Contribution ID: **56** Type: **Poster**

Lamellar neutron diffraction sample environment: vapour atmosphere and temperature control with Raman spectroscopic monitoring of gas phase equilibration

Here we investigate the lipid membrane reorganization caused by sorption of ethanol from the gas phase. The physical effects of the short chain alcohols, e.g. ethanol & butanol, on cell membranes seem to be a fundamental limitation on the amount of alcohol that can be produced by fermentation. This technology is already an important renewable alternative to fossil fuels. We hope that information from neutron spectroscopy and molecular dynamic simulations, will help tailor organisms with appropriate bilayer composition for enhanced and more efficient alcohol production from fermentation. Lamellar neutron diffraction and contrast variation of stacked lipid bilayers provides a means to analyze scattering length density compositional information of bilayer systems in the direction normal to the stack (Kucerka et al., 2008) and the nature of disorder in these stacks (Hamley, 2022). Such insights have provided indispensable in understanding the interaction of small solute molecules with bilayers (Kent et al., 2015) and provide high quality structural data for refinement of molecular dynamics force fields (Dickson et al., 2014). Here we present a new sample environment developed at the Heinz Maier-Leibnitz Zentrum which allows us to measure low-background lamellar neutron diffraction in the Bragg-Brentano geometry with controlled temperature and vapor composition at the sample position. A Raman spectrometer provides real time monitoring of the chemical and isotopic composition of the sample. This capability has been used for: contrast variation of the absorbed moisture vapor phase used for phasing of the Fourier reconstruction from intensity data at three contrasts; and analysis of the changes in structure of a fluid phase dipalmitoylphosphatidylcholine with adsorption of ethanol from the gas phase.

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Primary authors: Dr GARVEY, Christopher J. (1. Forschungs-Neutronenquelle, Heinz Maier-Leibnitz Zentrum (FRM II), Technische Universität München); Dr STAHN, Jochen (Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut); Dr WOLF, Marcell (Forschungs-Neutronenquelle, Heinz Maier-Leibnitz Zentrum (FRM II), Technische Universität München); Mr WANG, Peixi (Technical University of Munich, TUM School of Natural Sciences, Chair for Functional Materials); Mr SCHWAIGER, Dominik M. (Technical University of Munich, TUM School of Natural Sciences, Chair for Functional Materials); Prof. MÜLLER-BUSCHBAUM, Peter (Technical University of Munich, TUM School of Natural Sciences, Chair for Functional Materials); Dr GEORGII, Robert (Forschungs-Neutronenquelle, Heinz Maier-Leibnitz Zentrum (FRM II), Technische Universität München); Dr SKOULATOS, Markos (1. Forschungs-Neutronenquelle, Heinz Maier-Leibnitz Zentrum (FRM II), Technische Universität München)

Presenter: Dr GARVEY, Christopher J. (1. Forschungs-Neutronenquelle, Heinz Maier-Leibnitz Zentrum (FRM II), Technische Universität München)

Session Classification: Clip Session