

Advanced School in Soft Condensed Matter 'Solutions in the Spring'

3–6 April 2016
Homerton College, Cambridge, UK

Organised by the IOP Liquids and Complex Fluids Group

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Advanced School in Soft Condensed Matter “Solutions in the Spring”

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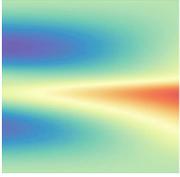
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Advanced School in Soft Condensed Matter 'Solutions in the Spring'

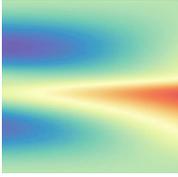
Programme

Sunday 3 April 2016

- 11:00 Arrival and refreshments
- 12:30 Lunch
- 14:00 Introductory lecture
- 14:45 Lecture – Self Assembly 1
- 15:30 Refreshments
- 16:00 Networking session
- 18:30 Dinner
- 20:00 Free Time

Monday 4 April 2016

- 08:00 Breakfast
- 09:00 Lecture – Self Assembly 2
- 09:45 Lecture – Micro-rheology 1
- 10:30 Refreshments
- 11:00 Lecture – Self Assembly 3
- 11:45 Workshop – Self Assembly
- 12:30 Lunch
- 14:00 Lecture – Confined Fluids 1
- 14:45 Lecture – Neutron Reflectivity 1
- 15:30 Refreshments
- 16:00 Poster Session
- 18:30 Dinner
- 20:00 Free Time



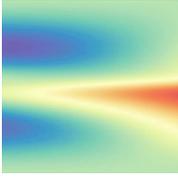
**Advanced School in Soft Condensed Matter
'Solutions in the Spring'**

Tuesday 5 April 2016

- 08:00 Breakfast
- 09:00 Lecture - Confined Fluids 2
- 09:45 Lecture - Micro-rheology 2
- 10:30 Refreshments
- 11:00 Lecture - Confined Fluids 3
- 11:45 Lecture - Neutron Reflectivity 2
- 12:30 Lunch
- 14:00 Workshop - Confined Fluids
- 14:45 Lecture - Neutron Reflectivity 3
- 15:30 Refreshments
- 16:00 Free time in Cambridge
- 17:30 Punting - Cambridge River Tour (Thompson Lane, CB5 8AQ)
- 18:30 School dinner in Cambridge, La Mimosa restaurant (Thompson Lane, CB5 8AQ)

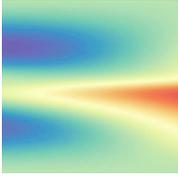
Wednesday 6 April 2016

- 08:00 Breakfast
- 09:00 Workshop - Neutron Reflectivity
- 09:45 Lecture - Micro-rheology 3
- 10:30 Refreshments
- 11:00 Workshop - Micro-rheology
- 11:45 Prize Award Session
- 12:00 Lunch and depart



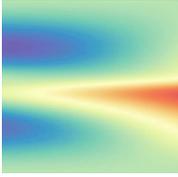
Poster programme

- P01. Vitrification of colloids as a connectivity transition**
Ruben Higler, Wageningen University, The Netherlands
- P02. Encapsulation and release using ethyl cellulose microcapsules**
Javier Otero Marquez, University of Edinburgh, UK
- P03. Small angle scattering of soft matter assemblies: A need-case for coarse-graining**
Andrew McCluskey, University of Bath, UK
- P04. Squeezing an emulsion with two continuous phases: centrifugal compression of the bijel**
Katherine Rumble, University of Edinburgh, UK
- P05. What would Pickering think of protein-based emulsions?**
Marion Rouillet, University of Edinburgh, UK
- P06. Chocolate rheology and taste - role of surfactants**
Iva Manasi, University of Edinburgh, UK
- P07. Modelling the unbinding of membranes tethered randomly to a network substrate**
Sthembiso Gumede, Stellenbosch University, South Africa
- P08. Collective dynamics of bundles filaments in the contractile ring**
Stanard Mebwe Pachong, Stellenbosch University, South Africa
- P09. A microtubule dynamics and signaling feedback-loop induced cell self-polarization**
Yao Li, FOM Institute AMOLF, The Netherlands
- P10. Hard-sphere binary crystals**
Beatriz Iozzin Rios de Anda, University of Bristol, UK
- P11. Crystallisation in a modified Kob-Andersen glassformer**
Peter Crowther, University of Bristol, UK
- P12. The self assembly of amphiphilic peptide I₃K**
Henry Cox, University of Manchester, UK
- P13. Three-phase flow and fracturing of deformable granular media**
Deren Ozturk, Swansea University, UK
- P14. Emulsion generation and interdroplet force characterization**
Jun Dong, University of Bristol, UK



**Advanced School in Soft Condensed Matter
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- P15. Lattice Boltzmann simulation for lubricant impregnated surfaces**
Muhammad Subkhi Sadullah, University of Durham, UK
- P16. Phase behavior of two-dimensional colloidal fluids exhibiting pattern formation**
Blesson Chacko, Loughborough University, UK
- P17. Investigating the discrepancy between simulated and experimental hard sphere crystallisation rates**
Nicholas Wood, University of Bristol, UK
- P18. Phase inversion of Pickering emulsions**
Laura Sawiak, University of Edinburgh, UK
- P19. Designing peptide-based biomaterials: structure and related properties**
Maddalena Daniele, University of L'Aquila, Italy / La Sapienza University of Rome, Italy
- P20. "Self-shaping" drops**
Diana Cholakova, Sofia University, Bulgaria
- P21. Avalanche mediated devitrification in pseudo hard-sphere glasses**
Pablo Rosales, Universidad Complutense de Madrid, Spain
- P22. Colloids as an experimental model for proteins at liquid-liquid interfaces**
Rudi Mears, University of Edinburgh, UK
- P23. "Self-shaping" multi-component drops**
Zhulieta Valkova, Sofia University, Bulgaria
- P24. Recovering energetic landscapes in the presence of motion blur**
Michal Bogdan, University of Cambridge, UK
- P25. A phenomenological model for dense, non-Brownian suspension microstructure**
Rahul Chacko, Durham University, UK
- P26. The ice-water interface in the vicinity of a wall**
Siyu Chen, University of Oxford, UK
- P27. Driven colloidal spheres and rods in optical landscapes**
Josh Abbott, University of Oxford, UK
- P28. Microscopic study of the isotropic-nematic interface of a colloidal liquid crystal**
Louis Cortes, University of Oxford, UK



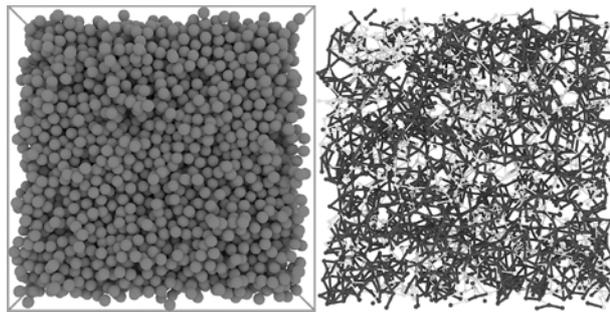
Poster abstracts

P01. Vitrification of colloids as a connectivity transition

R Higler¹, J Krausser², J van der Gucht¹, A Zaccone² and J Sprakel¹

¹Wageningen University, The Netherlands, ²University of Cambridge, UK

Both structural and dynamic precursors to the glass transition have been identified in recent years. Yet, establishing the relationship between liquid structure and its slowing down remains challenging. A resolution to this long-standing issue was recently proposed, by extending the elastic theory of the glass transition^[1] with the microscopic connectivity theory of disordered networks^[2]. While appealing, it remains to be proven directly in experiments. Here we study the glass transition of charged colloids using three-dimensional microscopy. We first quantify the liquid structure by determining the number of rigidly-bonded neighbours; establishing the validity of the network theory and the existence of an isostatic point. From this we reformulate the theory of Dyre to predict, without adjustable parameters, the growth of structural relaxation time from directly-measurable structural properties alone. We find an excellent quantitative agreement between this parameter-free microscopic theory and the experimental data. These results demonstrate a system in which vitrification can be described microscopically and quantitatively as a connectivity transition.



- [1] Dyre, J. C., Christensen, T. & Olsen, N. B. Elastic models for the non-arrhenius viscosity of glass-forming liquids. *Journal of Non-Crystalline Solids* 352, 4635 - 4642 (2006).
- [2] Krausser, J., Samwer, K. H. & Zaccone, A. Interatomic repulsion softness directly controls the fragility of supercooled metallic melts. *Proceedings of the National Academy of Sciences* 112, 13762-13767 (2015).

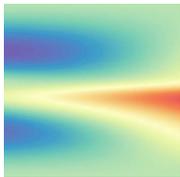
P02. Encapsulation and release using ethyl cellulose microcapsules

J Otero Marquez, A Pawsey and P Clegg

University of Edinburgh, UK

Ethyl cellulose microcapsules have been prepared and their encapsulation efficiency (%EE) and release profile (RP) studied. These can be used for weight management, as an alternative to gel capsules as they increase satiety after eating. In this experiment, only food approved ingredients via double emulsification have been used.

Capsules have been made with water-in-oil-in-water emulsions, using ethyl cellulose, ethanol and the following surfactants: Tween60, Span80 and PGPR. The performance is being corroborated using Red Nile as a dye for



confocal microscopy. Sodium acetate has been encapsulated, and its %EE and RP are being measured using Nuclear Magnetic Resonance Spectroscopy (NMRS).

Initial results suggest that this is a straightforward and valid way to create edible microcapsules for controlled release, and that NMR is a fast and simple method to determine the acetate release behaviour.

P03. Small angle scattering of soft matter assemblies: A need-case for coarse-graining

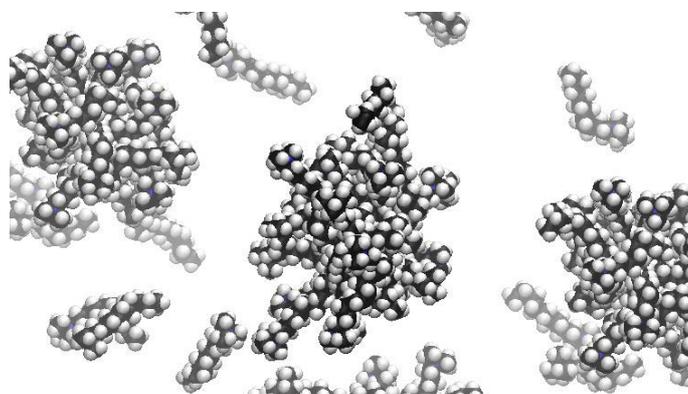
A R McCluskey¹, J Grant¹, D T Bowron², S C Parker¹ and K J Edler¹

¹University of Bath, UK, ²STFC-ISIS Neutron Scattering Facility, UK

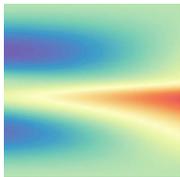
One of the most powerful techniques for the structural examination of micellar species is neutron and X-ray scattering. This work aims to improve both the efficiency and efficacy of experimental analysis, by improving the computational methodologies associated with soft matter modelling, in particular the coarse graining of self-assembly processes.

For the generation of a scattering profile, it is necessary to have an all-atom model of a self-assembled surfactant micelle, itself a non-trivial computational task due to the large system size. Herein, we have simulated the self-assembly of a single decyltrimethylammonium bromide (CTAB) micelle (see image). The simulated scattering pattern from this micelle was compared to experimental neutron scattering data obtained at the ISIS neutron source, to determine the accuracy of the computational modelling. The comparisons allow us to improve our understanding of the requirements for a computational protocol to utilise sophisticated computational modelling for the elucidation scattering patterns of self-assembled species. In particular the necessity of modelling larger systems with many more micelles is the need to obtain the necessary structure factors to generate the low- Q region of the scattering profile, as the structure factor is dependent on the interactions between different micelles.

In order to obtain systems large enough to give micelle-micelle interactions with long-enough time-scales to allow the surfactants to self-assemble "naturally", it is necessary to apply coarse-graining to the system. In addition to applying a bead-based coarse graining, we are deriving parameters to allow us to use the statistical approach, previously applied to study indented colloid systems^[1]. In this case each surfactant molecule is treated as a "*director*" with interactions accounted for by an effective potential. This approach will allow for a significant decrease in simulation time for many micelles forming; the all-atom surfactants can be mapped onto the *directors* and the scattering pattern can be generated.



[1] D.J. Ashton, R. L. Jack, and N. B. Wilding. Porous liquid phases for indented colloids with depletion interactions. Phys. Rev. Let., 114, 237801 (2015).



P04. Squeezing an emulsion with two continuous phases: centrifugal compression of the bijel

K A Rumble, J H J Thijssen, A B Schofield and P S Clegg

University of Edinburgh, UK

Bicontinuous interfacially jammed emulsion gels (bijels) are a class of soft material where two partially miscible liquids are quenched into the demixed region and phase separate via spinodal decomposition. This results in a short-lived bicontinuous structure; the interface can then be stabilised by solid particles which jam causing a long-lived stable structure to be formed^[1]. We have investigated the mechanical response of bijels using centrifugal compression (as for droplets in ^[2]). Macroscopically, we find that the bijel yields at relatively low angular acceleration and both continuous phases escape from the top of the structure rendering any compression irreversible. Microscopically, the bijel becomes anisotropic with the domains aligned perpendicular to the compression direction which inhibits further liquid expulsion; this is in complete contrast to the sedimentation behaviour of colloidal gels. The original structure can, however, be preserved close to the top of the sample and thus the change from bicontinuous to anisotropic suggests structural yielding. Any air bubbles trapped in the bijel are found to aid compression by forming channels aligned parallel to the compression direction which provide a route for liquid to escape. The expulsion of liquids appears to have a key role in the compression of the bijel.

- [1] E. M. Herzig, K. A. White, A. B. Schofield, W. C. K. Poon, P. S. Clegg, *Nature Materials*, 6, 966-971 (2007).
- [2] L. Maurice, R. A. Maguire, A. B. Schofield, M. E. Cates, P. S. Clegg, J. H. J. Thijssen, *Soft Matter*, 9, 7757-7765 (2013).

P05. What would Pickering think of protein-based emulsions?

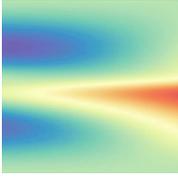
M Rouillet^{1,2}, W J Frith¹ and P Clegg²

¹Unilever, UK, ²University of Edinburgh, UK

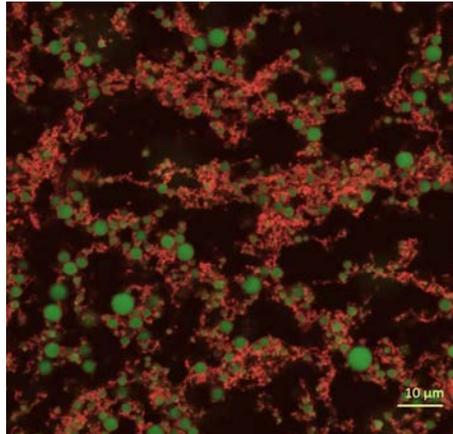
Water-soluble proteins are macromolecules that derive their usefulness in food applications from their ability to stabilise emulsions, as their flexible backbones carry both hydrophilic and hydrophobic residues and thus enable a strong adsorption at oil/water interfaces, and a good stabilisation of droplets by steric and electrostatic repulsion. They can also form gels, either of protein molecules or protein covered droplets. This double functionality is also shared by particles, which are used as stabilisers in Pickering emulsions and form colloidal gels, but is far less common in small molecule surfactants.

The similarities between particles and proteins leads us to ask how close is the behaviour of these two systems. The aim here is to examine analogous protein and particle gels and emulsions to probe the extent of this likeness in behaviour and to better understand the nature of both systems. Initial work is focused on the development of a suitable model protein system that forms both emulsions and gels.

Sodium caseinate, a milk protein with a singular molten globule state, is part of the ingredients of many commercial food emulsions, e.g. ice cream. An acidification of the solvent will cause the decrease of electrostatic repulsion and, under suitable conditions of concentration and time, the gelation of the protein in solution. Similarly the progressive decrease in pH of a caseinate stabilised emulsion will lead to an emulsion gel. Both can be seen as sticky spheres systems, although the micelle-like aggregate of caseinate and the coated oil droplets are different in size and composition.



A first step is to compare the gelation of caseinate when in solution and when coating oil droplets, using rheological measurements and confocal microscopy. Preliminary experiments showed that the moduli of the caseinate-coated oil droplets gel are considerably higher than those obtained for caseinate suspension gels, even if the droplet size was around 150 nm, very similar to the size of micelle-like aggregates of caseinate in water. The influence of the droplet size is soon to be explored.



Aggregated particle gel made of sodium caseinate coated emulsion droplets observed under confocal microscopy. Nile Blue is used to stain proteins (in red) and oil droplets (in green).

P06. Chocolate rheology and taste - role of surfactants

I Manasi and S Titmuss

University of Edinburgh, UK

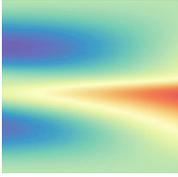
The aim of this work is to study the observed co-operative effect that lecithin, which is predominantly C16:0-C18:1 phospholipid, and polyglycerol polyricinoleate (PGPR), a comb copolymer comprising a backbone of polyglycerol with polyester side chains, has on the rheology of molten chocolate. Chocolate is a complex suspension of solid particles (sucrose, milk solids and cocoa) in a continuous fat phase stabilised by surfactants. In this work, we are attempting to understand the role played by the Lecithin and PGPR in stabilising the sucrose/oil mixture (model chocolate) and modifying its rheology by determining the structures formed by them at the interface using Tensiometry, QCM-D, neutron scattering and reflectivity. By understanding the polymer physics that controls the rheology, alternatives to the current additives can be proposed, leading to healthier chocolate and lower energy costs in processing.

P07. Modelling the unbinding of membranes tethered randomly to a network substrate

S R Gumede and K K Müller-Nedebock

Stellenbosch University, South Africa

In erythrocytes the plasma membrane is coupled to the underlying spectrin network. We develop a model to treat the detachment of a membrane from such a substrate, which might be a model for structural failure of the red blood cell. We consider a flexible membrane elastically linked at random points to a substrate. This quenched randomness requires the use of the replica formalism, which we investigate from both replica symmetric and weakly



broken replica symmetry perspectives. Criteria for detachment under an applied pressure differential across the membrane are derived. We also sketch how a more detailed spectrin network can be included in this model.

P08. Collective dynamics of bundles filaments in the contractile ring

S Mebwe Pachong and K K Müller-Nedebock

Stellenbosch University, South Africa

During cell division, the equatorially located contractile ring leads to the physical division of the cell by eventually pinching off the membrane. The main components of the ring are the filaments arranged as a bundle network into a hoop-like structure and the motor protein myosin II used as cross-linker agent. The behaviour of this actomyosin network has been shown^[1] to significantly affect the physical division of the cell. However, for the contractile ring, the precise mode of how is achieved is still not well understood. Models suggest that the force generated by the motor protein is achieved by mutual concert between the filaments and the motor protein. We develop a minimal model suggesting how the contractile behaviour occurs inside the ring. The idea used has been borrowed from "the sliding filaments theory" first established by Huxley et al. (1953) for muscle contraction. The analytical model developed here, predicts that the "*pushing / pulling*" behaviour of the chains leads to the "*repulsion / contraction*" behaviour of the bundle network. We show that the orientations of the overlapping filaments to each other are very crucial at initial condition to determine whether the ring (system) will experience contraction or not. The analytical theory of the model predicts that the active force due to the activity of the myosin motor cannot be the only force that maintains the integrity of the ring. We therefore think of two forces influencing the ring contraction: The networking and the active forces, both of which can be provided solely by myosin cross-linkers. The analytical model is complemented with molecular dynamics simulation. Both calculations clearly show and distinguish the *clumping* (explaining the contraction of the ring) and the *overtaking* (when the filaments pass each other) that the filaments experience inside the bundle network. Using the Random Phase Approximation via the Martin-Siggia-Rose formalism we have been able to study the stability of the contractile system by making use of collective variables of the filaments^[2,3 4,5].

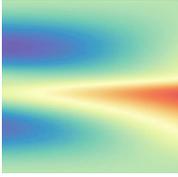
- [1] M. Lenz et al. "Contractile units in disordered actomyosin bundles arise from F-Actin buckling", Phys. Rev. Lett. 108, 238107 (2012).
- [2] R. V. Jensen "Functional Integral Approach to Classical Statistical Dynamics", J. Stat. Phys. 25, (1981).
- [3] G. H. Fredrickson and E. Helfand "Collective dynamics of polymer solution", J.Chem.Phys. 93, (1990).
- [4] K. K. Müller-Nedebock and T. A. Vilgis, "Collective dynamics of random polyampholytes", J.Chem. Phys. 110, 4651 (1999).
- [5] K. K. Müller-Nedebock and T. A. Vilgis, "Dynamics of condensed polyelectrolyte solutions", Macromol. 31, 5898-5903 (1998).

P09. A microtubule dynamics and signaling feedback-loop induced cell self-polarization

Y Li and P R ten Wolde

FOM Institute AMOLF, The Netherlands

The importance of the intricate interplay between membrane pattern formation and transport along cytoskeletal filaments is now increasingly being recognized. Yet, our understanding of these processes is still highly limited, largely because of the complexity of a living cell. Here, first, we propose a bottom-up minimal model combines protein signalling and protein shuttling inside a vesicle, establishing a feedback-loop through signalling protein transports, activations and microtubule dynamics, namely Pak-stathmin-microtubule loops. We then present a novel



particle-based simulation tool developed by us, which can efficiently treat the coupling between protein reaction-diffusion and dynamics of filaments. By systematic investigation of this minimal representation of a cell *in silico*, a self-polarized state with one protein cluster is found, and rich variety of protein pattern and microtubules structures emerge by tuning the signalling magnitude, microtubule density and instability. These theoretical results illustrate how feedback interplay between microtubule dynamics and signalling protein in cell could break symmetry and further direct future experiments in our collaboration group.

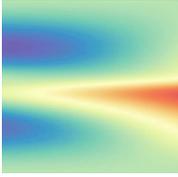
P10. Hard-sphere binary crystals

B I Rios de Anda¹, F Turci¹, R Sear² and C P Royall¹

¹University of Bristol, UK, ²University of Surrey, UK

Crystals made of binary mixtures have potential applications in photonics, optics and structure design, and are ideal models to study the kinetic mechanisms of salt formation^[1,2,3,4]. With the interest of studying the crystal evolution and structure at the particle resolved level, we aim to track the nucleation and crystallisation processes of a mixture of sterically-stabilised fluorescently-labelled poly(methyl methacrylate) (PMMA) particles with a size ratio of 0.39. Dry particles were suspended separately in a saturated saline solution in a solvent mixture matching the particles' density and refracting index. This was done so to prevent sedimentation and to allow hardsphere-like behaviour^[2]. These particles were mixed together at different volume fractions, confined to flat rectangular glass capillaries, then studied by confocal laser scanning microscopy. It was observed that an equal number density and volume fractions above 0.52 yielded crystals through heterogeneous nucleation, whose crystallisation rate decreased as the volume fraction increased. Further particle tracking allowed crystal structure analysis^[4,5]. This showed that the crystals were a mixture of fcc and hcp lattices for the big particles, while the small ones occupied the octahedral holes of the lattice. Such structures correspond to NaCl and NiAs configurations, respectively. The resolved structural analysis carried out in this study has enabled us to confirm previous hypotheses concerning the crystal structure of a related system with the same size ratio^[6]. However, the structures are not perfect: voids between the big particles can be observed throughout all the samples. This phenomenon has already been reported for related systems and was attributed to impurities, polydispersity, and differences in sedimentation rates. This resulted in fluctuations in the size and particle number density ratios, which in turn prevented perfect crystal formation^[2]. We aim to apply the same structural analysis for homogeneous crystallisation, which will be possible by sintering the capillaries.

- [1] P. Bartlett, R.H. Ottewill, P.N.Pusey, Phys Rev Lett, 68: 3801 (1992)
- [2] Esther Vermolen. Manipulation of Colloidal Crystallization. PhD thesis, Utrecht University, 2008.
- [3] K.P. Velikov, C.G. Christova, R.P.A. Dullens and A. van Blaaderen. Layer-by-layer growth of binary colloidal crystals. Science, 26 (2002)
- [4] Alexei Ivlev, Hartmut Löwen, Gregor Morfill, and C. Patrick Royall. Complex Plasmas and Colloidal Dispersions: Particle-resolved Studies of Classical Liquids and Solids. World Scientific Co., Singapore Scientific, 2012.
- [5] Taffs J, Williams SW, Tanaka H and Royall CP, "Structure and kinetics in the freezing of nearly hard spheres", Soft Matter, 9, 297 - 305 (2013)
- [6] N. Hunt, R. Jardine and P. Bartlett. Superlattice formation in mixtures of hard-sphere colloids. Physical Review E, 62:1 (2000)



P11. Crystallisation in a modified Kob-Andersen glassformer

P Crowther, F Turci and C P Royall

University of Bristol, UK

Geometric frustration is an approach to the glass transition which proposes that glassiness is caused by a locally favoured structure (LFS) that does not tessellate in Euclidean space. In order to transition between a LFS-rich glassy state and a crystalline one, a large amount of particle rearrangement would be required. This results in a high energy barrier between the metastable glassy state and the thermodynamically favoured one. The Kob-Andersen (KA) binary mixture, a common model glassformer, is a special case however. The locally favoured structure is the KA mixture is a bicapped square antiprism ^[1] which does geometrically tessellate in Euclidean space to form the Al_2Cu crystal ^[2].

The KA binary mixture is a model glass former which is homologous to $\text{Ni}_{20}\text{P}_{80}$, a metallic glass. It is composed of 80% large and 20% small particles that interact with non-additive Lennard-Jones potentials ^[4]. We are able to identify local structures, in molecular dynamics simulations of the KA mixture using the Topological Cluster Classification (TCC) algorithm. The TCC algorithm uses a neighbour network to hierarchically identify local structures of up to 13 particles and is explained in detail elsewhere ^[3]. Using the TCC we identified that the LFS for KA has 3 common compositions, each consisting of different proportions of the binary particles, as shown in Fig. 1. Only the A_8B_3 form of the LFS is, a priori, able to tessellate to form the Al_2Cu crystal. However, even though energy minimisation of the structure shows it to be the lowest energy of the three, the A_8B_3 is the least common form of the LFS in a normal KA mixture at 3%. From this result, we propose that the nature of the frustration in the KA mixture is compositional rather than geometric.

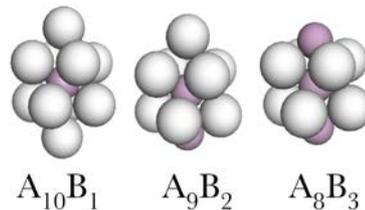


FIG. 1. The three common configurations of the LFS in a KA liquid. Only the A_8B_3 form tessellates

In order to favour the formation of the A_8B_3 form of the LFS and encourage the growth of an Al_2Cu structure, we modified the ratio of large to small particles in the KA mixture from the standard 4:1 to 3:1 and 2:1. This does serve to increase the relative fraction of A_8B_3 LFS in the mixture though the overall amount remains low at 7% and 25% of the total LFS for the 3:1 and 2:1 systems respectively.

We then conducted molecular dynamics simulations using a 2:1 KA liquid and a Al_2Cu crystal seed at a number of different temperatures. Using a distance based clustering method we were able to identify the LFS clusters which were members of the Al_2Cu crystal and so track the growth of the crystal over time as shown in Fig. 2. For an NPT simulation of 19236 KA liquid particles surrounding a 1500 particle Al_2Cu crystal seed at $P = 0$, the melting temperature is found to be $0.447(2)$ ^[5].

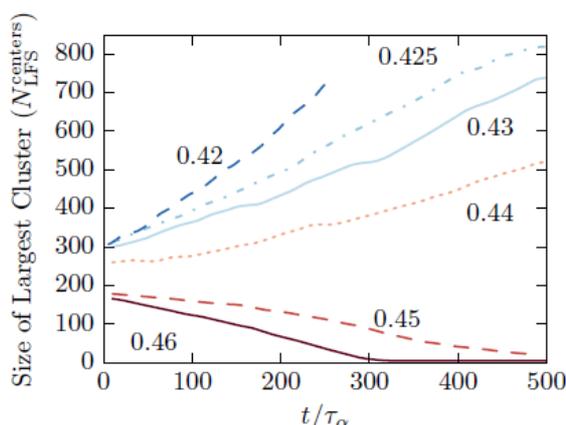
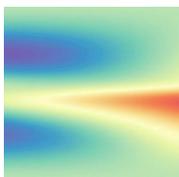


FIG. 2. Graph showing growth of the largest cluster of LFS in a molecular dynamics simulation as a function of the relaxation time of the equivalent KA liquid at 6 different temperatures.

This work was carried out using the computational facilities of the Advanced Computing Research Centre, University of Bristol.

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P12. The self assembly of amphiphilic peptide I₃K

H Cox, T Waigh and J Lu

University of Manchester, UK

I₃K is a small amphiphilic peptide whose self-assembly we hope to understand through experimental observations such as micro-rheology. I₃K contains a hydrophobic tail of three isoleucine residues and a positively charged lysine head, which is hydrophilic. Initial studies^{[1], [2]} have shown I₃K forms twisted nanotubes when immersed in water which can go on to form a physically crosslinked hydrogel. Hydrogels are a subject of ongoing research for therapeutic applications such as drug delivery^[3] and tissue engineering^[4]. Through the understanding of the self-assembly and gelation of I₃K we hope to help improve the design and scope of synthetic peptides for therapeutic use. Passive particle tracking micro-rheology is used to determine the properties of I₃K solutions and gels. Due to the very low forces involved, physical disturbance of the peptide is minimised and preliminary results suggest that a phase change occurs between 1 mM and 10 mM concentrations in pure water as shown in Figure 1. Moreover, we see evidence of pH mediated sol/gel phase transitions between pH 3 and 9.

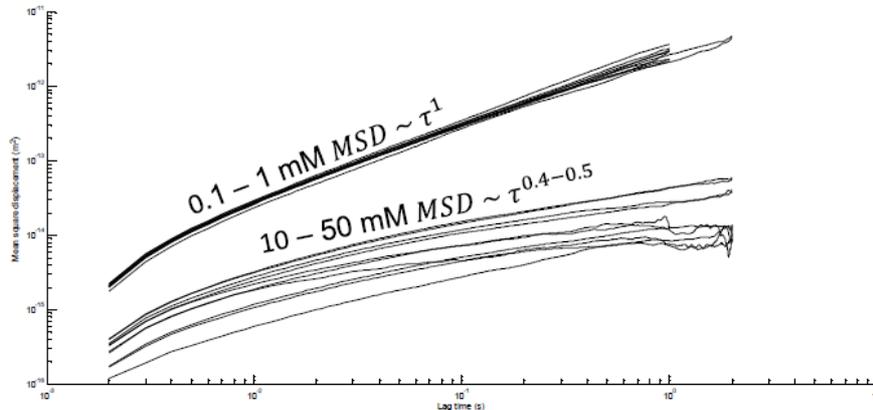
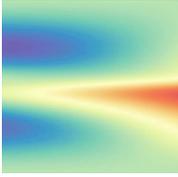


Figure 1 showing the mean square displacement (MSD) against lag time (τ) for concentrations 0.1 – 1 mM which are characteristic of a Newton fluid and 10 – 50 mM characteristic of a viscoelastic material.

- [1] H. Xu, Y. Wang, X. Ge, S. Han, S. Wang, P. Zhou, H. Shan, X. Zhao, and J. R. Lu, "Twisted nanotubes formed from ultrashort amphiphilic peptide I3K and their templating for the fabrication of silica nanotubes," *Chem. Mater.*, vol. 22, no. d, pp. 5165–5173, 2010.
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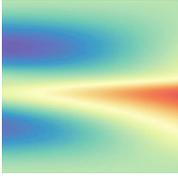
P13. Three-phase flow and fracturing of deformable granular media

D Ozturk¹, J M Campbell² and B Sandnes¹

¹Swansea University, UK, ²University of Leeds, UK

The invasion of gas via fractures into a water-saturated porous medium is a process that occurs in numerous geo-engineering and natural circumstances: fracturing for enhanced contaminant remediation, stimulation of hydrocarbon reservoirs, fracturing of soft tissue in arterial walls, soil drying and outgassing of crystal rich magmas for example. However, it is challenging to typify and predict complex flows through deformable fractured media. This is particularly true for multiphase flows in which the fluid dynamics are governed by interactions between gas, liquid, and granular phases.

We create a simple model system to illuminate these processes. A wet unconsolidated granular packing confined in a Hele-Shaw cell is subject to a slow invasion of gas, causing fractures. We study the influence of granular properties (size/shape), and gas injection rate on the system, as well as the layering of different granular material. We image the complete fracture pattern as it forms, allowing us to investigate the dynamics of its growth and the properties of the resulting pattern (fracture density, branching frequency etc.).



Fractures are triggered by initial pore invasion followed by fluidization of the compaction front and they grow in an intermittent, stick slip manner, interspersed with inactive periods. Growth is impeded by friction from local compaction fronts that form around the growing fracture branches. We describe a simple analytical model that predicts the fracture density from basic granular medium properties, and also demonstrate a transition from fracturing to capillary fingering in the presence of less permeable layers.

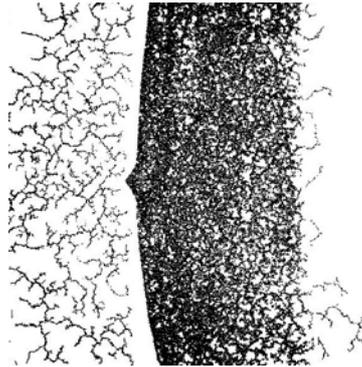


Fig. 1: Gas fractures and capillary fingering in wet granular packing of different grain sizes.

P14. Emulsion generation and interdroplet force characterisation

J Dong¹, M A Faers² and C P Royall¹

¹University of Bristol, UK, ²Bayer CropScience, Germany

In the study of the mechanical properties of gels, understanding the force chains represents a key aspect, which has been extensively investigated in granular materials^[1]. To study the force chains within gels which have been prepared by the mixture of emulsions and non-absorbing polymers, we first analysed the interdroplet forces of emulsions^[2]. Two methods, microfluidic devices and a homogeniser, were used to prepare the oil-in-water emulsions. Norland optical adhesive (NOA81) microfluidic devices were employed to generate monodisperse emulsions with diameter of a few micron whereas emulsions, which were efficiently prepared by the homogeniser, shown higher polydispersity. By applying fluorescence technique, emulsions with fluorescent dye can be characterised under confocal microscopy. In the confocal images (Fig. 1), compared with the brightness of emulsion droplets, brighter areas were observed at the contact parts where droplets are pressing each other^[3]. The contact areas were then extrapolated by adjusting the brightness threshold of the images in order to calculate the interdroplet forces using the force model^[4].

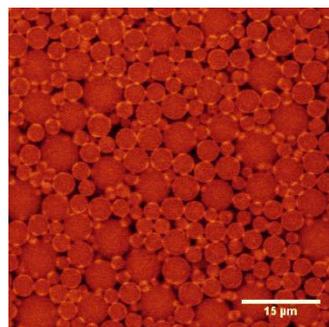
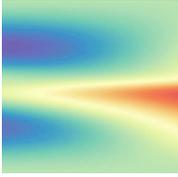


Figure 1. A confocal image of the oil-in-water emulsion where interdroplet contacts show higher brightness.



- [1] Majmudar, T. S. & Behringer, R. P. Contact force measurements and stress-induced anisotropy in granular materials. *Nature* 435, 1079–1082 (2005).
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P15. Lattice Boltzmann simulation for lubricant impregnated surfaces

M S Sadullah¹, C Semprebon² and H Kusumaatmaja¹

¹University of Durham, UK, ²University of Edinburgh, UK

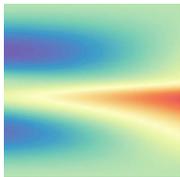
Lubricant Impregnated Surfaces (LIS) are liquid repellent surfaces made of porous surfaces infused with lubricant. Compared to superhydrophobic surfaces, LIS have been demonstrated to have superior range of liquid repellency as well as better robustness. Given such advantages, LIS have many promising applications varying from foods and beverages packaging to energy harvesting systems. Investigating such system empirically is demanding as it is subject to surface texturing, surface energy manipulation, and the availability of the lubricant. To complement experiments, a powerful numerical approach is therefore needed. In this contribution we present a ternary free energy lattice-Boltzmann model suitable for simulating such system. The distinctive feature of this free energy model is that we are able to predict analytically and capture the relevant physical parameters such as contact angles, liquid-liquid and solid-liquid interfacial tensions. The model is exploited to reconstruct possible wetting states in LIS system and then to study the dynamic of LIS for each wetting state. We then discuss how the mobility of water droplets on LIS may depend on the wetting states and the physical parameters of the system.

P16. Two-dimensional colloidal fluids exhibiting pattern formation

B Chacko, C Chalmers and A J Archer

Loughborough University, UK

Fluids with competing short range attraction and long range repulsive interactions between the particles can exhibit a variety of microphase separated structures. We develop a lattice-gas (generalised Ising) model and analyse the phase diagram using Monte Carlo computer simulations and also with density functional theory (DFT). The DFT predictions for the structures formed are in good agreement with the results from the simulations, which occur in the portion of the phase diagram where the theory predicts the uniform fluid to be linearly unstable. However, the meanfield DFT does not correctly describe the transitions between the different morphologies, which the simulations show to be analogous to micelle formation. We determine how the heat capacity varies as the model parameters are changed. There are peaks in the heat capacity at state points where the morphology changes occur. We also map the lattice model onto a continuum DFT that facilitates a simplification of the stability analysis of the uniform fluid.



P17. Investigating the discrepancy between simulated and experimental hard sphere crystallisation rates

N Wood, P Royall and J Hallett

University of Bristol, UK

Colloidal dispersions provide a valuable model system for investigating the phase behaviour of atomic and molecular systems. The simple model of hard spheres - particles which do not interact at range but are prohibited from overlapping - has been realised in colloidal models^[1]. This includes a rich phase behaviour, moving from fluid to crystal to glass phases as the control parameter, volume fraction, is increased. Despite the simple, one parameter phase behaviour, the experimental hard sphere systems do not agree with simulation, with discrepancies in crystallisation rates at low volume fraction of many orders of magnitude^[2,3]. It is possible that this discrepancy is due to the role of the slow sedimentation in experiments, which may introduce hydrodynamic fluctuations that are not accounted for in simulation. By performing experiments with controlled sedimentation, we examine the structural difference between sedimenting and non sedimenting fluids, aiming to explore how this affects the energy barrier to nucleation.

- [1] Palberg, J Phys Condens Matter. 26, 333131, (2014)
- [2] Auer, Frenkel Nature 409, 1023 (2001)
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P18. Phase inversion of Pickering emulsions

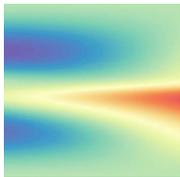
L Sawiak and P Clegg

University of Edinburgh, UK

Oil and water can be mixed and stabilised using solid particles to form a Pickering emulsion. The particles reduce the surface energy of the interface by reducing the interfacial area. Whether oil or water becomes the dispersed phase is thought to be determined by the wetting characteristics of the particles. When the particle preferentially wets a medium, it sticks further out into it, making it more likely to be the continuous phase. Experimentally, this can be measured using the contact angle of the particles at the oil-water interface, taken through the water phase. The emulsion is unstable far from 90°. Slightly below 90°, an oil in water (o/w) emulsion is expected, and above it a water in oil emulsion (w/o).

However, it has been observed for some particles with intermediate wettability that as the particle concentration is increased while the relative amount of water to oil is maintained that catastrophic inversion can occur. Where the emulsion was o/w, it is now w/o.

This work looks to understand the underlying mechanism through studies of the morphology of the stabilising particles, and any structures they may form between particles or droplets. Confocal microscopy will be the main technique used. The particles used are hydrophobic silica, with varying numbers of silanol groups to study the effects of hydrophobicity.



P19. Designing peptide-based biomaterials: structure and related properties

M Daniele^{1,3}, S Sennato², L Chronopoulou¹, F Domenici¹, C Palocci¹, S Lupi¹ and F Bordi¹

¹La Sapienza University of Rome, Italy, ²CNR-ISC Institute for Complex Systems, Italy, ³University of L'Aquila, Italy

Recently, scientific as well as technological interest in the synthesis of novel peptide-based hydrogel materials have grown dramatically. Applications of such materials mostly concern the biomedical field with examples covering diverse sectors such as drug delivery, tissue engineering and production of scaffolds for cell growth, thanks to their biocompatibility and biodegradability^[1].

In this framework, we have explored the phase diagram of molecular gels produced from a solution of the aromatic polypeptide derivative fluorenyl-methoxycarbonyl(poly)phenylalanine (Fmoc-polyPhe)^[2]. Our experiments indicate the importance of phenylalanine in the gel formation, suggesting that different combinations of Fmoc-polyPhe promote the formation of gels with different strength and fluidity. Furthermore, we have characterized the kinetic of gelation demonstrating its reversibility. By combining Dynamic Light Scattering and Fourier Transform Infrared Spectroscopy techniques we have revealed that the gel structural details strongly depends on temperature suggesting a specific mechanisms of formation. The complex self-assembled networks formed by nanofibers has been investigated by Atomic Force Microscopy investigation on hydrogels deposited on mica, and the structural details of the nanofibers have been determined.

This information can be used for a rational optimization of the design and of the applications of novel hydrogels.

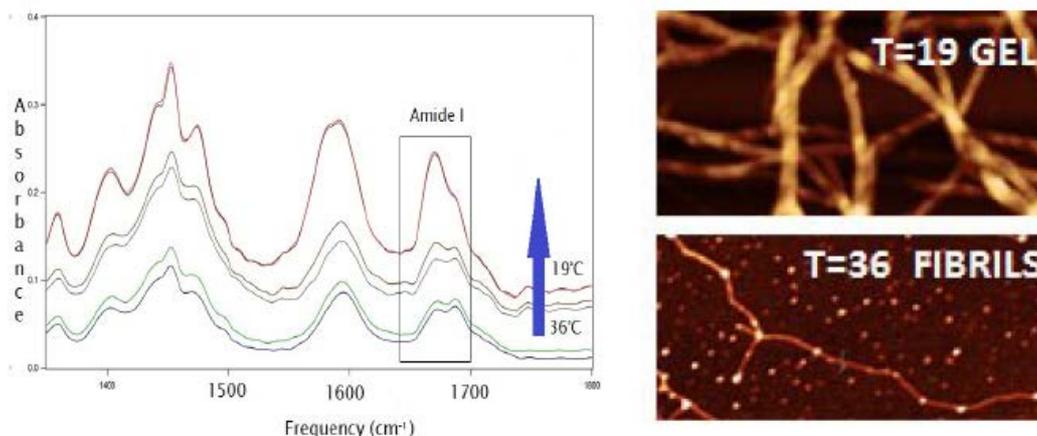


Figure 1. Fourier transform infrared spectroscopy and atomic force microscopy investigation on hydrogel to different temperature

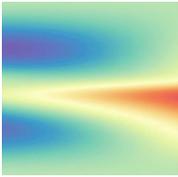
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P20. "Self-shaping" drops

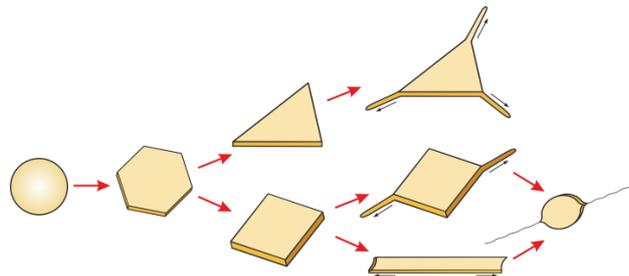
D Cholakova¹, N Denkov¹, S Tcholakova¹, I Lesov¹ and S Smoukov²

¹Sofia University, Bulgaria, ²University of Cambridge, UK

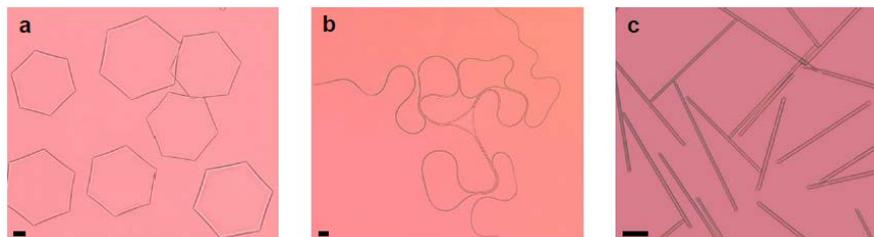
Linear hydrocarbons are known to pass through a series of stable and metastable rotator phases before freezing. In our recent studies^[1,2] we showed that, by using appropriate cooling protocols, we can harness these phase transitions to control the deformation of liquid hydrocarbon droplets and then freeze them into solid particles,



permanently preserving their shape. Upon cooling, the droplets spontaneously break their shape symmetry several times, morphing through a series of complex regular shapes owing to the internal phase-transition processes. In this way we produce particles including micrometre-sized polyhedra, various polygonal platelets and fibres of submicrometre diameter, which can be selectively frozen into the corresponding solid particles. The main factors which can be used to control the drop "self-shaping", before their freezing into solid particles, are the surfactant type and chain length, cooling rate, and initial drop size. As a rule, the smaller drops, stabilized by surfactants with longer chain-length, and subject to slower cooling, evolve easier to shapes with higher aspect ratio. The mechanism explaining all these transformations offers insights into achieving complex morphogenesis from a system with a minimal number of molecular components.



Schematic of the evolution process showing the main stages through which the drops pass upon cooling.



Deformed drops from hexadecane: (a) hexagons, Tween 60; (b) triangle, Brij 58; (c) rods, Tween 60. Scale bars, 20 μ m.

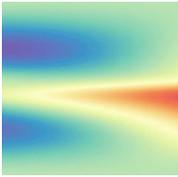
- [1] N. Denkov, S. Tcholakova, I. Lesov, D. Cholakova, S. K. Smoukov, „Self-shaping of oil droplets via the formation of intermediate rotator phases upon cooling“, *Nature* 2015, 528, 392-395.
- [2] D. Cholakova, N. Denkov, S. Tcholakova, I. Lesov, S. K. Smoukov “Control of drop shape transformations in cooled emulsions”, 2016, in preparation.

P21. Avalanche mediated devitrification in pseudo hard-sphere glasses

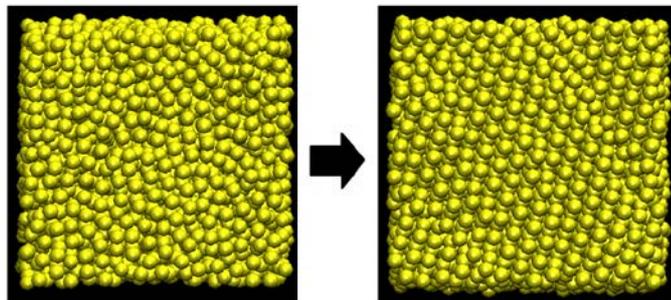
P Rosales, C Valeriani and E Sanz

Universidad Complutense de Madrid, Spain

By means of Molecular Dynamics we analyze several aspects of the avalanche-mediated devitrification mechanism recently reported^[1] for hard sphere (HS) glasses using a continuous version of the HS potential we refer to as pseudo-hard spheres (PHS)^[2]. We observe that the crystallization mechanism in HS and PHS is the same, although PHS glasses crystallize earlier for a given density because the development of avalanches is eased by the small degree of overlapping allowed in the PHS potential. Increasing the density retards crystallization due to a decrease of the avalanche emergence likelihood.



We also study the effect of both simulation ensemble and temperature coupling on the devitrification pathway. The observed avalanche mechanism and its density dependence do not substantially change with the employed ensemble (NVT vs NpT). Neither the use of a velocity-rescale thermostat (that changes the velocity moduli) nor that of a Langevin thermostat (that changes both moduli and directions) alter the main features of the avalanche-mediated devitrification mechanism. Finally, we analyze the coupling between momenta and configuration in the development of avalanches. While avalanches can be averted by changing the momenta distribution in configurations immediately prior to the avalanche, once the avalanche develops it cannot be stopped by momenta reassignment.



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- [2] J. Jover, A. J. Haslam, A. Galindo, G. Jackson, and E. A. Muller, "Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules," The Journal of Chemical Physics, vol. 137, no. 14, p. 144505, 2012.

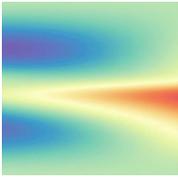
P22. Colloids as an experimental model for proteins at liquid-liquid interfaces

R Mears, J Thijssen and C MacPhee

University of Edinburgh, UK

Proteins stuck to liquid-liquid interfaces are ubiquitous: consider the liquid, membrane bounded world of cells where they perform structural, transportational and chemical functions, or the protein-stabilised emulsions of the food and cosmetics industries. Hence, understanding their behaviour is crucial to a range of interfacial systems such as the waterproof coat worn by filamentous fungi cells^[1,2].

There are a number of techniques available to investigate the interfacial rheological properties of protein layers adsorbed to liquid-liquid interfaces depending on whether shear or dilational rheology is being probed. However, models for the dynamics of these interfaces are scarce due to some difficulties such as inconsistent data across different experiments, the highly non-ideal equation of state (surface pressure is not proportional to surface concentration), the complexity of the protein intermolecular interactions and intramolecular rearrangement and the effect of irreversible adsorption^[3,4]. Instead we aim to use hard-sphere colloids – poly(methyl methacrylate) (PMMA) sterically stabilised by poly(12-hydroxystearic acid) (PHSA) – as an experimental model system to attribute certain protein properties to certain protein characteristics. The first step in this process is to use oscillating pendant drop tensiometry – where the shape of a hanging fluid drop tells us its surface tension and the changes under volume oscillation tell us about its viscoelasticity – to characterise the dilational rheology of a model particle laden liquid-liquid interface. We may then vary the properties of the particles to explore the effects of doing so.



Our first choice of independent variable is particle size: typical proteins (~5nm) are far smaller than typical colloids (~100nm). The preliminary results of this investigation indicate that interesting changes in behaviour exists over the 1000-200nm range of particle radii.

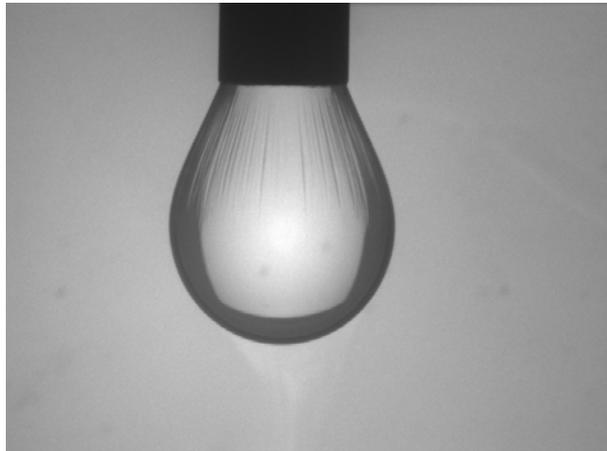


Figure 1: Wrinkling of a film of PHSA stabilised 264nm radius PMMA particles adsorbed to a water drop in dodecane

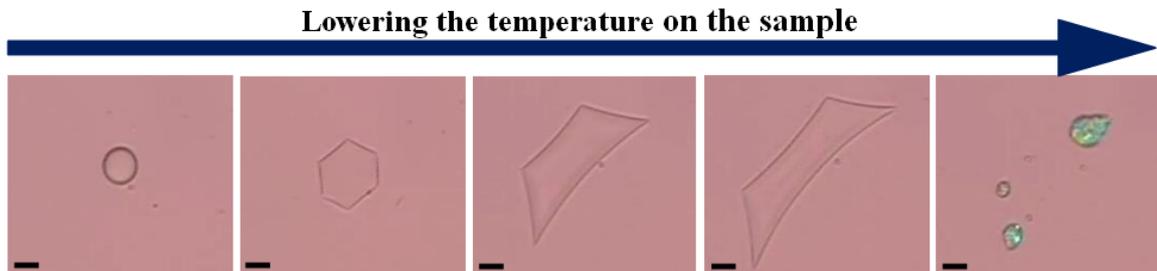
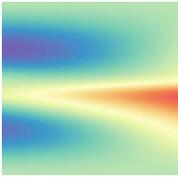
- [1] Linder, M. B., Szilvay, G. R., Nakari-Setälä, T., & Penttilä, M. E. (2005). Hydrophobins: the protein-amphiphiles of filamentous fungi. *FEMS microbiology reviews*, 29(5), 877-896.
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P23. "Self-shaping" multi-component drops

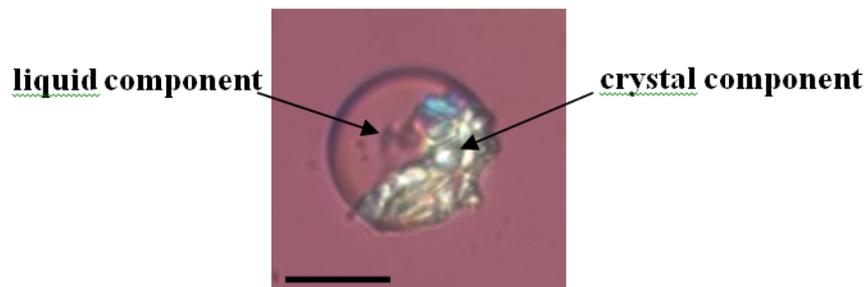
Z Valkova¹, D Cholakova¹, S Tcholakova¹, N Denkov¹ and S K Smoukov²

¹Sofia University, Bulgaria, ²University of Cambridge, UK

In our recent studies^[1,2] we showed that single alkane drops, stabilized with proper surfactant, can spontaneously break symmetry and transform into various shapes during cooling. However, most of the common substances used in the industry are not pure chemicals, but are mixtures of molecules. For example, mixtures of alkanes with lengths between 14 and 50 carbon atoms are used in cosmetics as "Vaseline". To check whether the "self-shaping" phenomena with drops, composed of alkane mixtures, follow the same trends as with drops of a single alkane, here we present a systematic study of emulsions made from alkane mixtures (alkanes are premixed to form homogeneous oily phase prior to emulsification). The observed trends can be summarized as follow: (1) The general drop-shape evolution for multi-component droplets during cooling is the same as with single-component drops; (2) Depending on the weight composition ratio and lengths of the mixed alkanes, conservation of the shape of the deformed drop may or may not be possible upon crystallization; (3) At high cooling rates, phase separation inside the drop interior can be observed; (4) Melting happens over a broad temperature range instead at a fixed temperature, allowing some transformations not only upon cooling (as observed until now) but during the heating process as well.



Microscope images showing multi-component drop evolution during cooling- the general drop shape evolution is the same, as with single alkane, but the final shape could not be preserved upon freezing. Scale bars, 20 μm .



Phase separation during moderate cooling, inside the drop volume due to different melting temperatures of the alkanes. Scale bar, 20 μm .

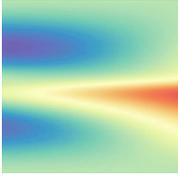
- [1] N. Denkov, S. Tcholakova, I. Lesov, D. Cholakova, S. K. Smoukov, „Self-shaping of oil droplets via the formation of intermediate rotator phases upon cooling“, *Nature* 2015, 528, 392-395.
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P24. Recovering energetic landscapes in the presence of motion blur

M Bogdan and T Savin

University of Cambridge, UK

We analytically show that finite exposure time during video camera measurements of positions of Brownian particles results in systematic errors of the measured probability distributions and mean squared displacements of these positions, systematically biasing, as a result, the indirectly measured energy landscapes the particles probe. We derive precise mathematical formulas for quantifying this bias and determining the relationship between the true potential and the naively measured apparent potential in one, two and three dimensions in two orders of approximation, and provide examples of specific applications for quadratic potentials, double wells, and DLVO potentials between moving particles. The predicted results of motion blur include measuring higher values of spring constants in optical traps than their true values and the appearance of non-existent local maxima and minima in DLVO potentials. We propose that manipulating shutter time could be used to evaluate local diffusion constants and energetic landscapes in complex cellular and biological environments. We verify the results with Brownian Dynamics simulations. We believe our work can explain discrepancies in reported experimental results.



P25. A phenomenological model for dense, non-Brownian suspension microstructure

R Chacko¹, R Mari², S Fielding¹ and M Cates²

¹Durham University, UK, ²University of Cambridge, UK

Dense suspensions, such as the Oobleck mixtures that are sometimes walked on at science outreach events, demonstrate surprisingly rich rheological behaviour. These systems still lack a constitutive model to describe their bulk rheology, even in the relatively simple case of a time-dependent shear flow. In this poster, we describe an approach, based on the work of Hand^[1], that allows one to derive a phenomenological nine-free-parameter model for the anisotropy of a high volume fraction, non-Brownian, density-matched, hard-particle suspension in a simple shear flow. This approach is valid in the zero Reynolds number limit with assumptions on the amount of system information contained in the anisotropy and on the size of the anisotropy. An extension to the model allowing one to relax the assumption on the latter is also discussed.

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P26. The ice-water interface in the vicinity of a wall

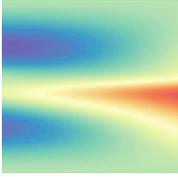
S Chen, J Schollick, R Dullens, R Style and D Aarts

University of Oxford, UK

When freezing the solvent of a colloidal suspension, the colloidal particles may either segregate from the solidifying solid or be captured in it, depending on the growth conditions. This is particularly important in fundamental research (the behaviour of bacteria or cells in cryopreservation¹), engineering (freeze-casting of porous ceramics²) and food industry (the trapping of fat by ice in ice-cream³). The shape of the ice-water interface near a wall has so far largely been ignored, but might play an important role in determining the behaviour of colloidal particles engulfed by the ice. In this project, we first focus on the ice-water meniscus for pure water (without colloidal particles).

We have derived a theory to predict the shape of the ice-water meniscus; surprisingly, this problem is analogous to that of a gas-liquid meniscus under gravity, with the temperature gradient playing the role of gravity. Then, to determine the exact three-dimensional shape of the ice-water interface under low temperature gradients, we use confocal laser scanning microscopy, together with a solidification cell with extremely accurate temperature gradients and separate control of temperature gradient and freezing velocity. This enables us to obtain the three dimensional profile of the ice-water interface under different conditions. The profile was then fitted with the mathematical model and we are currently interpreting the resulting typical length scales.

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P27. Driven colloidal spheres and rods in optical landscapes

J L Abbott, J Spiers, Y Gao, D Aarts and R P A Dullens

University of Oxford, UK

Optical trapping allows precise manipulation of particles on the colloidal scale, which can be used to probe both the static and dynamic behaviour of micron-sized objects. Here, we combine optical trapping with bright-field microscopy to explore the static behaviour of colloidal rods in optical traps. We compare this with the well-known behaviour of an optically trapped sphere. Next, we create an optical potential energy landscape using multiple optical traps and introduce motion by driving the sample precisely, and at known velocities, relative to the optical landscape. In particular, we analyse the particle dynamics both below and above the critical driving velocity that characterises the pinned-to-sliding state.

P28. Microscopic study of the isotropic-nematic interface of a colloidal liquid crystal

L Cortes, D Aarts and R Dullens

University of Oxford, UK

Since the seminal work of Onsager^[1] the bulk phase transition of colloidal rods has been studied in detail with joint contributions from experiments, simulations and theory; revealing the role of colloid's charge, flexibility and finite aspect ratio. The interface between coexisting isotropic and nematic phases has also received considerable theoretical and simulational attention; however, experimentally it has received less.

Here we study the interface of a phase separated colloidal dispersion of model silica rods, following the synthesis as described by Kuijk et al^[2]. This powerful method allows tuning the aspect ratio of the silica rods with accuracy, enabling quantitative confocal laser scanning microscopy. We use this system and technique to image the interface between the isotropic and nematic phases, and between the nematic and smectic phases. We measure the order parameter through the interface in the vicinity of a vertical hard wall with degenerate planar anchoring and focus on the capillary rise. Result are interpreted in light of emerging theories.

This project has received funding from the European Unions Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No 641839.

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