Soft X-ray spectroscopy at small to medium phase angles: Theoretical and empirical studies

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Abstract

A study of phase-angle, particle-size, and packing-density-related phenomena affecting soft X-ray spectroscopy of atmosphereless planetary bodies is presented. Both numerical modelling and laboratory measurements are included in the study. The surface properties, such as particle size and illumination geometry are found to have an effect for the total emission from the surface observed and on the measured fluorescent characteristic elemental ratios.

1 Introduction

Soft X-ray spectroscopy is a tool that has been used in planetary research since the Apollo 15 lunar mission [1]. It is used for providing global maps of elements such as silicon, iron, and calcium, which have characteristic fluorescent emission lines in the soft X-ray energy region (~0.5-10 keV, i.e., wavelengths of 2.5-0.12 nm). These maps are then used to deduce the rock types and even mineralogy of the surface, with the help of instruments from other wavelengths. The standard practice is to normalize the elemental abundances in the spectrum to some characteristic emission line, e.g., Si Kα.

The fluorescent emission from atmosphereless planetary surfaces is induced mainly by solar emission which, although highly variable in soft X-rays, is weak compared to visible wavelengths. Therefore, soft X-ray spectroscopy is useful only for inner solar-system bodies, i.e., Mercury, the Moon, and near-Earth objects (NEOs).

Spacecraft-based X-ray spectroscopy is limited to small phase angles (the angle between the light source and observer as seen from the surface), i.e., close to the backward direction. The most noticeable phenomena in soft X-rays take place close to the forward direction, e.g., Bragg scattering and by anomalous diffraction. Therefore, the backward direction has been left relatively unstudied.

Historically, the detectors used aboard the planetary missions for measuring the X-ray spectrum have been quite limited in both spectral and spatial resolution. However, with the advent of the next-generation space-based imaging X-ray spectrometers, such as MIXS aboard the ESA mission to Mercury BepiColombo (launch due in 2013), the resolution will improve dramatically imposing new challenges on the data analysis. One of these challenges is the fact that the instruments will begin to observe the surface elements with well defined illumination geometries. As is well known in the visible wavelengths, surface properties such as regolith grain size (distribution), packing density, as well as illumination geometry etc. affect scattering from the medium.

In the soft X-ray wavelengths, the situation is complicated due to the high energy (short wavelength) of the radiation, introducing a new realm of physics compared to visible wavelengths. The physical interactions occur mostly between photons and single atoms in the regolith. Therefore, the bulk elemental composition of the material plays an important role.

Some work has been carried out to understand the particle-size and phase-angle-related phenomena in soft X-ray spectroscopy (e.g., [2], [6]), but more detailed analyses are needed to allow a correct use of future high-spatial-resolution soft X-ray spectrometers in planetary science.

2 Theoretical modelling

We have developed a Monte Carlo ray-tracing code for modelling X-ray scattering and fluorescence phenomena in atmosphereless planetary regoliths[4] [7]. The current model assumes a medium consisting of spherical particles, a good assumption considering the very short wavelengths, with fixed particle size and packing densities. The code computes the first-order fluorescence from the particles induced by incident radiation. We use a simulated solar X-flare spectrum as input spectrum to allow realistic simulated spectra. At the moment, the code allows two different elements in the same medium with arbitrary elemental ratios.

Our theoretical work and the first results were introduced in Näränen et al.[4]. They reported a strong dependence of the fluorescent radiation on the particle size, smaller particles producing more fluorescence, as well as a smaller dependence on the phase angle. An opposition effect was also seen to arise due to shadowing. An interesting result for planetary research is also that elemental ratios seemed to change as a function of the viewing geometry. All of the simulations were performed with the illumination source fixed in the direction of the normal of the surface.

Scattering, which produces most of the background signal in soft X-ray spectroscopy, has not yet been included in the simulation. It will soon be implemented, as it is required for the correct evaluation of the fluorescent lines. Secondary fluorescence (characteristic emission is allowed to induce fluorescence at lower energies), realistic particle size distribution, and capability to produce spectra instead of integrated output will also be addressed.

We exclude particle processes such as particle-induced X-ray emission (PIXE) from our modelling, at least at this phase, to limit the amount of free parameters in the simulations. For comparing the theoretical results with those from the laboratory measurements (see next section) this is a valid assumption. However, for analysing the data from planetary missions, also the particle processes need to be included.

3 Laboratory experiments

To complement the theoretical work, we started laboratory experiments in multiangular soft X-ray spectroscopy in March 2007. The experimental setup used was originally built for the scientific ground calibration of ESA SMART-1 lunar mission X-ray Solar Monitor (XSM)[3]. It consists of a cylindrical vacuum chamber (63 cm in diameter, 30 cm tall), inside of which all the measurements are performed, and a titanium light source (0.5 mA and 10 kV for the initial measurements). Near vacuum (4 mbar) is necessary, as soft X-rays are readily absorbed in air. The X-rays are directed inside the vacuum chamber through a collimator tube which has two apertures and an aluminium window. The experimental setup is illustrated in Figure 1.

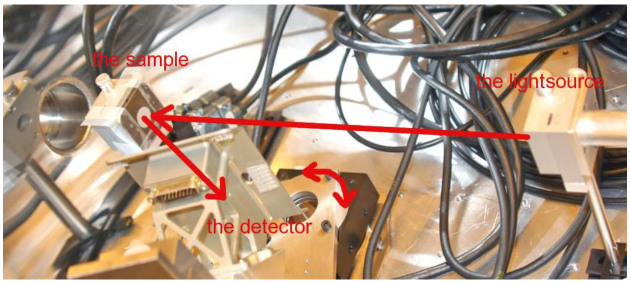

Figure 1: The experimental setup used for the initial measurements. The distance between the light source and the sample is 33 cm and the distance between the sample and the detector varied between 12.8 and 18 cm. The detector can be rotated remotely along the rotation axis indicated.

The first measurements that are reported here were performed on two samples of the same material but different grain size distributions ($< 75\mu$m an $75 - 250\mu$m). The sample material was basalt with olivine, which is considered to be a good spectral lunar highlands analogue material in the visible wavelengths. We have studied the sample materials previously in the visible wavelengths for, e.g., effects of extremes of packing density and surface roughness on the opposition effect [5]. Due to the present experimental setup restrictions, the samples had to be compressed into pellets with a packing density of 0.6±0.05. We measured the samples at four different phase angles; 16.6, 22.8, 30.2, and 38.8 degrees. For the first measurements, we limited the studies to nadir illumination geometries. In order to gain acceptable photon statistics, we measured each angle for more than 5 hours. The only measureable characteristic fluorescent lines in the samples were iron and calcium Kα lines (Fig. 2).

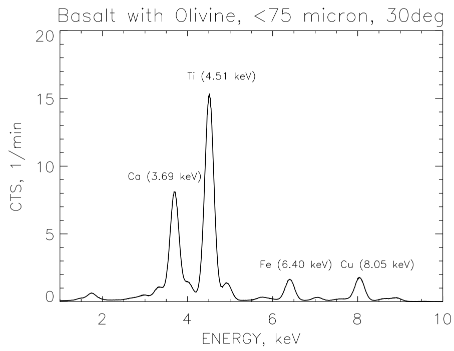

Figure 2: Spectrum measured for olivine-rich basalt sample (< 75μm) at phase angle of 30 degrees. The titanium line is produced by the light source and the copper line by the sample holder.

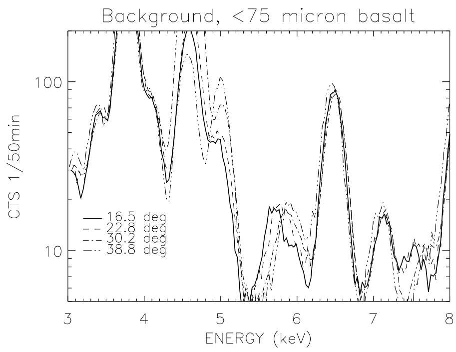

Figure 3: The scattering background of the < 75μm sample at different phase angles. There are systematic phase-angle dependent scattering phenomena. Note also the dependence of fluorescence on the phase angle.

The data were analyzed using custom-written IDL programs. The spectral lines were modeled with Gaussian functions and the maximum values of the functions were taken as data points. The effective area of the detector as a function of off-axis angle and energy was corrected for.

During 2007, we aim to continue the measurements with significant improvements in the experimental setup, including moving the sample to the center of the detector field of view.

4 Results

We report new theoretical results, including nadir-pointing simulations (observing direction normal to the surface) and results of changing the mixing ratio of elements in the medium. Even a small addition of iron in calcium-rich medium can cause a noticeable increase in the observed characteristic X-ray flux as illustrated in Fig. 5.

The initial results from the laboratory measurements are also reported. A significant increase in observed iron abundance relative to calcium is observed as a function of phase angle (Fig. 4). The results are qualitatively similar to those reported by Okada[6]. The results, if confirmed in more detailed studies, can have profound implications for the analysis of high spatial resolution soft X-ray planetary spectra.

Assessing the particle-size effect in the laboratory requires a more careful analysis and calibration of the data (as it deals with absolute values) than studying the relative intensities of elements.

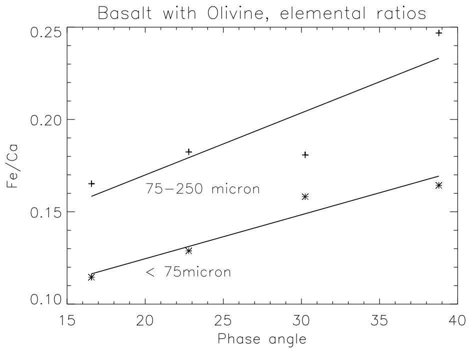

Figure 4: Measured elemental ratios of the two samples as a function of phase angle. The line represents the best linear least-squares fit to the data.

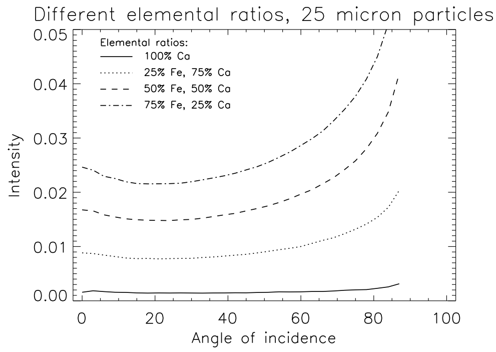

Figure 5: Total fluorescent emission from media with varying elemental ratios. Iron dominates the total output flux which can be at least partly explained by the fact that iron has over twice the fluorescent yield of calcium.

5 Conclusions

Our results show that in order to obtain accurate information from planetary soft X-ray spectroscopy, viewing-geometry-relatedphenomen need to be understood and taken into account. Particle size, packing density, and phase-angle-related phenomena in the spectrum create basis for solving the direct problem, i.e., of how to best calibrate the effects out of the data. But, in addition, they can also be used as input for the inverse problem (with data from other wavelengths as well) of actually gaining geometrical information of the surface. Our theoretical modelling and laboratory experiments are part of that endeavour that is just beginning.

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