In-Situ Monitoring Of Water-Rock Interaction By Micro FT-IR- An Example Of Calcium Silicate Hydrate Formation-

HIROKI BESSHO¹*, SATORU NAKASHIMA¹, MAI HAMAMOTO¹, NAOKI NISHIYAMA¹, RYOTA TONOUE¹, YUSUKE KIRINO¹, TADASHI YOKOYAMA¹ AND HIROSHI SASAMOTO²

¹1Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan (*Corresponding author: hbessho@ess.sci.osaka-u.ac.jp)
²Japan Atomic Energy Agency. Tokai 319-1194, Japan

In the geological disposal of high level radioactive wastes, cementitous grout materials are planned to be used and Calcium Silicate Hydrates (C-S-Hs) are supposed to be formed by water-rock interactions. The current study presents a new methodology of monitoring the C-S-H formation *in situ* by micro Fourier transform infrared (FT-IR) spectroscopy.

An *in situ* hydrothermal cell was constructed from titanium alloy with a diamond window to allow the transmission of an IR beam (Fig.1). In this study, thin sections of quartz were placed in the cell, with the remaining space filled with saturated Ca(OH)₂ solution. The *in situ* hydrothermal cell was then sealed and heated at 140 °C at a pressure of 3 MPa. IR spectra were collected every 5 minutes for 24 hours using an IR microspectrometer.



Fig.1 The schematic figure of the *in situ* hydrothermal cell Fig.2 Infrared spectral changes with time for 5 hours at 140 $^{\circ}$ C. The absorption band around 970 cm⁻¹ (C-S-H) increased with time.

An IR absorption band around 970 cm⁻¹ due to stretching vibration of Si-OH increased with time indicating the increasing formation of C-S-H (Fig.2). The temporal changes with 5 minute intervals of the peak heights in the first 240 minutes can be used to determine apparent formation rate constants of the C-S-H. Based on these experimentally determined kinetic parameters, mechanisms and rates of the C-S-H formation processes can be discussed.

Water in Na montmorillonite - A neutron scattering study

M. BESTEL^{14*}, F. JURANYI¹, T. GIMMI²⁴, M. A. GLAUS², L. R. VAN LOON², M. ZAMPONI³ AND L. W. DIAMOND⁴

¹Laboratory for Neutron Scattering, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

(*correspondance: martina.bestel@psi.ch)

²Laboratory for Waste Management, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

³Forschungszentrum Jülich, Centre for Neutron Science at FRM II, 85747 Garching, Germany

⁴Institute of Geological Sciences, University of Bern, 3012 Bern, Switzerland

Swelling clays, like Na montmorillonite, are important sealing materials for radioactive waste repositories. The negative charge of crystalline layers is compensated by cations surrounded by water in interlayers. At low hydration, all water is located in interlayers in up to 2 molecular water layers; at higher hydration, interparticle pores between clay particles also contain water.

To model and understand transport properties, e.g. water diffusion, it is important to know the water distribution at different hydrations and densities. Relative fractions of water in the two pore environments were measured directly and for the first time using Fixed Window scans on a neutron backscattering spectrometer. The decisive parameter was found to be the water content (total water / dry clay). In the range from 0 to 0.7 g/g the obtained water amount in the interparticle pores increases monotonically, but not linearly from 0 to 64%. These results were compared with values obtained based on surface area measurements.

They were also used to derive local diffusion coefficients from quasielastic neutron scattering. In the literature local diffusion coefficients can be found only for low hydrations (1 or 2 water layer) because of the difficulties in interpretation of the spectra when more than one water population exists. Here, from our combination of methods (quasielastic neutron scattering and fixed window scans) we can present local diffusion coefficients for up to 4 water layer in the interlayers.

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