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Influence of the Size of Cation on the Structure and Tribological Properties of Ionic Liquids Studied with Molecular Dynamics

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Ionic liquids (ILs) are two-component systems composed of large asymmetric and irregularly shaped organic cations and anions. Physical properties of ILs like negligible vapour pressure, high-temperature stability, high ionic conductivity and also a great variety of ILs and their mixtures highlight them as potentially relevant to lubrication [1, 2]. A large number of variations in IL composition is possible, estimated at the order of magnitude of 10^{18} different ILs. From their variety stems the possibility of tuning their physicochemical properties which can affect lubrication, such as viscosity, polarity, surface reactivity. Hence, it would be advantageous to figure out general relations between the molecular structure and tribological properties of ILs.

In this study, we investigate a generic tailed-model (TM) of ILs which includes: an asymmetric cation consisting of a positively charged head ($\sigma_C = 5$) and a neutral tail of variable size ($\sigma_T = 3, 5, 9$) and a large spherical negatively charged anion ($\sigma_A = 10$). It represents a more realistic model compared to the simplest one, the so called Salt Model (SM) [3, 4]. We figured that, although simple, TM model results in striking differences in equilibrium bulk structure of IL governed by the tail size relative to cationic head: (i) simple cubic lattice for the small tail, (ii) liquid-like state for symmetric cation-tail dimer, and (iii) molecular layer structure for the large tail. A mutual feature of all investigated model ILs is a formation of the fixed (stable) layer of cations along solid plates.

We have investigated the influence of the size of the cationic tail on the response of three ILs to confinement and mechanical strain, using molecular dynamics simulations in the *LAMMPS* code [5]. Tribological properties of three IL models are compared in and out of equilibrium. We have related the evolution of normal force with inter-plate distance to the changes in the number and structure of confined IL layers. A mutual feature of all investigated model ILs is a formation of the fixed (stable) layer of cations along the solid plates. The fixed layer formation is a result of strong Lennard-Jones interaction between the plates and ions. A consequence of the fixed layer stability is a steep rise of the normal force at small interplate gaps. The steep rise of the normal force is an effect useful for preventing solid-solid contact and accompanying wear.

Understanding the interplay between different processes in thin lubricant films is important due to the conflicting demands imposed on how IL lubricant should behave in dynamic confinement: high load-carrying capability requires strong adsorption to the surface, while low friction requires low viscosity.

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