

IR spectroscopy of Water at Mineral interface under High Temperature and High Pressure conditions

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We have investigated dissolution behavior of granite at sub- and supercritical hydrothermal conditions. As a result, we found occurring of granite fracture under hydrothermal conditions. In our previous fracturing experiments using granite and quartz, rock fracturing were initiated by quartz fracturing, and quartz were well fractured at specific hydrothermal conditions such as about 350 - 500 °C and in relatively low pressures under dry steam conditions, which had been termed as Hydrothermally Derived Fracturing (HDF). In addition, this phenomenon was also observed to occur under natural hydrothermal conditions. Hydrothermal solution have shown great role to generate and accelerate fractures in rock and rock-forming mineral. In order to investigate effects of molecular behavior of water at interface on the rock surface for HDF, High Temperature-Pressure cell (up to 400 °C and 50 MPa) was developed. Using the cell and FT-IR and Raman spectrometer, which was attached with optical microscopy, therefore, in situ microscopic spectroscopy of interface between water and rock became possible at high temperature and pressure (HT & HP) conditions.

As results of IR spectroscopy of water on a metal, broad peaks at ca. 3400 cm⁻¹ attributed to OH stretching vibration of water molecules were detected. The peak shifted with changes in temperatures and pressures. With increasing temperature, the peak position shifted higher wavenumber. And the peak position shifted lower wavenumber with increasing pressure. This indicated that the peak wavenumber became to be close to the wavenumber of vapor (3700 cm⁻¹) with increasing temperature and shifted to the number of ice (3200 cm⁻¹) with increasing pressure. As results of IR spectroscopy of interfacial water on quartz, peak position shifted to higher wavenumber with increasing temperature but slightly effected with pressure. Compared with the result of IR absorption properties of water on a metal, IR absorption properties of water on quartz exhibit different trend. We infer surface structure of quartz surface may give effects on vibration of OH stretching and structure of water molecules. As results of IR spectroscopy of synthetic solution of quartz, IR properties of solution of quartz and water on a metal exhibited the same trend; peak position shifted higher wavenumber with increasing temperature and shifted lower wavenumber with increasing pressure. Compared with the result of IR spectroscopy of water on quartz, IR absorption properties of quartz solution exhibit different trend. Although slight peak shift of water on quartz was considered as influence of changes of water structure induced by quartz dissolution. IR properties of solution of quartz and water on a metal exhibited the same trend, therefore slight peak shift of water on quartz was considered as influence of not dissolution of quartz but water-quartz interaction.

As results of IR spectroscopy, it can be recognized that the peak of water molecules was changed by environmental conditions such as temperature, pressure and substrate. Surface structure of quartz surface may give effects on structure of water molecules. We can consider on a possible structure of water molecules on quartz surface. Interfacial water molecules interacted via hydrogen bonding with surface silanol molecule of quartz. This water-quartz interaction might influence water structuring on quartz surface. Thickness of structured water layer is uncertain, however the thickness was presumed thicker than it was assumed. Such water, interacted with solid surface at HT & HP conditions, is considered to accelerate HDF phenomena. Interfacial water at solid surface under HT & HP conditions should be studied to reveal the details of the change of the water molecules interacted with the surface of solid materials, and then the mechanism of dissolution and fracturing of mineral induced by water-rock interaction might be revealed.