

Book of Abstract INTERM 2023



10th International Congress on Microscopy & Spectroscopy

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Microscopy & Spectroscopy
(INTERM 2023)**

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10th International Congress on Microscopy & Spectroscopy

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PLENARY SPEAKERS

Id-652

**Beam-sensitive Nano-crystals:
a Double Challenge for Crystallographic Structure Solution**

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Abstract- The determination of the crystallographic structure of a material is essential for the comprehension of its properties. It is therefore evident that the development of new materials with optimized properties is possible only if there are methods that allow elucidating their structures. For materials that can be grown to stable single crystals of at least a few tens of micrometers in diameter the crystallographic gold standard is single crystal X-ray diffraction (SCXRD).

However, there is a wealth of materials that are beam sensitive and only exist in nanometric crystals, because the growth of bigger crystals is either impossible or so complicated that it is not reasonable to spend enough time and resources to grow bigger crystals before knowing their potential for research or applications. In these cases, SCXRD is no longer an option and new characterization methods need to be optimized to get the most information out of these particles before the radiation damages them to a point where their structure is altered.

Both, the small size and beam sensitivity, call for electron diffraction as a privileged investigation tool. The strong interaction of electrons (as compared to X-rays) with matter allows single crystal diffraction experiments on nanometer-sized crystals and for the same amount of beam damage, electron diffraction yields more information than X-rays. These inherent advantages of electron diffraction are optimized in the recently developed low-dose electron diffraction tomography (LD-EDT).

Here we present three examples of beam sensitive nanometric crystals: the notoriously beam sensitive metal organic framework Mn-formiate $[\text{Mn}(\text{HCOO})_2(\text{H}_2\text{O})_2]_\infty$, a garnet structure exhibiting partial site occupation and the mineral bulachite $[\text{Al}_6(\text{AsO}_4)_3(\text{OH})_9(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$. In all these cases, even small electron doses of a few $\text{e}^-/\text{\AA}^2$ are enough to damage the structure. Therefore, the total dose for the data acquisition had to be chosen well below the onset of visible damage.

In the case of Mn-formiate we recorded a dataset of 60 electron diffraction frames corresponding to a total dose of $0.15 \text{ e}^-/\text{\AA}^2$. The obtained data quality is high, allowing not only the solution of the structure, but also its refinement taking into account the dynamical diffraction effects.

The NaMnGeO garnet contains the volatile Na and only decreasing the total dose to $0.13 \text{ e}^-/\text{\AA}^2$ yielded the correct solution of the partial occupation of the Na site.

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Likewise, on bulachite the electron dose had to be drastically reduced in order not to destroy the structure and conserve the free water molecules. We acquired a LD-EDT data set containing 105 frames with a total dose of 3 e-/Å². The obtained structure solution contained all non-hydrogen atom positions including the free water molecules. The charge valence sums calculated from the model allowed distinguishing the O²⁻, OH⁻ and H₂O. A dynamical refinement improved the accuracy of the atom positions with an average distance to the XRD refined positions of 0.1 Å for bonded oxygen (Figure 2).

In this contribution we show that beam sensitive crystals need the extremely low doses that can be obtained by LD-EDT to obtain the correct structures of complex crystals.

Keywords: Electron Crystallography; Beam Sensitive Materials; Structure Solution; Structure Refinement; 3D Electron Diffraction, Low Dose.

INVITED SPEAKERS

Id-651

Recent Progress in Understanding of Low Energy Electron Interaction with Solid Surfaces

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Abstract- Understanding the interaction of low energy electrons (LEEs) with solid materials is important both from a fundamental point of view as well as for important technological applications, such as the secondary electron (SE) microscope, electron optics and charged particle detection, particle accelerators and charged particle storage rings, spacecraft charging, the plasma-wall interaction in a fusion reactor, radiation damage in biological tissue etc. Several aspects of LEEs interaction with and emitted from surfaces are not yet sufficiently understood quantitatively or even qualitatively. In the present lecture we present recent results elucidating various aspects of LEEs near surfaces obtained with secondary electron electron energy loss coincidence spectroscopy (SE2ELCS). These include: (1) role of plasmons in emission of LEEs from surfaces; (2) influence of unoccupied states for SE emission from 2D materials; (3) assessment of the values of the electron inelastic mean free path below 50eV; (4) measurement of the surface potential barrier in metals and polymers, comparison with electron holography in the TEM (carried out at Forschungszentrum Jülich) and absolute secondary electron yield data (measured at CERN).

Keywords: Secondary low energy electrons imfp inner potential

INVITED SPEAKERS

Id-653

Correlative in situ Surface Microscopy of Rhodium Catalyzed Hydrogen Oxidation

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Abstract- Nanostructured metals are important functional materials for energy-relevant catalytic reactions. The oxidation of hydrogen to water by solid catalysts enables energy generation without combustion and without pollution, e.g., in fuel cells. For future developments of new green energy production technologies, it is important to monitor ongoing catalytic reactions by in situ microscopy of working catalyst surfaces. Two examples are presented, covering meso-scale planar Rhodium surfaces and a single Rh nanoparticle (single particle catalysis).

Several different microscopic techniques (see below) were combined for in situ imaging of catalytic H₂ oxidation on the same structures of the same Rh sample, i.e., in a correlative approach preferentially operated in a single setup under truly identical reaction conditions.

i) Using a correlative microscopy approach, H₂ oxidation on polycrystalline Rh foil was studied by scanning photoelectron microscopy (SPEM) and photoemission electron microscopy (PEEM), which allow local surface analysis and visualising the heterogeneity of ongoing reactions on a μm -scale. This revealed an anisotropy of surface oxidation, yielding an oxidation map, as well as the reaction mechanism involving subsurface oxygen. In situ PEEM imaging of ongoing H₂ oxidation directly compares the local reactivity of metallic and oxidised Rh, revealing a high transient activity of Rh surface oxide. Higher spatial resolution and chemical sensitivity were provided by low energy electron microscopy (LEEM) and XPEEM, revealing a new front propagation mechanism.

ii) Using the apex of a Rh-nanotip as model structure, single particle catalysis was studied on the nm-scale by field emission microscopy (FEM) as imaging tool. Novel effects were revealed, such as nanoscale multifrequential oscillations and limited interfacet coupling. Using ionized water as imaging species, the active sites on the metal nanotip were directly imaged by field ion microscopy (FIM).

The obtained insights may stimulate new ways of metal catalyst design and operation.

Research funded by the Austrian Science Fund (FWF) (SFB TACO und P32772-N). Cooperation with the groups of M. Stöger-Pollach, H. Grönbeck, L. Gregoratti and B. Roldan Cuenya are gratefully acknowledged.

Keywords: Photoemission electron microscopy, field emission microscopy, rhodium, hydrogen oxidation, reaction fronts, oscillations, single particle catalysis

INVITED SPEAKERS

Id-660

Computational Biomedical Imaging : Inverse Problems

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Abstract- This talk presents some recent advances in computational biomedical imaging, and how, many complex imaging challenges can be tackled. The talk focus on restoration topics. Different examples are shown throughout the talk.

Keywords: Image processing, restoration, inverse problem, denoising, deconvolution, super-resolution

INVITED SPEAKERS

Id-663

Mechanism of RNA-DNA Primer Synthesis Termination by Human Primosome

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Abstract- The human primosome, a four-subunit complex of primase and DNA polymerase alpha (Pol α), synthesizes chimeric RNA-DNA primers for DNA polymerases delta and epsilon to initiate DNA replication on both chromosome strands. Despite recent structural insights into the action of two catalytic centers, the mechanism of DNA synthesis termination is still unclear. Here we report results of functional and structural studies, revealing how the human primosome can count the length of RNA-DNA primer and timely terminate DNA elongation. Using single-turnover primer extension assay and cryo-electron microscopy single-particle analysis, we found that the primer length counting mechanism is based on three factors: 1) a tight interaction of the C-terminal domain of the DNA primase large subunit (p58C) with the primer 5'-end, 2) flexible tethering of p58C and DNA polymerase alpha catalytic core domain (p180core) to the primosome platform domain (p49-p58N-p180C-p70) by extended linkers, and 3) a transient interaction between p180core and the platform domain. These factors determine the mature primer length (~35-mer) and prevent DNA synthesis restart by blocking Pol α access to the completed primer. Our data revealed that all steps of RNA-DNA primer synthesis are regulated by p58C. The above findings provide new insights into the molecular mechanism of DNA synthesis termination by eukaryotic primosome, a key process for successful primer handover to replication DNA polymerases.

Keywords: DNA replication, cryo electron microscopy, structural biology

INVITED SPEAKERS

Id-665

Computational Modeling of Condensed-state Infrared and Raman Vibrational Spectra as a Tool for Analysis of Molecular and Supramolecular Structure of Liquids, Amorphous Solids and Their Solutions

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Abstract- Nowadays experimental IR and Raman spectra are almost routinely interpreted by comparison with spectra quantum chemically simulated for isolated molecules. This gas-phase approximation often fails in the case of spectra of solids, liquids and solutions, especially if hydrogen bonds (HBs) are in action, because HBs strongly influence vibrational spectra. This problem may be tackled within the framework of ab initio molecular dynamics, but such computations are extremely time- and resource-demanding. Recently we have proposed an efficient protocol for accurate quantum mechanical simulation of IR spectra of condensed-state systems in which (A) implicit and (B) explicit treatment of media effects are combined. (A): possible structural forms of the compound under consideration are computed with the use of the recently developed efficient CENSO protocol to implicit quantum mechanical modeling of non-rigid molecules in solution; (B) Boltzmann populations calculated with CENSO for each implicitly solvated single structural form are used to weight the IR or Raman spectra of such forms explicitly solvated by the first shell of solvent molecules. An automated cluster generation algorithm was applied to construct these “solute-solvent” clusters that were re-optimized at a reasonable but efficient level of DFT. Our protocol ensures an accuracy, comparable to experiment, for the theoretical prediction of condensed-phase vibrational spectra and, being computationally efficient, can be used in everyday spectroscopic practice. The simulations followed by comparisons of the computational predictions with the experimental spectroscopic data allow, apart from complete interpretation of the spectra, conclusions regarding the structure of molecular and ionic liquids, hydrogen bonding, conjugation, etc. Possible applications of the developed technique in IR/Raman spectroscopic analysis will be discussed.

Financial support from Russian Science Foundation (grant 22-23-00970) and ideological and technical support from Prof. S. Grimme are gratefully acknowledged.

Keywords: Infrared and Raman spectra; quantum chemistry; condensed state; hydrogen bonding

INVITED SPEAKERS

Id-668

Solid Wastes Recycling into Hierarchical Porous Carbon Materials for Supercapacitors – Microscopic and Spectroscopic Study

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Abstract- As a key energy storage device, the carbon-based supercapacitor (C-SC) has already been widely explored in different fields e.g. hybrid vehicles, and energy harvesting due to their great power density, rapid charge-discharge response, high capacity and durability. Among different electrode materials hierarchical porous carbons (HCPs) have been deeply explored. However, the commercial porous carbons, especially activated carbons, showed weak electrochemical performance with low capacity and weak rate capability. Therefore, it is of huge importance to tune and control the physicochemistry of HCPs, to fulfill the required characteristics of ideal electrodes for C-SC, with use of microscopic and spectroscopic tools. In this contribution, various HCPs designed from different carbon precursors (biomass, flame retardants, and polymer) were prepared through facile strategies and their microscopic/spectroscopic characteristics and electrochemical response will be presented.

The conducted research demonstrated that the physicochemical properties (2D/3D morphology, SBET, micropore volume, meso-/macropore volume, doping with heteroatoms and combining metal oxides) play key roles on the electrochemical response of these porous carbons and composites. Tuning these properties of porous carbons brings improvement in the charge storage capacity, rate capability, pseudocapacitance contribution, energy density, long-cycle stability and reversible specific capacity. What is worth to emphasize the optimization of one of the physicochemical property alone does not efficiently boosts the electrochemical properties. The synergy of these optimized physicochemical properties delivers: (i) increased charge storage capacity, (ii) a continuous electron pathway to benefit to ion transport via short diffusion pathways for a high rate capability, (iii) charge storage sites to create a large electric double layer for great charge storage capacity, (iv) doping heteroatom into carbon matrix to enhance electronic conductivity and surface wettability for pseudocapacitance.

Keywords: Supercapacitors, solid wastes conversion, added-value materials, TEM/SEM

INVITED SPEAKERS

Id-670

**Advanced Visualisation and Evaluation of Smart Nanostructured Materials
Preferably Derived by Simple Methods**

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Abstract- The chemical composition unquestionably lies behind the beneficial behaviour for the case of many newly developed materials. However, in reality, in many of the mentioned cases the chemical composition proved only as a necessary condition for the desired performance, while performance beyond that was more or less enabled by the advances of the morphological features. In many examples the morphological features that proved particularly beneficial are related with the phenomenology of ordered organisation of the material constituting domains. So nanostructuring can further extrapolate the case of functional nanomaterials. The work covers the conceptual route from simpler chemical routes to those more complex and advanced, that enable preparing from just mixed metal oxide nanoparticles to mixed metal oxide nanostructured thin-films. Their properties can be either controlled by modifications in the course of synthesis or they can be designed to show some extent of smart behaviour i.e. adapt according to changing conditions. Accordingly, these are prepared from simple purely chemical routes or by multistep chemical routes supported by physically deposited seeds layers. Consequently, the issues are encountered during these steps, particularly for the case of more complex routes. This work elucidates these discrepancies and basically discuss the troubleshooting strategies. The work is wrapping around applications such as charge transfer layers in solar cells, anticorrosive coatings and biomaterials for implants. Particular attention is devoted in applied visualisation and evaluation methodology.

This work has been funded by the projects UIP-2019-04-2367 and PZS-2019-02-1555 by the Croatian Science Foundation, and KK.01.2.1.02.0316 by the European Regional Development Fund.

Keywords: Self-assembly, smart materials, nanomaterials

INVITED SPEAKERS

Id-673

**On Surface C-C Cross Coupling Reactions Investigated by Scanning Probe
Microscopy**

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Abstract- Bottom-up covalent assembly of molecular building blocks on surfaces by C-C cross coupling reactions is of great interesting for its potential in preparation the covalent architectures. For example, dendrimers are homostructural and highly branched macromolecules which exhibit many unique dendritic effects and lead to extensive use in multidisciplinary fields. Although thousands of dendrimers have been synthesized in solution, the on-surface synthetic protocol for planar dendrimers has never been explored, which limits the elucidation of the mechanism of dendritic effects at the single-molecule level. We described an on-surface synthetic approach to planar dendrimers, in which exogenous palladium was used as a catalyst to address the divergent cross-coupling of aryl bromides with isocyanides. This novel reaction enables one aryl bromide molecule to react with two isocyanide molecules in sequential steps to generate the divergent growth product composed of a core and two branches with high selectivity and reactivity. On this basis, a dendron with four isocyanide-derived branches and dendrimers with eight and twelve isocyanide-derived branches in the outermost shell have been synthesized on a surface. This work opens the door for the on-surface synthesis of various planar dendrimers and relevant macromolecular systems.

Keywords: On surface reactions, cross-coupling reaction, scanning probe microscopy

INVITED SPEAKERS

Id-674

**Monitoring the Response of the Immune System by Infrared Spectroscopy-based
Machine-learning Algorithms for Rapid Diagnosis of the Etiology of Patients'
Infections as Bacterial or Viral**

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Abstract- One of the leading causes of morbidity and mortality in humans has traditionally been infectious diseases. Although the immune system responds differently to a bacterial infection or a viral infection, the symptoms of these illnesses are in most cases the same. Modern etiology-diagnosis methods take two to four days and are accurate for accessible infections, but they are ineffective for inaccessible infections. Doctors regularly subjectively determine whether an infection is bacterial or viral in all cases for inaccessible infections and frequently for accessible infections based simply on symptoms, their experience, and medical measures. In many cases, they start unnecessary antibiotic treatment. Sensitive, focused, and speedy novel techniques are therefore required to ascertain the etiology of infections for both accessible and inaccessible illnesses. Along with machine learning (ML) techniques, Fourier transform infrared (FTIR) spectroscopy has become an effective diagnostic tool in the medical industry. According to our hypothesis, it is possible to detect modest changes in white blood cells (WBC) as well as more significant molecular alterations brought on by the different immune responses to viral or bacterial infections. In this work, we evaluated the potential of the mid-infrared spectroscopy technology for rapid and reliable diagnosis of bacterial and viral diseases based on straightforward peripheral blood samples. Peripheral blood samples were collected from patients aged 0 to 18 who had a fever: 113 controls, 54 bacterial and 27 viral of accessible infections, and 89 bacterial and 60 viral of inaccessible infections.

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The white blood cells were separated and their infrared absorption spectra were recorded and analyzed by a support vector machine (SVM), using a classification approach with four stages: data extraction, data pre-processing, feature selection, and classifier training and prediction. A binary classification was performed in two stages, the first of which classified the samples into healthy controls and infected patients (which includes both viral and bacterial samples). The second classification stage divided the infected samples into viral and bacterial classes. A five-fold cross-validation procedure was used to evaluate the SVM classifier's performance.

Based on our methodology, it was determined that >23% of doctors' subjective diagnoses of the causes of inaccessible infections were incorrect. This was accomplished by employing the accessible infection data to train the classifier, which served as the gold standard and was utilized to predict the etiology of inaccessible infections.

It was possible to determine the etiology of infection for both accessible and inaccessible illnesses as being bacterial or viral within one hour after the blood sample's collection with >94% sensitivity and >90% specificity.

Keywords: Immune-system inaccessible infections, accessible infections, Infection etiology infrared microscopy, machine learning

INVITED SPEAKERS

Id-675

Rapid Identification and Antibiotics Susceptibility Determination of Bacteria Isolated Directly from Patients' Urine Samples by Infrared Spectroscopy in Tandem with Machine Learning

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Abstract- Urinary tract infections (UTIs) are considered to be the most common bacterial infections worldwide, which are caused mainly by *Escherichia (E.) coli* (about 80%). *Klebsiella pneumoniae* (about 10%) and *Pseudomonas aeruginosa* (about 6%). Although antibiotics are considered as the most effective treatment for bacterial infectious diseases, unfortunately most of the bacteria already have developed resistance to the majority of the commonly available antibiotics. Therefore, it is crucial to identify the infecting bacteria and to determine its susceptibility to antibiotics for prescribing effective treatment. Classical methods are time consuming, require ~48 hours for determining bacterial susceptibility. Thus, it is highly urgent to develop a new method that can significantly reduce the time required for determining both infecting bacterium at the species level and diagnose its susceptibility to antibiotics. Fourier-Transform Infrared (FTIR) spectroscopy is well known as a sensitive and rapid method, which can detect minor molecular changes in bacterial genome associated with the development of resistance to antibiotics. The main goal of this study is to examine the potential of FTIR spectroscopy, in tandem with machine learning algorithms, to identify the infected bacteria at the species level and to determine its susceptibility to different antibiotics directly from patients' urine in about 30 minutes after receiving the patients' urine. For this goal 1600 different *E. coli* isolates, 600 different *Klebsiella pneumoniae* isolates and 250 different *Pseudomonas aeruginosa* isolates were isolated for different patients' urine sample, measured by FTIR microscopy and analyzed using different machine learning algorithm like Random Forest, XGBoost and CNN. We achieved 96% success in isolate level identification and 83-89% accuracy in susceptibility determination to different antibiotics.

Keywords: Urinary tract infections (UTIs), *E. coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, bacterial, antibiotic, susceptibility to antibiotics, infrared microscopy, machine learning

INVITED SPEAKERS

Id-677

**Application of Element and Molecule-based Imaging and Dosimetric Techniques
for Nanotoxicology and Nanomedicine.**

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Abstract- The degree and the mechanism of uptake, localization and distribution of nanomaterials (NMs) and nanocarrier loading with drugs (NDs) in cells and organs are major issues concerning risk assessment and therapeutic efficacy of the novel products. The application of these materials for diagnostic and therapeutic purposes requires monitoring of their interaction with cells. Label-free imaging techniques are therefore required.

The translocation of NMs across plasma membranes, their quantification and interaction with metabolic relevant cellular elements and biomolecules were studied in in vitro as well in vivo by means of label-free imaging methods based on element and molecule analysis. The two ion beam microscopy techniques as proton induced X-ray emission (μ PIXE) and Rutherford backscattering (μ RBS) were used simultaneously at the Leipzig Ion Nanoprobe LIPSION for cell and tissue analysis. These two techniques provide unique and powerful tools for element dosimetry and spatially resolved elemental analysis. The results of NM uptake in vitro were compared with in vivo study providing a tool for estimating the relevance of in vitro data for in vivo predictions. A quantitative analysis of minor and trace elements and their alterations due to NM loading at single cell level were performed and correlated with the cellular adverse response.

Furthermore, NM and ND subcellular localization and co-localization with cell compartments and biomolecules were investigated using confocal Raman microspectroscopy (CRM). CRM live imaging was additionally performed to follow the extra and intracellular fate of NM&NDs. The uptake kinetics as well as the intracellular dissolution behavior were studied as well. Specific cellular regions of interest have been screened for spectroscopic signatures by means of cluster analysis or principle component analysis. The early alterations of chemical fingerprints in cells upon exposure to nanomaterials were evaluated as chemical biomarkers regarding their predictive potential.

Keywords: Nanomaterials, nanodrugs, label-free imaging, single cell analysis

INVITED SPEAKERS

Id-678

**Time-Resolved Charge Observation by Tip-Synchronized Electrostatic Force
Microscopy**

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Abstract- The micro- or nanoscale generation, migration, and recombination of local charges (collectively referred to as charge dynamics) play essential roles in many natural and artificial systems or phenomena, including the brain, light harvesting, photosynthesis, catalysis, photovoltaic devices, and field-effect transistors. Charge tracking is intrinsically important for understanding the fundamental characteristics of these systems as well as the fabrication of functional materials and devices.

Time resolution in scanning tunneling microscopy (STM) was initially reported in 1990 by Hamers and Cahill, who applied the pump–probe method. Subsequently, Shigekawa and co-workers achieved femtosecond time resolution using terahertz pump–probe STM. Although these approaches simultaneously realized fast time resolution and nanoscale spatial resolution, the samples were limited to semiconductors because the STM measurement required a nonlinear tunneling current. Consequently, the observable phenomena were limited to the modulated densities of states and work functions. For tracking charge migration and recombination, the charge should be directly detected from the functional materials typically used in device applications, such as insulators, wide-bandgap semiconductors, and poorly conducting surfaces.

We previously proposed a tip-synchronized tr-EFM method involving the generation of pump pulses with a constant phase of cantilever vibration. In this method, the charge detection at the tip position closest to the sample surface corresponds to the probe detection in the pump–probe framework, improving the sensitivity and spatial resolution compared with standard EFM methods. Using a similar approach, Marohn and co-workers employed phase-kick EFM for time-resolved electrostatic force detection. Recently, we were able to obtain a video showing photoexcited carrier migration on an organic photovoltaic device with a time resolution of 0.3 μ s and sensitivity of 0.3 Hz.

The tip synchronization can be extended to dual-bias pump–probe measurements using constant-amplitude feedback control, frequency-shift electrostatic force detection, and lock-in detection of the probe pulse train modulation. This method permitted highly sensitive detection of the electrostatic force under a constant tip–sample distance, thereby enabling time-resolved observation of the charge dynamics for the conductive polymer SPAN, which is a relatively poor conductor. Comparison of SPAN thin films with different doping levels revealed the individual differences in carrier density and mobility. The obtained

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results demonstrate that time-resolved EFM is a powerful tool for elucidating the charge dynamics of hopping conductors such as thermoelectric materials containing metallic grains. In addition, the application to the plasmon induced charge separation will be also presented.

Keywords: Time-resolution, electrostatic force microscopy, charge migration

INVITED SPEAKERS

Id-680

Application of Attenuated Total Reflectance Infrared Spectroscopy (ATR) in Quantification: Determination of Hydroquinone in Whitening Facial Cream

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Abstract- Attenuated total reflection (ATR) accessories in conjunction with Fourier transform infrared (FTIR) spectrometers coupled with a simple preparation of the sample provide particularly well-suited quantitative analyses. The optimum solvent with suitable sample preparation can increase the precision of the quantification in FTIR technique. Determination of hydroquinone in whitening facial cream by ATR using a silver nanoparticles coated filter paper (Whatman no. 1) as a solid support has successfully developed. The intensity of 3 absorption peaks including C=C- stretching of aromatic at 1514 cm⁻¹, C-H bending and 1,4-disubstituted at 860 and 750 cm⁻¹ were linear relationship with hydroquinone concentration. The intensity of the IR peak at 1514 cm⁻¹ was used for quantitative determination of hydroquinone. The linear range were in the range of 300–60,000 ppm with r-square of 0.9976 and the detection limit of 200 ppm. The precision (%RSD) from 10 replicates of hydroquinone determination at 8,000 ppm was found to be 9.2%. Propyl paraben (10,000 ppm) and methyl paraben (10,000 ppm) were not interfered the determination of hydroquinone at 10,000 ppm.

Keywords: Hydroquinone; attenuated total reflection; silver nanomaterials

INVITED SPEAKERS

Id-684

**Imaging the Nanoscale World of Life: A Biophysical Approach to Studying
Microbes, Stem Cells, and Antibiotic Resistance**

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Abstract- The characterization of biological interfaces is critical for understanding biophysical phenomena and designing biomaterials. Biological surface science has been an active area of research for over two decades, but conventional methods require fixed or dehydrated samples studied in ultrahigh vacuum, which limits the ability to investigate the native structure and function of biological interfaces. This work proposes the use of Photoinduced Force Microscopy (PiFM) and Cryogenic X-ray Photoelectron Spectroscopy (XPS) as novel techniques for studying life's surfaces.

PiFM is used for the first time in the liquid phase to investigate the surface chemistry of stem cells, allowing characterization of their bulk and membrane chemistry. PiFM and XPS have penetration depths of 5-20 nm, enabling unparalleled examination of surface science in biological species. The presentation explores how PiFM can be implemented to map the nanoscale chemistry of nucleic acids, proteins, lipids, and other important spectroscopic groups in gram-negative, gram-positive, and fungal microbes, achieving a resolution of up to 20 nm. The PiFM technique provides unprecedented detail of the molecular vibrations associated with functional groups, including C=O and N-H stretches, which can be used to identify specific chemical species.

Furthermore, these new techniques have enabled mapping and spectroscopic explanation of the origin of mobile colistin resistance in *E. coli*. Colistin is an antibiotic of last resort that is used to treat serious infections caused by Gram-negative bacteria, but resistance to colistin has emerged due to the spread of the mobile colistin resistance (MCR) gene. The use of PiFM and XPS allowed for the determination of the chemical identity of MCR-1 and MCR-3, which are important proteins involved in the resistance mechanism. These techniques also enabled the identification of key bond stretches and the chemical environment surrounding the MCR proteins, providing insight into the mechanism of colistin resistance in *E. coli*.

Overall, the development and implementation of PiFM and XPS techniques provide a powerful toolset for examining the chemistry and function of biological interfaces at the nanoscale. The ability to study biological systems in their native state and with high spatial resolution will enable a deeper understanding of biological phenomena and will facilitate the development of new biomaterials and therapies.

Keywords: Photoinduced force microscopy (PiFM), cryogenic X-ray photoelectron spectroscopy (XPS), surface chemistry, nanoscale mapping, stem cells, microbes, colistin resistance, biomaterials

INVITED SPEAKERS

Id-688

Spectroscopic Methods in the Study of the Influence of Amino Acids on the Corrosion Process of Materials used for Implants

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Abstract- Metallic implants are a very significant component of biomedical treatments (i.e. bone fracture, reconstruction, replacement) that have improved patient quality of life. Among biomaterial implants, metallic implants are the main class of components and have achieved great success since the development of advanced stainless steel and titanium (Ti) alloys. However, despite these successes, there are certain materials-associated complications, such as implant corrosion, which induce various infections and allergic reactions in the human body. Modification of the surface of biomaterials can be a good way to improve corrosion properties. One of the methods is the deposition of nanoparticles (NPs) on the metallic surface. In addition, an extremely important aspect is analysis of the processes that occur on the metallic surface in the presence of biological compounds. After implementation in the human body, the adsorption of plasma proteins appears; this process is very complex and the sequence of amino acids influences the protein-metallic interaction. Considering a wide spectrum of amino acid functions, a detailed analysis of the adsorption process of threonine (Thr), tryptophan (Trp), and cysteine (Cys) on the metallic surface was investigated.

In our studies of the corrosion and inhibition processes we focus on application of spectroscopic methods such as Raman (RS) and Fourier-transform infrared (FT-IR) spectroscopy and techniques based on surface-enhanced effects such as surface-enhanced Raman spectroscopy (SERS), surface-enhanced infrared absorption spectroscopy (SEIRA), and novel technique which combine atomic force microscopy (AFM) with infrared spectroscopy (AFM-IR). The application of SERS and SEIRA techniques gives a detailed description of the adsorption of Thr, Trp and Cys on metallic surfaces such as iron, stainless steel, titanium and titanium with deposited copper NPs (CuNPs). Thr influenced the process of iron surface corrosion due to the strong interaction between the protonated amine and carboxylate groups and CuNPs deposited on the metal surface. Trp was adsorbed through the lone electron pair of the nitrogen atom of the indole ring and the protonated amine group on the corroded stainless steel surface. In an acidic environment, Trp acts as a mixed-type bioinhibitor and provided good inhibiting properties for stainless

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steel. Deposition of a thin CuNPs layer on the titanium substrate improves the corrosion resistance of the substrate. However, the addition of Trp to the corrosive environment provided the degradation of the CuNPs coating. In this case, Trp was adsorbed on the corroded CuNPs-Ti surface via the indole ring and the protonated amine group on the metallic surface. The application of AFM-IR proved that Trp coated the bimetal surface and provided significant degradation of the surface. In situ and ex situ Raman studies of Cys behavior on a titanium surface in buffer solution give detailed information of the adsorption process on this metallic surface in different systems. The data obtained confirmed that there is a very good dependence between the results recorded by different spectroscopy techniques such as SERS, SEIRA, and AFM-IR. This research was funded by the National Science Centre, Poland, grant number 2019/35/D/ST4/02703. The research was partly performed using the equipment purchased in the frame of the project co-funded by the Małopolska Regional Operational Program Measure 5.1 Krakow Metropolitan Area as an important hub of the European Research Area for 2007–2013, project no. MRPO.05.01.00-12-013/15.

Keywords: Corrosion processes, Raman spectroscopy, FT-IR, SERS, SEIRA, AFM-IR, Copper nanoparticles (CuNPs)

INVITED SPEAKERS

Id-690

Rapid Characterization and Identification of Primary, Pre-Malignant, and Malignant Cells: Raman Spectroscopy-Based Machine Learning Algorithms

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Abstract- The most prevalent deadly illness in the world is cancer. An estimated 19 million new cases of cancer are identified each year, and 10 million people die from it. Daily challenges for cancer patients include unpleasant treatments, a lack of effective painkillers, and difficult social and financial circumstances. To increase recovery chances and reduce the cost burden on the patient and society, early detection of the cancer condition is crucial. One of the most promising methods for reaching this objective is Raman spectroscopy, which is recognized as a quick, sensitive, and precise method for identifying and characterizing biological systems at the molecular level. Existing methods for cancer diagnosis take a long time, cause patients agony and anxiety, and generate a lot of medical waste. The main objective of this study is to assess the potential of Raman spectroscopy in tandem with machine learning for the identification and characterization of three biological systems that serve as representative models for the various stages of cancer development and to identify which region of the cell (cell center, cell cytoplasm, or cell membrane) contributes most to this differentiation. The main goal of this study is to evaluate the potential of Raman spectroscopy-based machine learning to identify and characterize three biological systems that serve as a model for the different stages of cancer development and to establish whether part of the cell—cell center, cell cytoplasm, or cell membrane—contributes most to this differentiation. Healthy cells are represented by normal mouse fibroblast cells (NFC), precancerous cells are represented by the fibroblast cell line NIH/3T3, and cancerous cells are represented by totally malignant mouse fibroblasts (MBM-T). It was feasible to identify between pre-cancerous and cancerous categories with 82.2% success and between normal and pathological (pre-cancer and cancer) systems with a success rate of 97.9% by analyzing the Raman shift Spectra using machine-learning algorithms. Also, our findings demonstrated that the three distinct cell components—the center, cytoplasm, and membrane—contributed rather equally to the differentiation between the various biological systems under study. Also, our findings demonstrated that

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the various cell regions—the nucleus, cytoplasm, and membrane—contributed rather equally to the differentiation between the various biological systems under study.

Keywords: Cancer, Raman spectroscopy, machine learning, normal fibroblast cells (NFC), NIH/3T3, MBM (cancerous cells)

INVITED SPEAKERS

Id-693

**Combining Impedance Spectroscopy with Environmental TEM for Solid State
Electrochemical Experiments**

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Abstract- Method development within operando TEM is necessary for developing our understanding of dynamical processes in green energy technologies such as solid oxide electrolysis/fuel cells (SOEC/SOFC) and batteries. This presentation describes a method that combines Electrochemical Impedance Spectroscopy (EIS) with environmental transmission electron microscopy (ETEM). With the EIS-TEM method, solid oxide electrochemical experiments can be performed in the TEM with applied electrical potentials, in reactive gassed and at elevated temperatures. With such a method it is possible to directly observe the active sites in electrochemical cells while measuring the electrochemical response.

Proof-of-concept of the EIS-TEM method is given via experimental results from the functional material $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95-\delta}$ (CGO). CGO can conduct both ions and electrons (or polarons), a so-called mixed conductor. The conductivity depends on the gas environment and temperature and therefore this material is a good test object for electrochemical dependencies on temperature and gas environment. It is shown that reliable EIS measurements can be performed in the TEM while recording HRTEM images and spectroscopy data of the sample.

Keywords: TEM, EIS, operando, in situ, SOEC, SOFC

INVITED SPEAKERS

Id-695

Novel Perspectives in Microscopy of Nanofibrous Materials

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Abstract- Nanofibrous materials are engineered materials that can find applications in healthcare and medicine, energy production and conversion, electronics, sensing, filtration, food, environment, etc. High surface-to-volume ratio, low diameters and interconnected porous network make them an ideal candidate for these areas. Typically, the ideal size of the nanofibers are accepted as 100 nanometers or below, but some communities accept nanofibers as nano-scale fibrous materials up to a size of 500 nm and the debate in this area is still ongoing. Therefore, imaging nanofibers and nanofibrous materials promise enormous research and development opportunities in both academia and industry area. Not only the advances and differentiation in microscopy areas such as the scanning electron microscopy, atomic force microscopy and x-ray diffraction microscopy, but the modifications and tailored apparatus developments also enlighten the way nanofibers could be characterized in an advanced and precise manner for further research and implementation. The present work presents a wide scope of microscopic studies carried out in the imaging morphology of nanofibers that can serve as a timeline and future prospects in terms of techniques and device developments. Microscopy of the nanofibers has been taken into consideration based on a two-way approach including material science and microscopy together. In addition to the traditional nanofibers, the microscopic analysis issues were examined for novel nanofibrous structures such as three-dimensional nanofibers and biomimetic nanofibers. Future improvement possibilities of the present techniques and devices were also discussed considering current drawbacks, challenges and demands pushed by scientists and industry. It was thought that the conclusions drawn from the present work can help nanofiber researchers and commercial producers in their imaging activities for the development of the next generation of nanofibrous materials.

Keywords: Nanofibers, microscopy, SEM, AFM, XRD

INVITED SPEAKERS

Id-696

Theoretical DFT and Vibrational (IR and Raman) Characterization of Biologically Active Lanthanide(III) Complexes

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Abstract- Metal-based complexes of biologically active ligands and their structural derivatives with outstanding chemical diversity have been the source of research for potential drugs for last decades. Many molecules are acknowledged with excellent cytotoxicity and antioxidant activity. This presentation highlights the role of lanthanide(III) complexes in cancer drug development.

Biologically active coumarin and uracil derivative ligands and a series of their lanthanide(III) complexes have been synthesized and thoroughly investigated. The physicochemical characterization of the newly obtained compounds has been performed using theoretical, spectroscopic and analytical techniques. Vibrational study gave evidence for the coordination modes and was in agreement with the other theory prediction.

In order to study the pharmacological profile of the compounds, anticancer and antioxidant activity of the tested compounds was investigated. The in vitro studies revealed that the synthesized compounds exhibit potent biological activity. Taken together the results from the cytotoxicity and antioxidant screening give us reason to conclude that the lanthanide(III) complexes proved to be active cytotoxic and antioxidant agents and necessitate further more detailed pharmacological evaluation.

Keywords: Lanthanide(III) complexes; DFT; vibrational characterization; cytotoxicity; antioxidant activity

INVITED SPEAKERS

Id-700

Unusual Magneto-optics of Europium Chalcogenide Magnetic Semiconductors

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Abstract- Magnetic semiconductors based on europium chalcogenides represent a compact group of materials with a great potential for applications such as spintronics, integrated optoelectronics and new functional electronics. Europium chalcogenides EuX, where X = O, S, Se, Te, are intrinsic magnetic semiconductors with unique electronic, magnetic, optical and magneto-optical properties. The electronic structure of Eu²⁺ ions having strongly localized 4f⁷ electrons determines many physical properties of EuX. Eu²⁺ ions have seven electrons half-filling the 4f shell, which are aligned according to the Hund's rule with a spin of 7/2 and a large magnetic moment of 7.9 MB and producing a strong energy separation between occupied and unoccupied states of the 4f shell through a local Coulomb interaction.

In this talk, unusual magneto-optical phenomena in europium chalcogenide magnetic semiconductors will be discussed. A strong magneto-optical phenomenon such as the quadratic Kerr effect in ferromagnetic epitaxial EuO films will be shown. Crystallographic and spin-induced contributions to the nonlinear process of second harmonic generation will be considered in the films EuTe and EuSe. Different aspects of nonlinear optical spectroscopy, such as polarization, temperature and field dependences, will be analysed. The possibility of photo-induced Faraday effect for detecting magnetic polarons with an extremely large magnetic moment in epitaxial films of europium chalcogenides will be shown. The phenomenon of optical orientation will be demonstrated as a mechanism triggering the precession of magnetization in epitaxial EuO films.

The Russian Foundation for Basic Research (project 19-52-12063-NNIO_a) and the Deutsche Forschungsgemeinschaft (grant ICRC TRR160, project C8) are acknowledged.

Keywords: Magneto-optical Kerr effect, photoinduced Faraday effect, second harmonic generation, magnetic semiconductors

INVITED SPEAKERS

Id-701

Mineral Textures – Key to Uncovering the Physical and Chemical Environment, and Precipitation Mechanism. A Case Study from the Eocene Epithermal, Low-sulfidation Surnak Gold Deposit, SE Bulgaria

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Abstract- The most significant part of the epithermal precious metal mineralization in the Surnak (or Sarnak) deposit is located along and near the contact between the metamorphic basement and overlying sedimentary cover and along steep faults cross-cutting this contact. Pyrite is the main ore mineral, while marcasite is sporadic. The main gangue mineral is quartz while adularia is present in the steep faults and along and near the contact but is absent far from the contact. Quartz and adularia are cross-cut by later carbonates. To constrain the paleoenvironment and precipitation mechanism in different locations relative to the contact we sampled the epithermal mineralization in drill hole cores from 1) the contact and nearby areas; 2) steep faults, and 3) far from the contact both above and below. Here, we present results from the mineral macro- and microtexture study.

The samples from steep faults represent hydrothermal breccia, which cements clasts of earlier hydrothermal quartz. These samples have a distinct macroscopic appearance: cryptocrystalline and porcelain-like outlook; dark grey quartz; black, powdery-like pyrite. The samples from and near the contact are microcrystalline; quartz is white, and pyrite aggregates are fine-grained. The mineralization far from the contact is scarcer. In the metamorphic basement, pyrite forms thin veinlets in brecciated gneiss or follows schistosity. In the sandstone far above the contact pyrite forms disseminated impregnation or thin veinlets in siltstone.

The microtextures of samples from steep faults include very fine-grained anhedral quartz grains of interpenetrating boundaries (known as a jigsaw or mosaic quartz) (a few microns across); quartz and pyrite spheres (a few microns in diameter); submillimetre-wide globular pyrite aggregates of patchy zonation; pseudomorphs of quartz and pyrite after platy calcite (known as bladed texture); as well as pyrite bands of whimsical shapes among anhedral quartz. Adularia is always present. The microtextures of samples from and near the contact include pyrite aggregates of weak patchy zonation; anhedral pyrite grains; porous areas in pyrite aggregates. In places adularia is present. The pyrite aggregates from the metamorphic basement, far below the contact, are zonal; the zonal textures comprise commonly a core, an oscillatory mantle, and a euhedral rim. The microtextures of samples far from the contact in the sandstone above it display very

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weak banded zonality as the bands are very thin. Vein adularia is absent far from the contact, both below and above.

The macro- and microstructures described above suggest different physical environment and precipitation mechanisms in the three groups of samples. We assume that the steep faults were connected to the surface and during hydrothermal brecciation, the pressure drop was very sharp and fluid flashing occurred. We expect a high supersaturation with respect both to amorphous silica and iron disulfide to be achieved in that event, resulting in the formation of colloidal suspension which later turned into mixed silica - iron disulfide gel through gelation. For the samples from and near the contact, we assume episodic boiling but of a lower degree: adularia is present but quartz and pyrite spheres, and globular pyrite are absent which suggests lower supersaturation which did not reach a supersaturation with respect to amorphous silica likely due to poor venting. Boiling in the deposit was previously proved by fluid inclusion data. For the samples far from the contact we propose steadier and gradual depositional conditions – cooling of the fluids along the Earth's geothermal gradient.

The authors thank Dundee Precious Metals Krumovgrad, Bulgaria for permission to sample and provided geological information. The study is supported by the Bulgarian National Science Fund, contract KP-06-N54/6.

Keywords: Gold, low-sulfidation, pyrite, adularia, mineral texture

INVITED SPEAKERS

Id-705

**Methods of Multivariate Classification of Industrially Produced Mineral Fertilizers
and "Manufacturer-quality" Model**

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Abstract- Modern industrial production is a complex process with many factors that affect the quality of the finished product. For example, these factors for mineral fertilizers are the content of nutrients (type and grade, e.g. NPK 15-15-15), solubility, granulometric composition, content of trace elements (B, Zn, Mg), content of heavy elements (Hg, Pb, Cd), etc. Each of these parameters are important for the consumer and determines the general criterion of quality (safety and efficiency of fertilizers). Therefore, it is important to ensure that the quality of fertilizers on the market is controlled rapidly and efficiently.

In the present work, the method of multidimensional classification of X-ray fluorescent spectra and optical recognition of industrially produced mineral fertilizers for the construction of "manufacturer-quality" model is proposed. The approach that allows to rapidly define the manufacturer of the unknown sample of mineral fertilizer and to draw a conclusion on a single concept of "quality" for the given object is described (as a set of physical and chemical properties of the object). The identification will help to recognize counterfeit products and defective mineral fertilizer in the sales markets. The energy dispersive X-ray fluorescent method and optical control were chosen as the methods of analysis, which possesses a number of necessary properties (quick and multi-element analysis, the spectrum depends on the chemical and physical properties of the sample, high resolution, etc.). The essence of the proposed approach is to compare the spectra of unknown samples with the previously built database of quality products of known manufacturers. For each sample, the spectrum was recorded, and each energy channel of the spectrum was used as a separate feature (about 3000 channels per one spectrum) as well as optical fertilizers data. These features are used to create a matrix of "object-features" (the basis of the database of quality products). Values of features are normalized by mean and dispersion. Then the algorithm of reduce the dimensional of data is carried out according to the projection on the main components algorithm and clusters are calculated according to the k-means algorithm. Each cluster corresponds to a well-known brand and manufacturer of the fertilizer. Furthermore, the χ^2 criterion (based on the set of energy channels) and the Euclidean distance to the center of the corresponding cluster in the space of two components were calculated for each spectrum. Unknown sample spectra are recorded and converted under similar conditions. Then, a custom χ^2 and Euclidean distance to the nearest cluster is calculated for the unknown sample. Based on the combination of these parameters, a conclusion is made about the manufacturer and quality of the fertilizer, and a numerical quality criterion of it is calculated. A set of five different fertilizer

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brands and four encrypted samples was investigated for experimental validation of the model. As a result, the brands of all encrypted samples were defined correctly and their numerical "quality" criterion were calculated. The analysis time of one sample did not exceed 5 minutes.

Keywords: Multivariate classification; data analysis; fertilizers; X-ray spectroscopy; optic spectroscopy

INVITED SPEAKERS

Id-706

Recognition of Crude Oil Samples based on Terahertz Time-domain Spectroscopy and Principal Component Analysis

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Abstract- In order to recognize multiple crude oils from different oil fields, terahertz time-domain spectroscopy (THz-TDS) combined with principal component analysis (PCA) is used to investigate 105 crude oil samples from different oil fields in several countries and regions. The refractive index and absorption coefficient of the samples in the range of 0.2 to 2.5 THz are extracted, and a univariate linear regression model is set up to analyze the relationship between crude oil density, carbon content, sulfur content and average refractive index and average absorption coefficient. The results show that the refractive index and absorption coefficient of crude oils are independent on every single factor such as density, carbon content, and sulfur content, but are determined by comprehensive factors. Principal component analysis (PCA) was applied for dimensionality reduction and feature extraction of the refractive index and absorption coefficient spectra, and being input into a convolutional neural network (CNN) for classification. The results show that for the training set containing 68 samples, the accuracy reached 100%, and for the test set containing 15 samples, the accuracy also reached 100%. Therefore, the combination of terahertz spectrum, principal component analysis, and convolutional neural network technology can quickly and accurately identify the origin of crude oil.

Keywords: Crude oil; terahertz time-domain spectroscopy; principal component analysis

REGULAR SESSIONS

Id-640

**High-resolution X-ray Diffraction Edge Geometry for Epitaxial Nanostructures
Characterization**

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Abstract- High-resolution X-ray diffraction (XRD) is the basic research method for the characterization of nanomaterials such as epitaxial layers and structures, quantum wells and dots, superlattices, and nanorods. The use of XRD methods makes it possible to determine, above all, the lattice parameters, composition, and thickness of individual layers. In addition, this nondestructive method allows for the analysis of strain/stresses or dislocation density in structures. In such investigations, the main difficulty is the measurement of planes perpendicular to the sample surface. In a standard XRD configuration, it is practically impossible to measure such planes for highly oriented samples. The application of measurements carried out from the edge of the sample allows investigation of planes perpendicular to the sample surface. This makes it possible to independently determine the in-plane lattice parameter, separate the tilt and twist mosaicity, and calculate the density of the edge dislocations or residual strains in the structure. Furthermore, XRD edge geometry measurements were used to estimate the QD asymmetry. It is a crucial property for the design of e.g. polarization-insensitive semiconductor optical amplifiers. The proposed method provides a nondestructive insight into crystal lattice disturbances reflecting in-plane quantum dot symmetry. In this method, we used XRD in the measurements of reciprocal lattice maps performed from the edge of the sample. This non-classical approach allows one to detect disturbances in the crystal lattice associated with the presence of QD in the structure. XRD measurements carried out on the two orthogonal edges of a sample allow observation of the lattice disturbances, providing at least quantitative information on the nanostructure in-plane geometry. This type of measurement was developed in the Structural Research Laboratory at Wrocław University of Science and Technology and has been used in the analysis of epitaxial structures - mainly mismatched III-N materials and low-dimensional QD structures of III-V materials.

Keywords: High resolution X-ray diffraction, edge scans, quantum dots, semiconductors

REGULAR SESSIONS

Id-647

Changes in RBCs Under Hypoxia: Spectrophotometry and AFM Study

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Abstract- Hypoxic conditions using noble gases, is potential prospect for long-term storage of donor packed red blood cells (pRBCs). Storage of pRBCs under hypoxia is expected to reduce the level of structural and biochemical alterations in RBCs resulting from oxidative processes during storage and consequently reduce transfusion-related complications. The aim of the present study was to investigate changes in RBCs under hypoxia using spectrophotometry and atomic force microscopy (AFM) methods. There were two methods of creating hypoxic conditions in the model experiment in vitro. The first one is storage of RBCs in glass tubes without the possibility of oxygen exchange. The second method is based on using noble gases, in particular xenon and argon, and also storage samples in glass tubes. The kinetics of changes in the concentrations of hemoglobin derivatives was studied using a Unico 2800 digital spectrophotometer (United Products & Instruments, USA) and the nonlinear curve fitting method for analyzing of optical spectra by Origin Pro 2019 (OriginLab Corporation, USA). For the analysis the dynamics of RBC morphology changes during hypoxia an NTEGRA Prima atomic force microscope (NT-MDT Spectrum Instruments, RF) was used. As a result, under hypoxic conditions there was a consistent increase in the deoxyhemoglobin concentration to 97%, and methemoglobin formation during storage. There was a change in cell morphology from discocytes to echinocytes, microspherocytes, codocytes, and ghosts. There were mostly irreversible forms by day 30 of storage: 80% microspherocytes and ghosts. The addition of nutrients such as SAGM to the solution has been shown to affect storage results under hypoxic conditions. Our results are important for studying the biophysical mechanisms of RBCs behavior under hypoxia.

Keywords: Atomic force microscopy; spectrophotometry; red blood cells; hypoxia; hemoglobin derivatives

REGULAR SESSIONS

Id-648

Using Confocal Laser Scanning and Atomic Force Microscopy to Assess the Effect of Activators on Neutrophils

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Abstract- Neutrophils are important effector cells in protecting the host from invading pathogens. One of the mechanisms they use to eliminate pathogens is the release of neutrophil extracellular traps (NETs). Although the release of NETs and subsequent cell death, known as NETosis, has been extensively studied, the cellular components and factors determining or contributing to NET formation remain incompletely explored.

Atomic force microscopy (AFM) and confocal laser scanning microscopy (CLSM) were used to monitor the number of altered cells and visualize their structure in three dimensions assessed the effect of activators (A23187, PMA) on neutrophil morphology and shape.

After isolation of human PMNs, cells were activated using A23187 and PMA, and recorded at different stages of activation, after 0, 30, 60, 120, 240 minutes. When exposed to A23187, 83% of cells with adherent membrane appeared after 30 minutes. By 60 minutes, cells with a swollen nucleus appeared. After 240 minutes, the number of cells that released NETs was 44%.

When exposed to PMA, adhesion cells appear after 30 seconds. After 60 minutes, 33% of cells with a swollen nucleus appear, 15% of adherent cells and only 11% segmented nucleus cells remain. At 240 minutes, the number of cells that released NETs was 66%.

The obtained result can be used in further studies of morphological changes in neutrophils in norm and pathology, as well as in clinical studies and pharmacology.

Keywords: Neutrophils; NETosis, AFM; CLSM

REGULAR SESSIONS

Id-649

**Comprehensive Study of Red Blood Cell Pathologies Using Atomic Force
Microscopy**

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Abstract- Atomic force microscopy (AFM) is the effective method for studying blood cells at micro- and nanoscale levels. Morphology and membrane nanostructure of red blood cells (RBCs) change under the influence of pathogenic factors. As a result, RBC deformability decreases and their gas transport function is disturbed. This study presents the results of a comprehensive study of various physicochemical factor influences on RBCs using an NTEGRA Prima atomic force microscope (NT-MDT Spectrum Instruments, RF).

The impact factors were pharmchemicals, in particular, hemin, free iron ions; ionizing radiation; long-term storage of packed RBCs; hypoxia. The objects of study were the cell morphology, membrane nanostructure, cytoskeleton nanostructure, membrane stiffness, cell aggregates in an ensemble, and hemoglobin derivatives. Image Analysis P9 software (NT-MDT Spectrum Instruments, RF) was used to process the AFM images obtained in the experiment, a spatial Fourier transform method was used for detailed representation of membrane nanosurface and quantitative assessment of its characteristics. To measure the stiffness of the native RBC membranes, the method of force curves with author's modification was applied. Also, spectrophotometry and Non-Linear curve Fitting method (OriginLab Corporation, USA) were used. It has been shown that, depending on the type and intensity of exposure factors, there are a significant change in cell morphology, the appearance of specific structural formations in RBC membrane, the emergence of cytoskeleton reorganization, the increasing of Young's modulus of the membrane, a violation of hemoglobin derivative ratio.

The original results of such a comprehensive study of RBCs using AFM are of scientific interest for biophysics, medicine, pharmacy, and materials science.

Keywords: Atomic force microscopy; morphology of red blood cells; membrane; cytoskeleton; membrane stiffness; pathologies; physico-chemical influence

REGULAR SESSIONS

Id-659

International Standards for Radiation Protection Instrumentation

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Abstract- The standards published by the International Electrotechnical Commission (IEC) and prepared by its Sub-Committee (SC) 45B "Radiation Protection Instrumentation" cover a very large scope. They address instrumentation used for the measurement and the quantification of ionizing radiation in the workplace, to the public and in the environment for radiation protection purposes. These standards cover also the detection of illicit trafficking of radioactive material and identification of radionuclides as well as the radiation-based security screening.

The IEC standards serve as basis for national standardization, as references when drafting international tenders and contracts and for conformity evaluation of instrumentation. It is to be noted that more than 80 % of all European (EN) standards are actually IEC standards that are transposed by CENELEC (the European Committee for Electrotechnical Standardization) without or with some minor modifications.

Among the various requirements in the standards, the different types of tests for photon, neutron, beta and alpha radiation and their characteristics are the heart of these documents. Dose (rate) response linearity evaluation, relative intrinsic error determination, energy and angular dependences of the response, radionuclide identification and overload tests are just a few examples. In addition, the standards have electromagnetic (EMC), electrical, environmental and mechanical requirements and associated tests to demonstrate compliance with the requirements.

The criteria and the compliance test methods in these standards are the result of an optimization and compromise between the participating experts from many countries searching for acceptable detection performance that reflects the positions of the national regulatory agencies, the scientific and technological progress of the industry, the testing laboratories capabilities, the end users, the instrument production cost and the compliance testing procedure.

This presentation will provide an overview of the international IEC standards that set the minimum performance requirements for all radiation protection instrumentation. They provide manufacturers with internationally acceptable requirements and provide the users with assurance of the rigorous quality and accuracy of the measurements.

Prepared partially by LLNL under Contract DE-AC52-07NA27344.

Keywords: Standards, radiation protection, radiation detection instrumentation

REGULAR SESSIONS

Id-662

Identification of Isomeric Molecules by Spectroscopy of Non-covalent Complexes

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Abstract- We make use of intermolecular hydrogen bonds to distinguish very similar isomeric glycans and isomeric lipids by fragmentation spectroscopy of cryogenically cooled complexes of the molecules with aromatic peptides. An aromatic reporter molecule changes its absorption differently in the complexes with different isomers of a host molecule. We detect these differences and use it for library-based quantifications of isoforms mixed together. The non-covalent complexes of the analyte molecules with a reporter aromatic molecule are readily formed in solution upon mixing. Soft mode of electrospray ionization allows for transfer of the complexes to the gas phase with little dissociation. The ions of interest are, first, m/z selected by a quadrupole mass filter and then transferred to an octupole ion trapped, where they are cooled to T=10 K in collisions with He buffer gas. Cooling suppresses inhomogeneous spectral broadening, making the spectra structured and more distinguishable. The cold complexes are then irradiated by a 5-ns pulse of UV or IR light, and the appearing fragments are detected by a quadrupole MS. Scanning wavelength of UV/IR laser light while detecting the appearing charged fragments generates a respective spectrum of the complex. Alternatively, ionized analyte can be electrosprayed retaining a molecule of solvent that can be used as a tag for IR photofragmentation spectroscopy. Such measured IR spectra of isomeric standards then can be used for quantitative identifications of these isomers in their complex mixtures. Currently, the practical implementation of our innovative method is hindered by a lack of a suitable commercial instrumentation. We will present a module under developing that can be added to commercial high resolution mass spectrometers for identifications of isomers by IR/UV cold ion spectroscopy.

Keywords: isomers, mass spectrometry, spectroscopy, biomolecules, non-covalent complexes

REGULAR SESSIONS

Id-669

Ball Milling as Facile Route for Borophene Nanoflakes Fabrication

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Abstract- Borophene as an encouraging new member of the family of 2D materials, due to the fact that it shows promising properties, focuses attention in regards of its synthesis. So far, the borophene has been fabricated via few routes such as: (i) atomic layer deposition (ALD), (ii) molecular beam epitaxy (MBE), (iii) chemical vapor deposition (CVD), (iv) sonochemical exfoliation, (v) modified Hummer's method or even (vi) electrochemical exfoliation. Two first approaches strongly limit investigations where e.g. grams or even milligrams are needed to be provided. Three latter approaches are still in their early stages but they are promising to provide larger-scale quantity of free-standing material. In our study we reveal, for the first time, the potential to use ball milling technique as an easy, facile and reproducible to be upscaled. Borophene nanosheets formation was monitored by changing the process parameters such as various rotation speeds, time and weight ration of bulk boron. Thickness, size and yield have been investigated as operating parameters. In the optimal conditions ball-milling at 400 rpm, 6 hours offers regular distribution of the thinnest borophene flakes. On the other hand, the increase in the speed of rotation contributes to well-known phenomenon as flake agglomeration. Our detailed study was based on microscopy and spectroscopy analysis. Atomic force microscopy (AFM) allowed to determine the thickness/size of the flakes (determining the height profiles of the flakes), transmission electron microscopy (TEM) made it possible to examine the morphology of the obtained materials (size of the flakes, their distribution and symmetry), using Raman spectroscopy, a qualitative assessment of the tested materials was carried out. Finest sample was also examined using X-ray photoelectron spectroscopy (XPS) for chemical structure and atomic composition.

Keywords: borophene, ball milling, atomic force microscopy

REGULAR SESSIONS

Id-685

**Energy-level Alignment of Ru Complexes Placed in Multi-layers Probed by
Frequency Modulated EFM**

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Abstract- Molecular electronics utilizes molecules as elements in electronic devices to exploit their diverse functions. Ru complex (N719) are one of the promising molecules to obtain stable electrical conduction. The charge transfer process in molecular devices is a key to understanding the charge-transfer process from the electrode in organic film layers. The charge transfer process in molecular devices is strongly influenced by the structure of the organic multilayer, the interaction between the layers, and the junction with the electrode. Previous studies have shown that multilayer systems of Ru complexes and self-assembled monolayers (SAMs) are unaffected by interactions with electrodes and directly reflect the electronic properties of the Ru complexes. However, it is not known how the applied voltage from the electrode is distributed across the multilayer to align the energy levels of the molecules in the multilayer. In this study, the alignment of the energy levels of the molecules in the multilayer was determined by frequency modulated electrostatic force microscopy (FM-EFM). In sample preparation, Au(111) substrates vacuum deposited on a mica surface were immersed in ethanol solutions of 6-amino-1-hexanthiol (6-AHT) or 11-amino-1-undecanthiol (11-AUT) for two hours. Subsequently, they were immersed in an ethanol solution of N719 for 1 day. When the voltage was swept using FM-EFM, the frequency shift of the 6-AHT showed a behavior that deviated from the parabola from around ± 5 V. A similar deviation from the parabola was also observed for N719 on the 6-AHT. On the other hand, no deviation from the parabola was observed in 11-AUT/Au and N719/11-AUT/Au. The deviation from the parabola was considered as a decrease in electrostatic energy and plotted against voltage. In the negative voltage region for N719/6-AHT/Au it was found to be simple tunneling, as it fitted the Simmons formula well. In the positive voltage region, the Simmons equation was not fitted. By taking resonance tunneling into account, the equation was fitted for the positive voltage region, and the results agreed well with the experimental values. This suggests that electrical conduction through the LUMO of N719 is taking place.

Keywords: Ru complex, multi-layers, resonant tunneling

REGULAR SESSIONS

Id-697

**Detection of Pathogenic Bacteria by Using Bacteriophages
and Plasmonic Nanoparticles by Surface Enhanced Raman Spectroscopy**

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Abstract- Food and water borne diseases are among the most serious and costly public health concerns worldwide. According to WHO millions of deaths occur annually due to food and water-borne diseases mostly caused by pathogenic bacteria including *Escherichia coli*, *Salmonella*, *Staphylococcus*, and many others, even in developed countries - which is a very scary scenery. In addition, the number of antibiotic-resistant bacteria is rapidly increasing - has already raised above very dangerous levels - which is even much more frightening. Monitoring food and water quality has therefore been recognized as one of the most important priorities globally. Current pathogen detection methods include: (i) microbiological techniques (conventional culturing); (ii) nucleic-acid based (e.g., PCR and DNA hybridization using oligonucleotides as bio-recognition elements - bio-probes) and (iii) immunological (e.g., ELISA - using specific antibodies as bio-probes). Using bacteriophages as bio-probes alternative to antibodies and nucleic acids for bacterial detection is a very unique approach and that have been proposed rather recently. Bacteriophages are viruses which only infect bacteria, with excellent host selectivity. Bacteriophages are not only the most abundant biological entities but also probably also the most diverse ones. They may be very specific even at serotype levels, could be easily propagated therefore quite in expensive and have long-shelf life. Bacteriophages have been used for specific detection of target bacteria by using different bio-sensing platforms which are mainly treated in two categories: (i) using labels (including fluorescent, luminescent, enzymes, electrochemically active labels, etc.), (ii) label-free systems (QCM, SPR, Ellipsometer, Raman and Mass spectrometers, etc.). Almost all of technologies mentioned above have been applied for detection of pathogens by using bacteriophages with different extent and success. The challenging objective is to develop enhanced detection technologies with high levels of reliability, sensitivity, and selectivity with short assay times. In recent year due to the "size and shape-dependent" properties metallic, especially gold and silver nanoparticles have been extensively studied in wide variety of applications. Gold nanorods (GNRs) are rod-shape nanoparticles which could easily produced with different aspect ratios (dimensions) - therefore different plasmonic properties. Their unique optical and physical properties have allowed using them for development of bio-sensing platforms mainly as surface signal enhancers. Here, we briefly review the detection of pathogenic bacteria by using bacteriophages as selective bio-probes together with gold

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nanoparticles by Surface Enhanced Raman Spectroscopy will be briefly reviewed using also our own experiences in the field.

Keywords: Pathogenic bacteria, detection, bacteriophages, raman spectroscopy, plasmonic nanoparticles

REGULAR SESSIONS

Id-702

EFM/KPFM Measurement of Plasmon-induced Charge Separation on Au Nanoparticle/ TiO₂ Interface

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Abstract- Surface plasmon resonance is one of the ways of using the energy of light. Although it is difficult to use the hot carriers generated by localized surface plasmon resonance in the plasmonic metal due to a quite short lifetime, Plasmon-induced charge separation (PICS) makes the lifetime of the hot carrier longer by use of the Schottky barrier between the metal and semiconductor interface. Whereas many applications of PICS are reported as photovoltaics and photocatalysis because of the long lifetime, the time scale of PICS phenomena was only estimated utilizing photocurrent or products of the chemical reaction, which are indirect way of observing the time change of PICS. The lifetime of the separated charge itself on the metal-semiconductor interface has not been directly obtained in previous researches. Our goal is the direct measurement for the dynamics of PICS on gold nanoparticle (AuNP)/TiO₂ interface by electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM). The system of AuNP/TiO₂ is the typical combination of materials for PICS. EFM and KPFM, which are methods based on the technique of atomic force microscopy can simultaneously obtain the topography and the charge distribution as electrostatic force and surface potential, respectively. The topography and the contact potential difference (CPD) image before and after the laser irradiation were simultaneously obtained by KPFM measurement. Although the topography did not change by irradiation, the CPD value on the AuNP region increased only after laser irradiation. This result indicates AuNP is positively charged when hot electrons are transferred to TiO₂. Because the feedback loop of KPFM requires a long measurement time, the time-dependent measurement of separated charge is suitable for using EFM rather than KPFM. The time change of electrostatic force on an AuNP obtained by EFM measurement revealed that the charge accumulation and decay takes the order of several 100 ms, and the amount of accumulated charge depended on the DC bias voltage applied between cantilever and samples. The annihilation process was discussed in a simple model based on the transient Schottky barrier, and the result indicates the decay constant for the annihilation of the separated charge on the AuNP/TiO₂ interface was directly determined to be about 150 ms. The lifetime of PICS on the AuNP/TiO₂ interface directly obtained in our result is consistent with previous researches, which indicate the process of the chemical reaction requires the lifetime of the separated charge of microseconds to seconds.

Keywords: plasmon, atomic force microscopy, electrostatic force microscopy

REGULAR SESSIONS

Id-711

Mast Cells through the Lens of Microscopy: From Structure to Precision Medicine Concepts

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Abstract- The state of a specific tissue microenvironment represented by vessels, a cellular component, and an extracellular matrix, is critical in the formation of the pathological focus. Each organ has specialised cellular clusters that use proper regulatory mechanisms to maintain local homeostasis. Mast cells are key regulatory players in the organ-specific tissue microenvironment. MCs actively participate in the management of cellular cooperations, monitoring most of the key parameters of the cellular microenvironment. The uniqueness of MCs lies in the extraordinary combination, on the one hand, of an adapted sensory apparatus to informationally significant signals of the integrated-buffer metabolic environment, and, on the other hand, of a multifunctional effector apparatus represented by a secretome. The changes existing in the tissue microenvironment are recorded by MCs using a wide range of receptors, including surface IgG receptors, toll-like receptors, C-type lectin receptor, retinoic acid-inducible gene-1 like receptors, and a lot more. In case of non-allergic activation of MCs adequately to the challenges of the cellular microenvironment, MCs are able to secrete with high selectivity a rich arsenal of biologically active substances, which can be divided into preformed mediators and mediators newly synthesized in the process of MC activation. Pre-accumulated secretome products are represented by biogenic amines, proteases, including specific proteases chymase, tryptase and carboxypeptidase A3, enzymes, proteoglycans, cytokines, chemokines, growth factors, as well as numerous regulatory peptides. Resynthetic products include cell-derived cytokines, growth factors, and mitogens, MC-derived chemokines, and various lipid metabolites, in particular prostaglandins and leukotrienes. MCs are closely integrated into the genesis of adaptive and pathological conditions through secretome components, representing not only an informative marker of disease progression, but also a promising therapeutic target. Of particular importance are specific MC proteases – tryptase, chymase, and carboxypeptidase A3. The secretory pathways of proteases and other components of the secretome represent various options for the

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excretion of substances with high selectivity into the extracellular matrix, forming a wide range of biological effects. MCs have a great potential for tissue remodeling through induced collagen fibrillogenesis, angiogenesis, wound healing, etc., without reaching high quantitative indices per unit area of tissue. Studies of mast cells in translational medicine, including multiplex immunohistochemistry technologies, also at the ultrastructural level, make it possible to use mast cells not only for new algorithms for diagnosing pathological conditions, but also for new protocols for personalized therapy.

Keywords: mast cells, a specific tissue microenvironment, the cellular microenvironment

POSTER SESSIONS

Id-658

Development of Radiation Data Format for Streaming Data in Real-Time

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Abstract- Smartphones and handheld tablets are used often in connection with radiation detection instruments. Their graphical user interface, radiation data processing and display capabilities, situational awareness and network interfacing capabilities make them valuable components in any radiation detection scheme. The use of these devices is rapidly increasing for the real-time streaming of data over short and long distances. The development of an international standard for the format of radiation data to be streamed in real-time from radiation detection sensors to smartphones or tablets is presented. Representatives from instrument manufacturers, universities, and government agencies and laboratories are participating in this effort. The goal is to develop a fast and compact format applicable to as many radiation detection platforms as possible, that is easy to use and simple to implement. Additionally, the standard is designed to provide room for future expansion and inclusion of developments in the fields of radiation detection and wireless transmission. The specification of the radiation data is written in Abstract Syntax Notation One (ASN.1); a joint international standard by ISO, IEC and ITU. The presentation will describe the current status of the draft standard, its basic principles, the mandatory and optional data fields, and future development plans. Upon completion, the final draft will be distributed for comments through the Institute of Electrical and Electronics Engineers (IEEE) process. The standard is expected to be published as IEEE N42.61 standard with the title "Radiation Data Format for Streaming in Real-Time Data from Radiation Detection Instrument to a Smartphone or Tablet".

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Keywords: radiation data, real-time streaming, ASN.1 notation

POSTER SESSIONS

Id-686

Utilization of Infrared Spectroscopy based Machine Learning for Rapid Identification of Extended-Spectrum β -lactamase-producing Bacterial Isolates Purified Directly from Patient's Urine

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Abstract- The most effective treatment for bacterial infections is antibiotics. Unfortunately, most bacteria have already acquired resistance to a wide range of antibiotics due to their uncontrolled use. One of the most common classes of multidrug-resistant bacteria is the producing Extended-Spectrum Beta-Lactamase (ESBL). It is crucial to develop a technology that can quickly identify bacterial isolates that produce ESBL for effective treatment. Fourier transform infrared (FTIR) microscopy is a sensitive method that can rapidly detect minor molecular changes in cells. In this study, we examined the potential of the FTIR spectroscopy-based machine learning algorithms for the rapid detection of ESBL producing bacterial isolates obtained directly from the patient's urine. 591 ESBL producing and 1658 ESBL non-producing samples of *Escherichia coli* (*E. coli*) and *Klebsiella pneumoniae* were investigated. Our findings demonstrate that, 40 minutes after receiving the patient's urine sample, FTIR spectroscopy-based machine learning can successfully identify the ESBL-producing bacteria with a success rate of 80%.

Keywords: *E. coli*, *Klebsiella pneumoniae*, bacterial resistance to antibiotics, extended-spectrum beta-lactamase (ESBL), infrared microscopy, machine learning

POSTER SESSIONS

Id-687

Infrared Spectroscopy in Tandem with Machine Learnings as a Rapid Method for the Identification of Resistant Pseudomonas Aeruginosa Isolates to Antibiotics in Twenty Minutes After The First Culture

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Abstract- A serious concern in hospital-acquired infections is Pseudomonas (P.) aeruginosa bacteria, which causes severe infections. Because of P. aeruginosa inherent resistance, and extraordinary ability to develop additional resistance mechanisms to many classes of antimicrobial drugs, it is very challenging to treat nosocomial infections caused by this organism. Thus, it is crucial to rapidly determine the susceptibility of P. aeruginosa isolates to antibiotics for effective treatment. The currently used methods for susceptibility determination are time-consuming. Therefore, it is important to develop new methods for this manner. Fourier-transform infrared (FTIR) spectroscopy is a sensitive and rapid method with the ability to detect minor abnormal molecular changes, including those associated with the development of resistant bacteria to antibiotics. The main goal of this study is to evaluate the potential of FTIR spectroscopy to determine the susceptibility of P. aeruginosa to different antibiotics in ~20 minutes after the first culture. For this goal, 590 isolates of P. aeruginosa, which obtained from different infection sites of various patients. These isolated were measured using an FTIR spectrometer and analyzed by Random Forest. With an 82–90% accuracy for different antibiotics, we have effectively determined P. aeruginosa susceptibility to them.

Keywords: pseudomonas aeruginosa, antibiotic, bacterial susceptibility to antibiotics, infra-red microscopy, machine learning

POSTER SESSIONS

Id-708

Influence of Laser Power on Microstructure of Laser-induced Graphene

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Abstract- Graphene has unique properties. It has a single layer of sp² hybrid carbon, which makes it very good at conducting electricity and heat. Graphene can be synthesized by various methods. Among them, laser-induced graphene is an alternative method for producing graphene. Compared to other fabrication methods, laser induction does not require chemicals or special instrumentation. Laser induction is performed on a surface with a photothermal incidence. Usually, polyimide substrates are used for this method. Polyimide is an aromatic compound with many functional groups. When the laser beam is directed onto the surface, the functional groups are removed from the system and only the hexagons remain. These hexagons then form as graphene on the surface. Laser-induced graphene has a porous structure, and the amount of graphene formation depends on the laser power. In this work, graphene films were prepared on polyimide using a laser-induced method with 7.5W, 9W, 10.5W, and 12W laser power, respectively. Microstructure and phase analysis were performed using scanning electron microscope (SEM) and X-ray diffraction (XRD). Elemental properties were studied by X-ray photoelectron spectroscopy (XPS) and the atomic ratio of carbon and oxygen was determined. Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy were used for chemical characterization. This work showed that with increasing laser power, the crystallinity of graphene increased. Also, as the laser power increased, the atomic ratio of the C/O ratio decreased. In chemical characterization, we found that all the bonds in the polyamide structure were broken. We also observed in the Raman spectra that the intensity of the 2D/G peak was higher at lower laser power. This indicates that the number of layers in the graphene increases with laser power.

Keywords: laser power, 2D/G peak ratio, laser-induced graphene

POSTER SESSIONS

Id-709

The Conformational Change Optimization of PEDOT:PSS Chains by Secondary Doping Treatment

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Abstract- PEDOT:PSS has recently attracted much attention due to its easy doping, high transparency, high mechanical flexibility, excellent thermal stability and easy processing in solutions. PSS increases the solubility of the solution, but also transforms the orientation of the polymer chains into coiled structure, which reduces the overall electrical conductivity. Therefore, PEDOT:PSS needs to be treated with polar organic solvents to change the arrangement of the polymer chains are arranged from coiled to a linear or extended coiled structure. In the literature, various organic solvents are used to treat PEDOT:PSS, such as ethylene glycol (EG), dimethyl sulfoxide (DMSO), isopropyl alcohol, N-N-dimethylformamide, ethanol, methanol, acetonitrile and so on. Among them, EG and DMSO are the most preferred ones, which can also be used as co-solvents. In this study, PEDOT:PSS was treated with 5 vol% EG. To see how well these two solvents work together, EG was used to treat another sample, which was washed with DMSO at the end. For microstructural characterization, SEM/EDS was also performed to see how the atoms of the elements were distributed across the cross section. AFM was used to determine surface roughness at a scan size of 5 µm. UV-Vis-NIR measurements were performed in the wavelength range of 200-350 nm. XPS analysis was performed for chemical analysis. Curve fitting of these XPS spectra was performed using CasaXPS. The results show that the sample treated with EG and washed with DMSO has a smoother surface and thus a more linear chain alignment. Also, the PSS content decreased the most for the sample treated with EG and then washed with DMSO. The thickness of the films was measured to be about 9 µm.

Keywords: PEDOT:PSS, ethylene glycol, secondary doping, organic solvent treatment

POSTER SESSIONS

Id-710

The Effect of Pore Size on Optical, Structural and Mechanical Properties of Porous Ecoflex Sponges

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Abstract- Ecoflex is a biocompatible silicon-based elastomer with very high stretchability and is widely used in many applications such as soft robotics, human implants and strain sensors. The sugar templating process is a simple method for fabricating porous 3D structures. In this technique, particles such as sugar, salt or starch are used as templates. In this study, macroporous Ecoflex sponges were fabricated using sugar particles of different sizes. Characterization techniques such as scanning electron microscopy (SEM) and UV-Vis-NIR spectroscopy were used to study the microstructure and optical properties of the Ecoflex sponges. Mechanical tests were performed to investigate the flexibility and deformability of the Ecoflex sponges. We have shown that we can fabricate porous structures with different pore sizes in a single step using the sugar templating process. It has also been shown that porous structures can be used to produce materials that are easier to stretch and last longer. After compression tests, the elongation of the Ecoflex sponge with large pores reached about 70-80% at low load. As the compressive load increased, it was found that the pore spaces began to shrink and the material gradually began to harden. According to the Tauc's plot slopes obtained from the transmission spectra, a decrease in the band gap value from 4.90 to 3.86 eV was observed with the decrease in pore size. Considering all the characterization results, we believe that these materials prepared by sugar templating method can be used as substrates or insulating layer for various applications.

Keywords: ecoflex, porous structure, sugar templating process

POSTER SESSIONS

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A Preliminary Work of Magneto-resistive Sensors on Flexible and Transparent Substrate as a Buffer Layer

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Abstract- The use of flexible and transparent (light-permeable) polymer substrates instead of Silicon substrates, which are widely used in magnetic sensors to be prepared within this study. The reason for this is that polymer substrates have been used in many academic and industrial applications in recent years. Polyethylene Terephthalate (PET) structures are one of the most notable among the flexible polymer substrates that have been widely used. The widespread use of these structures in flexible and organic electronic studies has paved the way for them to come to life in many industrial applications. In this study, we worked on cleaning process of PET substrates. After that, we coated Platinum at 10W to each other (all of their thickness are about 10 nm) in Ultra High Vacuum by Magnetron Sputtering Deposition Techniques.

Keywords: flexible substrate, PET, magnetron sputtering deposition, buffer layer

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