IONIC LIQUIDS UNDER CONFINEMENT: THE ROLE OF ANISOTROPY ON FRICTIONAL PERFORMANCE

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ABSTRACT
Understanding the lubrication mechanisms in engineering systems is important for developing new concepts that can reduce friction. Such an interesting research topic is the use of Ionic Liquids (ILs) for lubrication, which has been shown to have a positive impact on friction loss reduction.

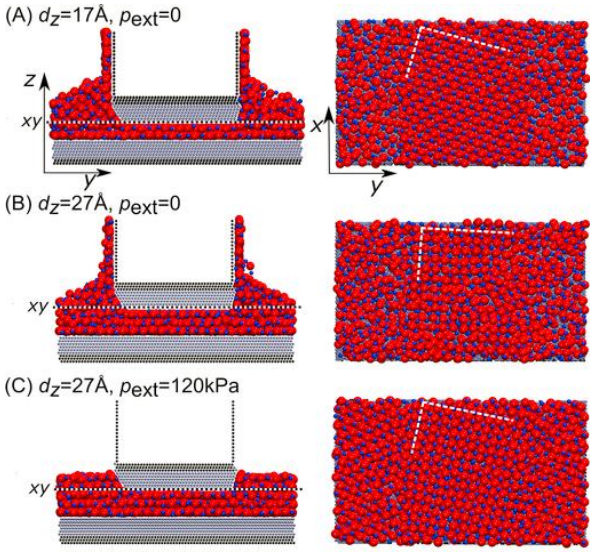

Fig.1 Side (yz) and top (xy) views of snapshots of MD simulations of IL under confined shearing.

Recent results from Molecular Dynamics simulations of IL lubrication [1] have shown the impact of confinement resulting in IL layering and solidification under high pressure. As shown in Fig. 1, layered ordering is observed in the transverse direction, while crystalline structures can be observed in the lateral direction, consistent with results known in literature [2, 3, 4].

In the current work we attempt to quantify the role of such anisotropy on the tribological properties of ILs. We employ equilibrium and non-equilibrium MD simulations of coarse grain IL molecules and correlate the ordering of bulk and confined liquids with their frictional behavior. The solidification of the liquid under isotropic and anisotropic loading is a topic of special interest and will be studied in detail.

We expect that the deep insight of such fundamental processes through the use of numerical methods, should result in more accurate description of the underlying physico-chemical mechanisms that control lubrication and guide us towards developing optimal engineering concepts.

REFERENCES
[1] Gkagkas, K., Ponnuchamy, V., Dašić, M. and Stanković, I., "Molecular dynamics investigation of a model ionic liquid lubricant for automotive applications," Tribol. Internat., 2016, In press.
[2] Capozza, R., Vanossi, A., Benassi, A. and Tosatti, E., "Squeezout phenomena and boundary layer formation of a model ionic liquid under confinement and charging," J. Chem. Phys., 142, 2015, 064707.
[3] Fajardo, O. Y., Bresme, F., Kornyshev, A. A. and Urbakh, M., "Electrotunable Lubricity with Ionic Liquid Nanoscale Films," Sci. Reports, 5, 2015, 7689.
[4] Fajardo, O. Y., Bresme, F., Kornyshev, A. A. and Urbakh, M., "Electrotunable Friction with Ionic Liquid Lubricants: How Important is the Molecular Structure of the Ions?" J. Phys. Chem. Lett., 6, 20, 2015, 3998-4004.