

Quantification of ordering in confined lubricants

I. Ristic¹⁾, M. Srbulovic^{1,2)}, K. Gkagkas^{3)*}, and A. Vernes^{1,4)}

¹⁾AC2T research GmbH, Wiener Neustadt, Austria

²⁾Institute of Engineering Design and Product Development, TU Wien, Austria

³⁾Advanced Material Research Division, Toyota Motor Europe NV/SA, Zaventem, Belgium

⁴⁾Institute of Applied Physics, TU Wien, Austria.

*Corresponding author: konstantinos.gkagkas@toyota-europe.com

The main goal of the present contribution is to quantify and visualize the ordering in highly confined lubricants, namely the formation of near-wall layers and their evolution in time.

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1. Introduction

It is a well-known and widely accepted experimental fact that confined lubricants, like ionic liquids (ILs) – for example, tend to form layers near the confining walls, and that this feature is properly reproduced by molecular dynamics (MD) simulations [1].

2. Computational details

Both equilibrium and non-equilibrium coarse-grained MD simulations have evidenced the solidification of confined lubricants under various loading and shearing conditions [1]. Based on these MD data, then various structure factors and order parameters are calculated and utilized to capture the formation of layering and its stabilization.

The structure factors are generalized response functions used for disordered systems, e.g., liquids, for quantifying the linear response of a density, such as the concentration or that of charge, to a weak external perturbation [2]. Formulas for computing the bond-orientational order parameters (BOOPs) are derived from the spherical harmonics expansion of the bond-density, which quantity in turn is a rather positional than chemical one [3].

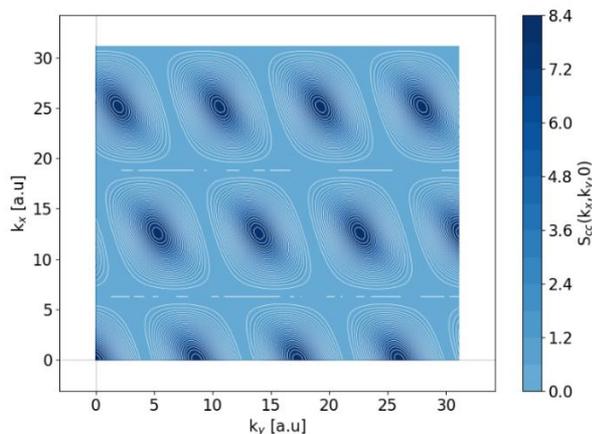


Figure 1: Structure factor $S_{cc}(k)$ obtained by ensemble averaging the concentration-concentration correlation function visualizing and quantifying a 2D ordering.

3. Results and discussion

As shown in Fig. 1, the structure factors are directly aiming the global crystallographic characterization of near-wall layers. In fact, the second-order rotational invariant of the global BOOP is much better to use together with the third-order one, since both are independent of the right-handed Cartesian coordinate system. As illustrated in Fig. 2, a combination of the rotational invariants unambiguously identifies the crystallographic symmetry of any particle in accordance with its surrounding beyond the global symmetry identified by the structure factors.

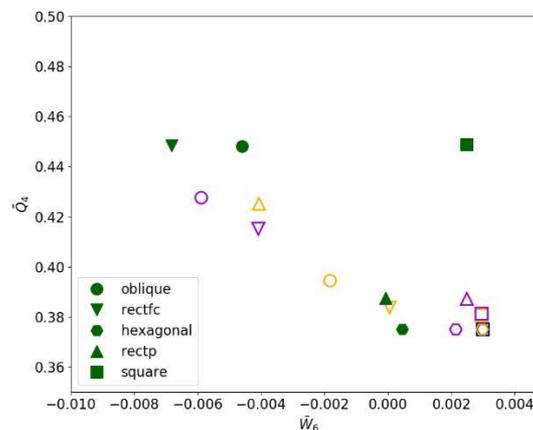


Figure 2: Identification of all five 2D Bravais lattices up to the 3rd (green), 4th (yellow) and 5th (violet) shell.

4. Acknowledgments

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5. References

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