12. Studentská vědecká konference fyziky pevných látek a materiálů (2023)

Monday 04 September 2023 - Thursday 07 September 2023

Pension Kamínek

Book of Abstracts

…..sorted by order of lectures…..

Contents

Deposition techniques / 21

Ionized Jet Deposition method basic principles and influence of deposition parameters

Author: Jakub Skočdopole[1]

[1] *CTU FNSPE*

Corresponding Author: jakub.skocdopole@fjfi.cvut.cz

The Ionized Jet Deposition (IJD) method is classified as a pulsed electron deposition (PED) method. IJD uses several physical processes to function. In this presentation, these processes will be presented together with the deposition parameters. Deposition parameters are quantities that influence the prepared thin layers.

Deposition techniques / 25

Příprava tenkých vrstev vysokoteplotních supravodičů typu RE-BCO na monokrystalických substrátech metodou IJD

Author: Martin Kolář[1]

[1] *CTU FNSPE*

Corresponding Author: kolarm34@fjfi.cvut.cz

Příprava tenkých vrstev vysokoteplotních supravodičů typu REBCO na monokrystalických substrátech metodou IJD

Deposition techniques / 16

Optimal Substrate Temperature for Thin Film Deposition of High-temperature Superconductors Based on YBaCuO Using Ionized Jet Deposition

Author: Michal Jůza[1]

Co-author: Jakub Skočdopole [1]

[1] *CTU FNSPE*

Corresponding Author: juzamich@fjfi.cvut.cz

This research paper is focused on the dependence of phase composition according to the substrate temperature during the IJD deposition. Samples prepared with different substrate temperatures were analyzed using X-Ray spectroscopy and Atomic Force Microscopy in order to determine the chemical composition and presence of superconducting phase as well as thickness of the layer, which ranged between 500 and 1000 nm. In two of the samples superconducting phase was found.

Deposition techniques / 8

Preparation and analysis of High Entropy Alloys thin films deposited by Ionized Jet Deposition method

Author: Jáchym Lis[1]

[1] *CTU FNSPE*

Corresponding Author: lisjachy@fjfi.cvut.cz

The aim of my work was to investigate the preparation of high-entropy alloys thin films using the Ionized Jet Deposition method. In the theoretical part, high-entropy alloys are described, the IJD method is introduced and other analytical methods used in the thesis are briefly explained. In the experimental part of the thesis the preparation of the target for deposition of FeNiCoCuCr alloy by IJD method is described. A total of six layers were subsequently deposited from this target, two of which were test layers and the subsequent four were aimed at studying the effect of the deposition voltage. This series of four samples was analysed by AFM, SEM, EDS and XRD to determine the layer thickness, surface homogeneity, elemental and phase composition and their dependence on the deposition voltage. The analyses showed decreasing layer thickness, slightly decreasing homogeneity and approximately constant elemental composition with increasing deposition voltage and FCC content of phases with a small proportion of oxides. At the same time, the oxygen content was detected both in the layers and target. Future research should focus on increasing the homogeneity of the layers and modifying their elemental composition, especially the removal of oxygen.

Quantum technologies and material modelling / 27

Quantum technologies

Author: Ivan Richter[1]

[1] *CTU FNSPE*

Corresponding Author: ivan.richter@fjfi.cvut.cz

Quantum technologies and material modelling / 22

Nonlocal response of plasmonic nanostructures

Author: Milan Burda[1]

[1] *CTU FNSPE*

Corresponding Author: milan.burda@fjfi.cvut.cz

Plasmonic nanostructures with characteristic dimensions in the nanometer range exhibit behavior different from classical predictions due to nonlocal response. In our contribution, we focus on the nonlocal interaction of fundamental structures, such as metallic spherical particles, thin metallic layer, and bilayer.

Quantum technologies and material modelling / 20

Anomalous transport and Berry curvature in Fe3Ga

Author: Jaroslav Hamrle[1]

[1] *CTU FNSPE*

Corresponding Author: jaroslav.hamrle@fjfi.cvut.cz

The anomalous Nernst effect (ANE) is a member of the extensive family of topological effects in solid state physics. It converts a heat current into electric voltage and originates from the Berry curvature of electronic bands near the Fermi level. Recent results established the Fe3Ga alloy as one of the most promising candidates for applications, due to its flat band structure consisting of a rich web of nodal lines. In this theoretical work, we study the effect of deformation of Fe3Ga on the anomalous Nernst effect, which naturally occurs in thin films. Furthermore, we demonstrate that doping, which effectively shifts the position of the Fermi level, can also significantly modify the strength of the effect. Lastly, we provide detailed analysis of the origin of ANE in the electronic structure of Fe3Ga which yields a deeper insight into the generating mechanisms, the understanding of which can lead to substantial enhancement of the effect in the future.

https://doi.org/10.1103/PhysRevMaterials.7.084403

Material modelling and structure analysis / 29

Nanostruktura a nanomateriály

Author: Aruzhan Almazova[1]

[1] *CTU FNSPE*

Corresponding Author: almazaru@fjfi.cvut.cz

Nanostruktura a nanomateriály

Material modelling and structure analysis / 17

Implementace algoritmu optimalizace hejnem částic do programu FOX

Author: Milan Kočí[1]

[1] *CTU FNSPE*

Corresponding Author: kocimil1@fjfi.cvut.cz

V rámci oblasti řešení krystalové struktury z práškového difrakčního záznamu, která může působit značné komplikace, je program FOX jedním z významných nástrojů. Tento program, specializující se na řešení krystalových struktur v přímém prostoru, využívá algoritmů pro globální optimalizaci. Tento příspěvek se zaměřuje na konkrétní implementaci a jemné doladění algoritmu optimalizace hejnem částic s cílem jeho začlenění do programu FOX.

Material modelling and structure analysis / 12

Electronic structures of quasiparticle self-consistent *GW* (QSGW) in ferromagnetic Heusler alloys Ni_2MnX (Al, Ga, In)

Author: Jakub Luštinec[1]

[1] *CTU FNSPE*

Corresponding Author: lustijak@fjfi.cvut.cz

The quasiparticle self-consistent *GW* method is an advanced *ab-initio* method for electronic structure calculations. A short explanation and a basic understanding of this method will be presented, with an example of an application and comparison with DFT calculations for Heusler alloys Ni_2MnX (Al, Ga, In). One of the electronic structure properties calculated is generalized susceptibility, which provides insight into possible intrinsic system instability.

Material modelling and structure analysis / 13

Residual Stress Analysis of Additively Manufactured AlSi10Mg Alloy

Author: Jiří Čapek[1]

Co-author: Karel Trojan [1]

[1] *CTU FNSPE*

Corresponding Author: jiri.capek@fjfi.cvut.cz

Additive Manufacturing, precisely Selective Laser Melting (SLM) technology, is a promising metal powder consolidation method and offers outstanding parts production opportunities. It is based on selectively melting parts of a thin flat powder bed in layers using a scanning energy source to produce 3D parts. The intricacy of the SLM process results in the magnitude and orientation of residual stresses (RS) being highly dependent on laser power, scanning speed, scanning strategy, and other processing parameters. A correlation was observed between the RS and the formation of surface fatigue cracks for welded materials.

Material modelling and structure analysis / 23

Rentgenová difrakce na Katedře inženýrství pevných látek

Author: Karel Trojan[1]

Co-authors: Jiří Čapek [1] ; Kamil Kolařík [2] ; Nikolaj Ganev [2]

[1] *CTU FNSPE*

[2] *Katedra inženýrství pevných látek, Fakulta jaderná a fyzikálně inženýrská, České vysoké učení technické*

Corresponding Author: karel.trojan@fjfi.cvut.cz

Laboratoř strukturní rentgenografie od loňského prosince využívá nový práškový rentgenový difraktometr Empyrean od firmy PANalytical, který významně rozšířil možnosti a kapacitu pracoviště. Tématika problémů řešených v Laboratoři strukturní rentgenografie jak v rámci projektů základního a aplikovaného výzkumu, tak i na žádost našich i zahraničních pracovišť a smluvních partnerů je neobyčejně pestrá. Za projekty základního výzkumu lze například zmínit projekt „Mechanické vlastnosti funkčních vrstev submikronových tloušťek“, v rámci aplikovaného výzkumu v současnosti běží projekt „Vysoce produktivní stroje pro prostředí digitálních továren“. Laboratoř spolupracuje s dalšími výzkumnými organizacemi a také se podílí na výzkumu průmyslových partnerů jak těch velkých jako například UJV Řež, a.s. nebo UJP Praha a.s., tak těch menších, avšak neméně důležitých, jako třeba NEVA – TST s.r.o., což je malý podnik v jižních Čechách zaměřující se na výrobu strojů a nástrojů pro zpracování dřeva. V rámci přednášky posluchače seznámím jak s výše zmíněným přístrojovým vybavením, tak také s aktuálně řešeními problémy a zajímavými výsledky.

Advanced materials / 1

Photo-active liquid crystalline materials: effect of lateral substitution far from the chiral center.

Author: Sergej Mironov[1]

Co-authors: Martin Cigl [2] ; Tomáš Suchánek [3] ; Jan Marhoul [3] ; Věra Hamplová [2] ; Alexej Bubnov [2]

[1] *CTU FNSPE, Institute of Physics, Czech Academy of Sciences, 182 00 Prague, Czech Republic*

[2] *Institute of Physics, Czech Academy of Sciences, 182 00 Prague, Czech Republic*

[3] *Gymnázium Christiana Dopplera, 150 00 Prague, Czech Republic*

Corresponding Author: mirnoser@fjfi.cvut.cz

Photo-active liquid crystalline (LC) materials attract considerable attention as they give an exciting possibility to drive, tune and control the optical properties of soft systems in a contactless way. To contribute to better understanding of the effect of lateral substitution on the self-assembling behaviour, several new materials with lateral substituents are studied. These materials can be used as dopants for photo-active LC mixtures targeted for optoelectronic and photonic applications.

Advanced materials / 7

power output optimization from complex laser systems: solution for Yb:YAG laser rod in crystallographic orientation [111]

Authors: Dominika Jochcová[1] ; Ondřej Slezák[2]

[1] *CTU FNSPE*

[2] *HiLASE, Fyzikální ústav AV ČR, v. i. i. Za Radnicí 828, 252 41 Dolní Břežany*

Corresponding Author: jochcdom@fjfi.cvut.cz

A novel approach to optimize power output from a complex laser system is presented. The proposed method employs the formalism of second-order coherence theory and is applied to power characterization. It addresses the optimization of power output for non-uniformly and completely polarized beams by selecting suitable input and output ideal elliptical polarizers. The method is demonstrated using the Yb:YAG laser rod cubic crystal with the crystallographic orientation [111].

Advanced materials / 6

Testing of thermal barrier coatings using concentrated solar power

Author: Jonáš Dudík[1]

Co-author: Iosif Hulka [2]

[1] *CTU FNSPE*

[2] *Politehnica University Timisoara, Romania*

Corresponding Author: dudikjon@fjfi.cvut.cz

The multi-layered thermal barrier coatings (TBC) are commonly used in systems exposed to extensive heat, such as jet engines. In service, the top-coat layer may be exposed to so-called CMAS particles. In the hot environment, the CMAS particles melt and penetrate the coating microstructure, inducing crystallographic and volumetric changes therein. In this proceeding, the possibilities of using concentrated solar power to test the performance of TBCs with and without CMAS will be discussed.

Advanced materials / 15

Elastic anisotropy of strongly textured pure Ti determined by resonant ultrasound spectroscopy

Authors: Martin Koller[1] ; Karel Tesař[2] ; David Vokoun[2] ; Hanuš Seiner[3] ; Petr Sedlák[4]

[1] *Institute of Thermomechanics, Czech Academy of Sciences*

[2] *Institute of Physics, Czech Academy of Sciences*

[3] *CTU FNSPE / IT CAS*

[4] *CTU FNSPE*

Corresponding Author: koller@it.cas.cz

Resonant ultrasound spectroscopy (RUS) was employed to determine the elastic properties of commercially pure Ti grade 2 that was processed by room-temperature equal channel angular pressing (ECAP). The accumulated severe plastic deformation during the ECAP processing lead to an ultrafined grained material with a strong texture, which persisted even after annealing at various temperatures. The elastic properties of the as-processed Ti and three annealed samples were studied by laser-based RUS, where the full set of elastic coefficients was determined from resonant spectra of millimeter-sized samples. All the annealed samples were found to be strongly anisotropic in the elastic properties, where the maxima of Young's modulus align with the directions of the (0001) texture maxima. Moreover, the evolution of shear modulus and internal friction was measured across a temperature cycle from room temperature up to 590 ℃, providing valuable insights into the internal dynamics of the ECAP-processed Ti during annealing.

Advanced materials / 10

Apparent anisotropic thermal diffusivity measured in cubic single crystals by transient grating spectroscopy

Author: Jakub Kušnír[1]

Co-authors: Petr Sedlák [1] ; Hanuš Seiner [2] ; Tomáš Grabec [1] ; Kristýna Zoubková [1]

[1] *CTU FNSPE*

[2] *CTU FNSPE / IT CAS*

Corresponding Author: kusnijak@fjfi.cvut.cz

Transient grating spectroscopy (TGS) was used to measure the elastic and thermal properties of solid materials. Our measurements on cubic single crystals show anisotropic thermal diffusivity, which should be isotropic!
A finite element method (FEM) model was created to simulate the TGS measurements. The simulation with isotropic thermal diffusivity and elastic anisotropy leads to an apparent anisotropy of thermal diffusivity, which agrees with the measurements.

High Entropy and Shape Memory Alloys / 14

Applications of High Entropy Alloys

Author: Ladislav Kalvoda[1]

[1] *DSSE, CTU in Prague, FNSPE*

Corresponding Author: ladislav.kalvoda@fjfi.cvut.cz

As High entropy alloys (HEAs) are usually called equimolar metallic alloys composed of five or more elements, typically of similar atomic radius, forming a randomly distributed tough solution crystallizing in face centered cubic (FCC) or body centered cubic (BCC) crystalline lattice. Energetically, from the point of its Gibbs free energy of mixing, the solution is stabilized by the entropic contribution, dominating over the enthalpy term. Due to its distorted structure, properties of HEAs differ in many aspects from traditional alloys. The contribution is focused on the already advanced/elaborated practical applications of HEAs which have appeared nowadays and can be considered as the most promising ones.

High Entropy and Shape Memory Alloys / 28

Experiments with Neutron Tomography on the HK-2 Channel

Author: Martin Dráb[1]

[1] *CTU FNSPE*

Corresponding Author: martin.drab@fjfi.cvut.cz

In the Laboratory of Neutron Diffraction in Řež near Prague, on the HK-2 channel of the LVR-15 reactor, aside from classical neutron diffraction experiments, we have also been trying to experiment a little with transmission radiography as well. We have managed to acquire a new experimental equipment recently, consisting mainly of a new neutron camera and a one-axis goniometer and aside from significant resolution and image quality improvements we are slowly preparing for our first experiments with neutron tomography.

Shape Memory Alloys / 2

Tvorba meziatomárního potenciálu pro NiTi pomocí strojového učení

Author: Petr Jaroš[1]

[1] *CTU FNSPE*

Corresponding Author: jarospe7@fjfi.cvut.cz

Simulace molekulární dynamiky jsou silně závislé na potenciálu, který určuje meziatomární interakce, volba tohoto potenciálu ovlivňuje kvalitu a spolehlivost získaných dat. Meziatomární potenciály jsou v současné době vytvářeny pomocí analytických funkcí, které mohou přinášet kvalitní výsledky u partikulárních problémů, nicméně v obecných problémech často selhávají. Neuroné sítě nám nabízí možnost vytvořit potenciály zcela novým, více univerzální způsobem. V článku bude představen nově vytvořený potenciál pomocí metod strojového učení pro systém binární slitiny NiTi a jeho základní charakteristiky.

Shape Memory Alloys / 4

Resonant ultrasound spectroscopy for characterization of lattice instability in shape memory alloys

Authors: Hanuš Seiner[1] ; Petr Sedlák[2]

[1] *CTU FNSPE / IT CAS*

[2] *CTU FNSPE*

Corresponding Author: hanus.seiner@fjfi.cvut.cz

The lecture will summarize the advantages of using resonant ultrasound spectroscopy for ferroelastic alloys. Three recently studied cases will be discussed: i) single crystals of ferromagnetic shape memory alloys in which the instability-induced softening couples with magnetoelasticity; ii) the effective response of fine regular laminates in tetragonal martensitic lattices; iii) modulated crystals with highly mobile interfaces that act as strongly-nonlinear mechanical oscillators.

Shape Memory Alloys / 5

Shape Memory Alloy Exhibiting the Reentrant Austenite Behavior

Authors: Petr Sedlák[1] ; Hanuš Seiner[2]

[1] *CTU FNSPE*

[2] *CTU FNSPE / IT CAS*

Corresponding Author: petr.sedlak@fjfi.cvut.cz

During conventional martensitic transformation (MT) in shape-memory alloys (SMA), the parent (P) phase is stable at high temperatures, and the martensite (M) phase is formed during cooling. Very recently new class of SMA were discovered showing reentrant martensitic transformation back to austenitic phase at low temperatures. The occurrence of these novel phenomena originates from the reversal of phase stability between P and M phases connected with change in magnetic structure. In this contribution we will discuss lattice and magnetic contribution to this entropy reversal effect based on experimental study of elastic and magnetic properties.

Neutron diffraction / 18

Analýza struktur součenin boru (borany) pomocí RTG monokrystalové difrakce

Author: Monika Kučeráková[1]

[1] *CTU FNSPE*

Corresponding Author: monika.kucerakova@fjfi.cvut.cz

V posledních třech desetiletích je chemie sloučenin boru jednou z nejrychleji se rozvíjejících oblastí chemie nekovů. V rámci příspěvku budou prezentovány struktury vybraných sloučenin BnHm klastrů a jejich derivátů s uhlíkem (karborany). Budou představeny také kovové nanoklastry stabilizované pomocí výše zmíněných klecových systémů, což představuje novou třídu nanomateriálů.

Neutron diffraction / 11

Preferred orientation of the shells of the species Pseudanodonta complanata, Unio tumidus, Unio crassus and Anodonta anatina determined using X-ray and neutron diffraction

Author: Leonard Valko[1]

[1] *CTU FNSPE*

Corresponding Author: valkoleo@fjfi.cvut.cz

The research investigates the crystalline structures of the shells from four distinct species. By employing advanced X-ray and neutron diffraction techniques, the study delves into the preferred orientation of these shells, shedding light on their internal composition and arrangement. The findings are anticipated to contribute to our understanding of the speciesamp;39; adaptations and ecological roles, while also providing insights into the broader field of biomaterial characterization. This research offers valuable implications for material science and evolutionary biology, emphasizing the significance of non-destructive analytical methods in studying biological structures.

Defect structure and optical spectroscopy / 9

Translokační defekty krystalové mříže

Author: Petr Kolenko[1]

[1] *CTU FNSPE*

Corresponding Author: petr.kolenko@fjfi.cvut.cz

Translokační defekty krystalové mříže nazýváme takové defekty, kdy se jednotlivé části krystalu skládají z několika identických mříží, které jsou vzájemně posun
uté. Tento jev lze pozorovat na difrakčních snímcích, Pattersonově funkci a mnoh
dy také na zhoršené kvalitě map elektronové hustoty. Experimentální hodnoty lze
však oproti tomuto jevu korigovat.
V makromolekulární krystalografii jsou tyto defekty velmi vzácné, přesto jejejich řešení podstatnou součástí dalšího vývoje softwarových nástrojů.

Defect structure and optical spectroscopy / 3

Temperature dependence of silicon vacancy centers photoluminescence in polycrystalline diamond

Author: Irena Bydžovská[1]

Co-authors: František Trojánek [2] ; Karol Hamráček [2] ; Martin Hanák [2] ; Marián Varga [3] ; Alexander Kromka [4] ; Oleg Babčenko [4] ; Petr Malý [2] ; Lukáš Ondič [4]

[1] *FNSPE CTU, FZU CAS*

[2] *CUNI MFF*

[3] *FZU CAS, IEE SAS*

[4] *FZU CAS*

Corresponding Author: bydzovska@fzu.cz

The silicon vacancy (SiV) colour center in diamond is an optically active crystallographic point defect. Narrow band light emission of SiV centers makes them desirable in various fields such as quantum optics. In this work, we study SiV centers in polycrystalline diamond by using time-resolved low temperature photoluminescence (PL) spectroscopy. We investigate the spectral position, width and decay dynamics of the SiV zero phonon line in the temperature range 12-300 K.

Defect structure and optical spectroscopy / 19

Raman spectroscopy as a tool for rapid identification of UTI infections

Author: Kateřina Aubrechtová Dragounová[1]

[1] *CTU FNSPE*

Corresponding Author: katerina.aubrechtova@fjfi.cvut.cz

This contribution is devoted to the identification of bacterial pathogens by Raman spectroscopy with special reference to mixed infections. The advantages but also the current limitations of the method will be discussed.