How the Sub-Nanoscopic Rougness Affects the Hydrophobic Gap: X-Ray Reflectivity Experiment and Molecular Dynamics Simulation

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Solid/liquid interfaces are ubiquitous in the earth and our daliy life. Understanding the solid/liquid interface structure is essential for biology, chemistry, geology and engineering. Hydrophobic gap has been observed, with the help of high resolution X-Ray reflectivity study, on the strongly hydrophobic surface, where the water density is reduced to half the bulk density with a scale of ~0.5-1 nm. However, the situation has been less clear for a weakly hydrophobic surface.

On the other hand, Wettability is a very important physical property for solid/liquid interfaces, which reflects the interactomic interactions between different contacted phases. It is known that the roughness in meso- or microscopic scale (larger than 10 nm) can lead the wetting status into either Wenzel status or Cassie-Baxter status dependent on the surface geometry. Consequently, the hydrophobic surface will be more hydrophobic, and the hydrophilic surface will be more hydrophilic. However, There is no consensus on (1) how the sub-nanoscopic roughness affects the wetting properties; (2) how the sub-nanoscopic roughness affects the hydrophobic gap as detected by X-Ray Reflectivity; and (3) how the relationship develops between the hydrophboic gap and the wettability.

We have recently started two indepedent X-Ray reflectivity experiments for silicon wafer surfaces with an ultrathin SiO_2 films immersed in liquid water. The surface chemistry is almost equivalent and the roughness is within 1 nm for both cases. However, we observed a hydrophobic gap in one time, and did not observe the gap at all in another time.

To elaborate whether the observed difference results from different roughnesses, we have prepared various silica-water interface systems and investigated the interfacial structure in detail using molecular dynamics simulations. The weakly hydrophobic surfaces are obtained with a silica surface (or slice) with only siloxane Si-O-Si bridge. The roughness is then controlled with a sinusoidal-function-like shape via the period and amplitude. It was found that the water density at interface has been modulated by the surface shape. The density at hydrophobic caves was found to be much depleted. The results will help us understand the liquid-solid interface better with consideration of the roughness at atomic scale.