MM 29: Liquid and Amorphous Materials

Time: Thursday 12:00–12:45 Location: H10

MM 29.1 Thu 12:00 H10

Molecular Feuds and Fragment Tales: Exploring Cyanobiphenyl Liquid Crystals with Cryo Atom Probe Tomography — •Kuan Meng, Kang'an Wang, Sebastian Eich, and Guido Schmitz — Stuttgart University,Institute for Materials Science, Heisenbergstr. 3, 70569, Stuttgart, Germany

Liquid crystals exhibit the fascinating duality of liquid-like fluidity and solid-like long-range order, requiring nanoscale characterization techniques with high spatial resolution and chemical sensitivity. Atom probe tomography (APT) uniquely meets these requirements, offering unprecedented insights into the behavior of anisotropic organic molecules. This talk bridges liquid crystal science and APT by exploring cyanobiphenyl systems (5CB, 8CB, and 8OCB).

We investigated the field evaporation behaviors of these molecules, observing remarkable stability under high electric fields. Molecular signals dominated (90% for 5CB and 8CB, 70% for 8OCB), with fragmentation patterns influenced by oxygen atoms. The fragments were classified as alkyl chains, single phenyl derivatives, cyanobiphenyl residues, and cyano-hydrogen substitution pairs. Spatially, both molecular and fragment signals correlate strongly with laser orientation: fragmentation decreases from illuminated to shadowed regions, reflecting cleavage behavior under thermal gradient-induced field variations. Additionally, APT revealed the uniform mixing of 5CB and 8CB across various ratios, as well as the lattice plane of the crystal structure of pure 8CB. In the crystalline regions, we will discuss how the molecules field evaporate at specific angles relative to their intrinsic orientations.

MM 29.2 Thu 12:15 H10

Peptide Analysis at Atomic Resolution with Atom Probe Tomography — •Sakshi Sinha and Guido Schmitz — Department of Materials Physics, Institute of Material Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart

Atom Probe Tomography (APT) promise decisive advancements in nanoscale characterization of biomolecules, since it offers in principle single atom sensitivity in the study of organic molecular structures. In our experiments, we test the analysis of carnosine (β-alanylhistidine), in aqueous solution since water provides a natural biological environment. The investigated dipeptide is for example essential for brain and muscle function. By combining cryogenic sample preparation with advanced laser-pulsing techniques, APT enables three-dimensional mapping of carnosine's atomic composition and the distribution of various molecule fragments in the water matrix. Remarkably, the concentration of the solution controls the detected fragmentation behavior in the full range from single atoms to the full peptide molecule. So, the measurement conditions can be optimized to preferentially address the questions regarding the local stoichiometry or the different subunits of the molecule.

MM 29.3 Thu 12:30 H10

Fe self-diffusion in Fe-Al-Si melts - A combined ab initio molecular dynamics and experimental study — •Katharina Dammer[1], Fan Yang[1], Elke Sondermann[1], Florian Kargl[1], Andreas Meyer[1,2], and Noel Jakse[3] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institut Laue-Langevin (ILL), 38042 Grenoble, France — [3]Université Grenoble Alpes, CNRS, Grenoble INP, SIMaP, 38000 Grenoble, France

Understanding the structural, dynamic and thermophysical properties of binary and ternary Al-Fe-Si alloys in the liquid and supercooled state before solidification is crucial to ensure the desired microstructure and therefore ideal product properties. With an increasing iron content in the alloy, the liquidus temperature increases and exceeds 1000°C for most ternary Al-Si-Fe alloys. At these high temperatures, experiments are more delicate to perform, making it challenging to obtain information on transport coefficients and (partial) structure factors.

We present a combined first principle-based molecular dynamics (AIMD) simulations and experimental study of Al-Fe melts. Measurements were performed using quasi elastic neutron scatting (QENS) to obtain the self-diffusion coefficients of Fe at different Al-Fe compositions as a function of temperature. We intend to achieve in the future an improved simulation scheme using machine learning that realistically covers a larger range of the phase diagram, which cannot be easily assessed with experiments.