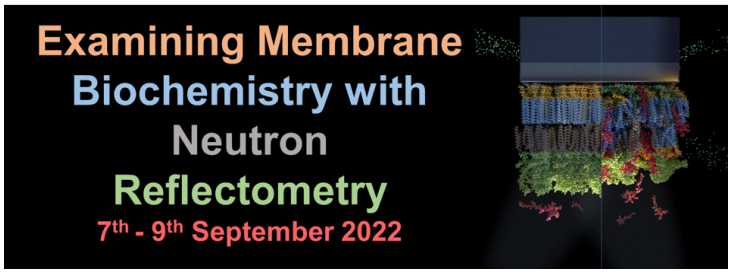


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# Fitting Reflectivity Data Using Molecular Dynamics Simulations

*Friday, 9 September 2022 12:20 (20 minutes)*

Reflectivity data is traditionally analysed using simple, layered approximations of the interface. Whilst these give a guide to the structure, fine details of the interface are often unresolved. Over the past 20 years, there has been a move to using more sophisticated models, using information from atomistic simulations to construct more refined descriptions of the interface. We have recently shown that excellent agreement between theory and experiment can be achieved by incorporating MD simulations directly into the model construction. Here we review those developments, and discuss how advancements in computing power and simulation sophistication mean that these methods are increasingly feasible approaches for data analysis over the timescale of a typical facility experiment, which from proposal to publication can span many months. In many cases, atomistic modelling could be considered as an analysis method for many experiments, but the barrier for users is often access. We discuss efforts at ISIS and SCD to facilitate these analysis approaches for the user community more widely.

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