The Ordovician Galiñeiro peralkaline gneiss complex, Vigo, NW Spain

PETER FLOOR¹, GUILLERMO CORRETGÉ² AND PILAR MONTERO³

¹van Beuningenlaan 24, 2334 CC Leiden, Netherlands (floor.p@planet.nl)

²Dept of Geology, Univ. Oviedo, 33005 Oviedo, Spain (corretge@geol.uniovi.es)

³Dept of Mineralogy and Petrology, Fac. Sciences, Univ. Granada, 18002 Granada, Spain (pmontero@ugr.es)

The Variscan mountain chain in Brittany (France), NW Spain, Portugal and SW Spain contains numerous orthogneiss complexes of early Paleozoic age, predominantly cropping out in the central zone of the orogen. Most have calcalkaline, alkaline and some peralkaline compositions. The first two are cut by numerous basic dikes.

The Galiñeiro peralkaline complex, situated mainly South of the city of Vigo near the Atlantic coast, is the largest and best investigated of these complexes. Fieldwork and petrographic studies done by the first author in the fifties and sixties of last century were followed in the eighties and nineties by detailed mineralogical and geochemical work by the third and second authors.

The results of both studies are highly complementary and give evidence of rock and mineral behaviour both at the intrusive stage and under Hercynian lowP, intermediateT metamorphic conditions leading to strong recrystallization, including total unmixing of the supposed original hypersolvus feldspar.

The rocks of the complex are enriched in REE and HFSE, present in a wide variety of accessories: bastnäsite, REE silicates (e.g., allanite, thalenite-yttrialiet), REE niobotantalates (aeschynite, fergusonite-formannite, samarskite, pyrochlore-betafite), REE phosphates (monazite, xenotime), Th-rich minerals (thorite, P-rich thorite), and zircon.

Magmatic fractionation, most likely from a mantle-derived volatile-rich alkaline basalt parent, led to peralkaline silicic differentiates with residual fluids extremely enriched in fluorine and other ligands, which complexed the REE and HFSE. Decrease in fluorine activity with falling temparature and the crystallization of F-bearing major minerals caused the breakdown of complexes, releasing the rare earths and the remainder of the high-field-strength elements, and formation of HFSE- and REE-rich minerals.

The elevated fluorine, CO_2 and sulfide contents of the Galiñeiro system, together with the energy inputs of the different phases of Hercynian metamorphism, caused episodic remobilisation, reflected by the zircon U—Pb concordant ages at 370 and 310 Ma, and the exotic geochemical features (Zr/Hf > 100, elevated levels of Be, Th, and HREE) of some samples.

Reference

Montero, P., Floor, P., and Corretgé, G. (1998) *Can. Miner.* **36**, 638–700.

The functional species of a mineral surface and their interaction with the adjacent water molecules – Determined by nonlinear optics and quantum chemistry

M. FLÖRSHEIMER,¹⁻³ K. KRUSE,^{1,3} R. POLLY,^{1,3} A. Abdelmonem,^{1,3} B. Schimmelpfennig,^{1,3} R. Klenze,^{1,3} and Th. Fanghänel²⁻⁴

- ¹Institute for Nuclear Waste Disposal, Forschungszentrum Karlsruhe, Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany (florshg@ine.fzk.de)
- ²Institute of Physical Chemistry, University of Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany

³Virtual Institute Functional Properties of Aquatic Interfaces, Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

⁴European Commission, Joint Research Centre, Institute for Transuranium Elements, Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

The functional species of the mineral surfaces, which control the mineral/water interaction, are not definitely known for most crystal faces because it is difficult to obtain chemical in situ information with interface selectivity. Here we apply interface selective vibrational sum frequency spectroscopy to the sapphire (001) surface. Additionally we carry out density functional theory and ab initio calculations on aluminium-oxide clusters as models for the sapphire (001) surface. The results of experiment and theory are well in agreement. This work is part of an ongoing fundamental study of the sorption mechanism of actinides on single crystal faces by various experimental and theoretical techniques. Sapphire serves as a simple model for natural clay minerals.

From the ideal termination of the bulk crystal structure, the (001) surface is expected to exhibit a single type of aluminol species with the OH group in a bridge position. We distinguish four OH species which are all doubly coordinated but exhibit different tilt angles of their OH bonds. Depending on the tilt, different geometries arise for hydrogen bonding with water molecules. At high pH the interaction of the mineral surface with the neighboring water molecules is dominated by electrostatic forces. The net dipole moment of these water molecules points into the direction of the mineral surface which is in agreement with the expected negative surface charge. In the pH range between 1.3 and 6 the interaction of the water molecules with the mineral surface is dominated by hydrogen bonds. Two populations of water molecules exist near the interface which are characterized by specific hydrogen bonding to the different aluminol species. Due to these bonds the net dipole moment of one water population points to the mineral surface, the net dipole of the other population points into the opposite direction. Since the relative concentrations of the different aluminol species depend on the pH, the relative concentrations of the two water populations changes also. In summary, a picture at the molecular level with surprising richness of details is obtained.