

How square ice helps lubrication

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The combination of water with graphite or graphene is under active investigation in several fields for a number of reasons. In the field of tribology, it is of interest due to the action of graphite powder as a solid lubricant, which is far more effective under humid conditions than in vacuum or dry air. This is opposite to the case for other solid lubricants, such as WS₂ and MoS₂ [1]. Moreover, water alone is a poor lubricant, due to its low viscosity-pressure co-efficient. While suggestions have been made as to the reason behind water's beneficial effects on graphite as a lubricant [2], this effect is not yet understood. We use atomistic molecular-dynamics simulations to investigate equilibration of water confined between graphene sheets over a wide range of pressures.

We demonstrate that, under the right sliding conditions, square ice can form in an asperity, and that it is similar to cubic ice VII and ice X. We find that thermal equilibration of the confined water is hindered at high pressures. We simulate sliding of the square ice on atomically at graphite and find extremely low friction due to structural superlubricity. The conditions needed for this equilibration correspond to low sliding speeds, and we suggest that the ice observed in experiments of friction on wet graphite [3, 4] is of this type.

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[3] K. B. Jinesh and J. W. M. Frenken, *Phys. Rev. Lett.* 96, 166103 (2006).

[4] K. B. Jinesh and J. W. M. Frenken, *Phys. Rev. Lett.* 101, 036101 (2008).

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