

Dynamics of Monolayer Water on a Single Crystalline TiO₂ Surface in Air by VSFG Spectroscopy

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Molecular dynamics on an oxide surface is a key process for various devices using oxide such as catalysts, solar cells, and electronic devices. We have been investigating the dynamics using picosecond vibrational sum-frequency generation (VSFG) spectroscopy suitable for in-situ observation. On a single crystalline TiO₂ surface, which plays important role in photo-catalytic reaction, we have succeeded in detecting monolayer water *in air* and revealing its photoinduced dynamics.

Figure 1 shows the VSFG spectrum of a TiO₂(110) surface measured in air at room temperature. Judging from their wavenumbers, the bands at around 2800 cm⁻¹ and 3300 cm⁻¹ are assigned to CH stretching modes of hydrocarbons and OH stretching modes of bulk water. In contrast to these bands, the 1600-cm⁻¹ band is fairly unique. The intensity is hundreds times higher and the width is much narrower than the others. According to the study on water-adsorption on a TiO₂(110) surface by HREELS in vacuum [1], HOH bending mode of monolayer water is located at 1605 cm⁻¹. In addition, the band strongly depends on the rotation of the sample. Thus, we assigned the band to the monolayer water on the TiO₂(110) surface in air. These features of the band are probably caused by the resonance not only to the vibrational mode but also to the electrically excited state of surface defect site. This strong and sharp band enables us to study ultrafast dynamics of monolayer water on an oxide surface, so we carried out pump-probe measurements.

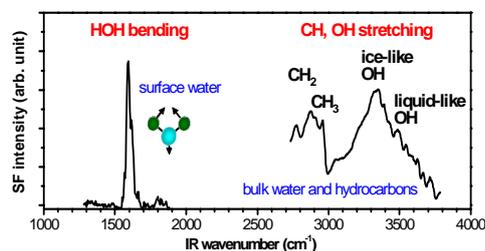


Fig.1. VSFG spectrum of TiO₂(110) in air.

[1] M.A. Henderson, *Surf. Sci.* **335**, 151 (1996).