MITT.ÖSTERR.MINER.GES. 149 (2004)

SPECTROSCOPIC EXAMINATIONS OF THE STRUCTURE AND ALKALI SORPTION OF HIGHLY POLYMERIZED C-S-H PHASES

Bornefeld, M.[1], Gasharova, B.[1], Garbev, K.[2], Mangold, S.[1], Beuchle, G.[2] & Stemmermann, P.[2]

[1] Forschungszentrum Karlsruhe, Institut für Synchrotronstrahlung (ISS), P.O. Box 3640, D-76021 Karlsruhe, Germany
[2] Forschungszentrum Karlsruhe, Institut für Technische Chemie, Wasser- und Geotechnologie (ITC-WGT), P.O. Box 3640, D-76021 Karlsruhe, Germany
e-mail: marc.bornefeld@iss.fzk.de

Cement is an inorganic hydraulic binder widely used in civil engineering, etc. By the reaction of cement with water Calcium-Silicate-Hydrate (C-S-H) gel is the principal hydration product (TAYLOR, 1964). For example, building materials based on Portland cement could contain up to 70 wt% C-S-H gel. Therefore, the structure of the C-S-H gel is responsible for the mechanical properties of the hardened cement paste.

The composition of the C-S-H gels within the $CaO-SiO_2-H_2O$ system varies over a large molar CaO/SiO_2 (C/S) range: from about 0.5 in older and partly carbonated hardened cement pastes up to 2.2 in fresh ones. Even lower C/S are probable due to weathering of hardened cement pastes and deteriorative reactions like alkali-silica-reaction (ASR). The latter leads to the formation of highly polymerized, alkali bearing C-S-H gels. The formation processes and the structure of these gels are widely unknown.

The existing models for the structure of C-S-H gel, mainly based on the structures of the crystalline C-S-H phases tobermorite and jennite, are suitable only for C-S-H gels with C/S ratios between 2/3 and 3/2. Despite the widespread occurrence of highly polymerized C-S-H gels there is still no proposal for a structural model for C-S-H gels with a C/S ratio < 2/3.

Due to the lack of long range order, spectroscopic methods such as FT-IR, XAFS and NMR are of great relevancy for structural investigations of the C-S-H gels. First results from these spectroscopic methods will be discussed and gain an insight in the structure and formation processes of alkali bearing highly polymerized C-S-H gels.

IR spectra of several C-S-H gels with C/S ratios varying between 0.2-1.5 and different alkali concentrations have been recorded at the IR-Beamline at ANKA (Angströmquelle Karlsruhe). The IR spectra of our samples clearly demonstrate systematical high frequency shifts of the Si-O-Si stretching vibrations with decreasing C/S ratio, thus indicating an increasing of the polymerization of the silicate structure (YU et al., 1999). In the OH stretching region a systematical shift of the broad absorption band provides useful information about changes of the H_2O environment upon varying C/S ratios. Additionally to the IR data, XAFS measurements at the Ca absorption edge provide detailed informations about the local environment around the Ca atom. ^{29}Si NMR data provide informations about the degree of polymerization of the SiO_4-tetrahedra in the gel structure.

References

TAYLOR, H.F.W. (1964): The Chemistry of Cements. Academic Press, London, New York. 168 p.

YU, P., KIRKPATRICK, R.J., POE, B., MCMILLAN, P.F. & CONG, X. (1999): J. Am. Ceram. Soc., **82**: 742-748.