Computer simulation evidence of the molecular mechanism of makeup removal using cleansing foam

～Is an "in silico formulator" superior to a human formulator?～

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Introduction:

Background

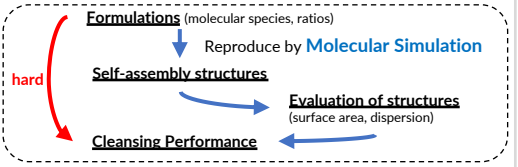
・Surfactant-type cleansing agents: cleansing foams have excellent rinsing properties and eco-friendliness but also weak removability, since they are water-based [1]. In this context, improving the cleansing performance of cleansing foams is a high demand issue. However, cleansing foams are typically composed of many ingredients, making it difficult to find the best formulation from numerous combinations.

・Molecular simulations can provide visualizations of the assembly structure [2,3] and the cleansing process at nano spatial-temporal scales, which are difficult to observe experimentally. To elucidate the molecular mechanism of cleansing will help reduce the high cost of formulation design.

Aim

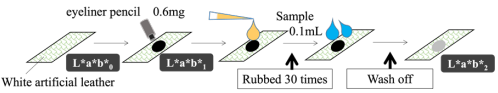
Clarifying the molecular mechanism of cleansing process by reproducing various formulations using molecular simulations and comparing their structures with cleansing capabilities.

Overview



Materials & Methods:

1. Evaluation of cleansing capability γ

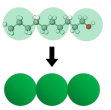


$$\text{Cleansing capability } \gamma\ (\%) = \frac{\sqrt{(L^*_1-L^*_2)^2+(a^*_1-a^*_2)^2+(b^*_1-b^*_2)^2}}{\sqrt{(L^*_1-L^*_0)^2+(a^*_1-a^*_0)^2+(b^*_1-b^*_2)^2}} \times 100$$

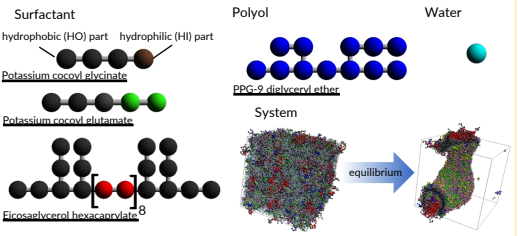
L*a*b* value were measured by a colorimeter (CM-2600d, Konica Minolta, Inc.) [4].

2. Dissipative Particle Dynamics (DPD)

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{f}_i = \sum_{j \neq i} -\frac{\partial U_{ij}}{\partial \boldsymbol{r}_{ij}}$$



Coarse-grained simulation models



Self-assembled morphologies

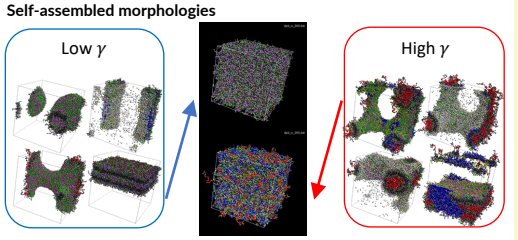


Figure 1: Representative snapshots and videos of equilibrium morphologies of cleansing foams. Water beads are eliminated for clarity. (γ : cleansing capability [%])

Results & Discussion:

▪ Correlations between performance and morphology

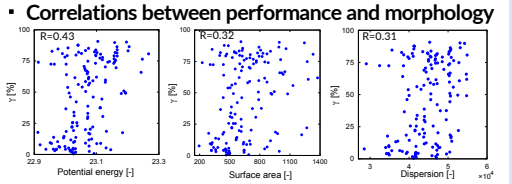


Figure 2: Scatter diagrams of the correlations between cleansing capability γ and simulation values which represent the aggregate state and structure. (R : correlation coefficient)

・Using these indexes, we were able to grasp the change of structures quantitatively.
・The more complex the self-assembled structure, the higher the performance.

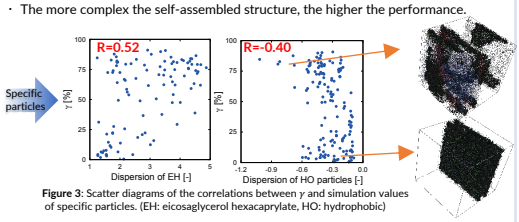


Figure 3: Scatter diagrams of the correlations between γ and simulation values of specific particles. (EH: eicosaglycerol hexacaprylate, HO: hydrophobic)

・Not only the entire structures, but also the distributions of particles contribute to the cleansing performance, such as non-ionic surfactant (EH), and HO particles.

▪ Self-assembled morphologies between oily stains

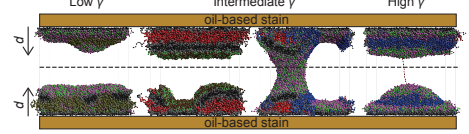


Figure 4: Representative snapshots of equilibrium morphologies of cleansing foams between oily stains. Water beads are eliminated for clarity. These equilibrium morphologies represent the state of the cleansing agent ingredients adsorbed on oil-based stains, before they were removed. (d: distance of particles from the oily stains)

Divide HO group to strongly hydrophobic **HO1** and weakly hydrophobic **HO2** (HO1: alkyl chain, HO2: ether bond, ester bond, and amido bond)

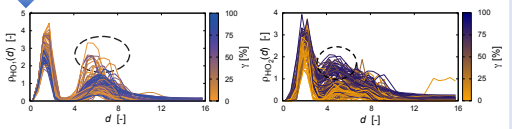
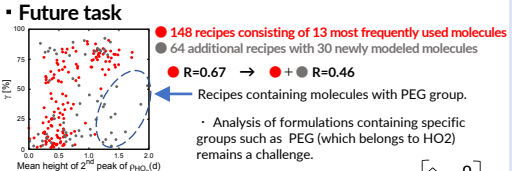


Figure 5: Density profiles of HO1, HO2 particles as a function of d for all formulations. The color indicates its cleansing capability γ.

・The heights of the 2nd peak of $\rho_{HO1}(d)$ are higher for the formulations with **low** γ.
・The heights of the 2nd peak of $\rho_{HO2}(d)$ are higher for the formulations with **high** γ .

▪ Future task



・Analysis of formulations containing specific groups such as PEG (which belongs to HO2) remains a challenge.

Figure 6: Scatter diagrams of the correlations between mean heights of 2nd peak of $\rho_{HO_2}(d)$ and γ.

Conclusions:

We investigated the mechanism of cleansing by simulating the self-assembled structures of cleansing foams.

・Various self-assembled structures were observed depending on the molecular species composing the system and their ratios.

・The complexity of a structure is one of the features of high-performance cleansing. However, the correlation between the performance of cleansing agents and their entire self- assembled structures are not strong enough.

・Focused on the inner distribution of aggregates, it was discovered that certain particles (molecules) such as EH or HO particles are crucial in cleansing process.

・The distribution of (HO1, HO2) particles when the cleansing foam is adsorbed on the dirt is also a significant clue to realize a high-performance cleansing.

References:

[1] K. Watanabe *et al.*, *IFSCC Magazine*, **7**, 310–318 (2004).
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