Mesoarchean hydrous upper mantle: Evidence from the Fiskenæsset Complex, SW Greenland

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The Fiskenæsset Complex, SW Greenland, contains the world's best preserved Archean (~2970 Ma) layered anorthosite, leucogabbro, gabbro, and ultramafic rock association. The ultramafic rocks consist mainly of olivine-pyroxene hornblendites, peridotites, dunites, and pyroxenites. The complex appears to have been emplaced into Archean oceanic crust (now amphibolite) and later intruded by tonalites, trondhjemites and granodiorites (TTGs). The complex and bordering TTG intrusions and mafic volcanic rocks were variably affected by granulite facies metamorphism and retrogressed under amphibolite facies conditions. Despite poly-phase deformation and amphibolite to granulite facies metamorphism, primary igneous structures and intrusive relationships are well preserved in many outcrops in the complex [1-3]. The Fiskenæsset ultramafic rocks share many petrographic characteristics of unmetamorphosed mafic to ultramafic layered intrusions and Alaskan-type ultramafic complexes. In ultramafic rocks, many orthopyroxene grains occur between amphibole and olivine grains and contain an intergrowth of symplectitic (vermicular) magnetite. These orthopyroxene-magnetite intergrowths appear to have grown at the expense of olivine. The origin of the orthopyroxene-magnetite symplectitic intergrowths is attributed to chemical reactions between residual, hydrous, hornblende-forming melts and olivine. In several locations, the Fiskenæsset ultramafic sills were intruded by a network of 5 to 40-cm-thick hornblendite veins. Given that horblendites and hornblende-bearing gabbros and peridotites are mainly restricted to Phanerozoic supra-subduction zone ophiolites and magmatic arcs, it is suggested that the Fiskenæsset Complex represents a relic fragment of a Mesoarchean oceanic island arc. The trace element systematics of the Fiskenæsset layered rocks and spatially and temporarily associated basaltic amphibolites and TTGs also indicate that these rock suites originated in an oceanic island arc setting. Petrographic observations and geochemical data provide strong evidence for a hydrous sub-arc mantle source for the igneous Fiskenæsset layered intrusion. Amphibole (mostly hornblende) occurs as an interstitial mineral to olivine, pyroxene, plagioclase, chromite and chrome-spinel and as inclusions in these minerals in the cumulates, consistent with an igneous origin. It is suggested that water was recycled to the source of the Fiskenæsset rocks through subduction of altered oceanic crust. Recycling of water to the upper mantle not only resulted in the generation of igneous amphibole in the complex, but it may also have contributed to the generation of neighbouring TTG-dominant continental crust by Archean subduction processes.

[1] Polat *et al.* (2009) *Precambrian Research* **175**, 87-115. [2] Polat *et al.* (2010) *Chemical Geology* **277**, 1-20. [3] Polat *et al.* (2011) *Lithos* **123**, 50-72.

Sorption and incorporation of radio-nuclides at mineral surfaces studied with quantum chemical methods

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The reliable long-term prediction of actinide migration in geological formations requires understanding of the adsorption/desorption and incorporation mechanism at the molecular level. The sorption and incorporation of metal ions at mineral surfaces is a very important process which leads to the retention/retardation of radionuclides such as actinide ions and fission products.

We present three different investigations in this talk: (1) the interaction of trivalent lanthanides and actinides with the solvated corundum (110) surface, (2) interaction of selenite with the hydrated calcite surface and (3) the incorporation of trivalent lanthanides and actinides in calcite. Study (1) is carried out with orbital based ab inito and DFT methods using TURBOMOLE, whereas (2) and (3) with plane-wave DFT, as implemented in the Vienna Ab initio Simulation Package (VASP).

The corundum (110) surface is a challenging task for a theoretical investigation because singly, doubly and triply coordinated aluminol groups are present simultanously. We used the $Al_{27}O_{75}H_{67}$ cluster in this study as a model system for the corundum (110) surface. In a first step, we determined the structure and deprotonation properties of this cluster and calculated the vibrational frequencies of the surface aluminol groups. These results are compared with experimental data to validate our cluster model. In a second step we determined the structure of the inner-sphere complexes of the trivalent lanthanides and actinides at the surface. Various multidentate surface bound inner-sphere complexes are found to predominate. They are characterized and compared with experimental results.

Se-79 is a fission product of U-235 with a long radioactive half life of $1.1x10^6$ years. Selenite (SeO_3^{2-}) and selenate (SeO_4^{2-}) interact only weakly with common mineral surfaces. Therefore they have been identified as crucial radio nuclides for long term safety assessments of nuclear waste disposal. We determined the structure of the water/calcit interface and identified surface sorbed and incorporated selenite species at the calcite/solution interface.

The last point tackles the incorporation of trivalent lanthanides and actinides into calcite. Earlier spectroscopic investigations suggest incorporation of lanthanide/actinide ions occupying Ca-sites in the calcite lattice. Charge compensation is achieved by the substiution of two Ca atoms by one trivalent lanthanide/actinide and one Na ion. Here, we studied modifications of the calcite structure induced by the substitution.