An infrared spectroscopic approach towards understanding the orientation of dangling OH bonds on amorphous solid water

T. Nagasawa,[1] T. Hasegawa[1] N. Numadate,[1] T. Hama[1]

[1]*Komaba Institute for Science, The University of Tokyo, Japan*

The surface reaction on amorphous solid water (ASW) is the key to figuring out the chemical processes in interstellar molecular clouds, where stars and planets are being born [1]. Macroscopic properties of ASW such as heat transfer coefficient [2], surface potential [3] have progressively become understood through intensive research. By contrast, our understanding about the microscopic structure of ASW is still at an early stage. For example, there is almost no experimental study about the molecular orientation in ASW, which is a key factor to control the physicochemical properties of organic thin films [4], due to the lack of direct measurement technique. Recently, we built an experimental apparatus for low temperature ultrahigh vacuum infrared multiple-angle incidence resolution spectrometry (IR-MAIRS [4][5]. IR–MAIRS is a spectroscopic method combining oblique incidence transmission measurements and multivariate analysis to retrieve both pure (in-plane; IP) IP and (out-of-plane; OP) OP vibration spectra for a thin sample. The method has the unique advantage that the average molecular orientation is determined by comparing the IP to OP band intensity ratio spectra on the absorbance scale. In this research, we report our recent IR-MAIRS results for dangling OH bands in ASW at 10 to 90 K. It is found that the average orientation angle of dangling OH bonds exhibit a drastic ice temperature dependence in the range of 10 to 90 K. The detailed results are presented in the poster.

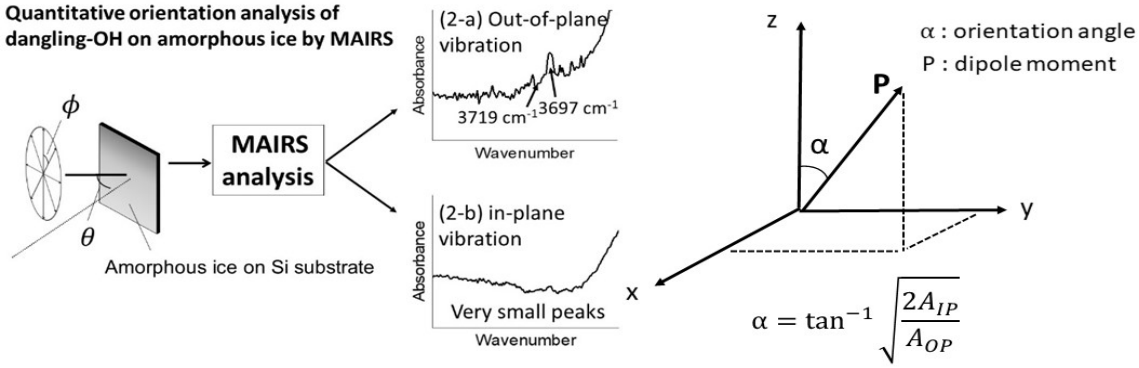

Figure: (left) Schematic illustration of IR-MAIRS. IR–MAIRS: Typical single-beam spectra measured at an angle of incidence of 45° at various polarization angles from 0° to 90° in 15° steps, and then extracting the IP and OP spectra by multivariate analysis.
(right) Molecular orientation analysis based on IR-MAIRS. The average orientation angle of molecules is determined by comparing the ratio of absorbance both IP and OP spectra.

References

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