Correlation Based analysis of SIMS Data from Meteorite Samples for Comparison with Cometary Grains

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Abstract

We used the reference model of COSIMA, the TOF SIMS on board Rosetta to compare different meteorite samples, using correlation analysis to find references which allows us to characterize the cometary grains and to put them into the context of meteorite data.

1. Introduction

COSIMA is a time-of-flight secondary ion mass spectrometer on board the Rosetta spacecraft and is analysing cometary grains ejected off the nucleus of comet 67P/Churyumov-Gerasimenko since August 2014 [1]. In our effort to understand the composition and the history of these cometary grains, we studied the characteristics of different meteorite samples with the COSIMA reference instruments at the Max Planck Institute for Solar System Research in Göttingen (Germany), with the goal to separate individual compounds and their fragmentation patterns.

2. Method and Meteoritic Samples

Different types of meteorite samples were prepared in the laboratory. Among these were one ordinary chondrite H4 (Ochansk), one unequilibrated ordinary chondrite H3 (Tieschitz) [3], one carbonaceous chondrite CR (Renazzo) [2], and a Martian shergottite (Tissint) [4]. Grains of sizes up to 100 μm were pressed into a blank gold metal target. The grains were identified with the instrument microscope and positive and negative secondary ion mass spectra were accumulated on different positions on selected grains. The mass spectra are accumulating all secondary ions up to mass 300 with reasonable detection efficiency and a mass resolution of 1400@ 100 u. This mass resolution is sufficient to separate organic (hydrogen rich) molecule peaks from minerals or elemental mass peaks.

The obtained mass spectra were aligned to a reference mass spectrum taken from the same target but pointing the ion beam at the gold substrate instead of at the meteorite samples. This involves the remapping of the time/mass scale for each single spectrum used. The cross calibration is mandatory to get meaningful correlations between time of flight channels across different spectra.

The rebinned spectra were processed with a centred moving average filter with a width of 3 bins and then used to construct a correlation matrix S in which each element $r_{ij}$ is the correlation of the counts in time slot i with the counts in time slot j across a specific sample. Taking an individual column or row of the matrix, yields the correlation of a single time slot with every other time slot. As the time slots translate to specific mass to charge ratios, this method allows to gain information on which elements and molecules are related in the investigated sample.

3. Results

In this abstract, we show the correlation analysis of samples from Tieschitz and Renazzo. Figures 1 and 2 show the Pearson correlations of counts at the time slots, which translates to the mass of $^{56}$Fe, with the counts across different time/mass ranges for the Tieschitz sample in Figure 1 and the Renazzo sample...
in Figure 2. To keep the text concise from now on, we just write of “correlation of ion abundance at mass x with masses from range y to z”.

## 4. Discussion and Conclusions

As can be seen from the figures, there are some subtle and some larger differences between the samples from the H3 chondrite and the CR chondrite. Especially the correlations of $^{56}\text{Fe}^+$ (mass 55.93 u) with different masses in the 50 u to 80 u range show that iron may be associated with different elements in Tieschitz and in Renazzo. Tieschitz shows some correlation of iron with masses 55 and 71, which might be associated with Mn and MnO, while Renazzo does not show the corresponding correlation peaks.

This single element already shows that the two distinct samples can clearly been distinguished from each other by correlation analysis. This makes us confident in our use of this technique to further characterize the spectra of the cometary dust particles. However, the correlation analysis is just one step to really identify compounds from the samples. Other methods are also needed, e.g., to look at absolute and relative abundance of specific elements, etc. We continue to apply and improve these tools for the use with cometary data.

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### References


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**Figure 1**: Correlation of ion abundance at mass 55.93 u (iron) with masses between 50 u and 80 u from the Tieschitz sample.

**Figure 2**: Correlation of ion abundance at mass 55.93 u (iron) with masses between 50 u and 80 u from the Renazzo sample.