

# **11. Studentská vědecká konference fyziky pevných látek a materiálů (2022)**

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FJFI ČVUT v Praze

## **Book of Abstracts**



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## 100. výročí Dolejškova objevu série N

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Přednáška zabývající se stým výročím Dolejškova objevu série N.

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## **Deformation processes under the nanoindenter tip**

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Nanoindentation was developed as an alternative to traditional hardness and microhardness tests based on the penetration of a tip into the material under investigation. Decreasing the penetration depths down to submicrometer range brings many experimental and theoretical challenges. The contribution shows several examples, where the evolution of plastic zone and deformation modes under the indenter must be taken into account for the correct interpretation of the measured data.

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## Effect of molecular structure on liquid crystalline behaviour for chiral lactic acid derivatives

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Liquid crystals are self-organizing materials that have great potential for practical applications. The relationship “molecular structure - mesomorphic properties” has not been fully established and understood despite numerous studies. We discuss a relatively broad subclass of calamitic chiral lactic acid derivatives and provide specific examples of effective tuning of their mesomorphic and electro-optical behaviour using various types of lateral substitution placed on the molecular core.

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## **Ga vacancies in GaN: challenge for theorists and experimentalists**

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Despite large spread of GaN-based devices in 1990s, several fundamental questions about GaN properties remain unanswered. One of them is a role or even a presence of Ga vacancies in GaN. According to the first-principle calculations, the Ga vacancy formation energy is too high for their presence in significant concentrations. However, this is in contradiction with experiments. In this work, new findings obtained by variable energy positron annihilation spectroscopy are shown and discussed.



## Generalized inverse problems in resonant ultrasound spectroscopy

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Resonant ultrasound spectroscopy (RUS) is one of the most precise and versatile methods used for the determination of elastic coefficients. The method is based on measurement of mechanical resonances of a solid body. However, determination of the elastic constants by RUS is an inverse problem so the experimentally obtained resonant frequencies cannot be directly recalculated into the elastic constants. Instead, an approximate spectrum is calculated from the known dimensions of the sample, its mass, and a set of 'guessed' elastic constants. Our main goal is to show the ability of the resonant ultrasound spectroscopy to precisely identify the anisotropy class, crystallographic orientations, and dimensions of the sample, in addition to elastic coefficient determination.

The reliability and robustness of our extended algorithm was tested on three differently oriented samples of Si-doped iron single crystal. Precision of the algorithm is discussed with respect to the number of resonances utilized during the procedure, and calculated crystallographic orientations are compared with the measurements obtained by Laue diffraction experiment. Our optimization procedure was then applied on room temperature measurements of 2 types of metastable  $\beta$ -Ti alloys (Ti15Mo and LCB) with an increased amount of secondary phase particles after additional heat treatment. The aim was to observe potential change of the symmetry of the material after the phase transformation. This procedure was performed by comparing the best possible inversion assuming cubic symmetry with full triclinic calculations.

Our results show no significant change of the symmetry of the material on macroscopic scale, which means that the material retained its cubic symmetry after the phase transformation. To further confirm our findings a transient grating spectroscopy (TGS) measurements are compared with the measurements obtained by RUS, showing a good agreement.

## **Jana2020 – the universe of crystallography in one software package**

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JANA is a crystallographic software developed to help users solve crystal structures from diffraction data. The first version of JANA software was developed in 1984 by Vaclav Petricek to solve modulated and composite structures from single crystal data. Over the years and versions (Jana94, Jana98, Jana2000, Jana2006 and Jana2020), the software has evolved to accept all types of diffraction data (powder and single crystal from x-ray, synchrotron, electron, time of flight or neutron sources) and solve many kinds of structures (simple, twinned, disordered, modulated, composite, magnetic).

Jana2020 is the newest version of JANA software. The graphical interface allows the user to solve the crystal structure interactively. It can be used by an experienced scientist as well as a student. The new interface makes it possible to understand complicated concepts such as magnetic or aperiodic structures without spending too much time by setting up simple constraints or restrictions. Using different examples, I introduce the new Jana2020 interface, its performance, and the new tools in this presentation.

## $K_{(1-x)}Li_xTaO_3$ - krystal s neobvyklou dynamikou feroelektrického fázového přechodu

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Za pomoci širokopásmové dielektrické spektroskopie, Ramanovy spektroskopie, generace druhé harmonické a měření pyroproudu byl potvrzen perkolační charakter feroelektrického (FE) fázového přechodu v krystalech  $K_{(1-x)}Li_xTaO_3$ . Tyto techniky umožnily studovat dielektrickou odezvu krystalu v oblasti 1 Hz – 20 THz a prozkoumat dynamiku měkkých fononových a relaxačních módů. Výsledky experimentů ukazují na vnitřní nehomogenitu FE fáze vykazující koexistenci FE domén a polárních nanoklastrů.

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## **Localization of martensitic transformation in shape memory alloys: 3D spatial reconstruction by X-ray diffraction/scattering computed tomography.**

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The stress-induced martensitic transformation in polycrystalline NiTi-based shape memory alloys often tends to localize in bands on the macroscopic scale. In this contribution, we will present utilization of one recent tomographic technique - X-ray diffraction/scattering computed tomography (DSCT) - for spatial reconstruction of austenite–martensite transition zones in superelastic NiTi wires subjected to stretching and twisting. The obtained localization patterns will be discussed with respect to current computational simulations and micromechanical models.

## Magnetocrystalline anisotropy of Ni-Mn-Ga-Co-Cu tetragonal martensite

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The martensites of Heusler alloys based on Ni-Mn-Ga exhibit magnetically induced reorientation resulting in giant field induced strain up to 12 % in Ni-Mn-Ga-Co-Cu with 4 at.% of Co and Cu. As the driving force of the phenomenon is the magnetocrystalline anisotropy (MCA), we studied the evolution of MCA in different tetragonal single crystalline Ni-Mn-Ga-Co-Cu and compared with pure Ni-Mn-Ga. The MCA of martensite was determined from magnetic hysteresis loops. No clear trends were observed.

## Metal Ion Exchange in Zn-Dependent S1 Nuclease: Effect on the Structure

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S1 nuclease is an enzyme commonly used in biotechnology applications. Its activity depends on the presence of three Zn(II) ions in the active site. In this work, we examine the possibility of exchanging the natively present Zn(II) ions to Cd(II). EDTA-treated S1 nuclease was successfully crystallized in the presence of CdCl<sub>2</sub>. The anomalous signal from three different energies confirmed the exchange of two Zn(II) ions to Cd(II). The residues of the active site remained structurally conserved.

## Morphological and Structural Changes of Ceramic Powders during Plasma Spraying

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Powders with spherical particles are utilized in various industries such as health, food, or in additive manufacturing due to their enhanced flow properties. Plasma spray spheroidization is an effective tool for manufacturing of such powders from angular or agglomerated powder feedstocks, namely thanks to its high feedstock throughputs. In this thesis, the formation process of spherical particles in hot gases, the in-flight behaviour of the particles, and several methods of powders' characterization were described. The collection chamber for powder spheroidization using the high-enthalpy hybrid water stabilized (WSP-H) plasma torch was designed and manufactured with emphasis on maximal collection efficiency. Spheroidization experiments with Al<sub>2</sub>O<sub>3</sub> and TiC powders were performed and the morphology, sphericity, flowability, particle size, and chemical and phase composition of resulting powders were observed. Successful spheroidization of Al<sub>2</sub>O<sub>3</sub> enhancing its flowability without significant phase changes was achieved. In case of TiC, significant refinement and oxidation into TiO<sub>2</sub> powder was observed.

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## **Numerical Study on Thermally Induced Birefringence in Yb:YAG Laser Rod: Power Output Optimisation**

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A traditional approach to study the birefringence induced under laser pumping is presented. Numerical study of thermally induced birefringence was performed based on material properties of Yb:YAG rod laser crystal in crystallographic orientation [001]. New method introduced here is devoted to optimisation of relative output intensity from the system containing a laser rod placed between two general polarizers.



## **Optimalizace depozičních parametrů tenkých vrstev vysokoteplotních supravodičů na bázi YBCO připravených pomocí IJD; Optimization of IJD deposition parameters of high temperature superconductors thin films based on YBCO**

**Author:** Michal Jůza<sup>None</sup>

Hlavním cílem této bakalářské práce byla optimalizace depozičních parametrů pro přípravu vysokoteplotních supravodičů na bázi YBCO pomocí metody IJD s přihlédnutím k využití v průmyslu. V teoretické části jsou vysvětleny základní principy samotné depoziční metody a analytických metod využitých pro studium nanosených vrstev.

V rámci experimentu bylo připraveno 6 různých vzorků ve dvou sériích. V každé sérii byly vzorky připraveny za třech různých teplot substrátu. Jednotlivé série se od sebe lišily dalšími zkoumanými parametry, konkrétně urychlovacím napětím a složením terčíku. Následně byla provedena analýza vzorků pomocí SEM, EDS a rentgenové difrakce. Kvalitativní fázová analýza přítomnosti supravodivé fáze v žádném ze vzorků neodhalila. Výsledky získané v rámci této práce mohou být využity pro budoucí výzkum zabývající se touto problematikou.

The main focus of this bachelor thesis is optimization of IJD deposition parameters of YBCO based high temperature superconductors with potential for application in industry. In the theoretical part basic principles of the deposition method itself and analytical methods used for study of prepared layers are explained.

During the experimental part 6 different samples in two series were made. Samples in each series were prepared using 3 different temperatures of the substrate. The two individual series differed in another examined parameters, namely accelerating voltage and target composition. SEM, EDS and XRD sample analysis was performed afterwards. The qualitative phase analysis did not reveal the superconductor phase in none of the samples. Results presented in this thesis might be used for future research dealing with this issue.

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## **Predikce krystalových struktur s pomocí experimentálních dat**

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Predikce krystalových struktur je metoda, při které se navrhuje nové struktury látek či se vytváří modely látek, které se nepodařilo vyřešit jiným způsobem. Výpočty přesných hodnot energie, podle nichž se struktury predikují, však mohou být časově náročné, proto se v práci věnujeme dvěma způsobům, jak predikci urychlit: úpravami algoritmu hledajícího krystalovou strukturu; zapojením experimentálních dat do procesu hledání krystalových struktur.

## **Preferred orientation of freshwater shells of the species *Sinanodonta woodiana* and *Anodonta anatina* studied by neutron and X-ray diffraction**

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Using neutron and X-ray diffraction, the texture of the prismatic and nacreous layer of several shells of the species *Sinanodonta woodiana* was studied and compared with the preferred orientation of the shells of the species *Anodonta anatina*. The shells of both molluscs were collected in freshwater streams in the Czech Republic. The neutronographic texture measurements were performed on the KSN-2 neutron diffractometer located at the research reactor LVR-15 in the Nuclear Research Institute, plc. Rez, Czech Republic. X-ray texture measurements were performed on a SmartLab Rigaku X-ray diffractometer (with Cu K $\alpha$  rotating anode) located at the Institute of Physics of the Academy of Sciences of the Czech Republic. It was found that during the growth of the shell the a and b axes of aragonite are reoriented and the direction of the c-axis does not change alignment. The texture strength is increasing with the shell growth.

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## **Příprava nanotyček ZnO na substrátech modifikovaných fokusem iontovým svazkem**

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Tato práce přináší nové možnosti pro úpravu morfologie a vlastností nanotyček při růstu metodou depozice z chemické lázně a pro studium vlivu různých reakčních podmínek na růst. To je velmi výhodné zejména pro výrobu polovodičových součástek, např. LD, solárních článků nebo piezoelektrických nanogenerátorů, jelikož pro různé součástky jsou vhodné různé nanotyčky. Pro možnosti studia a ovlivňování nanotyček je využito uspořádaných polí nanotyček připravených v reaktoru s kontinuálním průtokem.

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## Quantum Hyperion HPC Cluster - Status Update 2022

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A lot of work has been done on the new Quantum Hyperion cluster (obtained as part of the Quantum Technologies project at the faculty) in last year, mainly in the field of intra-cluster networking and parallel storage. This short talk is going to summarize the overview of what has been done and where are we currently also from the user point of view.

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## Quantum technologies

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Aim of the presentation is to provide a brief overview of scientific fields and topics referred to by the collective term “Quantum Technologies&39;”, with the emphasis laid on the areas that are close to the research conducted at the Department of Solid State Engineering FNSPE CTU in Prague, and might be thus of interest in terms of determining its future direction.

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## Rekonstrukce Landauovské energie feroelastického chování slitiny Ni-Fe-Ga(Co)

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Tento příspěvek popisuje sestavení energetické funkce popisující chování feromagnetické slitiny s tvarovou pamětí Ni-Fe-Ga(Co) v rámci Landauovy teorie. Monokrystalický vzorek byl podroben tahové zkoušce a rezonanční ultrazvukové spektroskopii v širokém intervalu teplot. Z naměřených křivek závislosti napětí na deformaci byly odvozeny konstanty landauovské volné energie 4. řádu. Tato energie věrně zachycuje klíčové vlastnosti slitiny, jako je například existence kritického bodu nebo vývoj Youngova modulu s teplotou.

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## **SHELIXIR: code development**

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The constant development of new experimental approaches goes hand-in-hand with the continuous improvement of data evaluation strategies, mainly software-based. When writing new software, the code writers should respect the needs of users, both experienced and novices. When possible, the software should serve universal purposes and use, decision strategies implemented, and novel metrics designed. Such approaches will be shown in the case of the program *SHELIXIR*, which automates experimental procedures using the *SHELX C/D/E* suite.



## Spektroskopie s přechodovou mřížkou tenkých vrstev NiTi

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NiTi is a shape memory alloy utilized in many applications thanks to its thermal stability, corrosion resistance and biocompatibility. In this work, surface waves propagation in thin epitaxial NiTi films is investigated with transient grating spectroscopy (TGS). It is demonstrated that the thin film thickness limits the amount of observable wave modes at given acoustic wavelength and influences the number of frequency measurements necessary for material characterization, e.g. determining elasticity of the film.

## Structural insight into antibiotic-inactivating enzyme from *Stenotrophomonas maltophilia*

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*Stenotrophomonas maltophilia* is an opportunistic bacterial pathogen responsible for a serious number of infections globally. It exhibits broad antibiotic resistance that has been further extended via the acquisition of antibiotic-resistance genes and mutations [1]. We carried out a bioinformatic analysis of its sequenced genomes to investigate not yet characterised antibiotic-inactivating enzymes. Several chosen proteins were expressed in *Escherichia coli* strain Lemo21 (DE3) and purified using Ni-NTA and size-exclusion chromatography. Their proposed function – enzymatic modification of antibiotics – was inspected with an activity assay. The enzyme with the confirmed activity was successfully crystallized and diffraction patterns were collected. The data exhibited serious anisotropy: a resolution cutoff determined in Aimless [2], according to the criterion of  $CC1/2 \geq 0.30$ , varied from 2.43 Å to 1.92 Å in different reciprocal space directions. Thus, the data were corrected with STARANISO [3]. After the solution of the phase problem in MoRDa [4], the model was refined in REFMAC5 [5]. The choice of the anisotropic high-resolution diffraction limit (1.88 Å) was confirmed with paired refinement in PAIREF [6].

The solved X-ray crystal structure reveals an atomic arrangement of the putative substrate-binding pocket that allows further structural analysis (in silico or in vitro) of complexes with potential inhibitors or antibiotic substrates. The overall fold is very close to the tetracycline destructases [7] or the reductase involved in the abyssomicin biosynthesis pathway [8]. However, the putative active site differs significantly. Our study leads to a better understanding of the involvement of this enzyme in the antibiotic resistance and could contribute to the development of new strategies of antibiotic therapies. Remarkably, the solved structure is composed of a homodimer linked with two disulfides. Nevertheless, further investigation using small-angle X-ray scattering, mass spectrometry and dynamic light scattering showed that the protein is monomer in solution.

1. T. Gil-Gil, J. L. Martínez, P. Blanco, *Expert Review of Anti-infective Therapy*, 18, (2020), pp. 335-347.
2. P. R. Evans, G. N. Murshudov, *Acta Cryst.*, D69, (2013), pp. 1204-1214.
3. I. J. Tickle, C. Flensburg, P. Keller, W. Paciorek, A. Sharff, C. Vonrhein, G. Bricogne. (2018). STARANISO (<http://staraniso.globalphasing.org/cgi-bin/staraniso.cgi>). Cambridge, United Kingdom: Global Phasing Ltd.
4. A. Vagin, A. Lebedev, *Acta Cryst.*, A71, (2015), s19.
5. G. N. Murshudov, P. Skubak, A. A. Lebedev, N. S. Pannu, R. A. Steiner, R. A. Nicholls, M. D. Winn, F. Long, A. A. Vagin, *Acta Cryst.*, D67, (2011), pp. 355-367.
6. M. Malý, K. Diederichs, J. Dohnálek, P. Kolenko, *IUCrJ*, 7, (2020), 681-692.
7. J. L. Markley, T. A. Wenczewicz, *Frontiers in microbiology*, 9, (2018), 1058.
8. J. A. Clinger, X. Wang, W. Cai, Y. Zhu, M. D. Miller, C. G. Zhan, S. G. Van Lanen, J. S. Thorson, G. N. Phillips Jr., *Proteins*. 89, (2021), pp. 132-137.

## Study of the real structure of laser-cladded steel

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The aim of this contribution is to describe the effects of laser additive manufacturing (cladding) on the real structure, microstructure, and mechanical properties of laser cladded H13 tool steel. Extensive experimental research combining X-ray, neutron and electron diffraction has been performed. Furthermore, the microstructure was described, the hardness and other mechanical properties were determined. Some results will be presented and discussed in the talk.

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## Superspace symmetry of Ni-Mn-Ga-based crystals

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The discovery of aperiodic crystals (crystals where three-dimensional lattice periodicity is absent) initiated crystallographers' journey into higher dimensions. Using (3+1)-dimensional superspace, we will introduce the world of incommensurate martensite structures with one-dimensional modulation and show how to deal with the lack of translational symmetry.

## The misfit layer compound PbSVS<sub>2</sub>: a composite structure with twins

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Transition metal dichalcogenides (TMD) have been attracting attention due to their promising use in photonic, biological, and chemical applications. As an alternative to the standard light-emitting devices (LEDs), which lacks the emission of chirally polarized light at room temperature, TMD semiconductors can be used to obtain controllable chiral LEDs. One of the configurations of chirally polarized LED configurations is the stacking of different types of semiconductors. The whole spectral range from the far-infrared to the ultraviolet can be spanned by creating heterostructures formed by superlattices of two layers of semiconductors. Misfit layer compounds (MLC) intrinsically form a superlattice consisting of stacking of a layer of a transition metal monochalcogenides (TMM) and one of a TMD, with a general composition of  $(MS)_{1+x}TX_2$ . Here, M is Sn, Pb, Sb, Bi, or a rare earth element; T is Ti, V, Cr, Nb, or Ta; X is S or Se;  $0.08 < x < 0.28$ .

In this work, single crystals of PbSVS<sub>2</sub> were prepared by chemical vapor transport and were measured using single-crystal x-ray diffraction. The crystal structure is an incommensurate composite with alternated stacking of the subsystems PbS and VS<sub>2</sub>, with the stacking perpendicular to the ab plane. The interaction between the sublattices corresponds to a perturbing potential, which causes the modulation of each of the sublattices, and consequently, satellite reflections are present on the diffraction patterns. The crystal structure will be described using the superspace group formalism, and I will present the trick behind scenes to elucidate the crystal structure of a composite with twins.

## Thin films of CsPbBr<sub>3</sub> nanocrystals on scintillating wafers

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There is a rising demand for new detectors with ultra-fast timing for the use of Time-Of-Flight measurements in medical imaging and high-energy physics. One way of tackling this challenge is a composite material of bulk inorganic scintillators with nanoscintillators exhibiting quantum confinement effect. In this work, thin films of CsPbBr<sub>3</sub> nanocrystals were prepared on various substrates and their radioluminescent and timing properties were tested. Enhancement in radioluminescence intensity and addition of ultrafast decay components was observed by applying CsPbBr<sub>3</sub> thin film on scintillating wafers. Significant improvements in detector time resolution of composite materials in comparison with pure inorganic scintillating crystals were observed.

## Towards biomedical applications of Heusler alloys

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Heusler alloys are alloys of three or more metal elements with specific atomic ordering that enables reaching properties very different from those of pure metals. Typically, the Heusler alloys can be ferromagnetic, despite of being composed of three non-magnetic elements. The Heusler ordering can also affect the lattice stability, leading to acoustic phonon condensation and diffusionless phase transition. Recently, the Heusler alloys have attracted a lot of attention as promising candidates for biomedical applications, in particular for bone tissue replacements, combining bio-mimetic elastic properties, high flexibility and surprising corrosion resistance. The lecture will summarize the current achievements in this direction, and especially the research carried out at the Tohoku University in Sendai (Japan) in collaboration with the Institute of Thermomechanics, Czech Acad Sci..

## Ultrasonic characterization of inner defects in cold sprayed coatings

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Pure Fe coatings were deposited by cold spraying onto Al substrates with machined notches. Scanning acoustic microscopy (SAM) was utilized to study the mechanical properties of Fe coatings around the notches, where an increased porosity was revealed by SEM. The resulting distributions of ultrasonic wave velocities and their attenuation show that the area affected by the non-perpendicular impact of Fe particles is more complex than observed in the micrographs. Besides that, a bimetal sample was cut along the planar Fe/Al interface, and it was gradually heated to 500 °C and then cooled back to room temperature. Due to the formation of the brittle FeAl<sub>3</sub> intermetallic phase, a crack initiated and propagated during the cooling, and its shape after the thermal cycling was determined by SAM.



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## **Understanding Antiphase Boundaries – Path to New Multiferroic Functionalities in Ni-Mn-Ga Magnetic Shape Memory Alloys**

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The presence of antiphase boundaries (APBs) can be expected in any chemically ordered compound. In Ni<sub>2</sub>MnGa, magnetic shape memory alloy, the transition between partly disordered B2' and ordered L21 structure occurs above 1000 K and the transition is fast and weakly of the first order. Understanding the nature of APB is important as it affects the magnetic hysteresis and also magnetically induced reorientation and thus it affects and also promotes new functionality of the materials.

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## Upřesňování jako nezbytný nástroj při studiu vazby mezi proteinem a ligandy

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Rentgenová strukturní analýza umožňuje studovat vazby mezi ligandem a proteinem na atomární úrovni, čímž může nejen významně přispět k objasnění funkce studovaného proteinu, ale i identifikovat jeho potenciální inhibitory. Tato práce se věnovala dvěma komplexům ligandu s nukleasou ze *Stenotrophomonas maltophilia*. Především pak upřesňování strukturních modelů a vlivu upřesňování na nalezení pozice ligandu v aktivním místě této nukleasy. Postupným upřesňováním strukturních modelů bylo možné přesně identifikovat místo a způsob vazby studovaných ligandů. Správnost určení pozice ligandu byla diskutována vzhledem k mapám elektronové hustoty vypočteným několika způsoby.

## Vliv teploty substrátu na vlastnosti tenkých YBCO vrstev připravených metodou IJD

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Příprava tenkých vrstev vysokoteplotních supravodičů je velmi aktuální problematiku, protože se v současné době vysokoteplotní supravodiče stále častěji uplatňují v praxi a je potřeba optimalizovat jejich výrobu ve všech formách. Metoda Ionized Jet Deposition (IJD) by mohla být vhodný způsob jak tyto vrstvy připravovat v průmyslovém měřítku. V současnosti je vyvíjen postup jak tyto vrstvy pomocí IJD připravit. Studium vlivu teploty substrátu během depozice je zásadní parametr, který ovlivňuje fázové složení připravené vrstvy vysokoteplotních supravodičů na bázi YBCO.

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## Využití neuronových sítí při tvorbě potenciálů pro molekulární dynamiku.

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V posledních dekádách jsou neuronové sítě čím dál častěji skolňovaným tématem. Díky jejich schopnosti přesné a věrohodné predikce nacházejí uplatnění v mnoha oborech včetně materiálového inženýrství. Jedna z možností jejich využití se nachází v molekulární dynamice, která nabízí možnost simulovat časový vývoj velkých systému, nicméně její přesnost je značně omezená. V této práci se budeme zabývat využitím neuronových sítí při tvorbě potenciálů pro molekulární dynamiku a následné použití vytvořeného potenciálu na monoatomární systém křemíku.

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## Vývoj substrátů pro spektroskopii založenou na povrchem zesíleném Ramanově rozptylu

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Spektroskopie založená na povrchem zesíleném Ramanově rozptylu (SERS) je vysoce citlivá metoda pro určování chemického složení. Principem je využití substrátů ve formě tenkých metalo-dielektrických nanostrukturovaných vrstev. V těsné blízkosti povrchu kovu dochází k řádovému nárůstu intenzity EM pole a tím i k zesílení Ramanova rozptylu na molekulách, které se zde nacházejí. Pro praxi je klíčové vyvinout substráty s vysokým zesílením, dobrou reprodukovatelností a nízkými výrobními náklady.

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## **X-ray tomography – first experiences**

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In the spring of this year, an *Xradia Versa 610* x-ray tomograph was installed in the Institute of Physics of the Academy of Sciences of the Czech Republic. In this post, I would like to summarize my first experiences with this equipment from common things to scientific samples. The device create a 3d object from thousands of x-ray images. For small objects, the size of one voxel (pixel in 3D) can reach approx. 250 nm.