Neutrons answer shampoo formulation puzzle

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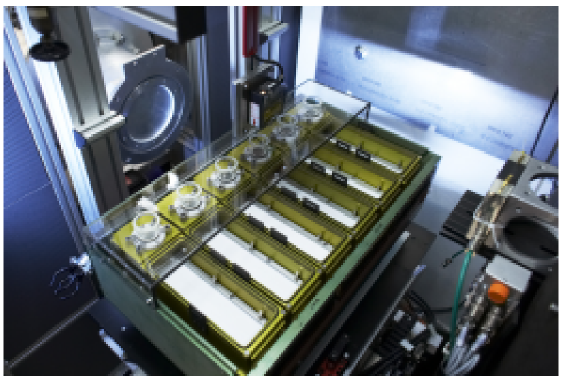

Adsorption trough assembly of the FIGARO neutron reflectometer at the ILL on which these air/liquid interface measurements were carried out. Credit: ILL/Alexis Chézičre

(PhysOrg.com) -- Scientists at the Institut Laue-Langevin have used neutrons to solve a long-standing mystery about the surface properties of polyelectrolyte/surfactant mixtures, such as those used in many detergents, paints, shampoos and conditioners. Their new findings, recently published in the Journal of Physical Chemistry B, could improve production and optimize the performance of these products, and could even lead to the development of new targeted drug or gene delivery applications.

A research team at the Institut Laue-Langevin, the flagship centre for neutron science, has demonstrated quantitatively the science behind an anomaly in the surface tension of polyelectrolyte/surfactant mixtures. Their findings show that the dramatic increase in surface tension that affects the production of various pharmaceutical and cosmetic formulations is caused by the comprehensive aggregation of active ingredients. They have outlined a way to reload interfaces with functional components simply by tuning the way the materials are handled.

Surface tension is a property of liquids resulting from the cohesion of their molecules that helps them resist an external force. It is responsible for the shape of liquid droplets and the reason why insects can run on the surface of ponds.

Surfactants are substances that lower the surface tension of a liquid and can capture other substances, such as oil or grease in cleaning products. They are often combined with polyelectrolytes, made of long charged molecules, to improve the efficiency of detergents, wetting agents, emulsifiers, foaming agents, and dispersants in paints, shampoos and conditioners, and are used throughout the food industry. Also, the strong attractive interactions of surfactants with natural polyelectrolytes, such as proteins or DNA, play an important role in many biological processes, as well as in medical applications, such as drug and gene delivery.

The commercial production and performance of polyelectrolyte/surfactant mixtures, however, is affected by a peculiar phenomenon, first investigated in depth a decade ago. Whilst adding a surfactant to a polyelectrolyte solution initially causes the surface tension to decrease, as further surfactant is added the surface tension dramatically increases again. This feature, known as a ‘cliff edge peak’, is accompanied by a change in the appearance of the mixture, with the eventual loss of the cloudiness that is present as soon as the materials first interact.

From an industrial production point of view, this rise in surface tension reduces the performance of the additive, often requiring the introduction of further surfactant at extra cost. As a result, there is a lot of interest in understanding the interactions between these mixtures at the atomic level both in solutions and at surfaces. Of particular interest are the primary causes of the cliff edge peak and ways to prevent, lessen or delay its effects that could lead to more efficient formulations and reduce the effects of many pollutants in our environment.

To investigate this problem, Dr Richard Campbell (Institut Laue-Langevin), Dr Imre Varga (Eötvös-Loránd University, Hungary) and their co-workers looked at a system studied widely in the literature – an oppositely charged poly (diallyldimethylammonium chloride)/sodium dodecyl sulfate (Pdadmac/SDS) system.

The international research team, which also includes members from the UK and Sweden, used neutron reflectometry, a reflection technique used for measuring the composition and structure of thin films, to monitor the surface properties with respect to the slow generation of the cliff edge peak. The instrument used was the brand new FIGARO reflectometer (Fluid Interfaces Grazing Angles ReflectOmeter) at the Institut Laue-Langevin, which was constructed during the Institute's innovative Millennium Programme. The researchers showed quantitatively for the first time that this striking feature in the surface tension results from the slow precipitation of particles into sediment from the aqueous solution. The precipitation depletes the solution and consequently the surface of its active ingredients, and also accounts for the loss of cloudiness observed.

As well as uncovering the reasons behind the rise in surface tension, the team were also keen to investigate methods to prevent its impact, which could directly benefit commercial applications. In the literature, researchers have suggested that the way these mixtures are handled could affect the nature of the material in the solution - a phenomenon called “non-equilibrium effects”.

To test whether the re-dispersion of surface-active material could actually switch off the cliff edge peak effect, the team carefully agitated a series of mixtures after the settling process had finished. A small mechanical stress provided just enough energy to re-disperse some of the sedimented particles and re-supplied the air/liquid interface with enough material to lower the surface tension once again.

“By approaching the problem in a different way, we have shown that the way you handle polyelectrolyte/surfactant systems can produce a variety of tuneable surface properties,” says Dr. Richard Campbell. “We hope that our findings will allow future industrial chemists across the pharmaceutical, detergency and cosmetic industries to generate better product output from their raw materials by learning to handle them in a smarter way, and create optimum surface properties on demand, rather than simply buying in more material to improve performance.”

There is hope also that this work can lead on to novel drug or gene delivery applications where one could apply an external stimulus to a stable biomacromolecule system in order to trigger the delivery of proteins or DNA to a given target.

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