Understanding Hair Friction using Coarse-Grained Molecular Dynamics

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We present a coarse-grained molecular dynamics framework in order to study hair friction and adhesion effects. We study the friction between individual hairs as well as between atomic force microscopy (AFM) tips and the hair surface. Different components relevant to hair care formulations are included at the contact interface to identify the physicochemical mechanisms yield desirable modifications to the tribological behavior of human hair.

Keywords: hair friction, coarse-grained, molecular dynamics, formulations

1. Introduction

The understanding of nanoscale interactions on the surface of the human hair is a key objective in the development of hair care products. AFM experiments indicate significant differences of the coefficient of friction and adhesive forces between virgin hair, damaged hair and hair treated with hair care formulations [1,2]. The intact hair epicutle (outmost layer of the hair) is covered predominantly by a 18-methyleicosanoic acid (18-MEA) fatty acid layer, which is covalently bound to a protein base through thioester bonds [3]. Atomistic molecular dynamics (MD) simulations of this fatty acid layer have been conducted by Cheong et al. [4] to predict the separation distance between fatty acid chains. In the proposed work, we further extend this approach to study tribological effects with the addition of aqueous polyelectrolyte-surfactant formulations.

2. Methods

Despite increasing computational resources, atomistic MD studies are restricted to relatively short timescales and small computational domains. Coarse-grained (CG) models have proven their capability to capture relevant physicochemical phenomena in many applications on larger domains and timescales, which is of particular use in biological systems. In this work, a coarse-grained (CG) force field is adapted to investigate friction behavior of the hair surface. We present a parametrization of the 18-MEA layer on the hair surface in the MARTINI 2.0 CG force field [5]. The proposed conceptual framework is shown in Fig. 1.

3. Outlook

The proposed modeling framework will be used to obtain detailed insights on the adsorption of coacervates (polyelectrolyte-surfactant mixtures) onto the hair interface. Furthermore, the friction and adhesion behavior of healthy and damaged hair surface will be quantified in systems with and without coacervates at the contact interface. Several mechanisms such as the long-range Coulombic interactions of polyelectrolytes with the hair epicuticle will also be investigated. We aim to provide a comprehensive study on how coacervate formulations could provide a modification to the hair friction behavior in hair-to-hair contacts and haptics.

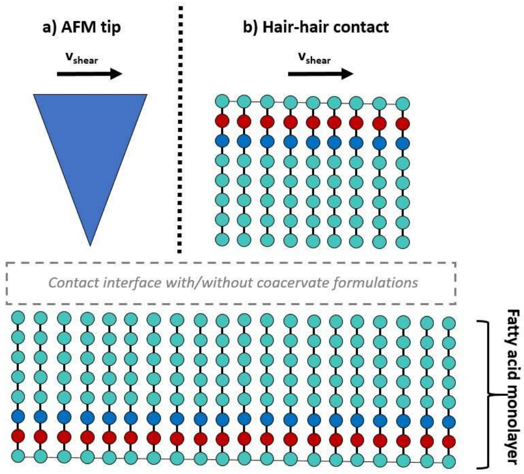

Figure 1: Proposed framework representative of a single hair contact with another hair or an AFM tip.

4. References

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