An Active X-Ray Spectrometer for the SELENE-2 Rover

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The Active X-ray Spectrometer (AXS) for the Japanese SELENE-2 rover has been proposed for elemental analysis on the lunar surface to measure the major elements: Mg, Al, Si, Ca, Ti, and Fe; the minor elements, Na, K, P, S, Cl, Cr, and Mn and the trace element Ni, all depending on their concentrations at a landing site. The elemental data of the AXS allow us to not only classification but also quantification of surface rocks on the Moon. The AXS is a compact low-weight instrument for elemental analysis based on the principle of X-ray fluorescence spectrometry using an X-ray spectrometer and two (four) pyroelectric crystals as X-Ray Generators (XRG). This paper introduces the current status of the pre-project to develop an AXS for the SELENE-2 Rover including the investigations on the generation of X-ray flux of the XRG, required surface roughness for the XRS measurement, and a thermal design of the AXS.

Key Words: SELENE-2 Rover, Active X-Ray Spectrometer, The Moon, Elemental Analysis

1. Introduction

Active x-ray spectrometers using radioactive sources have been frequently used to chemically characterize planetary surfaces. An alpha particle x-ray spectrometer (APXS) has been successfully used for Mars rover missions such as Pathfinder, Mars Exploration Rover, and Mars Science Laboratory¹⁻³⁾. Also, there are a few active x-ray spectrometer planned for the prospective lunar rover mission such as Chandrayaan-3⁴⁾. For all of these cases, a radioactive isotope was used to generate X-rays on the surface of a rock on Mars.

The Active X-ray Spectrometer (AXS) is designed to make X-ray measurements on the extreme environment of the lunar surface with respect to the conditions of the high radiation and temperature variation for the Japanese SELENE-2 rover. A new technique with an X-ray generator using a pyroelectric crystal has been proposed for the SELENE-2 rover for an AXS to investigate the composition and classification of lunar rocks. An AXS is mounted on the arm of the lunar rover of the SELENE-2 mission.

The AXS data will be used to determine the element concentrations of various samples: rocks, regolith samples, and breccias encountered at the landing site and along the traverse of the rover. The AXS can measure the major elements: Mg, Al, Si, Ca, Ti, and Fe; the minor elements, Na,

K, P, S, Cl, Cr, and Mn and the trace element Ni, all depending on their concentrations.

The composition of the measured samples will contribute to their classification. The samples will be compared with other lunar material (Apollo lunar samples and lunar meteorites). These data will be used to characterize the geochemistry of the landing site and the subsequent traverse of the rover.

Depending on the landing site, new insight into the lunar geochemistry and evolution can be obtained. As the Moon is an atmosphere-less body, the mechanical and thermal effects (melting) of impacts by micro-meteorites, small and large asteroids can be studied. The combined effect of bombardment and irradiation by visible light, ultra-violet light, cosmic-ray radiation from the sun and the galaxy is called “space weathering” and can be investigated during this mission. If there is a grinding tool attached on the rover arm, the comparison of AXS data of natural surfaces and abraded surfaces can provide profound insight in the effect of space weathering.

If the products of lunar volcanic activities can be encountered, these specimens can be measured by the AXS and compared with other lunar samples. Besides rocks and regolith, the specific results of impacts can be studied in the form of breccias, which range from glassy melt rocks, to glass-rich breccias, to regolith breccias.

All lunar rocks are thought to come from the crust. None seems to have come from the mantle. Spectroscopic data from the Japanese lunar satellite Kaguya show evidence that the mantle of the Moon may be exposed on certain areas of its surface. Depending on models of the lunar evolution certain mantle compositions can be expected, such as olivine-rich rocks. The AXS analysis can support the search for mantle material.

Together with other instruments of the rover, the AXS will provide basic geochemical knowledge of the landing site, which will be used to derive a more complete understanding of the present-day lunar surface and its formation long time ago.

Currently, six landing site candidates for the SELENE-2 mission have been selected to be Tycho, Apollo 14, Marius Hills, Copernicus, Zucchini, Mare Humorum. The AXS can play a vital role in characterizing the major element geochemistry of these rocks and testing hypotheses based on remote sensing.

2. Scientific Goals of AXS

There are many scientific goals that can be addressed with the data obtained by the AXS. However, the results will depend on the nature of the selected landing site. The lunar crust can be divided into three major terrains: Feldspathic Highlands Terranes (FHT), Procellarum KREEP Terrane (PKT), and South Pole-Aitken (SPA) Terrane⁵⁻⁸⁾. The term KREEP is an acronym for lunar material rich in potassium (K), rare-earth elements (REE), and phosphorus (P).

The different terranes are represented by (1) the formation of the feldspathic lunar crust by accumulation from the magma ocean, (2) intrusion into the crust (or mixing into the crust and underlying mantle) of the residual KREEP liquid from the last stages of crystallization of the magma ocean, (3) the subsequent excavation of the ca. 2500 km diameter South Pole-Aitken basin, an event that stripped off most of the upper crust over that region, and whose ejecta contributed significantly to the thickness of the farside anorthositic crust, north of the basin⁹⁾. Superimposed on these large-scale events, are episodes of mare (or basaltic) volcanism, impact events on all scales, and space weathering. Large bodies of basaltic flows are visible in basins of the lunar near-side, but volcanic flows also occur in the lunar highlands, where they have been concealed to varying degrees by subsequent impact deposits^{10,11)}. Impact events caused brecciation and ejecta deposits, dramatically reshaping lunar topography. Space weathering has affected all surfaces on the air-less Moon and has implications for interpretation of spectral data as well as the understanding of lunar surface processes.

The Apollo landing sites were concentrated in the PKT, which is enriched in incompatible elements compared to the rest of the Moon. Thus, the data returned from the Apollo missions include a sampling bias that can lead to erroneous conclusions about the structure, composition and origin of the

Moon as a whole. For example, the compositions of impact breccias collected during the Apollo 14-17 missions were used to infer that the feldspathic highlands were underlain by a mid- to deep-crustal layer of Th-rich, mafic rock (low-K Fra Mauro Formation, or "LKFM")^{12,13)}. Subsequent remote sensing observations and re-assessment of the Apollo sample data in light of lunar meteorites show that LKFM composition is associated with regional impact history of the PKT, rather than a Moon-wide feature¹⁴⁾. However, how many biases remain in our understanding of the Moon? Hence, landing in a terrain different from the one where the Apollo missions landed would be beneficial in this respect.

The *in situ* determinations of the AXS will characterize the new site geochemically, provide ground-truth for orbiting instruments, and lay the ground for a future sample return mission collecting rocks that we do not have in our terrestrial laboratories. Depending on the nature of the landing site, new insight into the lunar geochemistry and evolution can be obtained.

Table 1. Elements detectable by AXS and significance for rock and regolith classification and origin.

Element, parameter	Significance for classification, geologic origin
Al	highlands (anorthositic) components
Fe, Fe+Mg	Mare (basaltic) components
K, P, Cl	KREEP (or KREEP-like, incompatible element-rich) components.
Ti	Mare basalt classification Apollo samples show discrete clusters, but remote sensing data suggest a more continuous variation in Ti.
Ca	In combination with Na, Al, and Mg+Fe+Ti, can be used to constrain feldspar composition as a measure of alkali-enrichment. Also constrains ratio of high-Ca to low-Ca pyroxene.
Si	Essential for evaluating data quality. Shows little variation on a remote sensing scale, or in whole-rock compositions of lunar meteorites, but might be variable at a location where igneous differentiation occurred.
Na, K	Alkali enrichment.
S	Chalcophile element enrichment. May have been important volatile element for pyroclastic eruptions.
Ni	Siderophile element enrichment. High values could be a sign of meteoric material.
Mn	Silicates from the Moon expected to have near constant Fe/Mn (~70).
Mg' = Mg/(Mg+Fe)	Key parameter for primitive vs. evolved condition of all igneous rocks. Mg is compatible relative to Fe, so Mg' is high for early-formed, high-temperature rocks and decreases during crystallization.
Ti' = Ti/(Ti+Cr)	Reflects primitive vs. evolved condition of pyroxene-rich rocks. Ti is incompatible relative to Cr, so Ti' typically increases during crystallization.
principal components	Distinguish anorthositic vs. basaltic and weathered vs. unweathered regoliths

In the following, several scientific goals to be addressed by the AXS are described. However, one has to keep in mind the best AXS analyses cannot compete with analyses to be done in a terrestrial laboratory. The *in situ* analysis is an important first step. Sample return would be the logical next step. Returned samples have provided an irreplaceable source of data for understanding the origin and evolution of the Moon.

The AXS will provide data that are used to determine the element concentrations of various samples: rocks, regolith samples, and breccias encountered at the landing site and along the traverse of the rover. The AXS can determine the major elements, Mg, Al, Si, Ca, Ti, and Fe; the minor elements, Na, K, P, S, Cl, Cr, and Mn, and perhaps one trace element, e.g. Ni. The detection of each of the listed elements depends on its concentration in the sample and the given detection limit of the applied method (X-ray fluorescence). With a detection limit of mostly less than 1%, major elements of rock and soil composition can be determined. Characterization of soils and rocks can be determined not only using the abundance of each element but also elemental ratios which can categorize types of rock and process of chemical change. Detectable elements, key parameters, and significance to rock classification and origin are summarized in Table 1.

3. Instrument Description

3.1. X-ray spectroscopy (AXS)

The X-ray spectroscopy consists of two steps:

(1) Detection of emitted X-rays by a suitable X-ray detector and formation of a histogram of the recorded X-ray events (X-ray spectrum with characteristic sharp lines and a broad background).

(2) Determination of the energy of the recorded X-ray lines permitting the identification of the elements present in the sample and the determination of the abundance of each element in the sample based on a proper energy and concentration calibration.

3.1.1. Detection principle of chemical elements (XRS)

The general principle of sample analysis is the following in the active mode. The X-ray source, in this case an X-ray generator, bombards the surface of the selected sample spot with X-rays (Fig. 1). Due to the interaction of these X-rays with the shell electrons of the atoms in the sample, characteristic X-rays are produced based on the cross section of the interaction. The emitted X-rays carry information on the type of atom, i.e. the kind of element, which emits them and the number of these atoms in the investigated sample volume. In this manner, the different elements contained in the sample can be identified and the concentration of these elements can be determined provided a careful concentration calibration of the instrument was done.

In the active mode the AXS behaves as an *in situ* instrument, which means that its sensor head is hovering over the selected sample spot in such a way that the length axis of the head is positioned perpendicularly to the average surface plain (Fig.

1). For this manipulation a robotic arm is required, whose movements are controlled by a list of command sets sent from Earth to the rover on the Moon. In the passive mode, the AXS sensor head must be pointing into the direction of the selected sample as in vacuum distance plays no role, except that the field of view should be filled out by the investigated surface. The counting time in the passive mode is probably much longer than in the active mode and strongly depending on the intensity of the solar flare.

As the energies of the excited X-rays vary between 1 and 8 keV in the active mode, the associated penetration depths of the X-rays in the sample vary in a range of a couple of micrometers up to the several tens of micrometers (also depending on the density of the sample). This means that the AXS can measure rather thin layers of a sample. Hence, it would be very advantageous to have a grinding tool, as thus different layers can be removed and measured, each of them. Of special interest is the composition of the natural, untouched surface of a rock and in comparison its abraded surface, i.e. its un-weathered fresh surface.

In the passive mode, the energy range might be extended, so X-rays of energies higher than 8 keV might be measured if present. Remote lunar X-ray observations by ROSAT and Chandra Earth orbiting spacecrafts reveal mainly low-energy X-rays (< 2 keV) with a mean dominant energy of about 0.5 keV¹⁵⁾. The AXS has a lower threshold (LLD) of about 0.9 keV, hence, the oxygen K emission line of 0.52 keV cannot be seen.

Fig. 1. Preliminary cross-sectional view of the AXS sensor head (A) and schematic drawing of the pyroelectric X-ray generator (B). In the lower part of the housing, the X-ray detector is located in the center surrounded by two X-ray generators. The upper part contains the electronic boards. The sensor head is hovering in a typical distance above the ground to avoid contamination by dust.

3.1.2. Emission principle of X-rays (XRG)

A pyroelectric crystal X-ray Generator (XRG), or as a less attractive substitute a miniaturized X-ray tube, will be used to generate X-rays to avoid the disadvantages of radioactive sources (Fig. 1). Pyroelectricity is the ability of certain materials to generate a temporary voltage when they are heated or cooled. COOL-X (by the company Amptek) is a miniature X-ray generator which uses a pyroelectric crystal to

generate energetic electrons that produce X-rays in the crystal itself and in an attached target material (typically Cu).

The XRG operates in a similar manner. The hermetically sealed package has a thin beryllium window, which allows the X-rays to be transmitted to the sample. The XRG is a self-contained, solid state system which generates X-rays when the crystal is thermally cycled, typically between 20 and 100 °C. The XRG produces a dominant 8 keV peak, when Ta and Cu are used, and a bremsstrahlung continuum. The total XRG output flux is a function of time for several heating and cooling phases. The X-ray flux varies throughout the cycle, which can be chosen to last 2 to 5 minutes. Peak X-ray flux is found to be 10^8 photons/s and this is equivalent to a 2 mCi source. If necessary, multiple XRGs can be used to increase the flux. The size is 15 mm in diameter and 10 mm high and the weight is 3.9 g. With this X-ray generator, elements from Na to Ni and Pb (increasing atomic weight) can be detected depending on the used detector system.

Recent development of NASA shows that X-ray generation by UV LED is feasible via photoelectric effect (<http://nasa.olin.edu/projects/2011/dcom/?page=background>). Also, an X-ray tube is used for the CheMin instrument of MSL (<http://msl-scicorner.jpl.nasa.gov/instrument/CheMin/>). The X-ray tube provided a focused beam for XRD/XRF for the system. These recently developed techniques could be applied for future active X-ray spectrometer when a radioisotope is avoided to be used.

3.2. Principle of measurement

The Active X-ray Spectrometer (AXS) uses X-ray spectroscopy to determine the abundance of major and minor elements down to trace elements. The instrument provides a list of distinguished features: low weight, small size, low power consumption, high-energy spectral resolution, innovative X-ray production for X-ray excitation, and full-fledged X-ray spectroscopy.

3.2.1. General principle of AXS

The AXS consists of a sensor head that is mounted on a movable robotic arm and a main electronics unit located inside the rover's chassis. The instrument has two modes of operation:

(1) Active mode: The AXS is using a switchable X-ray generator to excite X-rays in the sample under question and counting X-rays emitted by the sample.

(2) Passive mode: The AXS is counting natural X-rays that are produced in the lunar surface by various processes and emitted from the surface material (no usage of X-ray generator).

In both modes the X-ray detector measures the energy distribution of the X-rays emitted by the sample atoms. These X-rays result from recombination of ionizations caused by the radiation either an onboard X-ray generator or solar X-rays or charged particles (galactic and solar cosmic rays), processes referred to as X-ray fluorescence (XRF) and particle-induced X-ray emission (PIXE), respectively.

In the active mode, the AXS is used as an *in situ* spectrometer which means that it is carried to the selected sample rather than the sample being collected elsewhere and brought back to the instrument. The active mode is based on the bombardment of the sample surface with X-rays from an X-ray generator. Measurements are taken by deploying the sensor head towards the desired sample, placing the sensor head over the selected measurement spot typically less than 2 centimeters away (hovering) to avoid cross contamination of sample material, and switching on the X-ray generator and detector. The X-rays emitted by the sample are counted for a predefined amount of time (about 20 (TBD) Minutes to several hours) without the need of further interaction by the rover.

In the passive mode, the AXS is located somewhere above the lunar surface and pointing to the selected object, regolith or rock, which can be at any distance as there is a high vacuum. The naturally occurring X-rays, emitted by the selected area, are counted for a longer period of time. No X-ray generator is used in this mode. To detect all possible X-rays in the lunar environment, the upper energy threshold may be raised to higher energies (TBD keV). As the thickness (450 μm) of the Silicon Drift Detector (SDD) is thick enough to detect high energy LX-rays (20 keV) from heavy elements.

At the end of each measurement in either mode, the rover retrieves the science, engineering, and housekeeping data. For longer (TBD) measurements, the internal AXS software splits the total measurement time into equal time slots with an adjustable cycle time parameter. This allows us to check for repeatability and to select spectra with sufficient spectral quality. These single X-ray spectra will be summed to improve the statistics of the peaks in the spectrum.

The AXS activates an internal Peltier cooling device for the X-ray detector chip. This device keeps the operating temperature of the detector below a preset temperature, typically below -5 °C (TBD). This results in a sufficient spectral resolution, measured as full-width-at-half-maximum (FWHM), of below 200 eV at 6.4 keV below ~ -5 °C and best FWHM of < 150 eV below ~ -15 °C (TBD) detector chip temperature. The active cooling allows us to operate at the elevated lunar day temperatures.

The sample area in the active mode is about 4 cm (TBD) in diameter when the sensor head is hovering 2 cm above the sample surface. A larger standoff results in gradually lower intensity of the X-ray flux and an increased diameter of the measured spot. Low Z (atomic number) element X-rays stem from the topmost 5 microns of the sample, higher Z elements like Fe are detected from the upper ~ 50 microns.

3.2.2. Sensor head of XRS

The sensor head has a shutter to protect the detector and generator from lunar dust (regolith). When the shutter is closed, a verification measurement can be performed by switching on the X-ray generator and measuring the X-rays emitted by the calibration material on the rear side of the

shutter. As the X-ray flux output of the generator is variable from cycle to cycle, the line intensity in the recorded X-ray spectrum will vary. However, the line shape is independent of moderate flux variations. Hence, the line shape parameters (FWHM, etc.) can be precisely determined. They are the best diagnostics of the performance of the X-ray spectrometer.

Besides natural surface measurements, sample preparations, such as brushing and grinding, are required. The AXS results average the elemental composition over the sampled area and the oxide abundances measured are renormalized to 100%, in the active mode. For the passive mode, the evaluation of the composition is more sophisticated as not all major elements are measured (solar XRF) and hence, no renormalization is possible.

3.2.3. Calibration of XRS

The AXS will be fully calibrated using certified and standard geological samples in the laboratory. An onboard calibration sample (well characterized rock slab) will be used periodically to check the performance and calibration of the instrument. The data analysis is theoretically well understood and delivers clear element identification and adequate accuracy for the determination of the elemental composition. After the extensive calibration of the instrument, the accuracy

Table 2. Comparison of different X-ray spectrometers dedicated for Mars with their specification^{1-3,16)}.

Mission	Type	Source	FWHM @ 6.4 keV	Element	Detection limit	Reference
Pathfinder	APXS	²⁴⁴ Cm	260 eV	Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe	0.1-1% wt	Brückner et al., 2003
MER	APXS	²⁴⁴ Cm, 30 mCi	160 eV	Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe, Ni	30 ppm(Ni) to 0.3 % wt	Gellert et al., 2006
MSL	APXS	²⁴⁴ Cm (sealed & unsealed)	155 to 140	Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, Cr, Mn, Fe, Ni	better than MER	Gellert et al., 2009
Viking	XRFS	⁵⁵ Fe, ¹⁰⁹ Cd		Mg, Al, Si, S, Cl, K, Ca, Ti, Fe	90% conf. level	Clark & Baird, 1973

Fig. 2. Temperature variation with respect to the lunar day time for five latitudes on the Moon, modified after the data of the Diviner instrument at LRO (<http://diviner.ucla.edu/science.html>).

for the different elements can be derived (major and minor elements will have different accuracies). The overall accuracy will be limited by microscopic sample heterogeneity (i.e., grain size effects). For the APXS on the MER Rovers, the accuracies were between of 5 and about 20 % depending on the element (Table 2)²⁾.

The calibration data together with the accuracies will be the guideline of “how long must we count a sample” to obtain a desired accuracy for certain elements. There will be a quick look (tens of minutes) of a sample and longer measurements, if minor and trace elements are of interest. The AXS data analysis is fast and allows a quick turnaround of results used for tactical rover operations.

3.3. Radiation environment on the Moon

The operation on the lunar surface requires that the AXS is space proof, which means it can tolerate the specific conditions of launch, cruise phase, landing, and lunar surface. For the Moon, the AXS will have to stand perfect vacuum, exposure to hard ultra-violet light, large temperature changes between night and day from 100 K up to almost 400 K, exposure to solar cosmic rays and galactic cosmic rays causing potential radiation damage in electronics and semiconductor devices, provided they are not radiation proof or at least tolerant (Fig. 2).

4. Current Development: Investigation on Surface Roughness

We performed investigations on surface roughness using artificially made rock samples because surface roughness of a sample could affect the quality of the determination of the chemical composition of the sample. It was suspected that a roughness effect of the surface of a sample would exist. Hence, the surface roughness of various samples was examined in order to find out the optimal surface roughness condition and how to minimize potential errors. For an investigation of elemental compositions as a function of surface roughness, we selected two basalt rock core samples, whose compositions were very uniform over a large volume.

4.1. Experimental setup for study on surface roughness

We cut each basalt core into eight disks of 5 cm in diameter and 1.2 cm thickness. Then we carved to make carved lines such as valleys and peaks (Fig. 3) using a portable cutter made by Bosch and/or polished each disk surface to obtain a different roughness using Showa Denko lapping materials. The surface roughness of each disk was quantified using a R1006 Surface Profile Gauge made by Paint Test Equipment. This digital gauge allows the peak-to-valley height of a surface to be accurately measured in accordance with the ASTM D4417 Standard. This surface profile gauge has a depth scale range of 0~1,000 μm with an accuracy of $\pm 2\%$. The roughness values of the samples ranged from 8.7 to 502.3 μm for Basalt A and 6.5 to 377.0 μm for Basalt B, respectively. The error associated with surface roughness measurement was counted for only instrumental accuracy of the surface profile gauge as

$\pm 2\%$. Average surface roughness was estimated by averaging 20 data points of roughness using a digital surface profiler.

4.2. Desirable camera image to examine surface conditions

Photos of the artificially carved samples were taken using a Olympus microscope with a camera (DIXI3000) attached (Fig. 3). Figure 3 shows samples with different surface roughness and this figure shows three surface samples taken with different image resolutions. In order to examine the surface roughness of a rock sample during *in situ* analysis, a camera with a resolution of lower than $14.7 \mu\text{m}/\text{pixel}$ can provide a clear image and sufficiently large area of the sample. The proposed Field Of View (FOV) of 25 mm for the SELENE-2 AXS and a camera with resolution of $\sim 20 \mu\text{m}/\text{pixel}$ was based on these experimental results. The cameras on board of MER and MSL have a FOV of $31 \times 31 \text{ mm}$ at $30 \mu\text{m}/\text{pixel}$ and $18.3 \times 21.3 \text{ mm}$ at $13.9 \mu\text{m}/\text{pixel}$, respectively.

Fig. 3. Three disks (ordered vertically) with very rough, little rough, and 'flat' surfaces are shown horizontally with different resolutions. About 20 to $30 \mu\text{m}/\text{pixel}$ seems to be appropriate for a planetary surface mission¹⁷⁾.

4.3. Findings from the preliminary study on surface roughness

The surface conditions of samples used for XRF analysis effects the results of the elemental analysis. In laboratory, making a consistent surface condition for an XRF sample is usually checked prior to the measurement. In the case of *in situ* XRF analysis on a planetary surface, it is difficult to meet a surface condition similar to the laboratory case. Therefore, understanding the X-ray flux emitted by elements in the sample with respect to surface roughness of the sample is very important. Hence, we performed experiments to investigate the issue. The laboratory setup consisted of a commercially available X-ray spectrometer (X-123 SDD) and an X-ray generator (Cool-X), both from Amptek Inc. (Fig. 4).

The peaks areas (counts per second) of the measured elements, Fe and Ca were determined for the eight different artificially carved disks mentioned above. Each sample was measured for 20 minutes, and before taking data, a warming time of 5 minutes was allowed to both stabilize the XRG and check the input of XRG for

a reliable measurement.

XRF analyses of Fe and Ca abundances in each basalt disk sample were performed. Errors quoted in this paper are solely based on XRS counting statistics and the uncertainty of the surface profile gauge. Other errors, such as the X-ray flux uncertainty associated with the XRG are not considered. Figure 5 shows the Fe counts as function of roughness. They deviate at 'very rough' or 'very smooth' from the general trend measured in the 20 to $200 \mu\text{m}$ roughness range. For very rough or very smooth surfaces, the measured elemental abundances would be systematically too low having a rock grinding tool on board a planetary rover, a medium roughness range would be sufficient for a lunar mission.

Fig. 4. Schematic diagram of experimental setting for XRF analysis for the investigation of surface roughness using basalt disk samples

The physics behind the decrease of X-ray fluxes for very rough or very smooth surfaces is known to be the effects of X-ray diffusion and reflectance off of the smoother surface and as well as grazing-incident small-angle scattering, of the rougher surfaces¹⁸⁻²¹⁾. X-rays exhibit total external reflection when incident on a sample at an angle below a critical incidence angle. As the angle of incidence is increased above the critical angle, X-ray penetration occurs and reflections from sub-surface layers interfere with surface reflected radiation causing interference fringes indicating thickness and interfacial roughness. (c.f. <http://www.ceriumlabs.com>).

Fig. 5. Results of Fe counts as a function of surface roughness for the Basalt A disk samples. Data points show that a suitable surface roughness ranges within $\sim 30 \mu\text{m}$ and $200 \mu\text{m}$ ¹⁷⁾.

Fig. 6. Comparison of X-ray mass attenuation coefficients (cm^2/g) for Fe and Ca ¹⁷⁾.

It was found that the surface roughness range within 20 to 200 μm shows consistent elemental ratios of Ca/Fe. A surface rougher than about 200 μm and smoother than 20 μm would cause lower Ca/Fe ratios than those in the range of surface roughness from 20 to 200 μm due to X-ray diffusion and reflectivity, respectively. This is caused by the difference of fluorescence X-ray production between Ca and Fe for the X-ray energy lower than 8 keV (from ~ 4 to ~ 6 keV) (Fig. 6). The results in this preliminary study are useful for the applications of *in situ* analysis using an AXS in both terrestrial and extraterrestrial applications. A further investigation similar to this preliminary study at various environmental settings with various vacuum and temperature conditions is under investigation at present.

5. Conclusions

An Active X-ray Spectrometer is one of core instrument candidates for a science payload on the Japanese SELENE-2 rover. An X-ray generator instead of a radioisotope will be used to generate X-rays for elemental analysis on the Moon. This requires major developments to meet the lunar challenge exceeding previous science payloads designed for Mars as the lunar environment is more severe than the Martian one. Because of the number of merits of a compact planetary science payload to study surface elemental composition, AXS is being considered on future lunar landing missions, such as Chandrayaan-2 and others. This study revealed that the required surface roughness of samples should range between ~ 20 and 200 μm . Outside this range a bias in the determination of elemental abundances could occur based on the X-ray interactions with the surface morphology. Further investigations under artificial lunar environment will be carried out as well studies of the stability of X-ray flux produced by the XRG.

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