THE ROSETTA ALPHA PARTICLE X-RAY SPECTROMETER (APXS)

G. KLINGELHÖFER[1,*], J. BRÜCKNER[2], C. D'USTON[3],
R. GELLERT[4] and R. RIEDER[2]

[1]*Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität,
Staudinger Weg 9, D-55099 Mainz, Germany*
[2]*Max-Planck-Institut für Chemie, P.O. Box 5060, D-55020 Mainz, Germany*
[3]*Centre d'Etude Spatiale des Rayonnements, 9, Avenue du Colonel-Roche,
BP4346, F-31028 Toulouse CEDEX 4, France*
[4]*Department of Physics, University of Guelph, N1G2W1 Guelph, On, Canada*
(*Author for correspondence: E-mail: klingel@mail.uni-mainz.de)*

Abstract. The Alpha Particle X-Ray Spectrometer (APXS) is a small instrument to determine the elemental composition of a given sample. For the ESA Rosetta mission, the periodical comet 67P/Churyumov-Gerasimenko was selected as the target comet, where the lander PHILAE (after landing) will carry out in-situ observations. One of the instruments onboard is the APXS to make measurements on the landing site. The APXS science goal is to provide basic compositional data of the comet surface. As comets consist of a mixture of ice and dust, the dust component can be characterized and compared with known meteoritic compositions. Various element ratios can be used to evaluate whether chemical fractionations occurred in cometary material by comparing them with known chondritic material. To enable observations of the local environment, APXS measurements of several spots on the surface and one spot as function of temperature can be made. Repetitive measurements as function of heliocentric distance can elucidate thermal processes at work. By measuring samples that were obtained by drilling subsurface material can be analyzed. The accumulated APXS data can be used to shed light on state, evolution, and origin of 67P/Churyumov-Gerasimenko.

Keywords: comets, general: instrumentation: detectors: methods: analytical: space vehicles: instruments

Introduction

One of the key issues in cometary research concerns the identification of the chemical composition of the comet surface. For the ESA Rosetta mission, the periodical comet 67P/Churyumov-Gerasimenko was selected as the new target comet since the originally selected comet 46P/Wirtanen could not be reached due to launch delay. Several ways of detection of chemical composition will be applied: remotely through measurements of emitted particles and gas by instruments on board the orbiter and in-situ through measurements of the comet surface by instruments on board the Lander PHILAE. One of the lander instruments is the Alpha Particle X-Ray Spectrometer (APXS) that can determine all elements from carbon to nickel. These

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compositional data will be used in conjunction with other data to obtain information on the composition of the comet surface.

Scientific Objectives

The goal of the Rosetta APXS experiment is the determination of the chemical composition of the landing site and its potential alteration when the comet approaches the Sun. The data obtained will be used to characterize the surface of the comet, to determine the chemical composition of the dust component, and to compare the dust with known meteorite types. These results will be brought into context with other measurements made on the lander and the orbiter to fully obtain a more complete picture of the present state of the comet, and to get insight into its evolution and origin.

Most theories assume that comets are pristine objects that have been formed from primordial material of the early solar nebular preserving chemical evidence for the fractionations that occurred in the solar nebula (see below). Comets are located either in the Oort cloud or the Kuiper belt (Weissman, 1995). Observations of the Hubble space telescope confirmed the existence of objects in the Kuiper belt (Cochran *et al.*, 1995). However, comets coming from the Oort cloud could originally have been formed in the giant planets' region of the early solar nebula, where temperatures and hence compositions varied greatly (Mumma *et al.*, 1993). The measured ice compositions of four comets (Halley, Hyakutake, Hale-Bopp, and Lee) are consistent with formation in the region beyond Uranus, while the composition of comet C/1999 S4 (LINEAR) suggests that its ices condensed from nebular gas, probably in the Jupiter-Saturn region (Mumma *et al.*, 2001).

In current models of the chemical composition of comets, two main components are assumed to exist – a volatile component consisting of ices and a non-volatile one, often called dust (Mumma *et al.*, 1993). The dust component may carry the signature of the compositions of regions of the early solar nebula, where the comet was originally formed, either in the Jupiter-Saturn region or beyond. There has been a long discussion of a simple compositional model of comets whether as a dirty snowball or as a snowy dirtball. Recent observations after the artificial impact of the Deep Impact mission favor the latter model for the comet Temple 1 (A'Hearn *et al.*, 2005).

The chemical elements of a planetary body can be categorized according to their behavior during the condensation of the solar nebula. Volatile elements have low condensation temperatures; moderately volatile elements have medium and refractory elements high temperatures. These temperatures define the condensation sequence of the elements (Wänke and Dreibus, 1988; Palme and Jones, 2003). For comets, it is assumed that the refractory and moderately volatile elements are contained in the dust component, while most of the volatile elements form the

different ice components (Jessberger and Kissel, 1991). However, some elements that are classically considered to be volatile, such as bismuth, would not be part of the icy component.

Carbonaceous chondrites are a subgroup of the chondrites, a class of meteorites that likely originated on small asteroids during the early solar system and hence, are contemporary with the comets. CI chondrites are of specific interest because their chemical compositions closely resemble that of the solar photosphere, neglecting the hydrogen and helium (Palme and Beek, 1993; Lodders, 2003). They have the most 'primitive' compositions of any meteorites and are used as a standard for assessing the degree of chemical fractionation experienced by materials formed throughout the solar system. Chemical fractionations are expressed in relation to some normalizing element – usually Mg or Si. Fractionations observed in chondrites are in refractory elements, moderately volatile elements, and metal from silicate (Palme and Jones, 2003). The APXS determines key element ratios that can be used to evaluate whether these same fractionations occurred in cometary material. Thus, Na/Mg, Ca/Mg, Ti/Mg, Fe/Mg or Ni/Mg (or other ratios) are diagnostic for testing of known nebular fractionations.

Because of their small mass, it can be assumed that comets are the least differentiated bodies in the solar system as they could consist of primordial 'rubble piles' (Weissman, 1986). Presumably, they accreted in low-gravity fields and spent most of their time at extremely cold temperatures. However, differentiation of a body depends on several critical parameters: abundance of short-lived radioactive nuclides which serve as an internal heat source and, of course, its size. In absence of any significant differentiation of comets, it can be expected that the elemental abundances of H, C, N, and O are more similar to elemental abundances of the Sun compared to carbonaceous chondrites. The question of the origin of comets and of their relationship to CI chondrites is very essential as CIs contain the most primitive material ever analyzed in terrestrial laboratories, except for some of the interplanetary dust particles (Delsemme, 1991). Based on these considerations, it could be assumed that the composition of the cometary dust component resembles that of some carbonaceous chondrites, while the elemental concentrations of its icy component may resemble more that of the solar photosphere, except for H and He. The compositional data of the APXS may confirm similarities of the dust component to elemental ratios of CIs or other carbonaceous chondrites. Solid matter that accreted from the solar nebula, which is assumed to be rather homogeneous before condensation, can vary in composition as function of heliocentric distance.

The chemical composition of the surface of a periodic comet is modified during its perihelion passes compared to its original pristine character. A crust could have been formed during these thermal cycles at perihelion, where the upper layers lose most of their volatile components. Due to the capability of the Lander to rotate and drill, the APXS may provide in-situ analysis of samples at different locations and from different depth layers. These data will characterize the topmost surface and possibly can compare them with a depth profile of the upper subsurface

layers. Repetitive measurements of the same surface spot as function of heliocentric distance of the comet will reveal the chronological changes of the chemical composition of the outer layer (crust), and support characterization of processes at work. In addition, APXS data can be compared with measurements of orbital instruments that determine the ratio of dust to ice in the coma as function of time (Keller, 1990).

Instrument Description

The Alpha Particle X-Ray Spectrometer (APXS) is an instrument that provides data on the elemental composition of the comet surface. The instrument consists of an alpha mode for alpha spectroscopy (Rutherford backscattering) and an x-ray mode for alpha-particle and x-ray induced x-ray spectroscopy. The APXS combines these methods in one single instrument while being low in mass and power consumption. Historically, there was also a proton mode that has been omitted in the new design in favor of an advanced x-ray mode. The acronym "APXS" stands for the old and new design.

INSTRUMENT HISTORY AND RESULTS

The design of the Rosetta APX spectrometer is based on the experience gained with the APXS built for Russian and American Mars missions. The Russian Mars-96 spacecraft together with two landers and two penetrates, containing a total of four APXS, was lost shortly after launch at 1996 (Rieder *et al.*, 1997a).

Mars Pathfinder APXS
After landing of the NASA Mars Pathfinder (MPF) spacecraft on July 4, 1997, the APXS was deployed by the small rover Sojourner to several soil sites and for the first time to rock surfaces and data of their chemical composition were derived from measured x-ray spectra (Rieder *et al.*, 1997b). In the preceding Viking lander missions (1976/77), x-ray fluorescence spectroscopy could only be applied to soil samples as no rock could be reached by the surface sampler of the lander (a 3-m retractable boom-and-scoop assembly).

The MPF APXS was the first of a series of instruments to be very low in mass and power consumption compared to older APXS (Rieder *et al.*, 1997a). This miniaturization made it a unique tool for in-situ analysis. The performance of the MPF APXS permitted chemical characterization of the landing site. Chemical composition of soils and rocks on the Martian surface were derived that could not have been obtained otherwise (Brückner *et al.*, 2003).

The MPF soil composition is rich in sulfur (2 to 3 wt.%) and confirmed the mafic nature of the surface as inferred from the results of Viking 1 and 2 data (Clark *et al.*,

1982). For all rock samples, a correlation of sulfur with other elements were noticed, illustrating that the rocks were covered with varying degrees of soil. The MPF rover Sojourner did not carry any tool to clean the rock surfaces. Therefore, sulfur was used as a tracer for the amount of adhering soil and the composition of a soil-free rock could be calculated. The MPF rock composition is high in Si and K and low in Mg and Fe compared to the soil, hence revealing a new type of rock on the Martian surface that is felsic in nature (Rieder *et al.*, 1997b). Using elemental data from MPF rock and Martian meteorites, a global estimation of the Martian crust composition was derived. The crust is of basaltic nature with a high abundance of incompatible elements (K, Rb, Nd, U, Th) and volatile elements (S, Cl), while carbonates are low or absent (Brückner *et al.*, 2003).

Rosetta APXS

Although Rosetta was launched after the landing of the Mars Exploration Rovers (MER) on Mars in 2004, the Rosetta APXS is actually a predecessor of the MER APXS instruments. The Rosetta APXS flight instrument was delivered in mid of 2002 and underwent all environmental test required to be integrated within the lander. Therefore, we will compare the Rosetta APXS to its MPF precursor rather than the MER successor.

Compared to the MPF APXS the Rosetta design incorporated for the first time a new silicon drift detector for x-ray detection (Lechner *et al.*, 1996) that delivers a greatly improved energy resolution (180 eV at 6.4 keV compared to 250 eV on MPF, both at temperatures below $-40\,^{\circ}$C) allowing a much better separation of low energy x-rays. The Rosetta x-ray detector was moved into the center of the sensor head surrounded by the curium sources. This concentric setup is favorable from a geometric point of view. The alpha detectors are now arranged as a ring around the sources.

Overall the improvements of the Rosetta design gained about a factor of 10 in sensitivity in the x-ray channel compared to MPF. The MER design gained another factor of two in sensitivity due to a 10 square mm detector compared with the 5 square mm one on Rosetta and a different collimator structure.

Besides the Rosetta APXS instrument itself several other technical issues had to be solved during the development. For the comet nucleus lander of the Rosetta mission, a dedicated deployment device was needed that lowers the sensor head to the comet's surface. The development of this device fell into the responsibility of the APXS team, which designed, built, and tested it. The environmental challenges for the mechanics and the electric motor – temperatures extremes between $+50$ and $-150\,^{\circ}$C in high vacuum – had to be met before delivery. The required data interface with the lander computer unit CDMS – using a tailored, non-standard interface protocol – had to be adapted to the electronics of the instrument.

Mars Exploration Rovers APXS

For the two Mars Exploration Rovers (MER), an upgraded APXS was designed and a unit built for each vehicle (Rieder *et al.*, 2003). On January 2004, Rovers Spirit

and Opportunity landed at two widely separated landing sites: Gusev crater and Meridiani Planum (Squyres *et al.*, 2004). For more than 1000 sols (Martian days) the rovers and their instruments have been working flawlessly (to date of writing). Many discoveries were made based on the measured chemical composition of many samples at the Martian surface, as briefly mentioned below (Rieder *et al.*, 2004; Gellert *et al.*, 2004, 2006).

APXS at Rover Spirit. There are two geological regions at the Gusev landing site, the plains and the Columbia Hills. The plains contain soils that are very similar to previous landing sites on Mars. Rocks in the plains revealed thin weathering rinds. The underlying abraded rock surface was classified as primitive basalt. One of the trenches, the rover dug with her wheels, showed large subsurface enrichments of Mg, S, and Br. Disturbed (by rover wheels) soils and rocks in the Columbia Hills revealed different elemental compositions. These hill rocks are significantly weathered and enriched in mobile elements, such as P, S, Cl, or Br. Even abraded rock surfaces have high Br concentrations. Thus, in contrast to the rocks and soils in the Gusev Plains, the Columbia Hills material shows more significant evidence of ancient aqueous alteration (Gellert *et al.*, 2004, 2006).

APXS at Rover Opportunity. The chemistry of the other landing site at Meridiani Planum shows similarities and differences compared to Gusev crater. Chemical compositions differentiate between basaltic rocks, evaporite-rich sedimentary rocks, mafic soils, and hematite-rich soils. Although soils are compositionally similar to those at previous landing sites, differences in iron and some minor element concentrations signify the addition of local components. Rocky outcrops are rich in sulfur and variably enriched in bromine relative to chlorine. The interaction with water in the past is indicated by the chemical features in rocks and soils at this site (Rieder *et al.*, 2004).

METHOD

The Rosetta APXS is able to determine in-situ concentrations of elements from sodium to nickel using the x-ray mode. Light elements such as carbon and oxygen can be detected using the alpha mode. However, the measurement of hydrogen (and helium) is excluded by the physics of the method of alpha backscattering. In contrast to a Martian environment, where a 10 mbar thin CO_2 atmosphere interferes with the detection of C and O in samples, the vacuum on a comet surface facilitates the application of an alpha mode as hydro-carbon or organic compounds are expected on a comet. Thus, concentration data will be obtained by the APXS for a broad range of elements that will provide together with data from other instruments an improved understanding of the composition of the comet surface.

The Rosetta APXS consists of a sensor head, a deployment device, and electronics. The sensor head contains Curium-244 alpha sources that bombard the sample with alpha particles of an energy of about 5.5 MeV and x-rays of about 14 keV

(emitted by the Plutonium-240 daughter). As a result, alpha particles are backscattered and x-ray radiation is emitted by the sample. The back-scattered alpha particles are measured by six alpha detectors and the x-ray radiation by one high-resolution x-ray detector. Energy dispersive alpha and x-ray spectra are recorded. The x-ray mode detects most elements from sodium to nickel depending on their concentration (usually about 0.1 to 1 weight percent), while the alpha mode is sensitive to elements with low atomic weight, such as carbon and oxygen (concentration levels above ~1 weight %). However, determination of hydrogen is excluded due to the physics of the analytical methods.

The x-ray mode makes use of two excitation processes simultaneously: alpha-particle induced x-ray spectroscopy or particle induced x-ray emission (PIXE) and x-ray induced x-ray spectroscopy or x-ray fluorescence (XRF). This permits to determine elements with low and high atomic weight with rather comparable sensitivities. X-ray lines of low-Z elements (Na, Mg, Al, Si, P, S, Cl, and K) are mainly the result of PIXE, while lines of high-Z elements (Mn, Fe, Ni and higher Z) are mainly the result of XRF; the elements Ca, Ti, and Cr benefit from both excitation processes (Rieder *et al.*, 2003; Gellert *et al.*, 2006).

In the laboratory, the instrument was calibrated in vacuum measuring a geological sample, called SSK-1 (already used for the MPF APXS) with known composition in a standard geometry (distance between sample surface and detector). The data from this sample are used to compare the performance and sensitivity of the Rosetta APXS with MPF APXS and MER APXS. This cross calibration mainly determines the response function of the x-ray detector, namely efficiency versus x-ray energy and energy resolution and line shape. Using these instrument specific properties, the calibration of the Rosetta APXS can be achieved using the extensive MER calibration and future new calibration measurements tailored to cometary samples.

Provided a flawless docking on the surface of the comet will occur, the comet data can be directly compared with concentrations derived from laboratory samples measured in the same standard geometry. If a different geometry will be encountered, which will be probably the case due to irregular surface morphology, then, element ratios can be determined, first hand. A larger distance than the standard one reduces the amount of received radiation because of the inverse distance law of radiation and hence, results in a seemingly lower concentration of all detected elements (fake dilution). If all elements of a sample could be determined then the so-called closure to 100 percent can be calculated (the weight percent concentration of all elements must sum up to 100%).

Oxygen is determined with the x-ray mode using default oxides of all elements. If there is sufficient information on the encountered geometry from other observations (camera images), a geometry correction can be applied and estimations of the absolute elemental concentrations will be performed as done successfully for Martian samples (Gellert *et al.*, 2006). However, if sufficient amounts of organic compounds (containing H, C, O, or N) will be present, a real dilution of the siliceous compound will take place. This can be observed for most primitive carbonaceous

chondrites, where the sum of oxides (excluding H and C) for type CI and CM are well below 100 wt.%, typically ~76% and ~87% respectively.

Hydrogen is an invisible element for both APXS measurement modes, but, in lower concentrations the error of neglecting H will be rather small (low atomic weight). Carbon and oxygen are invisible for the x-ray mode, however, detectable by the alpha mode. Future calibration work using samples containing ice and organic material will establish a suitable evaluation method. In any case, concentration ratios of elements can be derived directly because for element ratios distance and dilution cancel out in first order.

For the instrument calibration the used samples are usually homogenous within the field of view of the sensor head. 'Homogenous' means there is the same composition in each unit area of the sample surface, i.e. the composition is not sensitive to a lateral movements of the sensor head. However, if we have a mixture of rock and ice particles, then the assumption of homogeneity is no longer given because these objects with different composition are smaller than the field of view. If this rock-ice mixture is a checkerboard-type arrangement at the top surface, the rock fragments
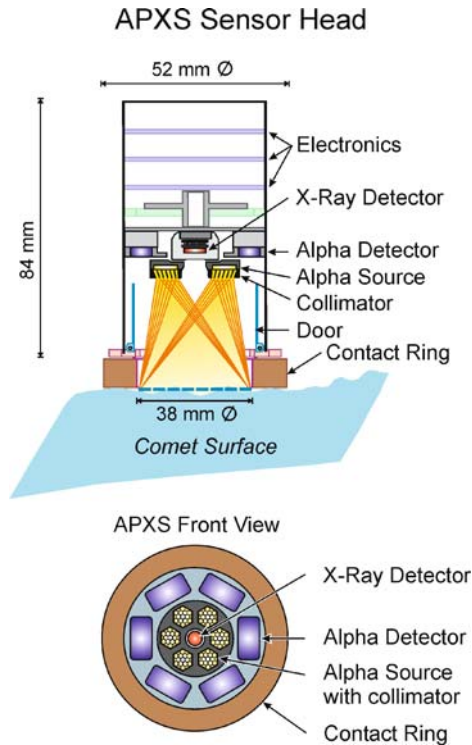

Figure 1. Functional scheme of the APXS sensor head in measurement position. The contact ring is retracted with doors in open position. The dotted line indicates the nominal sample distance from the detectors to the sample.

will yield 'true' element ratios. However, if rock fragments are positioned under a thin ice layer (thin enough with respect to x-ray penetration depth), elements with low energy x-rays will be attenuated more than the high energy x-rays. Thus, the Fe/Si ratio determined for the field of view will be incorrect. All cases where the sample is in-homogeneous with respect to lateral or vertical composition are strong caveats that have to be recognized by thorough imaging of the sample surface.

ROSETTA APXS DETAILS

The instrument performance, such as energy resolution and sensitivity, of the Rosetta APXS is greatly improved compared to the Pathfinder instrument, but, lower compared to the MER APXS. The arrangement of the Rosetta detectors and alpha sources is strictly concentric (Figure 1). The x-ray detector is in the centre of the front side. Six alpha sources (total of ca. 30 mCi $=$ 1.1 GBq of Curium-244) are placed on a circle around the centre of the sensor head at a movable holding device. On the outer periphery of the aperture, six alpha detectors are located concentrically to the alpha sources. The alpha detectors have a thickness of 300 μm, which makes them also sensitive to charged background particles. Therefore, they are
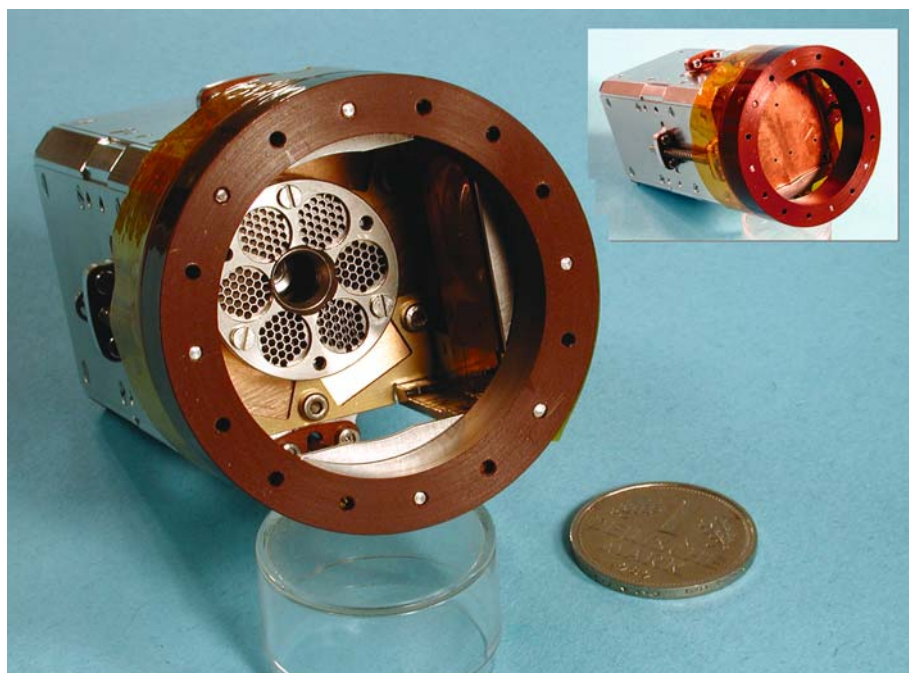

Figure 2. Front view of the APXS sensor head with doors open (contact ring retracted). Inset: doors closed (contact ring extended).

operated with lower than usual voltages so that they are not fully depleted (volume reduction). This decreases the sensitivity to cosmic or solar energetic particles.

The sensor head is located on the outside of the lander, mounted in an opening of the balcony's floor. To bring the APXS in contact with the comet surface, it is moved by the deployment device that can lower and raise the sensor head. The nominal working distance between detectors and sample is ~30 mm (standard geometry) and is defined by a cylindrical apron (Figure 2). The end is surrounded by a ring that moves inward when it is brought in contact with the surface and opens two protective doors. The backside of the doors (material composition is a copper-beryllium alloy: Cu98Be2) serves as a calibration target when in closed position. The nominal diameter of the surface sample is 25 mm. The sensor head and the deployment device are fully exposed to the environmental conditions of the comet.
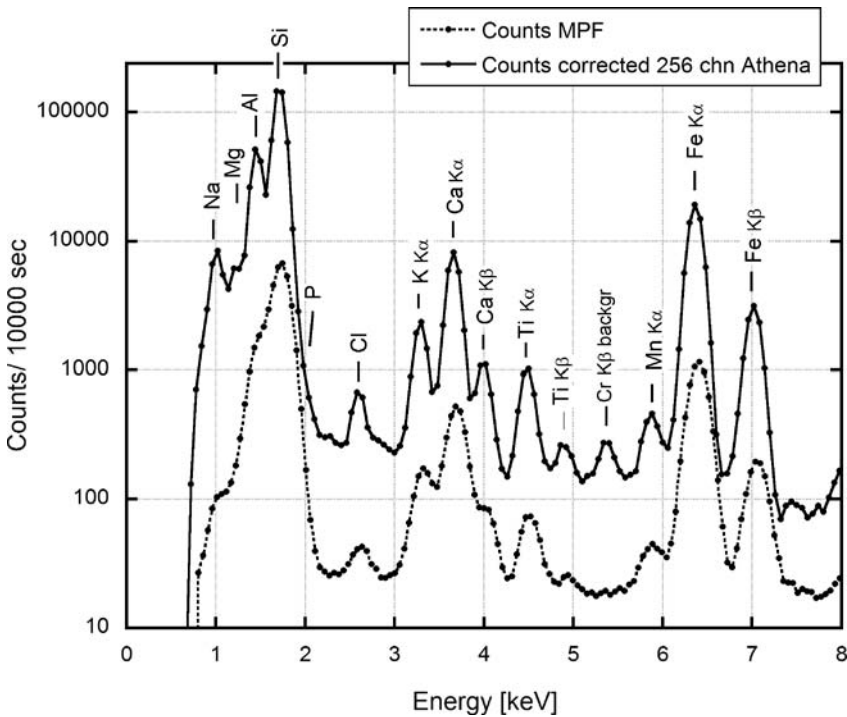

Figure 3. Comparison of two x-ray spectra, one obtained by a MPF-type instrument (dashed line) and one by a ROSETTA-type sensor head (straight line). The upper spectrum was compressed from 512 channels to 256 to permit a direct comparison with the lower MPF spectrum. Higher counting rates of the Rosetta APXS spectrum result from its higher sensitivity by a factor of 10 compared to MPF. The target was a terrestrial andesite (dubbed SSK-1) measured in a vacuum chamber at −40 °C. The energy resolutions of the 6.4-keV iron lines were: for MPF APXS 245 eV at −60 °C and Rosetta APXS 178 eV at −40 °C. Especially in the low-energy range (Na to Si), the improvement of the spectral resolution of the new APXS can be observed. Lower Z elements Na and Mg gain additionally from a custom made 5 μm Beryllium x-ray window compared to 8 μm for MPF.

The instrument was tested in a wide temperature range (down to $-150\,°C$) and the overall signal gain was found to be stable.

The energy resolution of the x-ray channel was significantly improved by replacing the previously used silicon pin diode by a newly developed high-resolution silicon drift detector system, originally described by Lechner *et al.* (1996). The energy resolution was improved from about 250 eV (MPF) to better than 180 eV. Advantages for the spectroscopy can be clearly seen in Figure 3. The energy range covered by the X-ray mode of the instrument has a adjustable lower threshold usually set to 1 keV, and a full scale energy increased from previously 12 keV (MPF) to 15 keV using the double amount of channels (512) in the x-ray spectrum (Figure 4). As a result of the new design the required integration time for x-ray could be reduced from about 10–12 hours to less than 3 hours for major and minor elements; trace elements as well as the alpha mode require more counting time to achieve sufficient counting statistics.

The alpha channel performance of the Rosetta APXS is significantly lower compared to the one of the MPF instrument (Figure 5). Nevertheless, the absence of an interfering CO_2 atmosphere (as in the Martian case) is in favor for determining C
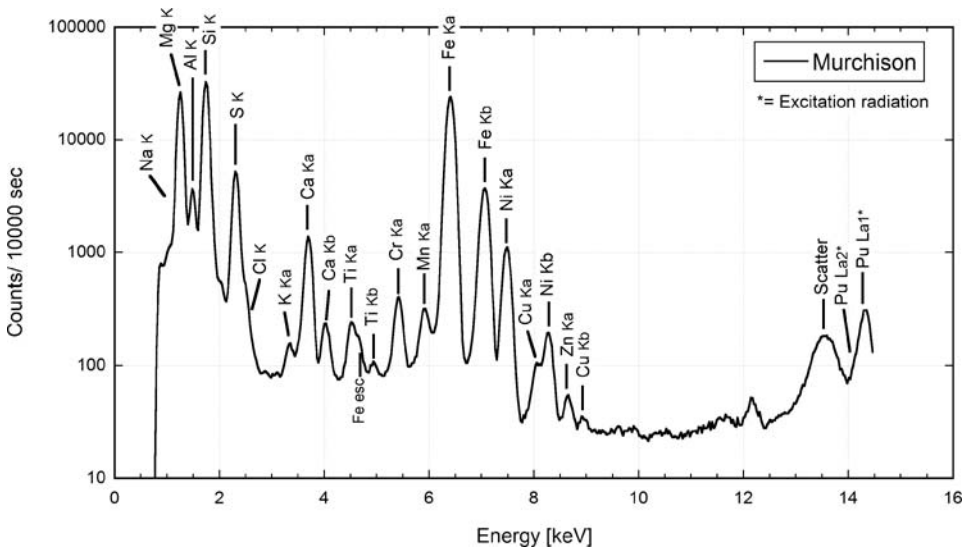

Figure 4. X-ray spectrum of the carbonaceous chondrite Murchison taken by a laboratory version of the MER APXS using the same x-ray detector as the Rosetta APXS. Only those major and minor elements that were analyzed can be seen. The excitation of the x-ray lines results from the alpha particles emitted by the curium source and the x-rays produced by plutonium, a daughter of curium, seen in the high-energy part of the spectrum. X-ray lines relevant for the analysis are produced in the K-shell of the atoms, hence there is the character 'K' behind the chemical key. Starting with potassium two lines per element can be visually separated, the $K\alpha$ and $K\beta$ lines (labeled Ka and Kb). The plutonium excitation lines result from the L-shell, $L\alpha1$ and $L\alpha2$ (labeled La1 and La2).
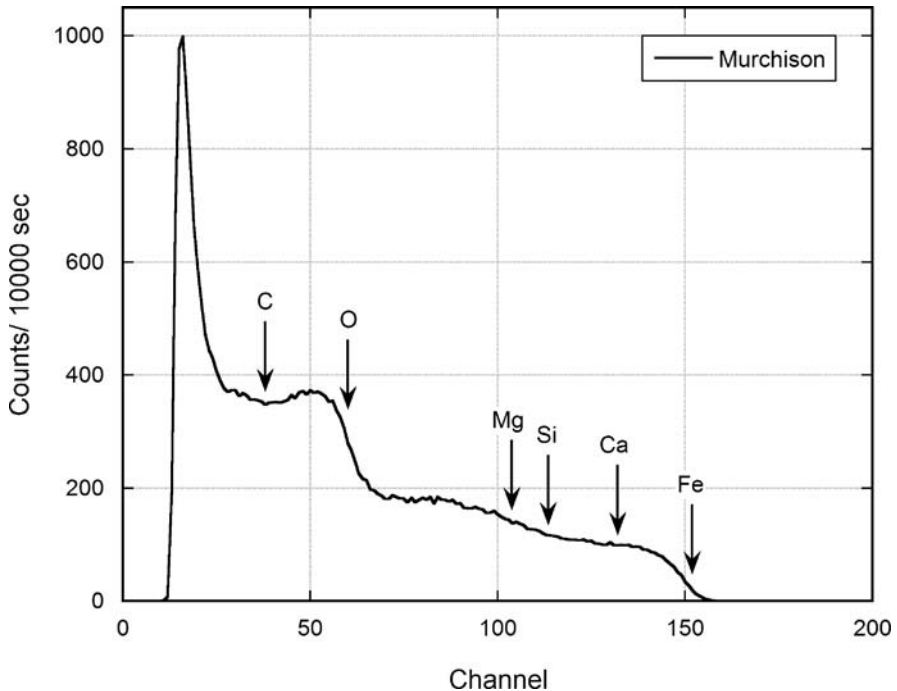
Figure 5. Alpha spectrum of the carbonaceous chondrite Murchison taken by a laboratory version of the MER APXS. In an ideal case (small detector acceptance angle and monoenergetic alpha beam), an element would be visible as a step function determined by its high-energy edge and the height of the plateau. In reality, the plateau is bended and the edge is a tailing curve. The positions of the edge of major elements are indicated by arrows. In front of the huge oxygen step is visible a small bump resulting from 1.7 weight-% carbon of Murchison. The low-energy peak results from the interaction of Cm-244 fission neutrons and high energetic gammas with the detector material and can be corrected for through the background measurement.

and O concentrations. The required integration times for alpha measurements range from at least 10 hours up to 24 hours or more depending on the desired statistical quality of the alpha spectrum.

In contrast to the MPF instrument, all preamplifiers are located in the sensor head reducing the pick-up of electrical noise, which results in lower background noise in the spectra. The total instrument mass is 640 g. The cylindrical sensor head is 84 mm long and 52 mm in diameter. The instrument uses 1.5 W of power when in operation.

For measurements, the Rosetta APXS sensor head will be lowered from the lander's balcony towards the surface by a special deployment device. As soon as subtle forces triggered by the surface material push the contact ring inwards, the doors will be opened and a contact switch stops the downward motion of the APXS sensor head and reports the successful deployment to the lander CDMS. Then,

spectra will be recorded in the harsh cometary environment. After the measurement, the sensor head can be retracted into its stowed position, which closes the doors again.

For onboard calibration of the x-ray and alpha channel measurements of the closed copper doors (stowed position) can be performed. Retracting the APXS sensor head half way up, which leaves the doors open after a surface measurement, permits to determine the sample independent signal background for both channels.

The ability to rotate the Lander will help to change the position of the APXS to measure several spots on the comet surface. This would allow characterizing local variation of surface material. The ability to rotate the lander could also be used to deploy the APXS over material extracted from the comet subsurface by the onboard drill; then the composition of subsurface material could be determined. Further, depending on the alternation of sunlight and shadow at different places (within reach of the APXS), the influence of temperature on the surface composition could be obtained at several locations. Repetitive measurements of the same spot as function of heliocentric distance of the comet (increasing mean surface temperature) will characterize surface processes at work in detail.

Conclusion

The APXS on board ROSETTA lander PHILAE has a long heritage from previous successful Mars exploration missions. The APXS will provide data on the chemical composition of the comet surface excluding the element hydrogen. With the help of the lander's rotation ability, drilling capacity, and longevity, data will be accumulated that together with results from other instruments will shed light on state, evolution, and origin of the comet.

Acknowledgements

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