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Imaging the invisible: resolving polymer brush structure through a freeform Bayesian analysis of neutron reflectometry data

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Surfaces covered with densely tethered polymer chains possess desirable properties and are ubiquitous in natural and human-made systems. These properties stem from the diffuse structure of these polymer brush interfaces; consequently, resolving their structure is key to better understanding and designing polymer brush systems. We have been using the *PLATYPUS* neutron reflectometer at the ACNS to achieve this structural resolution over the past six years, contributing to our understanding of brush structure, as well as fundamental polymer physics.

However, the analysis of collected reflectometry data is not without significant challenges; Inflexible models preclude viable structures and the uncertainty around accepted profiles (known as spread) is challenging to quantify. Furthermore, there is no guarantee of profile uniqueness in reflectivity analysis - multiple structures may match the data equally well. Quantifying profile uniqueness and determining the structures that agree with collected data (known as multimodality) has not been previously attempted on brush systems. Historically, data analyses have used least-squares approaches, which do not satisfactorily determine profile spread and bypass the possibility of multimodality.

Here we will briefly document our journey in modelling neutron reflectometry data collected from polymer brush systems, culminating in the presentation of our developed methodology. In this methodology, we model our brush with a freeform profile that minimises assumptions regarding polymer conformation while only producing physically reasonable structures. This model is built within *refnx*'s Bayesian statistical framework, which enables the characterisation of structural uncertainty and multimodality through Markov Chain Monte Carlo sampling. We demonstrate the rigour of our approach via a round-trip analysis of a simulated system before applying it to real data, examining the well-characterised collapse of a thermoresponsive brush. The method we describe is directly applicable to reflectometry experiments on soft and diffuse systems, but may also be generalised to other instruments where the "inverse problem" hampers data analysis.

Speakers Gender

Male

Level of Expertise

Student

Do you wish to take part in the poster slam

No

Primary author(s) : GRESHAM, Isaac (The University of New South Wales); MURDOCH, Timothy (University of Pennsylvania)

Co-author(s) : Mr EDWIN, Johnson (University of Newcastle); Prof. GRANT, Webber (University of Newcastle); Prof. WANLESS, Erica (University of Newcastle); PRESCOTT, Stuart (UNSW Chemical Engineering); NELSON, Andrew (ANSTO)

Presenter(s) : GRESHAM, Isaac (The University of New South Wales)

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