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Quantifying the robustness of neutron reflectometry for analysing polymer brush structure

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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 designing systems with better performance. NR has been widely used for studying these systems as it is the only technique that can resolve the detailed structure of these films, the polymer volume fraction profile.

However, the analysis of collected reflectometry data has significant challenges; inflexible models preclude viable structures and the uncertainty around accepted profiles (spread) is challenging to quantify. Furthermore, there is no guarantee of profile uniqueness in reflectivity analysis - multiple structures may match the data equally well (multimodality). Quantifying these uncertainties has not been attempted on brush systems, but is a vital part of validating the application of NR for structural characterisation. Historically, data analyses have used least-squares approaches, which can't satisfactorily determine profile uncertainty.

Here we outline the methodology we have developed for modelling NR data. We model our brush with a freeform profile that minimises assumptions regarding polymer conformation while enforcing physically reasonable structures. We employ a Bayesian statistical framework that enables the characterisation of structural uncertainty and multimodality through Markov Chain Monte Carlo sampling. The Bayesian approach lets us introduce prior knowledge into the analysis procedure; the amount of grafted polymer should remain constant under different conditions.

The rigour of our approach is demonstrated via a round-trip analysis of a simulated system, as well as data collected on thermoresponsive brushes. A low level of uncertainty was observed, confirming the validity of NR for examining polymer brush systems.

Level of Expertise

Expert

Presenter Gender

Man

Pronouns

Which facility did you use for your research

Australian Centre for Neutron Scattering

Students Only - Are you interested in AINSE student funding

Do you wish to take part in the Student Poster Slam

No

Condition of submission

Yes

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