

Water structure and hydration properties of imogolite nanotubes

A. FERNANDEZ-MARTINEZ¹, G.J. CUELLO²,
I.C. BOURG¹, M.R. JOHNSON¹, G.A. WAYCHUNAS¹,
G. SPOSITO¹ AND L. CHARLET³

¹Geochemistry Dept. Earth Sciences Division, Lawrence
Berkeley National Laboratory, Berkeley, USA

²Institut Laue-Langevin, BP 153, Grenoble, France

³Environmental Geochemistry Group, LGIT-UJF, Grenoble,
France.

Imogolite is a nanotubular aluminosilicate present in the clay fraction of volcanic soils. It has high specific surface areas (~500 m²/g) and is one of the few minerals reactive towards both anions and cations under the same soil physico-chemical conditions, properties which make it an important constituent of the soils where it is present. However, precise determinations of imogolite structure and geochemical reactivity have been hindered by its nano-crystalline character. Structural analyses, until now, were restricted to standard X-ray and electron diffraction techniques, the diffraction peaks being used mainly as fingerprints for the identification of the mineral in soils. In this work, we present a detailed structural characterization of the structure of synthetic imogolite using high-energy X-ray diffraction (HEXRD), neutron diffraction with isotopic substitution (NDIS), transmission electron microscopy (TEM), and molecular dynamics (MD) simulation methods.

Theoretical and experimental investigations of the structure of water at the imogolite – water interface revealed the presence of highly structured water shells both at the surface and inside the nanotubes. We used these structural inputs to develop a geochemical multi-site complexation (MUSIC) model of the acidity of surface Al₂-OH groups on the external surface of imogolite and compared this to the acidity of similar sites on the equivalent (but planar) surface of gibbsite. This comparison yielded insights into the influence of surface curvature on mineral reactivity. Our MD simulations also probed the energetics of water adsorption and revealed that the external surface of imogolite is more hydrophobic than that of gibbsite. Ongoing work involving the use of inelastic neutron scattering also will be presented and discussed.

Anisotropy of magnetic susceptibility of Triassic Red Beds, Central Portugal

C. FERREIRA¹, C. GOMES^{2*} AND H. SANT'OVAIA³

¹DCT, Universidade de Coimbra, Portugal

^{2*}CGUC, DCT, Universidade de Coimbra, Portugal

(*correspondence: romualdo@dct.uc.pt

³Centro de Geologia da U. Porto, DGAOT, FCUP, Porto,
Portugal.

Three sites in the Conraria and Castelo Viegas Formations, belonging to the "Silves Group" of Upper Triassic age, in the Coimbra region, central Portugal, were studied using the Anisotropy of Magnetic Susceptibility (AMS) methodology. The Conraria Formation is the lower unit and has mean thickness of 160 ± 15 m. The Castelo Viegas Formation is thicker (170-190 m) and the sediments are generally coarser and lighter than the sediments of the Conraria formation. The main goal of this study is to compare the AMS of the of the Conraria Formation, site A, with the two levels from the Castelo Viegas Formation, sites B and C. Site B is on a lower stratigraphic position than site C. AMS were carried out on 99 samples, 45 from site A, 10 from site B and 34 from site C. The magnetic susceptibility ranges between 40.6 and 239.7 x 10⁻⁶ SI in site A, between 64.4 and 100.0 x 10⁻⁶ SI in site C and between 51.5 and 58.4 x 10⁻⁶ SI in site B. Magnetic anisotropy (described by the parameter (k_{max}/k_{min}-1) x100) ranges between 0.4 and 8.3% in A, from 0.7 to 0.8 % in site C and between 2.3 and 3.0% in site B. The AMS ellipsoid is dominantly oblate in A and in site B, however site C present both oblate and prolate AMS ellipsoids. AMS fabric show different patterns in the studied sites: NW-SE subhorizontal magnetic foliations associated with subhorizontal N-S trending magnetic lineations in site A; N-S subvertical magnetic foliations associated to N-S trending magnetic lineations in site B; and scattered AMS ellipsoid axes in site C due to its lower anisotropy. Our results show that sites A and site C have higher magnetic susceptibility than site B which is related with mineralogical composition. Sites A and B have a magnetic foliation that probably underlines a primary sedimentary fabric however this foliation has tilted in site C. The N-S magnetic lineation probably materializes the paleocurrents. The general parallelism of the magnetic fabric with bedding indicates a composite fabric between a primary sedimentary fabric and an early tectonic event as is attested by the magnetic anisotropy of Conraria formation and site B of Castelo Viegas Formation.