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Poster Abstracts

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Investigating the Structure of Ethylene Glycol-Water Mixtures at Different Concentrations by Total Neutron Scattering

Luke Roebuck

University of Manchester, UK

The structure of ethylene glycol/water mixtures have been investigated by combined neutron diffraction and computer simulation. Total neutron scattering datasets of ethylene glycol and aqueous mixtures at 3 different concentrations (XEG = 0.11, 0.46, 0.9) were obtained on the Near and InterMediate Range Order Diffractometer (NIMROD), ISIS Neutron and Muon Source. These datasets were then used to refine simulations of the systems using empirical potential structure refinement (EPSR). Analysis of the refined simulations has revealed significant insight into the structure and hydrogen bonding of the mixtures. Initial analysis has shown that at molar ratios of 0.46 and above the tetrahedral structure of water is lost and molecules become increasingly isolated. When the molar ratio reaches 0.9 water molecules are completely isolated and exist as single molecules. These finding may explain the cryoprotectant properties of ethylene glycol/water mixtures.

EFFECT OF HEAT TREATMENT ON MICROSTRCTURE EVOLUTION AND CORROSION PERFORMANCE OF 316L SS

Tushar Dandekar

University of Portsmouth, UK

The current study seeks to understand the influence of a variety of heat treatments at a range of temperatures from 700 °C to 1200 °C on microstructure evolution, and corrosion behavior of as-built components of Stainless Steel (SS 316L) fabricated by selective laser melting. While interfaces are viewed as regions of segregation and therefore, an impediment to uniform concentration of desirable alloying additions, this study shows counterintuitive results. Electrochemical measurements showed that the As-printed (As-SLM) specimen exhibited the lowest corrosion rate (I_{corr}) and thus the best corrosion resistance amongst all conditions. The microstructural origins of this behaviour are explored in the present study using detailed characterisation. The role of Cr and Mo in the hierarchical solidification structure is elucidated. The results will allow for an informed interface engineering of AM alloys, specifically for corrosion resistance.

In-situ Studies of Cross Metathesis Breakdown of Rubbery Polymers

Richard Thompson

Durham University, UK

Cross-metathesis chemistry offers the potential of a simple room-temperature process to break down cross-linked rubbers, yielding oligomeric products. Our initial research showed that this process worked remarkably well, even in the absence of the diester that was assumed to be necessary to introduce chain ends (https://doi.org/10.1039/C5GC03075G).

We have recently addressed several of the shortcomings that we discussed in the original work and have considerably improved the initial process. Firstly, we demonstrate that the catalysts can enable significant breakdown at orders of magnitude lower concentrations than initially used. Secondly, by switching to a Grubbs–Hoveyda catalyst, the process is now tolerant to oxygen and can work well in air. Thirdly, we find that the process works equally well using a more benign solvent than the chlorinated solvent used in the original work. Small-angle neutron scattering enabled the rate of the breakdown process to be studied in situ and suggested that the catalysts are predominantly active near the polymer chain ends rather than via a random scission process. We present the new results using the SANS methodology, which could readily be applied to a wider range of materials' breakdown processes.

Neutron scattering, Raman scattering and molecular dynamics simulation study of supercritical fluid nitrogen

John Proctor

University of Salford, UK

We have performed neutron scattering experiments on supercritical fluid Nitrogen (N2) at 300 K (2.4 T_C) and 160 K (1.3 T_C), backed up by ab initio molecular dynamics simulations at 300 K. Very recently, we have performed Raman scattering from 300 K to 400 K and are currently extending our neutron scattering investigations to 90 K (0.7 T_C) to compare with recent computational predictions that the Frenkel line extends to the triple point [1].

We have been able to reliably characterize the Frenkel line in nitrogen using both diffraction (neutron scattering) and spectroscopy methods for the same substance, backed up by simulation, and obtain a broad overview of what parameters change, and what parameters do not change, when the Frenkel line is crossed. Furthermore, we have established characterization of the Frenkel line over a far wider temperature range than previously achieved and that characterization of the Frenkel line position via diffraction and spectroscopy methods yield findings that are – at least roughly – in agreement.

Finally, our investigation includes the temperature regime in which both the Widom lines and the Frenkel line are present. We find that behaviour of nitrogen remains gas-like until the Frenkel line is crossed, and our data support the hypothesis that the Widom line transitions are driven by density increase.

References

1. C.G. Pruteanu et al., J. Phys. Chem. Lett. 12, 11609 (2021).

Characterisation of Quantum Dot Ligand Shells by Neutron Scattering for Enhanced Triplet Exciton-Photon Interconversion in Organic-Semiconductor/Quantum-Dot Blend Films

Daniel Toolan

University of Manchester, UK

Blends comprising organic semiconductors and inorganic quantum dots (QDs) are relevant for many optoelectronic applications and devices. However, the individual components in organic-QD blends have a strong tendency to aggregate and phase-separate during film processing, compromising both their structural and electronic properties. Here, we demonstrate a QD surface engineering approach using electronically active, highly soluble semiconductor ligands that are matched to the organic semiconductor host material to achieve well-dispersed inorganic–organic blend films, as characterized by X-ray and neutron scattering, and electron microscopies. This approach preserves the electronic properties of the organic and QD phases and also creates an optimised interface between them. We exemplify this in two emerging applications, singlet-fission-based photon multiplication (SF-PM) and triplet–triplet annihilation-based photon up conversion (TTA-UC). Overall, we provide a highly versatile approach to overcome longstanding challenges in the blending of organic semiconductors with QDs that have relevance for many optical and optoelectronic applications.

Tackling local minima in the modelling of Inelastic Neutron Scattering experiments

Alban Bloor Riley

University of Manchester, UK

Inelastic Neutron Scattering experiments can directly probe the energies of crystal field and spin excitations. However, in order to interpret such observations a Hamiltonian model is typically required. Such models are typically constructed with Stevens operators and electron-electron exchange terms, where the coefficients of these operators are parameters to be found. This can be a challenging process, partly due to the existence of many local minima when trying to optimise the value of these parameters. In this poster, we will introduce two novel algorithms designed to tackle this problem using the technique of deflation.

Tribology Behaviour and Residual Stress of Thick Stellite 6 Thermal Spray Coatings

Federico Venturi

University of Nottingham, UK

The transition to renewable energy sources may require the existing fossil-fuel powered plants to work at an increased flexibility to supply power when intermittent renewable sources (e.g. wind and solar) are not providing enough. This puts critical power plant components, such as the boiler valve seat, at an excess of operational stress beyond the one predicted in their design. Stellite 6 is a cobalt-based superalloy which is extensively used as arc welded coatings in power plants boilers. This material has exceptional wear and corrosion resistance and is often used as a benchmark for hard facing surfaces in industry. However, when subject to thermal cycling at high temperatures and pressures, the residual stresses can cause delamination and cracking of the coating, which could lead to potential issues downstream to the steam turbine, causing downtime and maintenance costs. Therefore, improved coatings need to be provided to enhance lifetime and prevent operational losses, ultimately enabling a safe and reliable transition to NetZero. This work explores the tribology of a 1mm-thick Stellite 6 coating obtained by High Velocity Oxy-Fuel (HVOF) Thermal Spray, as well as the residual stress which originated from the deposition process, as a possible alternative which would improve components' reliability and lifetime.

Selective disruption of novel Serine-rich antimicrobial peptides

Anna Stephens

University of Manchester, UK

Selective substitution of serine residues into rationally deigned antimicrobial peptide G(IIKK)3I-NH2 promotes changes to peptide assembly and interaction with bacterial membranes. This work explores how serine-rich peptides interact with Gram-negative bacteria's inner and outer bacterial membranes by combining molecular dynamics (MD) simulations and neutron reflection (NR) to unravel how these selective replacements influence peptide behaviour.

The adsorption of surfactant-like ionic lubrication additive on stainless steel

Shilin Deng

University of Manchester, UK

To address the limitations of water-based lubricants—such as poor dispersion and dissolution stability, low reactivity, and high corrosiveness—ionic liquids (ILs) with surfactant-like structures were developed. These ILs exhibit amphiphilic properties that enable the formation of an adsorption layer on stainless steel surfaces, providing effective friction-reducing and anti-wear capabilities. However, the specific influence of this adsorption layer on the tribological properties of ILs remains unclear, warranting further investigation into its structure. In this study, we examine DEHP-TDAO (DEHP), a synthesized derivative that mimics commercial lubrication additives and has demonstrated promising tribological performance through its adsorption behaviour and aqueous structures. Using techniques such as surface tension measurements, ellipsometry, neutron reflection (NR), atomic force microscopy (AFM), dynamic light scattering (DLS), and small-angle neutron scattering (SANS), we gain valuable insights into the underlying mechanisms responsible for the superior performance of DEHP in lubrication applications.

Membrane-lytic Interactions of Short Arg- and Trp-Rich Lipopeptides with Outer and Inner Membranes of Gram-Negative Bacteria

Tianhao Ge

University of Manchester, UK

In this work, a series of lipopeptides rich in Arginine (Arg/R) and Tryptophan (Trp/W) is designed, namely C12RRWW, C12WWRR, and C12RWWR, where C12 denotes a lauroyl chain. All the lipopeptides were antimicrobial towards resistant and clinical Escherichia coli and Staphylococcus aureus strains, with C12RRWW showing MIC values lower than 10 μM against Escherichia coli strains and 5 μM against Staphylococcus aureus strains. C12RRWW and C12RWWR were also effective against clinical Pseudomonas aeruginosa strains. Dynamic killing assays revealed that these three AMPs could eliminate Pseudomonas aeruginosa within 10 min, much faster than antibiotic polymyxin B. Further fluorescence assays with N-phenyl-1-napthylamine, 3,3'-Dipropylthiadicarbocyanine iodide, and BODIPY-TR-cadaverine showed faster binding of C12RRWW and C12RWWR with lipopolysaccharides on the outer membranes of Gram-negative bacteria and greater efficiency at lysing these membranes, while C12WWRR was stronger in depolarizing their inner membranes. Neutron reflection and small angle neutron scattering techniques helped unravel how these lipopeptides interacted with bacterial membrane models, and the amount of removal of membrane lipids and extent of insertion of AMPs into the membranes were well correlated to the antimicrobial actions of the lipopeptides. These studies revealed that lipopeptides such as C12RRWW could offer potent antimicrobial efficacy and efficiency with low cytotoxicity.

Designed Dengue Virus Disordered Peptides Effect on Mimicry Bilayer of Bacteria Membrane

Yingyu Wang

University of Manchester, UK

Antimicrobial peptides hold promise as effective antimicrobial agents. Their cationic nature enables them to eliminate bacteria by disrupting bacterial membranes via electrostatic interactions and facilitating binding to the negatively charged bacterial membrane surface. This mechanism acts more rapidly than traditional antibacterial drugs, making it challenging for pathogens to develop resistance. The design of the peptide in this study was inspired by the conserved segment of the dengue virus (DENV) capsid (C) protein, Pep14-23 (NMLKRERNEV). Upon binding to negatively charged phospholipid membranes, this peptide displays an α-helical conformation and asymmetrically distributed charge structure. This peptide binds to lipid droplets (LDs) and successfully inhibits DENV C-LDs interaction. We will explore whether this peptide could rupture the bacterial membrane and achieve an inhibitory effect. Therefore, we designed several different cationic short peptides based on the sequence of pep14-23, to investigate how key amino acids and the hydrophilic and hydrophobic sequences affect the behavior of the short peptides.

Novel Fitting Routine for Kinetic Neutron Reflectivity Data and Its Applications for Polymer Dynamics

Stephanie Burg

University of Sheffield, UK

Continual upgrades to state-of-the-art instruments in the field of neutron scattering now allow us to access fast time scales with techniques that were previously impossible. This decrease in acquisition time opens up exciting possibilities for examining kinetics in various polymer systems on the order of seconds, but also results in a substantial increase in the amount of data collected. These large datasets still pose considerable time barriers to processing, even in the age of modern computing power. There is also the issue of error bars, as faster data is often noisier, making it even more important to fully account for this in the data analysis. Here, we propose a new fitting routine for neutron reflectivity data, which allows for a complete Bayesian statistical analysis of the fitting parameters, including error bars, and is capable of running in seconds on a standard laptop. We then demonstrate its capabilities by examining the thin film expansivity of polymer films in their liquid and glassy states, achieving highly accurate results consistent with the literature, with complete error propagation from the neutron counting statistics to the calculated expansivities.

Loading and release studies of amphiphilic antibacterial short peptides in hydrogel network

Ke Ding

University of Manchester, UK

Rationally designed, amphiphilic, cationic, short peptides have attracted extensive attention due to their excellent antibacterial properties and low cytotoxicity, but there are still many challenges in the development of their practical applications. This project explores the controlled loading and release dynamics, antibacterial effects, and cytotoxicity of the antimicrobial peptide G3 (G(IIKK)3I-NH2) in a hydrolysed cellulose hydrogel network. G3 is trapped in the network structure of the hydrogel and released slowly over time. As the loading of G3 increases, the released G3 will also increase, so the concentration of the effect can be adjusted within the range of effective sterilization and low cytotoxicity by controlling the load. The strength of HEC affects the drug release rate of G3, and the hydrogel with low cross-linking degree has a stronger release effect. HEC-G3 hydrogel showed better antimicrobial activity against bacteria than other commercial hydrogels. HEC acts as a diffusion barrier and regulates the release rate and the total released amount. For M-HEC gels, 83.14%G3 will be released in the 100h. Experiments from zones of inhibition showed that all zones of inhibition produced by HEC-G3 were larger than those of the control hydrogel. At the same time, cell experiments also showed that HEC-G3 has better cytocompatibility than the control hydrogel. The results are discussed in the context of literature studies using antimicrobial agents such as PHMB, octenidine. This work provides a valuable reference for the practical application of cationic antimicrobial peptide hydrogels in the direction of wound healing.