Skin creams aren't what we thought they were

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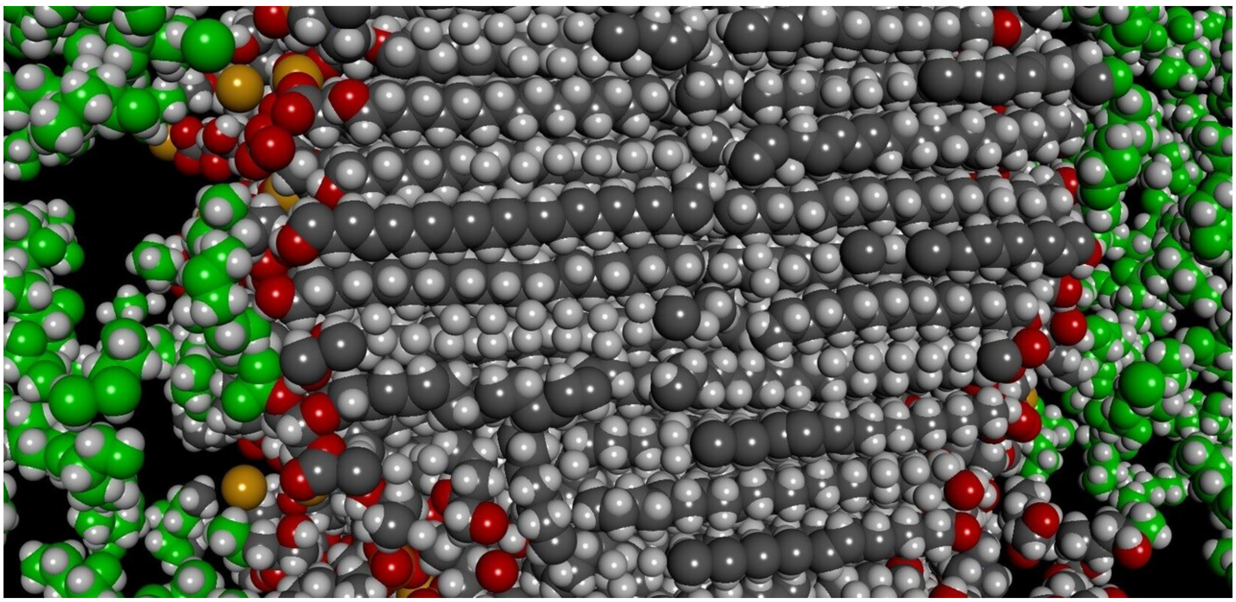

Model of the molecular structure of a cream, with the atoms of a surfactant and co-surfactant in the lamella shown in light and dark gray in the middle of the image, and atoms of a preservative in green and light gray along the edges of the image. The red and orange spheres are oxygen and sodium atoms, respectively. Credit: David Barlow and Delaram Ahmadi

Anyone who has gone through the stress and discomfort of raw, irritated skin knows the relief that comes with slathering on a creamy lotion. Topical creams generally contain a few standard ingredients, but manufacturers know little about how these components interact to influence the performance of the product. Now, researchers report the first direct glimpse of how a cream or lotion is structured on the molecular scale, and it's not quite what they expected.

The researchers will present their results today at the American Chemical Society (ACS) Fall 2019 National Meeting & Exposition.

"The long-term stability and clinical properties of a cream are determined by its fundamental structure," says Delaram Ahmadi, the graduate student who performed the study. "If we can understand the chemical microstructure of the cream and relate that to the structure of the skin, then perhaps we can better repair the compromised skin barrier."

One of Ahmadi's research advisors, David Barlow, Ph.D., adds, "We wanted to improve the science around cream formulation so that companies could more rationally formulate them to get exactly what they want. The most significant thing we found is that the textbook picture of the structure of a cream is very naïve."

Formulators have mostly inferred the structure of these emulsions based on indirect measurements, Barlow explains. But his group took a direct approach, with Ahmadi analyzing the cream using X-ray and neutron scattering techniques to determine how the ingredients were dispersed. Ahmadi and Barlow are at King's College London, and their co-investigator, Jayne Lawrence, Ph.D., is at Manchester University.

Cream is usually thought of as stacks of lamellae, or membranes, composed of surfactants and co-surfactants that maintain oil droplets dispersed within water (or vice versa). To reveal a cream's true structure, the researchers started with an aqueous cream formulation from the British Pharmacopoeia that contains two co-surfactants and a sodium dodecyl sulfate (SDS) surfactant. They also incorporated a diol known to act as a preservative. One by one, Ahmadi replaced each ingredient with heavier isotopic versions. The researchers then scattered X-rays and neutrons off the selectively isotope-labelled samples and, from the resulting patterns of scattering, determined the location of each ingredient and the aggregate it formed within the cream.

The results were surprising. Although they observed co-surfactants in the lamellar layers as predicted, the surfactant was not there. "The surfactant peak profile suggested that the molecule formed micelles in the cream," Ahmadi says. In addition, the preservative was not found in the aqueous layer, where scientists have always presumed it would be. It was, in fact, residing in the lamellae. Preservatives have an antimicrobial effect, thereby prolonging shelf-life. Formulators had assumed that to be an effective antimicrobial, the preservative had to be dissolved in the water layer. So, Ahmadi says this finding could mean the creams are essentially self-preserving.

The team is currently performing computer experiments to model the behavior of the preservatives in a bilayer system like a cream to understand why they are in the membrane layer. And they want to better understand the structure of the surfactant micelles dispersed in the layers. "I don't think anybody else has considered that there would be these micelles in the system at all," Barlow says. "This is new, and we need to think about where they are in the structure and what they are doing."

They also want to study different creams. Ahmadi says the formula from the British Pharmacopoeia is pretty basic, with only five ingredients. In addition, personal care companies have phased out SDS as a surfactant, so the researchers plan to analyze variations without SDS in the future.

More information: Simple creams, complex structures, the American Chemical Society (ACS) Fall 2019 National Meeting & Exposition.

Abstract

Objectives
Topical creams used to treat various skin conditions are typically semi-solid emulsions in which oil droplets are dispersed throughout a continuous aqueous phase containing an 'excess' of emulsifier - a mixture of surfactant and co-surfactant(s), which form lamellar structures and give "body" to the cream. Historically, structural details of creams have been inferred largely from indirect observations and the exact composition and structure of the lamellar phases present remain poorly characterized. Here we report studies conducted to secure a detailed understanding of the molecular structure of a simple cream and how this is influenced by additives like preservatives.

Materials and Methods
Aqueous creams containing cetyl and stearyl alcohol (co-surfactants), sodium dodecyl sulfate (surfactant, SDS), water and liquid paraffin were prepared as specified in the British Pharmacopoeia. The concentration of emulsifier was varied as either 4% or 10% (w/w), with the latter prepared with and without preservative, 1,5-pentanediol. The macroscopic properties of the creams were studied using rheology and microscopy and their molecular architecture determined via small-angle neutron and X-ray scattering (SANS and SAXS) and wide-angle X-ray scattering (WAXS) experiments.

Results
Evidence of a lamellar structure was seen in the 10% but not the 4% emulsifier creams - both directly as Bragg-peaks in SANS and SAXS profiles and indirectly as Maltese crosses in polarised-light micrographs. For the 10% emulsifier creams with and without preservative, the lamellar d-spacings varied as ~240 vs ~270 Å, with bilayer thicknesses of ~48 Å in both cases. The use of individually perdeuterated cream components showed that the co-surfactants along with the preservative

co-locate in the lamellar bilayers. The surfactant (SDS) however, appears to arrange (primarily) as a monolayer surrounding the oil droplets and also seems to combine with one or both of the co-surfactants to form mixed micelles. WAXS measurements indicated hexagonal close packing of the emulsifier alkyl chains, with the paraffin forming a liquid-crystalline phase. Rheological measurements showed that both the 4% and 10% emulsifier creams are shear-thinning with consistency indices of 58 and 113 Pa.s, respectively.

Conclusions
Details of the molecular architecture of a simple cream have been deduced, revealing the packing arrangements and loci of the component surfactant, co-surfactants, and preservative.

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