2D ^{29}Si{^{1}H} heteronuclear correlation NMR studies of sorption site in Calsium Silicate Hydrate

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Bentonite and cementitious materials are installed as engineered barrier in low level radioactive waste disposal facility in japan. Some chemical reaction will be caused on the boundary between bentonite and cementitious materials such as alkali redaction and generation of precipitations. Calcium Silicate Hydrate (C-S-H) is one of most important precipitations formed by ion interaction because C-S-H is expected to adsorb radioactive nuclides. Several possibilities for adsorption mechanisms of radioactive nuclide for C-S-H are proposed because to clarify the mechanisms are important to evaluate long-term durability of engineered barrier. 2D ^{29}Si{^{1}H} heteronuclear correlation solid state NMR is performed to understand the adsorption mechanism of C-S-H in this study. The spectrum of synthesized C-S-H (Fig.1) shows chemical environment of ^{29}Si and ^{1}H[1]. Si in C-S-H bond two types ^{1}H, One is -OH group which can be adsorption site and the other is -OHCa group which can not be adsorption site. The fraction of -OH group/ -OHCa group is different depending on Ca/Si of C-S-H: low Ca/Si C-S-H, which adsorb more cation than high Ca/Si C-S-H, has larger number of -OH group. Adsorption for -OH group should be one possible mechanism and the number of -OH group, which is calculated by this NMR method, can be good index to show adsorptive capacity.

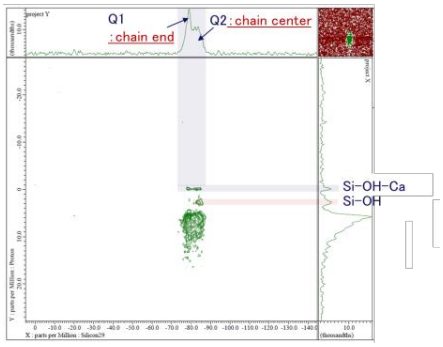

Fig.1 2D ^{29}Si{^{1}H} heteronuclear correlation solid state NMR spectrum of synthesized C-S-H

[1] Elizaveta Pustovgar, *et al.*(2016), Understanding silicate hydration from quantitative analyses of hydrating tricalcium silicates, Nature Communications 7, Article number: 10952