SYNCHROTRON LIGHT FINLAND 2025

27.-28.11.2025 Kumpula campus

UNIVERSITY OF HELSINKI

Day 1, November 27th

Registration – Chemicum lobby from 12:00-12:30		
12:30-12:40	General Introduction	Dr. Ryan Trevorah
Session 1 – Chair: Paavo Penttilä		
12:40-13:25	Neutron Scattering for Soft Matter: what lies ahead	Dr. Leonardo Chiappisi (ILL, France)
13:25-13:50	The European Synchrotron and Free Electron Laser User Organisation	Assoc. Prof Cormac McGuinness
13:50-14:05	Time-resolved small-angle X-ray scattering data analysis of the amyloid fibril formation process	Taïsiia Cheremnykh (JYU, Finland)
14:05-14:20	3D Imaging of nerve structure in pathologic synovium	Khaled Elkouly (University of Oulu, Finland)
14:20-14:35	Multiscale Characterization of Wood and Bamboo Using X-ray Scattering and Machine Learning	Enriqueta Noriega Benitez (JYU, Finland)
14:35-15:05	Coffee break (Chemicum foyer)	
Session 2 – Chair: Heikki Takala		
15:05-15:50	The free electron laser FLASH - new opportunities for ultrafast science	Dr Markus Guehr (DESY, Germany) (online)
15:50-16:10	Cryo-soft X-ray tomography studies of virus-induced changes in cells	Dr Maija Vihinen-Ranta (JYU, Finland) (online)
16:10-16:30	Probing the fate of lignin nanoparticles at the oil-water interface using X-ray and neutron scattering	Dr Felix Abik (University of Helsinki, Finland)
16:30-16:45	Multiscale structural characterisation of hierarchical materials via combined X-ray tomography and scattering	Dr Mira Viljanen (MAX IV, Sweden)
16:50-17:30	FSRUO annual general meeting	

Day 2, November 28th

Session 3 – Chair: Ryan Trevorah		
9:00-9:30	Coffee break (Exactum foyer)	
9:30-9:50	Soft X-ray absorption spectroscopy and microscopy in Ti3C2Tx nanocomposite for electrocatalysis	Dr Zhongpeng Lyu (Aalto University, Finland)
9:50-10:10	Catalytic reactor effluent analysis using photoionization mass spectrometry	Morsal Babayan (University of Oulu, Finland)
10:10-10:30	Versatile Operando Fuel Cell for Laboratory and Synchrotron Based Hard X-ray Spectroscopy	Dr Antti-Jussi Kallio (Aalto University, Finland)
10:30-10:55	The NEPHEWS project	Piotr Piwowarczyk (Jagiellonian University, Poland) (online)
10:55-11:00	Closing words	

Time-resolved small-angle X-ray scattering data analysis of the amyloid fibril formation process

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Processes such as the formation of amyloid fibrils and protein aggregation involve subsequent chemical reactions that occur under native conditions. Time-resolved small-angle X-ray scattering (TR-SAXS) is a structural characterisation method that allows one to capture conformational changes and measure the kinetics of macromolecules and complexes in near-native solutions. For functional biological complexes, it is important to observe not only structural changes, but also identify their biological implications. As analysing one-dimensional SAXS data in terms of three-dimensional (3D) models is an ill-posed problem and analysing kinetics requires detecting time-dependent changes, the characteristic times of structural changes also need to be defined in order to analyse large amounts of time-resolved data. In this study, the amyloid fibril formation process was structurally characterised using dimensionality reduction techniques. Processed TR-SAXS data revealed conformational polymorphism in the formation of amyloid fibrils by determining the shapes of the starting/final states and possible intermediates in the process.

References:

T. Cheremnykh. Automated SAXS data analysis of the amyloid fibril formation process. *Hochschulschrift, Hamburg*, Universität Hamburg, Hamburg, 2022.

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3D Imaging of nerve structure in pathologic synovium

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Pain perception in early osteoarthritis (OA) is believed to be connected to synovial inflammation (synovitis) rather than to the destruction of articular cartilage. Traditional nerve imaging techniques in synovial tissue are based on immunohistochemistry and immunofluorescence. They are inherently destructive and often fail to capture the full three-dimensional complexity of the tissue. This experiment aimed to visualize nerve fibers in human synovium by combining contrast-enhanced high-resolution synchrotron radiation X-ray phase-contrast (X-PCI) imaging with a novel application of heavy-metal isotope labeled (Cd110, Tm169 and Eu151) antibodies against neuron-specific proteins (PGP 9.5 and neurofilament) and a vascular marker (CD31), respectively.

Synovial biopsy samples were obtained after total knee replacement surgery. Prior to heavy metal immunolabelling, samples were fixed, permeabilized, and incubated with a penetration buffer and then a blocking buffer. Subsequently, the samples were incubated with the heavy-metal labeled antibodies mentioned above. Finally, samples were washed to remove excess reagent and embedded in agarose for the X-PCI imaging.

High-resolution X-PCI was performed at the DanMAX, MAX IV Laboratory (Lund, Sweden). A sample-specific mosaic tomography approach was employed to first scout full sample. Two or more scan positions were used depending on the sample size, and 4000 projections were collected with the ORCA detector at 4×4 binning (effective pixel size = 2.22 µm) and 2 ms exposure time under HDR mode. Subsequently, higher-resolution mosaic scans were acquired from the target region with 6000 projections at an effective pixel size of 0.55 µm, 1×1 binning, and an exposure time of 5 ms. Filtered back projection with a cosine filter and the Paganin phase-retrieval ($\delta/\beta = 365$ for lower-resolution and $\delta/\beta = 50$ for higher-resolution acquisitions) algorithm were used to reconstruct X-PCI images.

The scout X-PCI imaging allowed us to visualize synovial tissue structures, and high-resolution scans enabled 3D mapping of the nerve network. Furthermore, distinct higher intensities of the neural structures due to heavy-metal labeling made them easier to segment from the X-PCI images. The developed method of immunolabeling with heavy metals, combined with X-PCI, could provide novel insights into joint innervation.

Multiscale Characterization of Wood and Bamboo Using X-ray Scattering and Machine Learning

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Modern synchrotrons generate massive, high-resolution scattering datasets that capture the structural complexity of heterogeneous materials. However, the rapid growth in data quality and volume presents a major analytical challenge—large portions of valuable information remain underused due to time and resource constraints. Machine learning (ML) offers a powerful approach to automate and enhance the interpretation of these multidimensional datasets, enabling deeper structural insight across scales.

In wood, wide- and small-angle X-ray scattering (WAXS, SAXS) experiments on Norway spruce at the ESRF synchrotron produced detailed spatial maps of wet and dry samples. Principal component analysis (PCA) and clustering methods identified differences in moisture state and tissue type, while near-infrared (NIR) spectroscopic imaging provided complementary information for classification. This integration of scattering and statistical analysis demonstrates the potential of ML-supported approaches for multiscale materials characterization. [1]

Extending this work to bamboo, combined computed tomography (CT) and scanning WAXS are being used to investigate guadua bamboo. Random forest regression and autoencoder models can correlate scattering features with fiber cell wall mass derived from CT, effectively linking nanoscale scattering patterns to anatomical composition. These data-driven models show how ML could accelerate interpretation and reveal structure–function relationships in multimodal setups. [2]

Complementary to these ML-based studies, small-angle X-ray scattering tensor tomography (SAXS-TT) provides three-dimensional orientation information on cellulose microfibrils in wood tissues. Data collection on pine and birch samples and initial analysis are complete, with ongoing processing to extract quantitative orientation maps and integrate them with complementary imaging.

Together, these approaches establish a unified framework combining high-resolution synchrotron techniques, advanced data analysis, and computational modeling to better understand hierarchical plant-based materials.

References

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[2] Ahvenainen, P., Noriega Benitez, E., Jyske,T., Viljanen, M., Suhonen, H., Penttilä, P. Tissue-specific variation of softwood nanostructure revealed by scanning X-ray scattering and clustering analysis, submitted to Cellulose

Probing the fate of lignin nanoparticles at the oil-water interface using X-ray and neutron scattering

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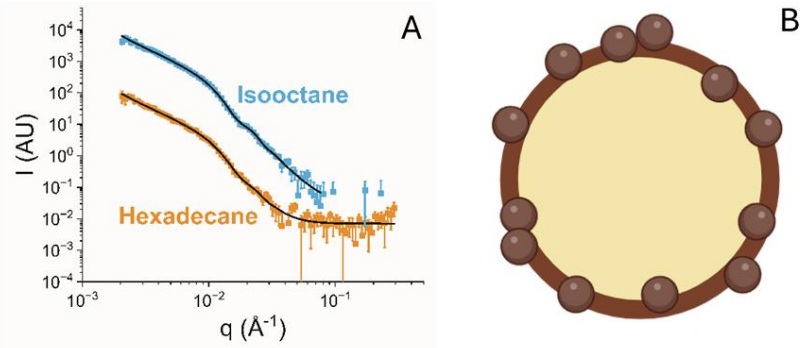
Lignin, a polymeric polyphenol occurring naturally in plants, is considered to be a frontrunner in the race towards sustainable renewable materials. By converting lignin into nanoparticles (LNPs), it can be dispersed into aqueous systems, expanding its use in various water-based applications. However, given the complexity of lignin's polymeric structure, including variations arising from its source and extraction methods, there is currently little correlation between lignin's behavior at the molecular level to its macroscopic properties.

One of the potential uses of LNPs is as emulsifiers. Given their generally compact, spherical structure, it has long been thought that LNPs act as Pickering emulsifiers, where they are adsorbed at the oil-water interface as solid particles. However, our results appeared to indicate otherwise. While SAXS results of the LNPs in their dispersions were consistent to their microscopic images, SANS of the emulsions indicated that the particles experienced deformations as they adsorb at the oil-water interface. Moreover, this deformation appeared to be influenced by the type of lignin and oil used in the emulsion. From these results, we are one step closer towards establishing an evidence-based rationale to tailor lignin functionalities in various emulsion systems.



Multiscale structural characterisation of hierarchical materials via combined X-ray tomography and scattering

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With the ever-increasing demand for renewable materials for product manufacturing sector, cellulose-based materials remain vital for creating sustainable alternatives for many everyday products. In wood and plant derived fibres renewability and sustainability are natively combined with superior mechanical properties which arise from the hierarchical arrangement of cellular structures and the ultrastructural characteristics of cellulose microfibrils [1]. By studying the behaviour and structural properties of such hierarchical materials at the micro-, nano- and atomistic scales, we gain essential insights into the fundamentals of natural hierarchical systems while supporting the innovation and development of new materials.

Combined X-ray microtomography and scattering techniques are provide an efficient way for obtaining multiscale structural information from wood and other hierarchical materials [2]. To showcase this approach, we present few examples of the multiscale and -modal experimental capabilities available at ForMAX beamline at MAX IV Laboratory.

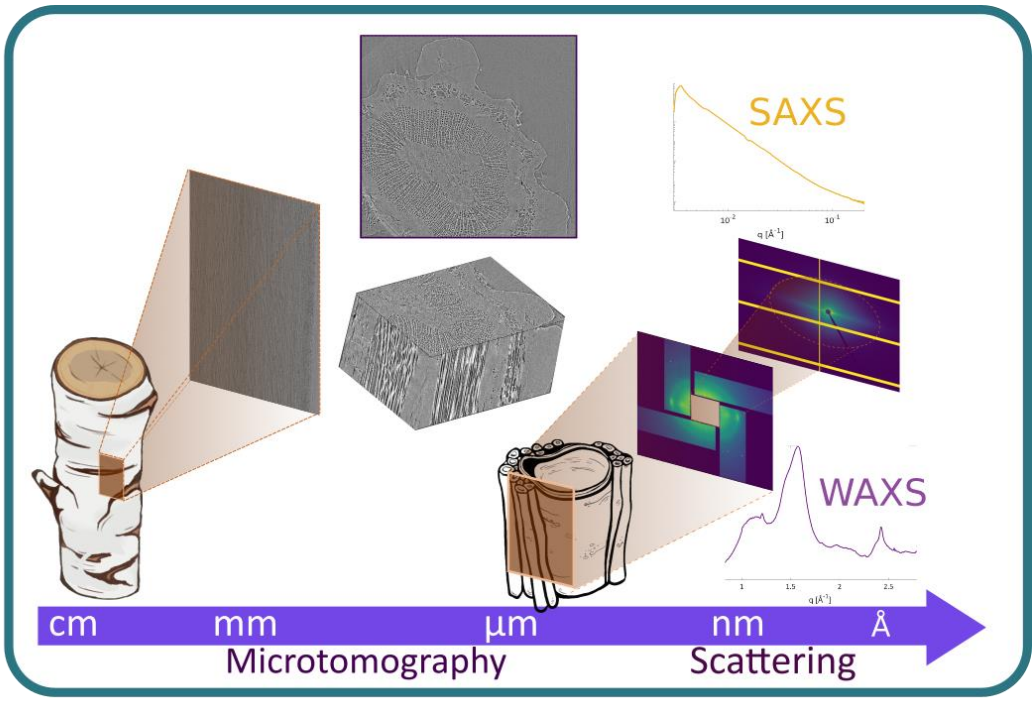

Figure 1. Schematic illustrating the kind of information obtainable from wood structures using a multiscale approach that combines X-ray scattering and microtomography techniques.

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Soft X-ray absorption spectroscopy and microscopy in $Ti_3C_2T_x$ nanocomposite for electrocatalysis

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MXenes have become versatile co-catalysts for enhancing the electrocatalytic performance of many transition metal layered hydroxides (TM-LHs) and layered double hydroxides (TM-LDHs), benefiting from their synergistic physical and chemical properties. Recent studies suggest that an effective coupling of the two materials enhances the overall OER performance in terms of overpotential, Tafel slope, and durability,[1] making the heterostructures of TM-LHs/LDHs-MXene promising candidates for low-cost earth-abundant electrocatalysts for, e.g., the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). The structural/electronic coupling and charge redistribution at TM-LHs/LDHs-MXenes heterostructure interfaces can boost the conductivity and active sites, which cannot be achieved by either pristine TM-LHs/LDHs or MXenes.[2] However, the interfacial chemistry and the synergistic effect between TM-LHs/LDHs and MXenes are complicated and still poorly understood. Detailed pictures of heterostructre formation, charge redistribution, and structure reconstruction are still missing.[3]

Here, we shown some preliminary attempt to probe the soft edge of Ti in $Ti_3C_2T_x$ MXene and its composites using scanning transmission X-ray microscopy (STXM) and X-ray Raman spectroscopy (XRS). We have performed the STXM measurement on Ti L-edge during the in-situ growth of CoFe LDH on $Ti_3C_2T_x$ flake. We found when Co2+ and Fe3+ were first absorbed on the -O or -OH terminations of $Ti_3C_2T_x$ and then exposed to the base solution, oxidation of Ti3C2Tx was revealed during CoFe LDH formation. This observation is consistent with our published work and provides a much deeper understanding of the heterstructure formation with both high spatial and chemical resolution.[2] XRS revealed bulk chemical state of $Ti_3C_2T_x$ MXene which cannot be acquired using conventional surface sensitive soft X-ray methods. With these preliminary results, we acquired a more detailed picture of the interaction among various LHs and LDHs and Ti3C2Tx MXenes with different surface chemistry.

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Catalytic reactor effluent analysis using photoionization mass spectrometry

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Heterogeneous catalysis is critical for novel industrial processes, such as Methanol-To-Hydrocarbons (MTH), which accelerates the transition from fossil fuels to sustainable resources and produces complex organic mixtures. However, our understanding of catalyst behavior under various operating conditions is limited [1, 2]. Under industrial conditions, the product analytics is based on Gas Chromatography (GC) which struggles to monitor highly reactive intermediates. While model studies under sub-ambient conditions like Temporal Analysis of Products (TAP) experiments are highly time-resolved and sensitive but limited when it comes to overlapping ion fragments and isomers [3]. Coincidence photoionization mass spectrometry (PIMS), which detects ions in coincidence with emitted photoelectrons, alleviates some of these limitations. Recently, synchrotron ultra-violet (SUV) PIMS has emerged as a powerful tool offering real-time, in-situ analysis of complex catalytic reactions [4].

Currently, a limited number of synchrotron beamlines are equipped to perform PIMS-based analysis of catalytic reactor effluents. Here, the development of such an instrument at the FinEstBeAMS beamline in MAX IV is presented. First, the prototypical model reaction of dimethyl ether (DME) on zeolite is studied using in situ/operando PIMS. We showed the isomer selectivity of this technique by quantitatively distinguishing xylene isomers using the photoelectron spectrum corresponding to the ionization channel of $C_8H_{10}+hv \rightarrow C_8H_{10}^+ + e^-$ [5]. Later, to check the feasibility of catalytic intermediate detection, we studied the conversion of methyl acetate (MA) over pentasil using photoelectron-photoion coincidence (PEPICO) and photoion-photoion coincidence (PIPICO) spectroscopy. In PEPICO, photons with 40 eV energy are utilized to excite the valance electrons of the effluent gas mixture. Then the correlated ions and electrons from the same ionization events are analyzed to characterize the effluent stream. In PIPICO, a higher photon energy (330 eV) is used to excite the core level C 1s electrons. Here, besides the correlated ion and electron coming from one ionization event, the secondary fragments (from the same event) are also detected, which provides an additional dimension in data. For this set of experiments, we detect ketene which is a highly reactive intermediate. There are limited number of beamlines worldwide working with low energy photons to perform PEPICO, however, PIPICO has the potential to be implemented at a wider range of beamlines, highlighting exciting new possibilities offered by PIMS-based effluent analytics for kinetic studies of complex chemistry.

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