A new interface-sensitive analytical method based on a combination of linear spectroscopy and informatics

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Processes at interfaces are paramount to understanding the most challenging questions in chemical reaction, biology, tribology, and geology. Recently, it has been revealed that the interfacial phenomenon is governed not only by the two-dimensional interface but also the interfacial region where molecules behave differently from the bulk system (1). Many surface-sensitive methods have been developed to investigate the interfacial properties, such as non-linear optical spectroscopy, surface-enhanced Raman/Infrared, etc. However, despite the high sensitivity of these methods, the lack of information from the entire interfacial region and the challenge of quantitative analysis make it difficult to investigate the interfacial region. For instance, sum-frequency generation (SFG), representative of non-linear optical spectroscopy, can detect only the non-center-symmetrically arranged molecular groups.

In this work, we developed a new surface-sensitive method based on attenuated total reflection infrared spectroscopy (Fig. 1a). By controlling the gap between sample and prism, a series of spectrums with different bulk and interfacial water ratios were recorded (Fig. 1b). Subsequently, the spectrum of interfacial water was extracted from the unresolved spectrums by the multivariate-curve resolution (MCR). Fig. 1c shows the spectrum of interfacial water on Poly(dimethylpolysiloxane), which displays sharp peaks from 3600 to 3750 cm^{-1}. The peaks in this region were assigned to the OH stretching modes of dangling OH bonds directing to the surface, demonstrating high surface-sensitivity of this method. The high surface sensitivity and the signal incorporating the entire interfacial region make this technique an ideal tool for the study of the interfacial phenomenon. In the presentation, we will introduce our results of interfacial water and compare previous results obtained by conventional surface-sensitive analytical techniques.

Reference: (1) T. Hayashi, Chemistry Letters **50** (6), 1173 (2021).

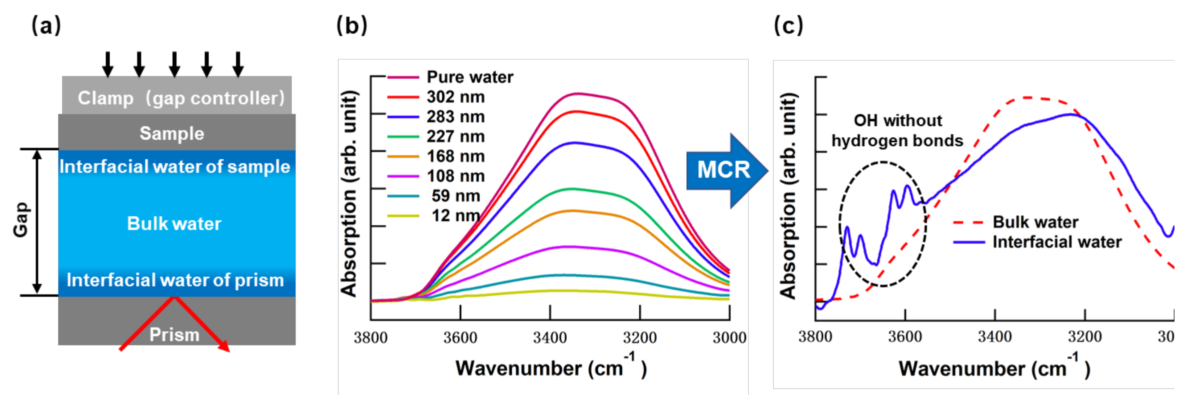

Fig.1 (a) The schematic diagram of gap-controlled ATR-IR, (b) the spectrum corresponding to different gaps were measured on Poly (dimethylpolysiloxane) (PDMS). (c) The spectrum of interfacial water is extracted by Multivariate Curve Resolution. (The thickness of Gaps are calculated from the intensity)