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IR Spectroscopic studies of Water on Mineral and Water in Mesopores at High Temperatures and Pressures

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Geofluids have a significant role in Earth processes such as geochemical and geophysical processes. In both of pure Earth science and geoscientific engineering, Water-Rock interaction is essential reaction system under various natural conditions, covering wide ranges of temperatures-pressures and fluid environment. Accurate understanding of Water-Rock interaction is most fundamental and essential issue for further progress of the Earth's crust environmental engineering and science. Additionally, as results of previous studies, IR and Raman properties of water at HT & HP were different from ambient condition. And, interfacial water configuration on solid surface was changed by effect of solid surface structure. Therefore, in order to resolve Water-Rock interaction at HT & HP, a molecular-level investigation at HT & HP must be effective. In this study, to resolve Water-Rock interaction, IR-Raman spectroscopic system at HT & HP was developed and applied to spectroscopy of Water-Rock interface. And then interfacial water properties on various solid materials were investigated at HT & HP using IR spectroscopy. In order to investigate the effect of solid surface on interfacial water, IR spectra of interfacial water on various solid materials were measured at HT & HP. As results of IR spectroscopy of water on metal, IR spectra attributing OH stretching vibration of water molecules were detected from ambient condition to HT & HP. The peak band shifted higher value with increasing temperature and shifted lower value with increasing pressure. On the other hand, the peak position of water on quartz slightly shifted depending on pressure. This indicated that the interfacial water configuration on quartz didn't changed with pressure condition. Therefore, interfacial water on quartz was restricted and formed structured water layer. Results of IR spectroscopy indicated that the water properties changed depending on substrate, including temperature and pressure. In addition, in order to investigate the effects of physical structure of substrate on interfacial water, IR spectra of water in mesoporous silica were measured. As results, the peak positions of water in mesoporous silica were detected lower value than water on quartz. This indicated that water molecules in mesospace were more restricted than water on quartz, and water configuration became more ice-like. Furthermore, in the case of small pore diameter (3-20 nm), the peak positions of water were detected at lower wavenumber (ca. 3300 cm^{-1}). On the other hand, those were detected at higher wavenumber (ca. 3500 cm^{-1}) in the case of large pore diameter (30-50 nm). Additionally, the peak position drastically changed between 20 nm and 30 nm. This indicated that degree of restraint of molecular vibration of water changed depending of pore diameter. Therefore, physical structure of substrate also affected interfacial water properties, not only on temperature and pressure.

Based on the results of this study and previous studies, the possible structure of interfacial water molecules on quartz surface and water molecules in mesoporous silica were considered. And the thickness of interfacial structured water layer was considered. As results the thickness of structured water layer might be 10-15 nm.

According to the above findings, it is suggested that interfacial water properties changed depending on temperature, pressure and chemical composition and physical structure of substrate. Such structured water, which interacted with solid surface at HT & HP, is considered to relate Water-Rock interaction (dissolution, precipitation, hydrolytic weakening and HDF phenomena). In the Earth's crust, it is considered that water exist at restricted space (e.g. aperture of rock, grain boundary) under high temperature and pressure conditions. And this water might be possible origin of the Earth activity (Earthquake, Volcanism, Fault activity).