Combining molecular dynamic simulation with neutron reflectometry to understand and predict friction

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Around 20% of global energy is used to overcome friction with an annual global cost of ~€2.5 trillion. Friction causes energy losses in motors and bearings which leads to material wear. Organic friction modifiers (OFMs) are small molecules that improve the energy efficiency and longevity of combustion engines, and in hybrid and electric motors. New fuels and motors are being introduced, and it is therefore necessary to develop lubricants and additives that are compatible with new chemistries and materials. To achieve this, it is essential to understand how lubricant additives work at the molecular level, enabling better molecules to be designed and synthesised on short time scales to keep up with the rapidly evolving transport sector.

It is challenging to reproduce the tribological conditions found within an engine and to probe the interfacial structure of adsorbed species in-situ. Hence, much of the research has been conducted under static or mild conditions. Neutron Reflectometry can determine the thicknesses of thin films on a sub-nm scale. We have built a novel tribometer rig designed for in-situ operation in the neutron reflectometer. In parallel, molecular dynamic simulations have been performed on the same systems and the simulated form factor is then compared with experimental results. This has facilitated the development of a predictive model for friction.