Meteorite classification by TOF-SIMS-chemometrics

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Introduction

Grains from eight different meteorites (ordinary and carbonaceous chondrites and a Martian meteorite) from the collection of the Natural History Museum Vienna were prepared on gold targets for time-of-flight secondary ion mass spectrometry (TOF-SIMS). The work is related to measurements of cometary particles by the COSIMA instrument [1] on board of the ESA spacecraft Rosetta.

Methods

(a) Mass spectra have been measured with a laboratory twin instrument of the COSIMA instrument on-board Rosetta. Main parameters are: primary ions ^{115}In, 6 ns pulses, 8 keV, 2 kHz; measurement spot 50 μm x 70 μm; secondary ions 3 keV; ion reflector; *m/z* up to ca 3000, positive or negative ions, mass resolution ca 1200. The built-in camera COSISCOPE makes pictures with 1024 x 1024 pixel (14 μm diameter) of the 1 cm x 1 cm targets.
(b) The ion counts of the signals in defined mass intervals for inorganic ions are summed to give peak heights at integer masses; e. g., at *m/z* 24 in the interval 23.896 - 24.017 (^{24}Mg has mass 23.985). Peak heights are normalized to a constant sum of 100 in each spectrum. For multivariate data analysis *m/z* 1-114, and 116-300 are considered (excl. ^{115}In). A set of 729 spectra, each with 299 normalized peak heights, was used.
(c) Chemometric methods applied were mainly principal component analysis (PCA) and k-nearest-neighbor (KNN) classification. KNN was applied together with the strategy repeated double cross validation (rdCV), allowing an independent optimization of the models and cautious estimations of the classification performances [2].

Results

KNN classification - evaluated with rdCV - yielded 93% correct assignment of the meteorite (mean of the results for all eight meteorites), which is similar to results for minerals using TOF-SIMS data from COSIMA [2]. Due to the heterogeneity (at a ca 50 μm scale) of the meteorite material the classification performance differs for the various meteorites. The spectra from, for example, the *Allende* meteorite are correctly assigned with 64% when reference spectra of this meteorite are only used from another grain. The available grains from the *Mocs* meteorite are very different from each other, allowing correct assignments only with reference spectra from the same grain.

Innovative aspects

(1) Signals from inorganic ions in TOF-SIMS data can be used for a preliminary classification of meteorites, provided appropriate reference spectra are available. (2) This classification is solely based on the inorganic contents of the sample surface. (3) Results are potentially relevant for the evaluation of spectra measured at the comet 67P/Churyumov–Gerasimenko.

[1] M. Hilchenbach et al.: Comet 67P/Churyumov–Gerasimenko: Close-up on dust particle fragments. *The Astrophysical Journal Letters*, 816:L32, 2016.
[2] K. Varmuza, P. Filzmoser, M. Hilchenbach, H. Krüger, J. Silén: KNN classification - evaluated by repeated double cross validation: Recognition of minerals relevant for comet dust. *Chemometrics and Intelligent Laboratory Systems,* **138**, 64-71 (2014).

This work is supported by the Austrian Science Fund (FWF), project P26871-N20.

Abstract for poster presentation at 27th Mass Spec Forum Vienna, 23-24 Feb 2016, Vienna, Austria