low absorption of neutrons, the bulk of the material and large-grain samples can be investigated, moreover - in many cases - in situ at elevated temperatures.

The sintered bars were processed by rotary swaging either at room temperature or at 900 °C into circular swaged bars with a diameter of 10 mm. The neutron diffraction patterns for structure and microstrain determination were collected at ambient temperature on the MEREDIT diffractometer of CANAM infrastructure at NPI Řež near Prague [3].

Two phases were identified in all samples of W-Ni-Co alloy. The main phase (denoted W-B2) had -W (B2) structure and was formed by the original tungsten powder grains. The second phase (denoted $NiCo_2W$ in what follows) with a weight fraction of 6%–7% and Ni-like structure (fcc) was present as well.

The analysis [4, 5] showed that the grains of the $NiCo_2W$ matrix refined significantly after the deformation treatments. The microstrain was higher in the cold swaged sample (44.2 × 10^{-4}) than in the hot swaged sample (41.2 × 10^{-4}). The evaluation of the modified Williamson-Hall plots showed that both the samples swaged at 20°C and 900 C exhibited the activation of edge dislocations with o {110} or n {111} slip systems, and/or screw dislocations with n slip system in the NiCo$_2$W matrix.

Dislocation densities in NiCo$_2$W phase were estimated from the diffraction peaks broadening. It was seen that the dislocation densities increased approximately 5 times after rotary swaging, and that it is 15 % higher for the sample swaged at room temperature than for the sample deformed at 900°C. It was concluded from the comparison with the stress-strain test that the increased dislocation density due to swaging is responsible for the observed substantial mechanical strengthening (larger for the cold swaged bar).

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The study was supported by the Czech Science Foundation (project no. 19-15479S). Measurements were carried out at the CANAM infrastructure of the NPI CAS Řež, and at the infrastructure Reactors LVR-15 and LR-0.

L21

ON OPTIMIZATION OF MAGNETIC NANOPARTICLES ARRANGEMENT IN PS-*b*-P4VP BLOCK COPOLYMER THIN FILMS

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The arrangement of inorganic nanoparticles in a polymer matrix or domains in block copolymer thin films has attached much attention due to their potential applications in diverse fields such as block copolymer lithography, nanostructured solar cells or advanced catalysts [1]. The key issue in all of these systems, which is to precisely control the spatial distribution of the nanoparticles, maintaining the thin film characteristics and polymeric domain's parameters, still remains a significant challenge [2].

In this work we demonstrate the effect of incorporating magnetite nanoparticles into polystyrene-poly-4-vinylpyridine (PS-*b*-P4VP) block copolymer thin films. The synthesized nanoparticles had a Fe$_3$O$_4$ core diameter of 7.2 nm and were coated by polyacrylic acid to improve affinity to P4VP block, giving overall hydrodynamic radius of 23 nm as measured by DLS. Solutions of the PS-*b*-P4VP were prepared in THF or THF/methanol mixture, where 2 wt. % of nanoparticles were mixed in. The films were prepared by dip-coating method with withdrawal speed varied in the range of 2 to 100 mm/min. The properties of the obtained films were characterized by the means of X-Ray Reflectivity, Grazing Incidence Small Angle X-ray Scattering, Atomic Force Microscopy and Transmission Electron Microscopy.

Thin films with thicknesses 9-70 nm were obtained. The V-shaped thickness dependence on withdrawal speed was validated for each system. For the films obtained from solvents mixture we have observed curve shift to lower dip-coating rates, but leading to possibility to achieve lower film thicknesses. Additionally, much better domain organization was obtained in the case of the films prepared from solvent mixture, especially in the capillarity regime (slow withdrawal speeds), while films prepared from THF solution showed an occurrence of particles aggregates on the surface. The addition of Fe$_3$O$_4$@PAA nanoparticles has been shown to induce the orientation of P4VP cylindrical nanodomains perpendicular to the surface. Domains of size in the range of 15 to 32 nm and spacing from 45 to 105 nm were obtained depending on the withdrawal speed. The optimal processing conditions have been found to fabricate long-range ordered hybrid organic-inorganic material without the need for further annealing or post-processing.

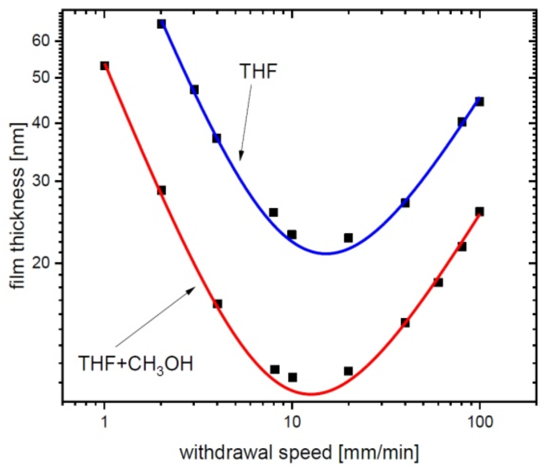

Figure 1. Film thickness as a function of the dip-coating rate. Red curve corresponds to the films, prepared from THF/methanol mixture; blue curve corresponds to the films, prepared from THF.

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L22

SPUTTERING ONTO LIQUIDS: THE BEHAVIOUR OF NANOPARTICLES UNDER THERMAL ANNEALING

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Metal nanoparticles (NPs) are extensively studied due to their unique physical and chemical properties rising from their high surface area and nanoscale size. NPs are suitable candidates for various fields, including catalysis, imaging, medicine, energy production and storage, and environmental applications [1].

The synthesis of metal NPs is divided into two main groups, i.e., physical and chemical. Each of these methods has pros and cons; the physical approach allows the production of pure NPs while the chemical one allows the fine control of the size, dispersion, and shape [2]. In order to improve the synthesis of NPs, the combination of methods is of interest. The sputtering onto liquid is an approach combining both the physical and chemical ways. In this approach, the solid substrate conventionally used during the sputter deposition of a thin film is replaced by a liquid withstanding low pressure. Thus, the metallic target is sputtered in a vacuum chamber. The sputtered elements reach the surface of the liquid. Then, the nucleation and the coalescence of the species occur, and ultimately, NPs are formed [3].

Since the first reported use of this approach in 1974, more than 125 scientific papers have been published based on this process. Most of them highlight the sputtering of monometallic NPs and the influence of parameters on the resulting morphology of the NPs. One of the most used liquid host for sputtering process are ionic liquids due to the higher control of the NPs size and dispersion compared to oil. Moreover, ionic liquid interacts weakly with the sputtered species, so the purity of the obtained NPs is very high. However, ionic liquids are quite expensive and often hygroscopic. Thus, the replacement of ionic liquids by stable organic oils is favourable. The use of such oils raises interrogation concerning the interaction between the metal surfaces of NPs and the oil molecules.

In this context, we report on the synthesis of monometallic NPs (Cu and Au) and alloy NPs (Au/Cu) onto an organic oil, pentaerythritol ethoxylate (PEEL). Moreover, we reveal the behaviour of these NPs under thermal annealing. The synthesis of NPs has been performed by magnetron co-sputtering of a copper and a gold target onto PEEL; these two targets can be simultaneously sputtered to synthesize alloy NPs. Five samples were synthesized: one using only the copper target, one with only the gold target, and three samples with both targets while varying the sputter power on the gold target to achieve different gold concentrations within each sample. The resulting dispersions of NPs in PEEL were analysed using UV-vis spectroscopy, Transmission Electron Microscopy (TEM), and Small Angle X-ray scattering (SAXS). The hypotheses drawn during this study were supported by quantum chemistry-based calculations carried out at the DFT level [4].

The study reveals the successful synthesis of Au/Cu alloy NPs when using both targets. Moreover, the oxidation of the Cu NPs, obtained by sputtering only the Cu target, is reported. As highlighted in previous work [5], the mean diameters of alloy NPs appear to be smaller than the one of the monometallic NPs, i.e., 2 nm for Au/Cu NPs against 6 and 4 nm for Au and Cu NPs, respectively. We explain this behaviour by the interaction energy between each metal (and alloy) with the PEEL molecules.

Following the synthesis of the NPs by magnetron sputtering, solutions containing the NPs were further annealed at 200 °C for 5h with aim to increase the mean NP size. By selecting different intermediate annealing temperatures, we were able to follow the behaviour of each metal and alloy NPs during the thermal treatment in PEEL solutions. First, the gold NPs, which are initially 6 nm-in-diameter spherical NPs evolve to an interconnected ligament structure with a ligament size around 140 nm. Then, for NPs obtained by sputtering a copper target, the diameter evolves from 4 to 80 nm with almost no change in shape. Finally, the diameter of the spherical Au/Cu NPs grows, without change of shape, from 2 to 16 nm. Moreover, the alloy NPs are still composed of homogeneous Au/Cu alloy after annealing.

This study provides an essential insight into the sputtering onto liquids process to synthesize NPs and their development. One of the main issues raised here is the significant growth of the NPs when dispersed in PEEL and further annealed. However, the difference in affinity between the crystallographic facets of a metal NP leads to non-spherical structures after heating treatments.

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Session V, Friday, November 27

L23

MICROSTRUCTURE ANALYSIS IN AlMnCu SAMPLES

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Due to the versatility, easy processing, and the multitude of applications of metals, an important number of research centres join their efforts seeking to improve the properties of this type of materials. Among the different mechanisms for improving mechanical properties, grain refinement achieved using severe plastic deformation (SPD) methods has been shown to be effective in increasing simultaneously the strength and toughness of the materials. A new method capable to produce ultra-fine grained tubular samples from bulk billets in one single step [1] has been employed to produce $Al_{0.98}(Cu, Mn)_{0.02}$ cylinders.

X-Ray measurements were performed on the lateral surface of the cylinder (see Fig.1a) carried out using Co K radiation with a point focus and Bragg-Brentano (theta/2theta) geometry. Following Rietveld refinement analysis was made providing a mean volume-weighted crystallite size Lvol-IB=248 nm with a microstrain of about 2%.

Then the sample was cut in order to make residual stress measurements on both outer and inner surfaces of the cylinder (see Fig. 1b). The sin^2 plot method has been used to evaluate the macroscopic residual strain of the sample which value is proportional to the observed slope. The measurements have been taken using Co K radiation and a graded multilayer mirror (Göbel mirror). The reflection from the plane (133) found at 2theta=148.65 degrees was

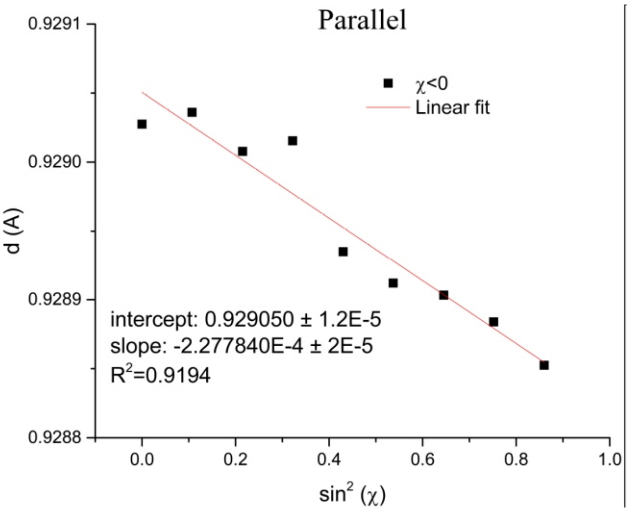

Figure 2.: sin^2 plot for the interplanar distance of planes (133).

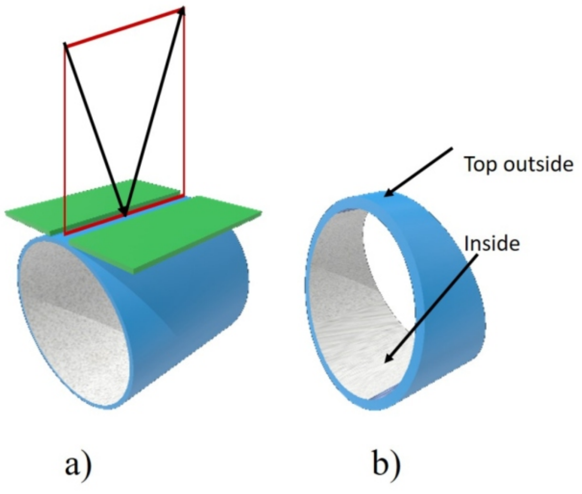

Figure 1. Setup for the X-ray measurements with the employed nomenclature .

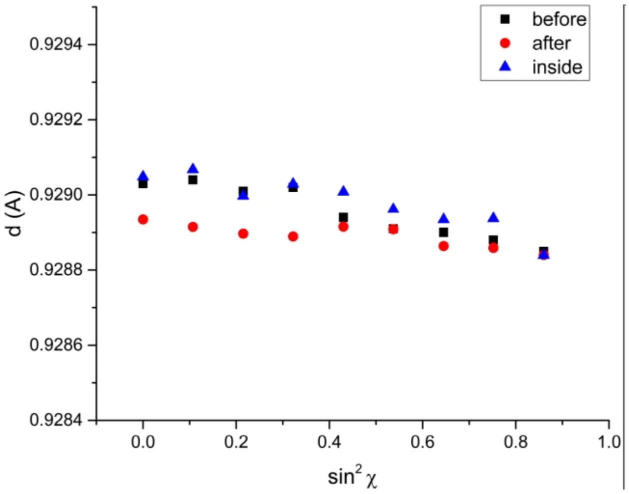

Figure 3. sin^2 plot for the interplanar distance of planes (133) measured in all the 3 different conditions.

selected for this study. The measurements have been performed using a geometry in pseudo inclination mode (measuring at different angles) at two different phi positions: with the diffraction plane placed along the axis of the cylinder (Fig 1a) and perpendicular to it. The measured diffraction peaks were fitted with asymmetric pseudo-Voigth functions in order to determine the position of the intensity maximum. In Fig.2 is shown one of the $\sin^2$ plot used in this study where can be appreciated the small slope from which a compressive stress in the order of tens of MPa has been calculated. This is a small value compared with other metals as steals which have values one order of magnitude higher.

Figure 3 shows the results obtained from the 3 different measurement conditions considered in this study.

It is noticeable that the cutting induce some relaxation of the residual stress while very small difference was observed between the outer and inner surfaces being the stress slightly smaller in the inner part.

Further investigations will be performed in order to determine the stress gradient along the wall of the cylinder.

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L24

X-RAY DIFFRACTION STUDY OF THE PREFERRED ORIENTATION OF SINANODONTA WOODIANA SHELLS

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Bivalve mollusks shells are of interest to leading experts in many areas of human activity, such as ecology, biology, paleontology, but also materials engineering. In recent years, much attention has been paid to studying the preferred orientation of biological tissues such as mollusks shells [1-4]. These polycrystalline materials are characterized by anisotropy of physical and mechanical properties, which are closely related to the preferred orientation (texture) of their grains. The above biological objects can serve as a bioinspiration for material scientists, because nature itself can create entities that are characterized by incredible mechanical properties using relatively small amounts of material. Therefore, the characterization of texture and its correlation with the above-mentioned properties is a cornerstone for understanding the properties of biological polycrystalline materials.

Preferred orientation and exact phase composition of two samples of freshwater shells of the species Sinanodonta woodiana collected from Czech freshwater steams were measured – (i) an adult shell and (ii) a young individual.

Pole figures were measured for planes (111), (021), (002), (211), (220) and (221). Texture data processing was done by MTEX (Matlab) [5]. All diffraction experiments were performed on the SmartLab Rigaku X-ray diffractometer (Cu K). Complete pole figures were calculated for planes (100), (010), (001), (101) and (110).

From the phase analysis it is clear that the Sinanodonta woodiana shells consist only of the aragonite phase. The c-axis of aragonite is perpendicular to the inner surface of the shell and crystallographic texture in all studied shells is strongly uniaxial. The sharpness of the texture is higher for young shells.

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L25

Structure of aluminothermy reduced deep-sea nodules

STRUKTURA HLUBOKOMOŘSKÝCH KONKRECÍ ZPRACOVANÝCH ALUMINOTERMICKOU REDUKCÍ

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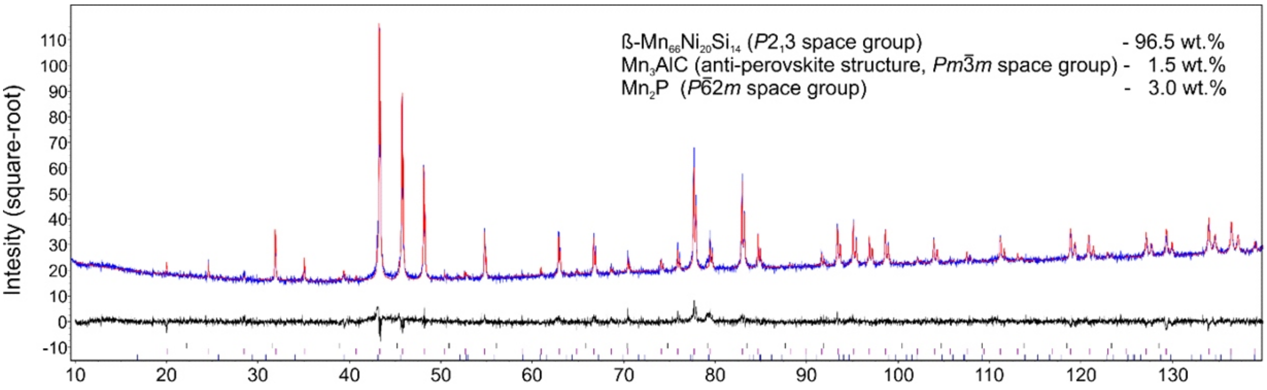
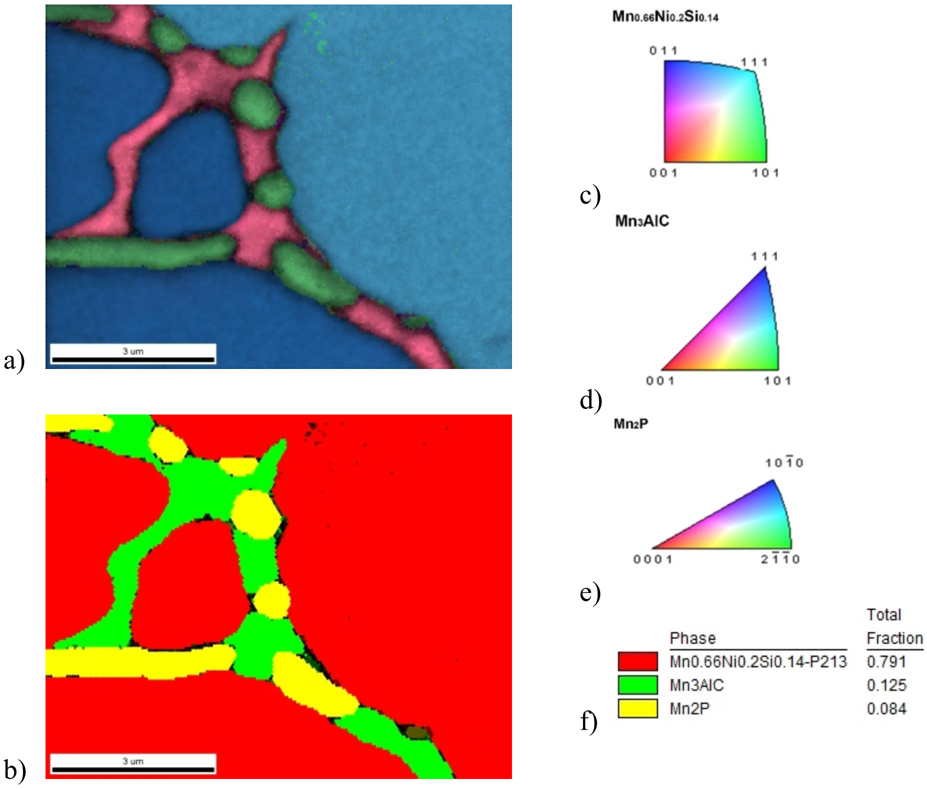
Hlubokomořské konkrece se zdají být zajímavým zdrojem barevných kovů, jejichž konvenční těžba je závadná nebo probíhá v nedostupných teritoriích. Novou myšlenkou je příprava přímo „přírodní slitiny“, nikoliv redukce konkrecí na čisté kovy. Konkrece ze zóny Clarion-Clipperton (Tichý oceán) byly aluminotermicky redukovány s 0, 10 a 20 %



Obrázek 1. Práškový difraktogram slitiny bez přebytku hliníku.



Obrázek 2. Slitina bez přebytku hliníku mapovaná metodou EBSD, a) barevná orientační mapa (IPF) proložená černobílým signálem image quality (IQ); b) barevná fázová mapa proložená černobílým signálem confidence index (CI); barevná orientační škála pro jednotlivé fáze (IPF) je zobrazena v c) – e); f) barevné kódování fází a obsah.

přebytku hliníku. Struktura takto získaných slitin byla následně studována kombinací XRD a SEM.

Struktura takto získaných slitin je složitá, pozorované fáze jsou nestechiometrické, případně jsou prvky ve strukturách substituovány. Slitina bez přebytku hliníku při aluminotermii obsahuje majoritní fázi - $Mn_{0.66}Ni_{0.2}Si_{0.16}$ a tři minoritní fáze; slitina s 10 % přebytku obsahuje sedm fází, z nichž tři mají přes 10 hm. %; slitina s 10 % přebytku obsahuje 9 fází, z nichž pět je minoritních. Je zajímavé, že majoritní fáze ve všech vzorcích je odlišná. Odhad fázového složení byl proveden pomocí XRD a následně jsme se snažili fáze potvrdit pozorován Kikuchiho obrazců metodou EBSD a zjistit jejich prvkové složení. Separace krystalograficky podobných nebo shodných fází byla možná jen kombinovaným měřením EDS/EBSD. Zcela minoritní fáze, např. MnS, byly pozorovány pouze pomocí EBSD.

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L26

COUPLING BETWEEN MAGNETISM AND CRYSTAL STRUCTURE IN THE ANTIFERROMAGNETIC UO_2

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Uranium dioxide is a major nuclear fuel and is an antiferromagnet with the Néel temperature T_N of 30.8 K [1]. The transition at T_N is accompanied by a static Jahn-Teller distortion of the oxygen cage, and strong magnetoelastic interactions that emerge from the face-centered cubic (fcc) structure. Very recent high field magnetostriction measurements showed that UO_2 is a piezomagnet and exhibits the abrupt appearance of positive linear magnetostriction, leading to a trigonal distortion [2]. In this work we observe peculiar behavior of sound velocity variation along the crystallographic axes of UO_2 at various temperatures. We employ first-principles calculations to prove a strong coupling between magnetism and crystal structure variations in UO_2. The results are compared with the thin films study where induce a tetragonal distortion in UO_2 by using different substrates [3].

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L27

XRD STUDY OF STRONGLY ORIENTED THIN FILMS OF HEXAGONAL FERRITES WITH POTENTIAL MAGNETOELECTRIC EFFECT

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X-ray diffraction and reflectivity techniques for analysis of thin polycrystalline thin films have been well-developed and they are routinely used when often low-angle incidence setup is applied instead or in addition to symmetrical scan. However, for strongly oriented films more different asymmetric scans and/or reciprocal space mapping are required. During study of nanocrystalline ZnO films [1] we have applied a combination of different scans to characterize both the so-called out-of-plane orientation and in-plane orientation. Strong out-of-plane orientations were found, and only basal (00l) reflections were available in symmetric scans. Therefore, the lattice parameters, profile analysis (crystallite size and strains) and residual stresses were studied by combination of several asymmetric reflections scanned at specific suitable angles of inclinations and (i.e. on the axis perpendicular to the film surface and axis perpendicular to the goniometer axis, respectively). For comparison of measured lattice parameters there was often a problem of either no data in the PDF-4+ database for specific phase or multiple but different data.

The methods were also used in later extensive study of M, Y, Z and W hexagonal ferrites with a potential of magnetoelectric effect. The films were prepared by chemical solution deposition (CSD) method and metalorganic precursor solutions prepared using the modified Pechini method. Number of processing parameters were tested and optimized with the aim to minimize the amount of impurities that could spoil the magnetic properties of final material. For preparation of highly oriented ferrite films, several substrates were used, and different substrate/seeding layer/ferrite layer architectures were proposed. From seven M phases with different chemical composition, magnetic character and lattice misfit values investigated in their use as template and buffer layers for Y ferrite growth, the best results were achieved when the misfit values between seed layer and substrate, and between seed layer and top Y-layer are approximately equal and when the surface of seed layers are formed by hexagons for which the surface area formed by top surface of hexagons is much larger than surface area formed by side walls of hexagons [2, 3].

New *Y-ferrite* phases were prepared with the composition $BaSrZnCoFe_{11}(Me)O_{22}$ (Me = Al, Ga, In, Sc). and it was found that for Me = Al, Ga the magnetic structure is of non-colinear ferrimagnetic type with unspecified helical magnetic structure. For Me = Ga this is a new system with potential ME effect. Moreover, these films could be prepared as well-oriented both out-of-plane and in-plane on STO - $SrTiO_3$(111) substrates directly without any seeding layers.

ME *Z-type ferrite* $Sr_3Co_2Fe_{24}O_{41}$ and $Ba_xSr_{3-x}Co_2Fe_{24}O_{41}$ thin films were prepared and characterized for the first time [4]. According to the XRD texture analysis the orientation relationship between Z ferrite and substrate can be expressed as (00l)Z || (111)STO || and Z || STO. However, in these films the analysis was complicated by the presence of M and S (spinel) phases that were also oriented (aligned with the substrate) and therefore also many asymmetric reflections were overlapped and many of them were weak. Therefore, a careful selection of reflections suitable for the analysis had to be made.

Composition series of *W-type* $SrCo_{2-x}Zn_xFe_{16}O_{27}$ hexaferrite thin films and powders were also successfully synthetized by CSD method. For successful growth of W hexaferrite films on $SrTiO_3$(111) substrate, annealing temperature and time falls into a very narrow interval of 1225 to 1250°C and 60 to 120 minutes, respectively, depending on the amount of substituting Zn^{2+} ion. The strong anisotropy of magnetic properties was confirmed. Currently, oriented *Y-Z* composites are studied that is another challenge for the analysis.

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L28

TEXTURE ANALYSIS OF STRONGLY ORIENTED LAYERS UTILIZING FAST RECIPROCAL SPACE MAPPING

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Polycrystalline layers of organic perovskites such as $CH_3NH_3PbI_3$ ($MAPbI_3$) are intensively studied in order to achieve high performance of solar cells. The final efficiency correlates with the defect density, size and morphology of the crystallites. These materials exhibit tendency to form strongly oriented layers with sharp fibre multi-component texture. In order to correlate the relevant physical properties of the layers with their crystallographic orientation, it is highly desirable to easily measure and describe the present texture.

As a classical and well-established approach, one can use pole figure measurement to fully determine the texture of the layers, however here the task is complicated by the fact that the low-symmetry unit cell of such materials is rather large. Consequently, the number of observable peaks is quite high and their diffraction angles are partially overlapping. Therefore it is necessary to increase the resolution in diffraction angle in order to discriminate different diffraction maxima during the pole figure measurement. As usual, it is at the expense of the collected signal making the pole figure measurement to be a time consuming. Another specific problem can be a presence of some strain influencing the peak positions.

Fortunately, fast 2D detectors are more and more available also in standard laboratory diffractometers that makes it possible to measure reciprocal-space maps very quickly. In this presentation, the measurements with 2D detector placed closely behind the sample are presented. Using the

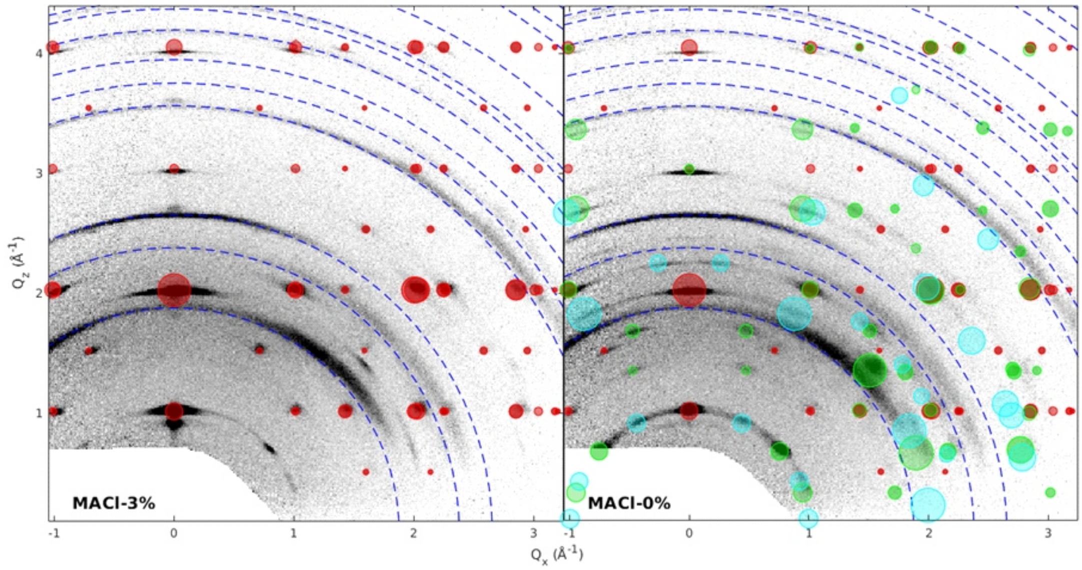

Figure 1. Wide Reciprocal Space Maps for the MAPbI3 thin layers grown with the presence of MACl additive. The concentration of MACl during the growth determines the final texture of the layer. A low concentration results in a multi-component texture whereas a high concentration enhances just one preferential orientation. Transparent spots represent simulated peak positions for the same MAPbI3 structure, the texture components are resolved by different colours.

shorter sample-detector distance, the resolution is partially sacrificed while the reciprocal space area observed by the detector is dramatically extended. In this configuration, the continuous theta-2theta scan fully probes a long stripe in a reciprocal space. By measuring several such stripes, it is easy to reveal the full planar cut of the reciprocal space, and surprisingly the total acquisition time can be only tens of minutes for strongly oriented layers. Moreover, such measurement can be performed for different sample azimuth in order to obtain different planar cuts. This is desirable for single-crystal substrates, for which the surface symmetry can be followed.

The obvious advantage of this approach is a possibility to quickly visualise the intensity in reciprocal space and to compare the obtained images with the simulations based on some expected phase/texture model giving semi-quantitative results. Therefore it is very suitable for the first-try characterization of the unknown samples.

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