GEOC: Division of Geochemistry

29 - Structural insights on Ni-Al LDHs using wavelet analysis

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Abstract: Nickel-aluminum layered double hydroxides (Ni-Al LDHs) serve as environmentally important minerals in contaminated soils. During Ni-Al LDH formation, Ni is removed from the soil solution and immobilized in the solid phase LDH. X-ray absorption spectroscopy (XAS) has often been used to identify Ni-Al LDHs and characterize their structure. In the Fourier transformed (FT) EXAFS spectra of Ni-Al LDHs, the first metal shell to the central absorbing Ni atom is a mix of two metals, both Ni and Al. Wavelet transformation (WT) of the k-weighted EXAFS data takes advantage of this property. In WT plots, two separate maxima at different wavenumbers confirm the presence of both “heavy” Ni and “light” Al backscattering atoms in the first metal shell and hydroxide layer. However, upon examining layered single metal hydroxide standards [e.g., $Ni(OH)_2$] using WT, the same WT plots as Ni-Al LDHs and a nickel phyllosilicate were found. This finding is opposite to the hypothesis that a single metal hydroxide should have just one maximum in the WT plot, not two. This presents a problem when using WT to identify or confirm Ni-Al LDHs found in soils or prepared in the laboratory. During LDH preparation, nitrate or carbonate groups may remain adsorbed to the hydroxide layer. In the WT plots, those groups may appear as a lighter backscatterer, similar to the effect of Al. Performing WT on the second and third metal shells of the Ni-Al LDH and $Ni(OH)_2$ reference spectra is a possible solution to this problem. Those shells are composed of focused multiple scattering involving both Ni and Al in the hydroxide layer and should not be affected by anions adsorbed to the hydroxide layer.