Biomaterial Surfaces & Interfaces
Room Naupaka Salon 4 - Session BI-WeE1

Bioimaging and Bionanotechnology
Moderator: David G. Castner, University of Washington

5:40pm **BI-WeE1-1 Machine Learning for Prediction of TOF-SIMS Spectra of Peptides**, ***Satoka Aoyagi,*** Seikei University, Japan **INVITED**

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is one of the most powerful surface analysis methods because ToF-SIMS provides molecular 3D imaging with high spatial resolution and detailed chemical structures. ToF-SIMS has extremely rich chemical information and so that it is often difficult to extract all of the important information from ToF-SIMS data by manual analysis. Multivariate analysis techniques such as principal component analysis have successfully been applied to TOF-SIMS data interpretation [1] and are generally useful for understanding TOF-SIMS results. Moreover machine learning and deep learning methods have been applied to ToF-SIMS data interpretation [2]. In order to interpret ToF-SIMS spectra, the processes of the data analysis should be opened, but most of the deep learning methods do not provide readable information on the analysis processes. Through a VAMAS (Versailles Project on Advanced Materials and Standards) interlaboratory study, the identification of peptide sample TOF-SIMS data by machine learning (Fig. 1) was investigated. In this study, unknow peptide spectra were predicted using Random Forest [3]. Moreover, this method can be applied to the prediction of other organic materials by improving the data format.

[1] M.S. Wagner and D.G. Castner, Langmuir 17 4649-4660 (2001).

[2] K. Matsuda and S. Aoyagi, Biointerphases 15 021013 (2020).

[3] S. Aoyagi, A. Takano and Y. Fujiwara, VAMAS TWA 2 A26, 2019:Identification of unknown peptide sample TOF-SIMS data by machine learning - Protocol for Analysis

6:20pm **BI-WeE1-3 Strategy for Constructing Accurate 3D NanoSIMS Depth Profiling Images of Cells Despite Lateral Variations in Surface Erosion**, *M. Brunet, B. Gorman,* ***Mary L. Kraft,*** University of Illinois Urbana-Champaign

We have developed a strategy for constructing accurate 3D NanoSIMSdepth profiling images of cells when the rate of surface erosion varies laterally. To accomplish this, we reconstruct the morphology of the cell each time a depth profiling image was acquired from the secondary electron images acquired in parallel with the negatively charged secondary ions during NanoSIMS depth profiling. Then the morphologies created for every imager plane in the depth profile are adjusted so the height of the cell at every x, y location decreases each time a new image was acquired. Finally, these reconstructions of the cell's morphology are used to shift the voxels in the 3D NanoSIMS images to the correct height. This strategy was validated by comparing morphology reconstructions for secondary electron depth profiling images acquired from a cell with focused ion beam - secondary electron microscopyand AFMdata acquired from the cell before depth profiling. The general shape and relative height of the reconstructed cell morphology was in good agreement with the AFM data. Application of this strategy to 3D NanoSIMSdepth profiling data of a metabolically labeled mammalian cell produced visually accurate 3D images of the intracellular ^{18}O-cholesterol and ^{15}N-sphingolipids distributions.Moreover, transport vesicles and organelle membranes containing ^{18}O-cholesterol and ^{15}N-sphingolipids could be more clearly visualized. Accurate 3D NanoSIMS images showing the distributions of molecules of interest within cells may now be constructed when the sputter rate varies laterally and without requiring the collection of topography data prior to depth profiling.

6:40pm **BI-WeE1-4 Multimodal Studies of Cellular Membrane Chemistry using GCIB-SIMS**, ***John Fletcher,*** University of Gothenburg, Sweden

Changes in the lipid membrane of cells has implications for cell survival, function and in the case of diseases treatment efficacy. For example lipid changes in secretory cells can alter exocytosis with implications for neuronal communication while cell membrane composition can effect permeability to pharmaceuticals, along with mechanical properties that may influence cell mobility, and in the case of cancer cells, metastatic potential.

Secondary ion mass spectrometry (SIMS) provides unique opportunities for analysing cells with both high spatial resolution, surface sensitivity and chemical specificity. The ability to characterise the cellular membrane lipid composition has been greatly enhanced by the introduction of gas cluster ion beams (e.g. $(CO_2)_{6k}^+$) that provide increased secondary ion signals for intact biomolecules. The presentation will illustrate the capabilities of GCIB-SIMS analysis of cell samples in studies of cancer and Parkinson's disease and highlight the complementarity of multimodal analysis using fluorescence microscopy and electrochemical analysis approaches.

7:00pm **BI-WeE1-5 Self-assembling Antimicrobial Peptide Coatings for Prevention of Infections**, ***Zhou Ye,*** The University of Hong Kong

Antimicrobial peptides (AMPs) are promising candidates as antimicrobial coatings due to its broad-spectrum activity, low bacterial resistance, and good biocompatibility. Previous works have explored the coatings of AMPs by covalent immobilizations or the introduction of an intermediate layer/nanoparticles. However, the fabrication processes were costly, complicated, and non-versatile, which limited the clinical applications. We have developed new strategies to form strong physical coatings by self-assembled AMPs and determined the significant roles of self-assembly and secondary structures in forming the AMP coatings. The dominant interactions between self-assembled AMPs and the substrate surfaces were studied to be hydrogen bonding, instead of electrostatic forces. We also correlated the self-assembly dynamics of AMPs to the antimicrobial activity by comparing L and D enantiomers of one model AMP, GL13K in aqueous solutions or interacting with phospholipid double layers and other bacterial envelope components. With the understanding of the coating mechanisms, we applied the self-assembled GL13K peptide coatings on various substrates, such as etched titanium implants, dentin, enamel, or mineralized collagen/hydroxyapatite. The AMP coatings presented excellent antimicrobial activities in mouse models or on *ex vivo* tooth with potentials in clinical settings.

7:40pm **BI-WeE1-7 Development of a Process for Flame Retardant Coating of Textiles with Bio-Based Anchor Peptides**, ***Rahel Krause,*** *I. Bettermann, R. Paul, T. Gries,* Institut of Textiltechnik of RWTH Aachen University, Germany*; M. Nöth, L. Feng, U. Schwaneberg,* Institute of Biotechnology of RWTH Aachen University, Germany*; C. Hummelsheim, L. Kampas,* Klevers GmbH & Co. KG, Germany

The fire protection of materials has an important role in our everyday life and covers a highly diverse spectrum of substances, materials and fields of application. Important fields of application for fire protection, especially in public areas, are construction and transport, electronic devices, furnishings and textiles (e.g. applications for occupational safety, carpets, curtains, upholstery, insulation and technical applications in outdoor areas). The efficient and durable finishing of the materials with flame retardant additives is crucial to ensure effective fire protection. Many of the flame retardant additives currently used are based on halogens, bromides, chlorides, phosphates or antimony. However, these flame retardants are harmful to the environment and/or health. Therefore, the use of these flame retardants is already being restricted by EU directives (e.g. REACH regulation) and it is foreseeable that they will be further restricted in the future. To keep up with this development, innovative and sustainable solutions must be developed in the short term. The amount of flame retardant additives that are harmful to the environment and health must be reduced. In the medium term these harmful additives must be completely replaced by sustainable flame retardant additives that are not harmful to the environment and health. This paper describes research results to reduce the amount of additives in the short term.

In order to reduce the amount of additives used, an innovative refinement process is being developed. In a first step, the flame retardant additives are combined with bio-based adhesion promoters (anchor peptides). Anchor peptides bind with high selectivity, binding strength and occupancy density to a broad portfolio of materials (e.g. synthetic polymers, metals, ceramics, natural materials) and enable the finishing of the materials with a broad spectrum of functional units (e.g. flame retardant additives). Material functionalisation by anchor peptides is energy-efficient and resource-saving at room temperature in aqueous solution and is scalable in its production.

Based on these developments, in this paper, a finishing process is presented with which flame retardant textiles can be equipped with bio-based anchor peptides. A requirements outline for the new finishing process is described. Established processes (e.g. foulard, coating machine, roller application) are compared with each other and evaluated with regard to the requirements and their suitability. The most suitable process is then designed and a laboratory scale as well as an industry scale concept are presented.

8:00pm **BI-WeE1-8 Impact of UV-C Exposure on Single-use Mask Integrity for Reuse to Address PPE Shortages Within At-Risk Communities**, *S. Ananthakrishnan, E. Rhoades-Clark, V. Mitchell,* ***Heather Canavan****,* University of New Mexico

The COVID-19 pandemic significantly disrupted supply chains in the global economy. The American Indian populations of the Southwest United States have been particularly hard hit, due to multi-generational housing, lack of access to running water, and insufficient protective personal equipment (PPE). The limited availability and price of commercial N-95 masks led the public to reuse their masks, rather than treating them as single-use equipment. In turn, this led users to experiment on their own on how best to sterilize their masks for repeated usage, including both low-tech (UV sterilization with sunlight, washing with detergent or soap) and high-tech approaches (fogging with disinfectant, UV lamp apparatuses, etc.). Recommendations by the CDC and mask manufacturers often contradicted each other on best practices; the CDC recommended reusing single-use masks through UV sterilization, while mask manufacturers indicated otherwise due to concern of material degradation. We hypothesized that exposure to UV-C (254 nm) would damage non-woven single-use mask fibers such as those found in N-95, KN-95, and surgical masks due to spalling, which would lead to increased mask pore size, and therefore decreased filtration efficiency. However, woven fabric masks should not suffer spalling from UV exposure due to a difference in the fabrication of the fibers. To test our hypothesis, we subjected N-95, KN-95, surgical, and fabric masks to UV-C exposure for appropriate time scales (0-24 hours) to simulate repeated exposure for sterilization followed by a close inspection of layers using Scanning electron Microscopy (SEM). We examined the pore sizes and density, fiber integrity, and surface morphology of the layers that comprised each mask and compared the resulting damage. We found that limited exposure to UV-C (15 minutes/4 exposure cycles) would result in significant damage to all the masks except for fabric masks. As the acute experiences of the pandemic have receded, the cost and availability of PPE have normalized, and well-funded populations have ceased to focus on the issue of sterilization and reuse. However, members of at-risk communities are still grappling with ways to best adapt to supply chain shortages and masking needs. Therefore, these results will be of interest to those seeking to understand how UV-C affects the reusability of various mask types.

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