

Detection of structured water on quartz interface by Raman-FTIR spectroscopy and its evaluation by molecular dynamics

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Molecular structure of water in thin film shows different characteristics compared with that of free water. Thin film water was observed at mineral grain boundaries, and its structure might be influenced by mineral surface.

High temperature-pressure cell for micro-Raman and Fourier-transform infrared (FT-IR) spectroscopy have been developed to investigate molecular structure of thin film water at high temperature and pressure conditions. As a result of micro-Raman and FT-IR spectroscopic measurements of water, the broad peak around 3400 cm^{-1} , attributed to OH stretching vibration mode of water molecular, was observed at ambient temperature and pressure. The broad peak shifted to higher wavenumber with increasing temperature on metal reflector. Compared with the result of IR properties of water on metal reflector, IR properties of water on artificial quartz surface exhibit different trend: the broad peak contained the peak component of the lower wavenumber (around 3200 cm^{-1}), even at high temperature.

In addition, molecular dynamics simulations were performed under the conditions of the experiment using MXDORTO. In the simulation, the water of a few nanometers of quartz near the surface was structured. The distribution of water density was different from the free water. These properties are discussed in the hydrogen bond between water molecular and silanol (Si-OH) of quartz.

Keywords: Raman spectroscopy, IR spectroscopy, interfacial water, subcritical, quartz, molecular dynamics