Experimental report

09/12/2021

Proposal: 9-13-1006 **Council:** 4/2021

Title: Adsorption to Biomimetic Thiol Surfaces

Research area: Soft condensed matter

This proposal is a new proposal

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Samples: D2O
NaCl
Deuterated Sodium Dodecyl Sulfate
Polyethylenimine
18 methyl eicosanoic acid

Instrument	Requested days	Allocated days	From	To
D17	5	0		
FIGARO	5	0		
SUPERADAM	5	4	24/05/2021 30/09/2021	26/05/2021 02/10/2021

Abstract:

The boundary of hair is formed by a lipid layer whose main component is the branched 18-methyl eicosanoic acid. How the lipid density and the amount of methyl branching affect the interaction properties of hair is not fully understood, given also the difficulty of direct study of hair. Such knowledge, though, is crucial for the design of products with protective and restorative properties, particularly in the current climate where there is an urgent need for new, sustainable materials to replace conventional additives which had years of optimisation. Adsorption models for coadsorbing polymers and surfactants to lipid surfaces based on Self-Consistent Field Theory exist, but these models require experimental verification and refinement. Neutron reflectance provides the ideal experimental window to understand how the unique branching of hair lipids affects self-assembly and adsorption in water. It is ideal for understanding hierarchical adsorption, where deuteration will provide the contrast. (This represents the first application with Serena Cozzolino, InnovaXn PhD student, L'Oréal supporting)

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From 24/05/21 to 26/05/21 and from 30/09/21 to 02/10/21 on SuperADAM

The performed experiments aimed at characterizing the adsorption of surfactants and polymers to biomimetic hair surfaces produced by self-assembly of thiols on gold. This information is important for the cosmetic industry to improve the formulation of hair care products.

These experiments are part of the thesis work for the InnovaXN PhD project of Serena Cozzolino "Adhesion and interaction with hair biomolecules – a cosmetic perspective".

A lipid layer covers the hair surface and makes it hydrophobic. Its major component is the molecule 18-methyl eicosanoic acid (18-MEA); damaged hair has a reduced lipid coverage and is hydrophilic.

Three types of surfaces have been produced by using commercial thiols with relevant features:

1. Octadecanethiol (ODT) or butanethiol layer – long or short straight chains giving hydrophobic surfaces (the short one has been used as a comparison for the surface in point 2.)

2. 2-methyl-1-butanethiol layer – short, branched thiol, which reproduces the characteristic antepenultimate methyl branch found in 18-MEA

3. a mixed layer of 2-methyl-1-butanethiol and sodium 3-mercapto-1-propanesulfonate – the latter molecule has a negative charge that reproduces the one found in damaged hair, where the outermost lipid layer is removed; this surface is then representative of a partly damaged hair surface with hydrophobic and hydrophilic patches.

The experiments in May involved the ODT and the mixed layer. Both surfaces have been characterized in:

— gold contrast matched water (GMW, 74:26 D_2O:H_2O), before and after the injection of the solutions below
— deuterated sodium dodecyl sulfate (dSDS) at the concentrations of 0.5 and 2 cmc in GMW
— 2 cmc dSDS + 100 ppm polymer in GMW (the polymer was chitosan for the ODT surface, but due to solubility problems we switched to pDADMAC for the other surface)

In September/October, one experiment was on the short, branched thiol layer, the second one involved again the mixed layer, and the final one was a shorter experiment on the butanethiol surface. In this case, the explored conditions were:

— GMW plus 100 mM NaCl (similar ionic strength of real formulations), before and after the injection of the solutions below
— 2 cmc dSDS in GMW + 100 mM NaCl (also the hydrogenated SDS was used in the first experiment to check for dSDS contaminants)
— 100 ppm chitosan oligomer (easier to dissolve than the polymer) in GMW + 100 mM NaCl
— 2 cmc dSDS + 100 ppm chitosan oligomer in GMW + 100 mM NaCl

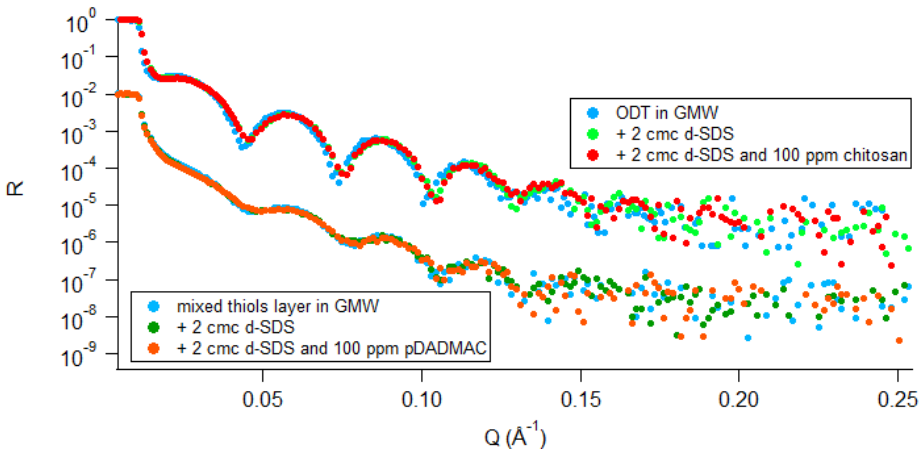

Figure 1. NR curves of the thiol surfaces produced in May, in GMW and after adsorption of dSDS or dSDS/polymer mixture. The difference in the fringes is due to different thickness and roughness of the layers composing the gold substrates, but within one set of measurements, the change in the signal depends on the amount of adsorbed species.

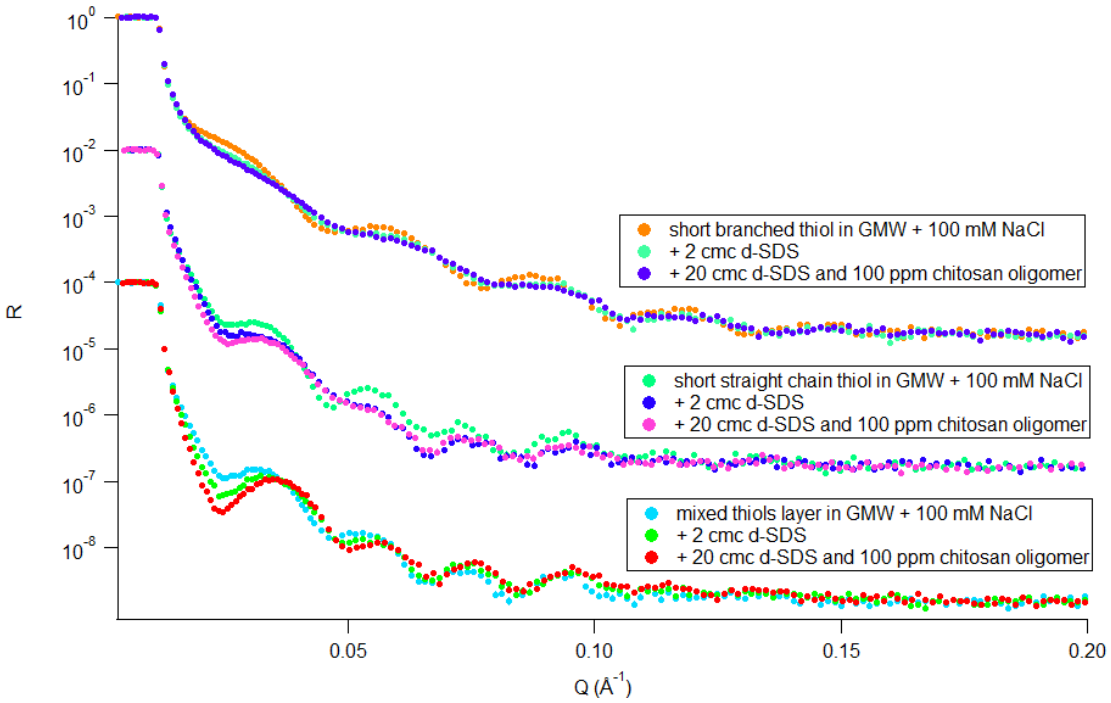

Figure 2. NR curves of the thiol surfaces produced in September, in GMW and after adsorption of dSDS or dSDS/chitosan oligomer mixture. The difference in the fringes is due to different thickness and roughness of the layers composing the gold substrates, but within one set of measurements, the change in the signal depends on the amount of adsorbed species.