S2PAM13 - 13. Studentská vědecká konference fyziky pevných látek, fotoniky a materiálů

Tuesday, 3 September 2024 - Friday, 6 September 2024

Pension Kamínek

Book of Abstracts

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Advances in signal processing, automation and construction of the transient grating spectroscopy

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Transient grating spectroscopy (TGS) is a non-destructive and non-contact optoacoustic method used to measure the elastic and thermal properties of solid materials. TGS can be used to measure samples over a wide range of temperatures. However, our TGS in its current design is not optimal for high and low temperature measurements with sample rotation. The new TGS design, measurement automation and signal pre- and post-processing will be presented.

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Simulations of SPM tip nanoindentation

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Methods of scanning probe microscopy (SPM) offer wide possibilities for basic and applied research. For example, tip-enhanced optical spectroscopy on single molecules performed with STM and AFM techniques offers a unique view into the world of fundamental photophysics at nanoscale. All SPM techniques have in common the need for atomically sharp tips as the probe. After more than four decades of SPM use on various problems in atomic and molecular physics, there is a consensus in the field that preparation of atomically-sharp tips is not easy and it involves shaping the apex at the mesoscopic and atomic scales. In this work, we simulate the tip-shaping by molecular dynamics in order to pave ways to better understanding and to develop more rigorous approaches to the process. We also aim to develop an algorithm to extract nanoscopic characteristics of real tips treated by nanoindentations and find a link to the simulations. This could ultimately lead to the much desired automation of the tip-shaping process and a significant benefit to the efficiency of SPM measurements.

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Nonlocal and quantum model of the response of a metallic nanostructure

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The focus of advanced simulations of the interaction between plasmonic nanostructures and electromagnetic waves is on phenomena associated with nanostructures with dimensions on the order of nanometers. From this perspective, the nonlocal response of the material is crucial. Quantum properties of the electron gas may also become significant, especially near the interface. An example is surface-enhanced attenuation. In our contribution, these topics will be briefly discussed.

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Introduction to Joint Life of Plasmons and Superconductors

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The role of plasmonic electronic excitation in formation of bosonic electron Cooper pairs and establishing a superconductive state is subjected to a long-lasting research. Still, many aspects of these interactions remain unclear and open for further theoretical as well as experimental examination. The contribution aims on introduction to important aspects of the coherent interplay between superconductivity and plasmonics, with a touch to existing and possible applications.

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Ke 100. výročí narození prof. Luboše Valenty, zakladatele KIPL FJFI ČVUT

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Profesor Luboš Valenta se narodil 26. ledna 1924 v Praze. Studium na Přírodovědecké fakultě UK ukončil v roce 1949 a akademický titul RNDr. mu byl udělen v roce 1951. V letech 1950-1953 absolvoval vědeckou aspiranturu u prof. Zdeňka Matyáše a získal hodnost kandidáta fyzikálně-matematických věd CSc. V letech 1953-1955 byl vědeckým pracovníkem Fyzikálního ústavu ČSAV. V letech 1955 - 1968 působil na Fakultě technické a jaderné fyziky ČVUT. V té době pracoval také ve Spojeném ústavu jaderných výzkumů v Dubně, na Fyzikální fakultě Moskevské státní univerzity a jako hostující profesor na Univerzitě Friedricha Schillera v Jeně.
V roce 1961byl pověřen založením a vedením katedry fyziky pevných látek na FTJF ČVUT. V roce 1969 přešel na Matematicko-fyzikální fakultu UK do funkce vedoucího katedry teoretické fyziky.
Těžiště vědecké práce prof. Valenty je v teoretických pracích o magnetizmu. Za originální teorii spontánní magnetizace tenkých vrstev byl v roce 1964 vyznamenán státní cenou. Inicioval a koordinoval vědeckou spolupráci mezi Přírodovědeckou fakultou UPJŠ v Košicích, Univerzitou v Lodži a Ústavem magnetických materiálů v Jeně.
Byl hostem mnoha zahraničních vědeckých ústavů. Byl často zván na mezinárodní konference k přednesení přehledných referátů a k řízení zasedání. Dlouhodobě působil v Komisi pro magnetismus Mezinárodní unie pro čistou a aplikovanou fyziku (IUPAP) a také jako předseda Mezinárodního výboru pro magnetické tenké vrstvy.
Pedagogická činnost prof. Valenty byla všestranná. Pod jeho vedením byla přeložena učebnice kvantové mechaniky A.S. Davydova. Se spoluautorem E. Jägerem vytvořil učebnici Festkörpertheorie : Eine Einführung.
Prof. Valenta se plně angažoval v akademických funkcích, v Jednotě čs. matematiků a fyziků a v redakci Československého časopisu pro fyziku.
Lodžská univerzita mu udělila v roce 1993 čestný titul dr.h.c. K 70. narozeninám mu slavnost uspořádala MFF UK a JČMF mu předala stříbrnou medaili a oborovou plaketu Fyzikální vědecké sekce.
Prof. Valenta byl výraznou osobností české fyziky ve druhé polovině dvacátého století.
Zemřel 21. října 1994 v Praze.

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Tailoring of UNCD films with incorporated SiV centres

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Ultrananocrystalline diamond (UNCD) films incorporating photoluminescent color centres have emerged as promising materials for quantum sensing applications due to their unique optical properties. This study investigates the synthesis, characterization, and enhancement of silicon-vacancy (SiV) centres in UNCD films. We successfully fabricated variously Si-doped diamond films using microwave plasma chemical vapour deposition (MPCVD). To enhance the photoluminescence (PL) of SiV centres, we employed oxidation treatment, which resulted in increased PL intensity compared to as-grown samples. Additionally, we utilized molten salt thermal etching (MSTE) to create nanoparticles from UNCD film, resulting in selective etching of the graphite phase while preserving nanocrystalline diamond particles with SiV PL. Surface characterization of the as-grown samples using contact angle measurements with deionized water droplets confirmed their hydrophobic nature. In an effort to further enhance PL, we conducted preliminary experiments exploring the surface plasmon resonance (SPR) effect using gold nanoparticles. While initial results did not show PL enhancement under the conditions tested, this approach warrants further investigation to optimize the experimental parameters. Our findings demonstrate a multi-faceted approach to UNCD growth and modification, offering controllable porous character and SiV center concentrations, and pave the way for advanced quantum sensing applications.

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Preparation of protein single crystals for electron diffraction experiments

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The use of electron crystallography in structural biology is gradually
increasing due to the properties of electrons such as strong interaction with matter. Procedures for the preparation of protein crystal samples for electron
diffraction as well as the subsequent processing of diffraction data are gradually
being standardized. This work deals with the optimization of crystallization conditions for growing microcrystals.

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IJD systems from laboratory to industry

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History and development of the IJD deposition method from laboratory prototypes to complex industrial systems

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Studium vlivu depozičních parametrů na vlastnosti tenkých vrstev vysokoteplotních supravodičů připravených metodou IJD

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V této práci jsme se zaměřili na přípravu a charakterizaci tenkých vrstev vysokoteplotních supravodičů YBCO připravených metodou IJD. V rámci výzkumu jsme připravili celkem 11 vzorků ve dvou sériích, lišících se použitým materiálem substrátu: MgO a $SrTiO_3$. Jednotlivé vzorky v rámci série se lišily teplotou substrátu během depozice. Ta se pohybovala mezi 480~℃ a 530~℃ pro MgO sérii a mezi 495~℃ a 515~℃ pro $SrTiO_3$ sérii.
Analýza tloušťky vrstev odhalila silnou závislost rychlosti růstu vrstvy na depozičním tlaku. Tloušťka připravených vrstev se pohybovala mezi 600~nm a 1400~nm.
Kvalitativní fázová analýza odhalila přítomnost fází $YBa_4Cu_3O_9$ a Y_2BaCuO_5 a po přežíhání vzorků byla u všech vzorků nalezena také supravodivá fáze $YBa_2Cu_3O_{7-x}$.
Měření elektrických vlastností potvrdilo supravodivý charakter vybraných vzorků s kritickou teplotou v rozmezí od 70~K a 85~K.

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Produkce a aplikace vysokoteplotních supravodičů

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Společnost CAN SUPERCONDUCTORS, s.r.o. je jediným průmyslovým výrobcem vysokoteplotních supravodivých materiálů v České republice. Společnost byla založena už v roce 1997 a nyní dodává produkty do více něž 45 zemí po celém světe. Hlavními produkty jsou supravodiče na bázi oxidů kovů vzácných zemin a mědi, jak v polykrystalické, tak i v jedno-doménové podobě. Jsme schopni vyrobit různé tvary i velikosti, abychom splnili i nejnáročnější přání zákazníka. Hlavní využití supravodičů můžeme nalézt v oblasti vesmírného výzkumu, částicové fyziky nebo ve vysokootáčkových ložiscích, které slouží k uchování velkého množství energie. Aplikací je několik a část z nich, stejně jako výroba a charakterizace těchto materiálů bude přiblížena v prezentaci.

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Superelastic bulk NiTi alloy samples prepared by spark plasma sintering

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NiTi alloys are widely used shape memory alloys due to their outstanding functional properties. Preparation of bulk NiTi with fine microstructures and high resistance to plastic deformation remains a challenge. Spark plasma sintering (SPS) theoretically enables to prepare such bulk NiTi. We synthesized, using SPS, bulk NiTi samples, exhibiting cyclic superelasticity in tension when sintering times were sufficiently long. Short times led to premature fracture in the elastic deformation regime.

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Preparation of thin films of silver using Ionized Jet Deposition and Magnetron sputtering methods for application in plasmonics

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Plasmonics is an advanced technology in the field of optical sensors. A methodology for the preparation of silver thin films suitable for plasmonics by Ionized Jet Deposition is developed. The RF Magnetron sputtering method is used for comparison as a well mastered technique. The roughness, relative permittivity and growth rate of the layers are analyzed using atomic force microscopy, attenuated total reflection and ellipsometry methods. Samples prepared by Magnetron Sputtering show slightly better properties, but the preparation by Ionized Jet Deposition can be further optimized.

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MOVPE grown AlGaN layers on sapphire substrates for UV applications

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Multiple applications (like LEDs) require growing high crystalline quality buffer layers before active region. These are the layers at the very bottom of structures, where on the boundary between sapphire and nitride many dislocations are created due to large lattice mismatch. It is important to improve the crystalline quality in this buffer layer, so that the active region has high internal quantum efficiency. We present preliminary results of AlGaN grown on sapphire with thin 3D GaN nucleation and coalescence layers.

Simulations and statistical analysis / 1

Alternative Methods of Fractal Analysis

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The presentation is focused on two original unbiased estimation techniques which are suitable for 2D and 3D image analysis. The first method is focused on the unbiased estimation of correlation dimension which is based on the Fourier image of given point set and its averaged power spectrum over all rotations in the Hilbert space. The second method is focused on the unbiased estimation of Renyi dimension using modified Renyi entropy and point neighborhood degeneracy.

Simulations and statistical analysis / 2

Statistical Analysis of Diffusion over Fractal Sets

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The work focusses on a statistical analysis of fractal diffusion and the estimation of fractal dimensions. We begin by introducing diffusion over fractal sets as subdiffusive anomalous diffusion characterised by statistical moments and return probability. We present butterfly diffusion and the constrained convolution schema, innovative approaches for analysis and numerical modelling. The results discussed offer significant insights for both theoretical research and practical use.

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Berry curvature in ferromagnetic materials

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Berry curvature expresses the curvature of the reciprocal space, in a similar manner as magnetic field express curvature of the real space, resulting in a curved transport of electrons in solids. Therefore, Berry curvature is a key to describe various transport phenomena such as anomalous Hall effect, anomalous Nerst effect, orbital magnetization, topological insulators or electric polarization. As those transports are lossless (also called bound current or topological current), they are interesting for various applications.
It is well known that Berry curvatures arise from close proximity of hybridizing bands, providing topological flows of Berry curvature in form of monopoles, one- (two-) dimensional flows, and or transitions between different dimensionalities [1] (Fig. 1). We use those features to identify and to visualize topological features of electronic band structure itself, such as dimensionality of avoided band degeneracy (e.g. where and at which dimensionality the bands approach each other or get degenerated). This provides a novel unique view on details of the electronic structure in whole Brillouin zone, inaccessible with traditional understanding of the band structure. Finally, we will demonstrate relation between Berry curvature and anomalous Hall effect in bcc Fe [1] and anomalous Nerst effect in Fe3Ga [2].
[1] Stejskal et al, Sci Rep 12, 97 (2022) [doi:10.1038/s41598-021-00478-1]
[2] Stejskal et al, Phys. Rev. Materials 7, 084403 (2023) [doi:10.1103/PhysRevMaterials.7.084403]

Neutron imaging technique / 31

Vývoj a výstavba zařízení pro neutronové zobrazování na reaktoru LVR-15

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České vysoké učení technické v Praze v současné době staví nové zařízení pro neutronové zobrazování na výzkumném reaktoru LVR-15. Projekt začal na jaře roku 2022 a jedná se o spolupráci mezi ČVUT v Praze, Helmholtz-Zentrum Berlin a Heinz Maier-Leibnitz Zentrum (FRM II). Zařízení je určeno pro techniky neutronové radiografie a tomografie s využitím tepelných neutronů. Očekává se, že zařízení bude dokončeno na podzim roku 2024 a poskytne přístup národním a mezinárodním uživatelům v různých výzkumných oborech v rámci otevřeného přístupu. Prezentace shrne základní komponenty zařízení, vysvětlí výběr filtrů a kolimátorů a upřesní možnosti využití zařízení.

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Optical and photothermal properties of TiN nanomaterials

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Transition metal nitrides (TMNs) have emerged as a promising alternative to precious metals thanks to their similar optical response and the additional advantages of refractory nature and compatibility with microelectronic industry fabrication process. This presentation will discuss the optical tunability of nanomaterials based on titanium nitride (TiN) in relation to their photothermal applications. A few selected case studies will be considered, including ultrathin planar films prepared by magnetron sputtering or atomic layer deposition (ALD), and titanium oxynitride nanotubes exhibiting broadband absorption for solar-thermal applications and photothermal catalysis.

Preparation techniques and analysis / 7

Optimisation of deposition parameters of Ionised Jet Deposition (IJD) created Titanium nitride thin films

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Titanium nitride is often used as a protective coating due to its hardness. Ionized jet deposition has a potential to improve and diversify ways of making TiN thin films. We optimised the nitrogen pressure in the IJD chamber to suppress concentration of titanium oxide in films. We manufactured a set of films using different deposition pressures. Based on the XRD data, higher gas pressure is preferable. In contrast, lower gas pressure contributes to higher film growth, based on AFM data.

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When crystal structure determination gets challenging

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Crystal structure analysis by diffraction methods is a standard, robust technique, that allows the solution of most new crystalline materials. It works even when the data suffers from systematic and statistical errors. However, some cases can be more challenging, and standard approaches do not easily solve the problem at hand. In this talk, we will show some examples of challenging structures that require a few advanced tools and a deeper understanding of crystallography.

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Study of the total structures of large metal nanoclusters by X-ray single crystal diffraction

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Atomically precise metal nanoclusters are nanoparticles less than 3 nm in size, which consist of a certain number of metal atoms protected by a specific number of thiolate ligands [1]. Such clusters of high number of atoms and atomically precise structure typical of molecular entities represent new emerging materials with numerous challenges related to understanding their molecular as well as supramolecular structure and their physical properties, and a correlation of the two. These species represent a transition from individual atoms, or their smaller arrays (several atoms) to the bulk form of the respective materials, and this transitional character makes them unique. Knowledge of the exact atomic structure represents an important milestone for understanding their physicochemical properties and thus for their possible use. For these reasons, single crystal X-ray diffraction is a very powerful tool.

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Simulace v nanofotonice

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Počítačové simulace v nanofotonice jsou nezbytným nástrojem pro návrh a analýzu optických systémů na nanometrické škále, kde analytické metody často selhávají kvůli složitosti interakcí světla s nanostrukturami. Tento příspěvek se zaměřuje na klíčové úlohy simulací v nanofotonice, jako je šíření, lokalizace a rozptyl světla. Tyto úlohy jsou řešeny numerickými metodami založenými na řešení Maxwellových rovnic, přičemž bylo vyvinuto mnoho pokročilých technik, což je výsledkem potřeby řešit širokou škálu specifických problémů, které nelze efektivně zvládnout jednou univerzální metodou. Představíme základní principy nejpoužívanějších metod, popíšeme jejich numerické vlastnosti a ukážeme jejich implementaci v moderních softwarových nástrojích.

Advanced materials / **19**

AA bilayer coupler

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Two non-interacting graphene sheets are deformed in a localized region where they form AA bilayer graphene. This theoretical model is called AA bilayer coupler. We show that the Hamiltonian of this system can be elegantly block-diagonalized. On the coupler, the scattering properties of Dirac fermions in two dimensions are analyzed through a partial wave decomposition. The differential and partial cross sections reveal us some interesting phenomena such as pouring particles from one layer to the other, filtering Dirac fermions with a given value of angular momentum or the formation of quasi-bound states. The coupler is further enhanced by electric and magnetic fields which provide an ability to manipulate the direction of scattered particles.

Semiconductors / 27

Onsemi –představení společnosti a možnosti spolupráce

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Onsemi –představení společnosti a možnosti spolupráce

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Karbid křemíku –budoucnost výkonové elektroniky právě začíná

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Karbid křemíku –budoucnost výkonové elektroniky právě začíná

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Upgrade of the Quantum Hyperion Cluster

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The Quantum Hyperion cluster currently runs CentOS 7 operating system, support of which have ended by June 30th, 2024. To continue running it safely an upgrade to a new system together with an overall upgrade of the software is needed. This talk is to summarize the changes that are currently being worked on and that will soon convert the Quantum Hyperion cluster into a new cluster called Quantum Hyperion 2.

XRD analysis / 9

Optimization of 3D printing parameters to minimize residual stresses in maraging steel

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Co-authors: Ivana Zetková [2]; Jiří Sika [2]; Jiří Čapek [1]; Nikolaj Ganev [1]; Petr Thurnvald [2]

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Fatigue crack initiation and propagation play an important role in fatigue properties, where they are shown to be strongly associated also with macroscopic residual stresses (RS). During additive manufacturing using the selective laser melting technology, a complex residual stress distribution is created that can significantly affect the printing itself and also the mechanical properties of the final product. The magnitude of these stresses may even approach the yield strength of the material. Thus, research has been carried out to optimize 3D printing parameters to minimize residual stresses in MS1 maraging steel. Macroscopic RS were determined using X-ray diffraction and hole drilling. It was found that the preheating temperature of the build platform significantly affects the residual stresses, especially in the vicinity of the building platform. For both samples, the tensile residual stresses near the surface still dominate, but a rapid decrease in residual stresses can be observed for the sample with platform preheating to 120℃.

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The real structure of γ-Fe phase of rolled 1.4470 duplex steel after shot peening

Authors: Marek Rušin[None]; Jiří Čapek[None]; Karel Trojan[None]; Nikolaj Ganev[1]

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Duplex stainless steels are grades composed primarily of α-Fe and γ-Fe phases. They exhibit better properties compared to single-phase steels and are widely used in many engineering areas. Shot peening is used to further improve the final properties of the materials. It is essential to know how this process affects the real structure. Using X-ray diffraction techniques, the impact of shot peening intensity on crystallite size, residual stresses, and preferred orientation of γ-Fe was studied. The depth distributions of these parameters with respect to distance from the sample surface are described.

XRD analysis / 8

X-ray diffraction analysis of additively manufactured AlSi10Mg alloy

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The paper deals with the analysis of residual stresses of additively manufactured AlSi10Mg alloy samples. The influence of the 3D printing strategy of the SLM (Selective Laser Melting) technology was proofed by X-ray diffraction. The phase analysis identified the intermetallic phase Mg2Si in addition to the major phases (solid solutions of Al and Si). The inhomogeneities of tensile residual stresses around the circumference of the tested samples were analyzed. Areas of steep changes in residual stresses (especially tensile) can be potential areas for crack initiation. Inherent anisotropy was studied by tracing the plasticity surface from which a yield stress of 160 MPa was determined. After tracing, a decrease in tensile residual stresses was observed.

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Systematic characterization of TaRhTe4 samples prepared by the exfoliation technique and fabrication of microstructures for spintronics

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Systematic characterization of TaRhTe4 samples prepared by the exfoliation technique and fabrication of microstructures for spintronics