

Institute of Mathematics and Physics,  
Aberystwyth University,  
Seminar Programme,  
Spring 2012

February 8, 2012

- Tuesday 31st January, 2.10pm, Room 231 (SEL/RfkaD)
- Dr Paul Staniec  
Diamond Light Source
- Title: The GI-SAXS Upgrade at I22, Diamond and  
GI-WAXS studies of Organic Photovoltaic Films

Small angle scattering (SAXS) is a non-destructive technique that can be used to probe the internal structure of condensed matter systems at the micron and nanometre length scales. Specifically, it measures the size, shape and distribution of inhomogeneities in the materials electron distribution.

In transmission mode, it is commonly used to measure particles, proteins, polymer chains or lamellar suspended in liquids or gels, within powders or bulk films. However, in this mode of operation it is not possible to measure thin films and interfaces, which scatter too weakly, or films that require thick substrates, which prevent the transmission of the beam. In such cases, performing SAXS in Grazing Incidence (GI-SAXS) is an excellent technique to work around this problem.

The soft-matter SAXS beamline at Diamond, I22, is currently dedicated to transmission mode, with only a limited GI-SAXS functionality and an upgrade programme is underway to develop full GI-SAXS capability. In particular, the programme will focus on performing high resolution imaging with samples in an evacuated or helium filled environment, with additional solvent vapour and humidity options. The proposed sample environment chamber will be designed to permit in-situ dynamic studies of soft matter systems: such as drying films (spread or dip cast) or thermal annealing. This includes the in-situ study of dip-coated ZrO<sub>2</sub> films by Dr Rudi Winters group. Additionally, the chamber will permit high throughput non-dynamic measurements of ex-situ prepared samples.

As an example of the science that will be possible with this upgrade some recent work on Organic photovoltaics (OPV) will be described. OPV's are an attractive and promising alternative to traditional silicon photovoltaic cells. The light adsorption and charge separation functionality of OPV devices occur in the active layer. This active layer is a blend between a conjugated polymer and a solubilised fullerene derivative, which should form a bulk heterojunction structure. The crystallinity, internal structure and vertical distribution of the blend materials play a major role in determining the performance of the device. These can be optimised for each material system by varying the blend ratio, the casting solvent, casting speed and thermal and / or solvent annealing.

The UKOPV collaboration (Universities of Sheffield, Cambridge and Cardiff, and Diamond) has studied the P3HT:PCBM and PCDTBT:PCBM blend systems with (grazing incidence wide angle x-ray scattering) GI-WAXS, both using ex-situ prepared samples (I16 beamline) and watching freshly cast (doctor bladed) films drying in-situ (I22 beamline). The dynamic studies were complimented with simultaneous ellipsometry measurements. Neutron reflectivity (CRISP, ISIS) was used to measure the vertical distribution of the materials, and dynamic mechanical thermal analysis (DMTA) to characterise the glass and melting transition phase behaviours.

A brief overview of some of the collaborations recent key X-ray related results and complimentary data will be presented.

- Thursday 1st March, 3.10pm, Room 321
- Prof. William R. Rossen  
Dept. of Geotechnology  
Delft University of Technology
- Title: Foam Generation for Improved Sweep Efficiency in Enhanced Oil Recovery

Injecting gases such as carbon dioxide, steam or hydrocarbon gases into oil reservoirs can recover nearly all the oil where the gas sweeps, but in practice sweep efficiency is poor because of reservoir heterogeneity, gravity segregation of gas and viscous instability when gas displaces oil. Creating a foam from injected gas can address all three problems. We review briefly some important issues in application of foam, and then focus on the question of foam generation.

A crucial issue use of foam is how and whether foam is created in the formation, and in particular whether foam that is created near the well at large pressure gradient can propagate far from the well where pressure gradient is smaller. We review experimental data and modeling of foam generation in porous media and implications for long-distance propagation of foam and improvement of sweep efficiency on the field scale.

William R. Rossen is Professor of Reservoir Engineering in the Dept. of Geotechnology at Delft University of Technology. He holds a BS degree in Chemical Engineering from MIT and a PhD degree, also in Chemical Engineering, from the University of Minnesota. His research interests include foams for well simulation and EOR, sweep efficiency in gas EOR, and modeling complex displacement and flow processes in porous media. In 2002 he received the Distinguished Achievement Award for Petroleum Engineering Faculty from the SPE. He is a Distinguished Member of SPE. In 2011 he was named Best Instructor at Delft University of Technology. In 2012 he will be named an IOR Pioneer at the SPE/DOE Symposium on Improved Oil Recovery in Tulsa, OK.

- Thursday 8th March, 3.10pm, Room 321
- Prof W.S.Kendall  
Department of Statistics  
University of Warwick
- Colloquium-style talk  
Title: Random lines and effective transportation networks.

Abstract: The theory of random lines has a celebrated history, reaching back 300 years into the past to the work of Buffon, and forming a major part of the field of stochastic geometry. Recently it has found application in the derivation of surprising non-stochastic results concerning effective planar networks [1]. I plan to present an account of this, accessible to non-specialists, and also to describe more recent work concerning flows in related networks [2,3] and to introduce a rather curious random metric space.

References:

1. David J. Aldous, WSK. Short-length routes in low-cost networks via Poisson line patterns. *Advances in Applied Probability* 40 (2008), no. 1, 1-21.
2. WSK. Networks and Poisson line patterns: fluctuation asymptotics. *Oberwolfach Reports* (2008), no. 5, 2670-2672.
3. WSK. Geodesics and flows in a Poissonian city. *Annals of Applied Probability* 21 (2011), no. 3, 801-842