

Investigation of Cement and Fly Ash samples by X-ray Absorption Fine Structure (XAFS) Spectroscopy and X-ray Diffraction

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ABSTRACT

Seven cement samples and one fly ash sample have been investigated by Ca and S K-edge x-ray absorption fine structure (XAFS) spectroscopy and by X-ray diffraction (XRD). The XRD analysis revealed that these samples are a complex mixture of three Ca-rich compounds, hannebachite, gypsum, and thaumasite, with a small amount of quartz. In view of the complex coordination chemistry of Ca in these compounds, it was difficult to obtain detailed information on the local atomic environment of Ca through direct computer analysis of the extended x-ray absorption fine structure (EXAFS). Nevertheless, it was possible to identify different Ca-containing phases through simple comparison of the Ca K-edge x-ray absorption near edge structure (XANES) and radial structure functions (RSF) of the cements to those of known reference compounds. Deconvolution of the S K-edge spectra indicates that sulfate and sulfite are the two major sulfur forms; these can be attributed to gypsum and thaumasite, and to Hannebachite, respectively. This is in agreement with our findings from Ca K-edge XAFS and XRD. Furthermore, the S XANES spectra exhibit a systematic increase in sulfate and a corresponding decrease in sulfite, as a result of gypsum and thaumasite formation with decreasing hannebachite content.