x2abundance local model for XSPEC

Chandrayaan-2 Large Area Soft X-ray Spectrometer (CLASS) maps the elemental abundances of major rock forming elements of the lunar regolith. It works on the principle of X-ray Fluorescence (XRF) where X-rays from the sun during a solar flare excite elements of the lunar regolith which then emit charactersitic X-rays measures by CLASS. From the energy and intensity of these emitted X-rays, quantitative abundances of the lunar soil can be estimated. x2abundance algorithm was developed by Athiray et al 2015 to derive elemental abundances from X-ray line intensities. We have adopted this algorithm as local model to be used in XSPEC which is standard X-ray spectral analysis software.

Modules in x2abundance

x2abundance local model module has the following scripts.

- **common_modules.py:** This file contains the common functions/methods used in this repository. Input and output classes of other dependant functions are also defined in this file.
- **get_xrf_lines_V1.py:** This script contains the function *get_xrf_lines*. Input variables are the atomic numbers of the elements of interest as well as the expected XRF transitions and shells involved. Currently only transitions involving K and L shells are considered. From the NIST atomic cross-sections database, photo-electric and scattering cross sections are obtained for these elements. Also, other constants like fluorescent yields, jump factors and radiative rates are computed. The output class (*Xrf_lines*) contains these variables as attributes.
- **get_constants_xrf_new_V2.py:** *get_constants_xrf* function of this script interpolates the NIST cross sections to the input energy scale and also takes into account the matrix effects i.e., the cross-sections are scaled by the weight percentage and edge energies of the elements. Input variables are energies, atomic numbers, weight percentages and *Xrf_lines* and the output class is *Const_xrf*.
- **xrf_comp_new_V2.py:** This script contains the function *xrf_comp* that computes the emitted XRF line intensities from a given matrix of elements from first principles. It takes into account both primary and secondary excitation effects. Inputs are incident spectrum, geometry of observation, *Xrf_lines* and *Const_xrf* and the output class *Xrf_Struc* has XRF line intensities for each element for all possible transitions.
- **define_xrf_localmodel.py:** This script contains the actual definition of the localmodel for XSPEC fitting. *xrf_localmodel* is the user-defined function which computes the XRF line intensities and does chi-square minimisation to derive weight percentages. *static_par_localmodel.txt* has the information about the incident spectrum as well as th geometry conditions. Currently, the localmodel is defined to derive only elemental abundance of Oxygen, Sodium, Magnesium, Aluminium, Silicon, Calcium, Titanium and Iron. Within this script, acceptable ranges for the weight percentages for these elements are also defined.

Using the local model

Running the local model requires installation of python modules like numpy, scipy, astropy and xraylib. Additionally, NIST cross-sections from FFAST database are available in the *data_constants* subdirectory. *static_par_localmodel.txt* is an ASCII file containing inputs necessary to run the local model. The parameters in this file should be updated by the user before running the localmodel. For fitting CLASS spectra, users need to choose appropriate background (pre-flare, postflare or long term average background)and generate scattered solar spectrum as table model. Users can modify the definition of the localmodel to include other elements too after updating the associated variables and parameters. Steps for fitting CLASS spectra are as follows.

- **Generation of CLASS spectrum:** 8 second CLASS spectra during the flare can be appropriately added in time to improve the statistics.

- **Identifying background:** CLASS spectra corresponding to either pre-flare or post-flare duration and on the nightside can be added in time to generate the background spectrum.
- **Modeling solar incident spectrum:** Solar spectrum corresponding to the UTC of CLASS can be obtained from X-ray Solar Monitor (XSM) onboard Chandrayaan-2. XSM data can be fit with standard solar plasma temperature and emission measure models and the modeled spectrum should be saved as an ASCII file with 3 columns (1st column: Energy in keV, 2nd column: Errors in energy scale, 3rd column: Solar spectrum in units of photons/(s cm^2 keV))
- **Modeling the scattered solar spectrum:** From the model of the incident spectrum, scattered component should be derived by applying appropriate cross section. The scattered component is currently modeled as a table model with multiplicative scaling factor as the fit parameter.
- **Spectral modeling in XSPEC:** CLASS spectr is fit in XSPEC with the scattered fraction as additive table model and the XRF component as local model. Sum of weight % of all elements needs to be tied to 100. Users can define ranges for weight % of each element and also freeze certain elements if necessary.

Sample files and script for fitting are provided in *test* subdirectory.