Characterization and identification of minerals in rocks by ToF-SIMS and principal component analysis

S. RINNEN[1]*, C. STROTH[1], A. RISSE[2],
C. OSTERTAG-HENNING[2] AND H.F. ARLINGHAUS[1]

[1]Physikalisches Institut, University of Muenster, 48149 Muenster, Germany
(*correspondence: stefan.rinnen@wwu.de)
[2]Bundesanstalt fuer Geowissenschaften und Rohstoffe, 30655 Hannover, German (Christian.Ostertag-Henning@bgr.de)

For a variety of geoscientific topics a technique which unambiguously identifies minerals in rock samples would be very advantegous. In addition to optical methods, chemical mapping on the element level with different techniques has gained importance during recent years. For investigating gas-fluid-rock reactions it is important to be able to detect small secondary minerals and mineral alterations formed during the reactions – in combination with a high spatial resolution this could be achieved by mapping the incorporation of isotope labels. Therefore, a method using time-of-flight-secondary mass spectrometry (ToF-SIMS) is being developed that aims at identifying minerals and mineral alterations.

ToF-SIMS has the advantage that the entire mass spectrum is recorded quasi-simultaneously, so that a great number of elemental and molecular ion signals can be used to characterize the minerals. Here, the statistical method of principal component analysis (PCA) is a powerful tool for identifying the ion signals with great differentiation potential between individual minerals. We have used ToF-SIMS and PCA to analyze various rock-forming minerals. A spectral library was produced for all minerals investigated. For this, positive and negative ToF-SIMS spectra were taken from polished grains of rock-forming minerals (silicates, carbonates, sulfates, oxides, etc.). Signals from elemental and molecular ions that allocate to at least one of the minerals were used for the PCA analysis.

Afterwards, we used ToF-SIMS to image areas of rock samples containing unknown minerals. Spectra from individual zones were extracted and used to identify these minerals either by comparing them with the spectral library or by PCA analysis. The data clearly show that the high lateral resolution achievable with ToF-SIMS is very advantageous for the detection and identification of e.g. small newly formed phases of minerals at the edges of other components. Additionally, PCA was successfully used to classify silicates according to their crystal structures by comparing SixOy signal ratios and chemical compositions.

Assessing the factors controlling the temporal variations of weathering fluxes in a tropical watershed: Mule-Hole (South India)

J. RIOTTE[1], J.J. BRAUN[1,2], J.C. MARECHAL,
A. VIOLETTE[1], P. DESCHAMPS[1,3], L. RUIZ[4], C. LAGANE[1],
M. SEKHAR[2], S. SUBRAMANIAN[2], C. KUMAR[2]
AND S. AUDRY[1]

[1]GET, UMR 5563, UPS-IRD-CNRS 14 av. E. Belin 31400 Toulouse, France
[2]IFCWS, Indian Institute of Science, Bangalore 560012 India
[3]CEREGE, CNRS-Aix-Marseille University, BP80 13545 Aix-en-Provence, France
[4]INRA, UMR1069, SAS, 35000 Rennes, France

We investigated the present-day and long term weathering and erosion fluxes in tropical forested watershed (Mule Hole, South India). The watershed, monitored since 2003, is located in the sub-humid zone (MAR = 1100mm/yr) of a sharp climatic gradient induced by the Western Ghats and mostly fed by the South West monsoon.

The present-day evapotranspiration from the forest accounts for 85% of the annual rainfall, with two major consequences: (1) limitation of groundwater recharge and disconnexion with the stream, and (2) limitation of the stream flow, which is highly ephemeral [1]. However, the stream deconvolution indicates that almost 80% of dissolved species but Na transited through the vegetation as a result of leaf recretion and litter decay. These results emphasis the ambigous role of the vegetation that limits the runoff but enhances dissolved fluxes in the stream.

The present-day denudation rate is 28mm/kyr. It is dominated by erosion, ~25mm/ky, and by groundwater flux, 3mm/kyr, whereas the dissolved flux in the stream is very low, 0.3mm/kyr. The long term -100kyr- denudation rate was measured by ^{10}Be on the stream bedload. It accounts for only one third of the present-day value which means that the watershed experienced much lower erosion fluxes during the last climatic cycle, likeky under drier climate. This is confirmed by the occurrences of pedogenic carbonates in the basin soils. Their U-Th datings reveal the coexistence of several generations, essentially during the Last Glacial Maximum and to a lesser extent during the Holocene [2]. Rainfall conditions during the carbonate formation were semi-arid (MAR= 400 to 700mm/yr), i.e. enough for deepening the weathering front, but not for maintaining erosion fluxes.

[1] Maréchal *et al.* (2009) *J. Hydrol.* **364**, 272–284.
[2] Violette *et al.* (2010) *Geochim. Cosmochim. Acta* **74**, 7059–7085.