The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
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A LIBRARY FOR SIMULATED X-RAY EMISSION FROM PLANETARY SURFACES

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ABSTRACT

The evaluation of the elemental composition of the crust of solar system objects (planets, asteroids and moons) represents an important clue to understand the formation of the solar system. A number of missions are planned in the coming years to measure the fluorescence spectra of Solar System objects, as a method to ascertain their composition.

A Geant4-based application for the simulation of X-ray emission spectra from rock samples is presented. The application is based on Geant4 Atomic Relaxation package, which provides accurate models for X-Ray fluorescence emission. This application demonstrates Geant4 capabilities to generate the fluorescent spectra resulting from complex materials, such as geological samples.

The simulation has been validated with comparisons to experimental data taken at Bessy by a team of the European Space Agency (ESA), exposing several rock samples of astrophysical interest (anorthosite, hematite, dolerite, gabbro, obsidian, basalt, Mars-stimulants, etc.). The simulation development, accurately validated by experimental results, has open the possibility to create a library of simulated rock spectra, to be used as a reference in the studies of several planetary missions, such as Smart-1, BepiColombo (Mercury) and Venus Express.

Key Words: X-Ray, fluorescence, Monte Carlo, Geant4

1 INTRODUCTION

The elemental crust composition of rocky bodies such as asteroids and planets, in particular the inner ones, is directly connected to the composition of the primordial nebula from which the Solar System was born[1]. In this context precise measurements of elemental crust composition are planned to be performed by future planetary space missions. These measurements will be performed to obtain high-definition spectra of X-ray emission induced by incident radiation on the planetary surface.

The measurement will be performed with solid-state detectors, since their characteristic such as the fast counting rate, high stopping power and high efficiency, make them the most appropriate instrument for the scientific goal to be reached.

In parallel to detector development, Monte Carlo simulations for these new detectors are and developed to support these planetary missions. Monte Carlo simulations are very important for space missions, since they give a powerful instrument to implement mitigation strategies against high-level risk. On the other end, precise Monte Carlo simulations are very useful as an instrument for physic reach studies.

In this paper the development of an application for the simulation of X-ray emission from complex materials such as rock samples is presented.

2 ATOMIC DEEXCITATION

2.1 Geant4

Geant4[2] is a toolkit for the simulation of the passage of particles through matter. It uses advanced techniques of software development that ensure great flexibility and power. The use of the object-oriented technology in Geant4 gives a high degree of modularity to the toolkit; moreover, Geant4 is developed following a rigorous software process, that guarantees rigorousness and reliability.

These features lead us to develop our simulation using the Geant4 toolkit and in particular its Atomic Deexcitation package.

2.2 Atomic Deexcitation Package

X-Ray emission is a product of the atomic deexcitation process: one vacancy, created in the electronic structure of an atom, is filled by electrons from outer shells, with consequent emission

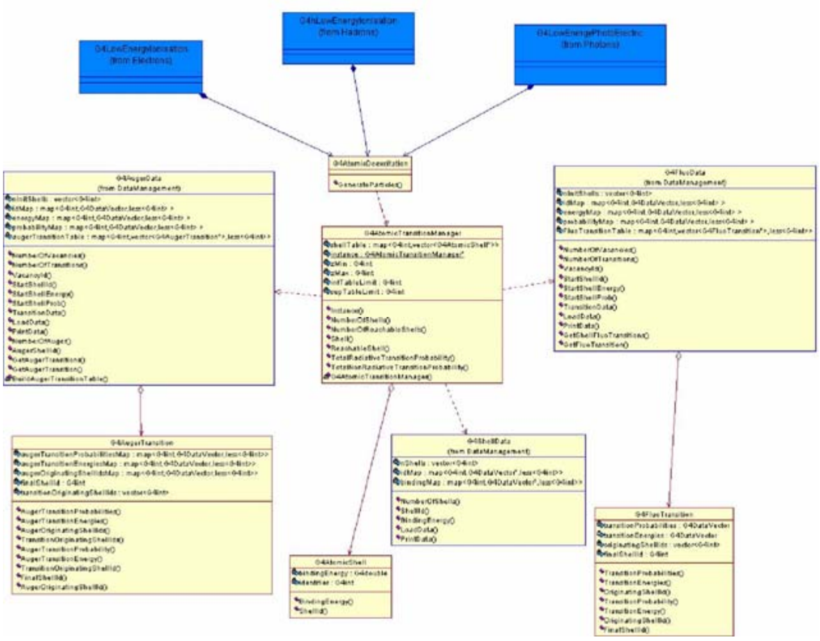

Figure 1: Design of Atomic Deexcitation Package

of photons (fluorescence). There are cases where photon emission does not take place, but the extra energy is given to atomic electrons, that leave the atom (Auger electrons).

The energy of the emitted photons or electrons depends only on the electronic structure of the atom.

The Geant4 Atomic Relaxation Package models both fluorescence and Auger emissions. The model is data-driven and is based on the EADL[3] library to get the probabilities of the transitions and the energy of the emitted particles. A vacancy in a specific shell can be filled from electrons coming from different shells: every transition has its probability and generates a photon or an electron with a defined energy. EADL reports data for a great number of transitions for elements with an atomic number greater than 5.

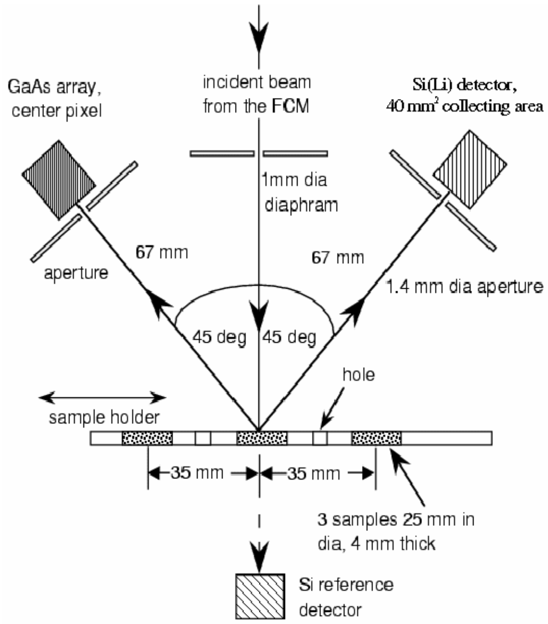

Figure 2: Bessy test beam setup.

The development of the Atomic Deexcitation Package followed a rigorous software process. The package was validated trough various tests: unit, system, and integration tests concerning software functionality and reliability, and physics tests regarding the correct modeling of physics processes. The physics test consists in comparing simulation results against available experimental data. The physics validation of the package has been accomplished both for Auger and fluorescence emission.

2.2.1 Fluorescence validation

Fluorescence emission validation was performed comparing original experimental data to simulated ones. Two kinds of analysis were undertaken: a parametric one for the emission lines of pure materials and a second one concerning simulated spectra from complex materials.

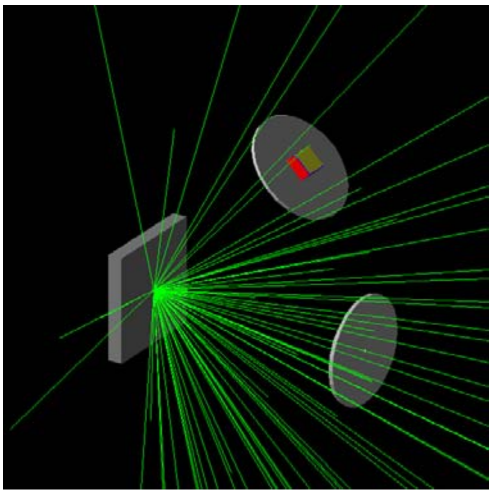

Figure 3: Visualization of the simulated geometry

Data were acquired by the European Space Agency, at Bessy laboratories, for composite materials. Samples of materials were irradiated with monochromatic photon beams; the induced photon emission was measured with a solid state X-Ray detector.

A Geant4 application was developed to model the experimental set-up shown in figures 2, 3, in terms of geometrical components, materials and response of the detector. The Geant4 application was used to reproduce the X-Ray emission from a set of rock samples, irradiated with monochromatic photon beams of various energies. This study was specifically addressed to validate the production of fluorescence spectra from complex materials, such as planetary surfaces rocks. The Anderson-Darling test[4] has been applied as statistical tool to compare the Geant4 simulation results and the corresponding experimental measurements. The test was adopted because of the complexity of the shape of the datasets and

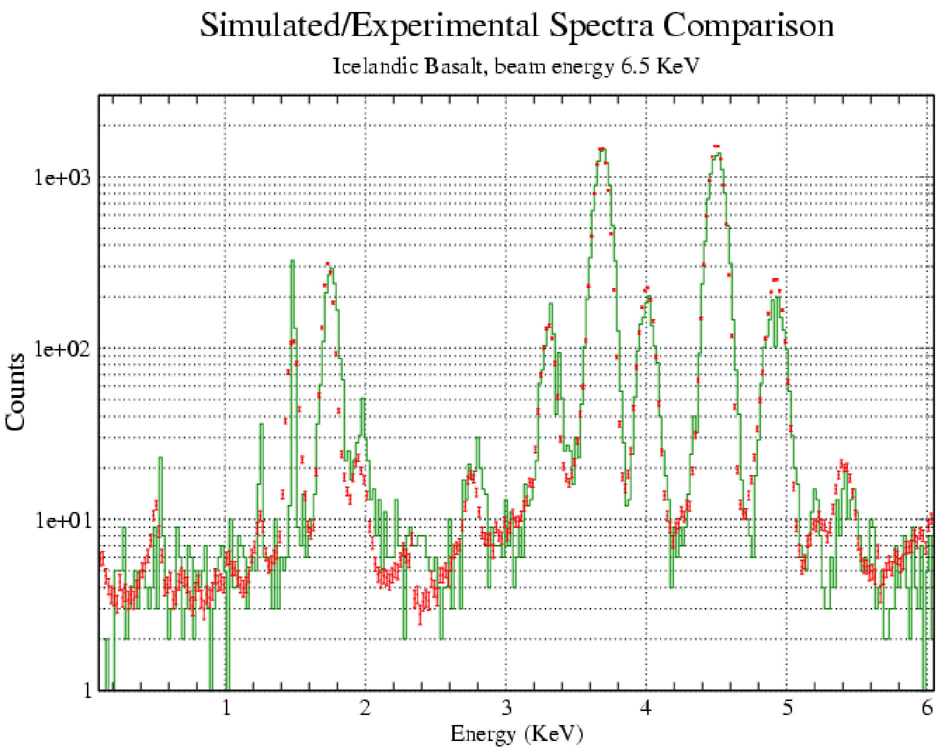

Figure 4: Mars simulant simulated and experimental X-Ray spectra comparison

the need to compare experimental and simulated data in their wholeness, even in low population bins. Test-Statistic of Anderson Darling test is

$$A^2 = \max\left\{ \frac{(F_1 - F_2)^2}{F_2 - (1 - F_2)} \right\}.$$

The A^2 values for the comparison of irradiation of a mars soil simulant at various energies are reported in Tab. 1 and validate the Atomic Deexcitation Package The two distributions are compatible at a C.L of 95%; all A^2 values are less than the critical value A_0= 0,752.

Table I - Anderson Darling Test Results

Beam Energy (KeV)	A^2
9,5	0,42
8,3	0,21
6,5	0,01
4,9	0,04

A graphical comparison of simulated and experimental data is presented in fig. 4. Another statistical test was performed to double-check the previous results, a Pearson's correlation test, whose results are described in tab. II. Results of this test indicate a high statistical correlation between experimental and simulated data: the probability that the correlation obtained by the comparison comes from statistical fluctuations is lower than 0.01%.

Table II – Pearson's correlation test results

Beam Energy (KeV)	Correlation coefficient (p)	p-value
9,5	0,93	<0,0001
8,3	0,94	<0,0001
6,5	0,99	<0,0001
4,9	0,99	<0,0001

3 CONCLUSIONS

The Geant4 Deexcitation Package has been fully validated to guarantee its rigorousness, reliability and the correct modeling of the physics processes. This study supports the use of

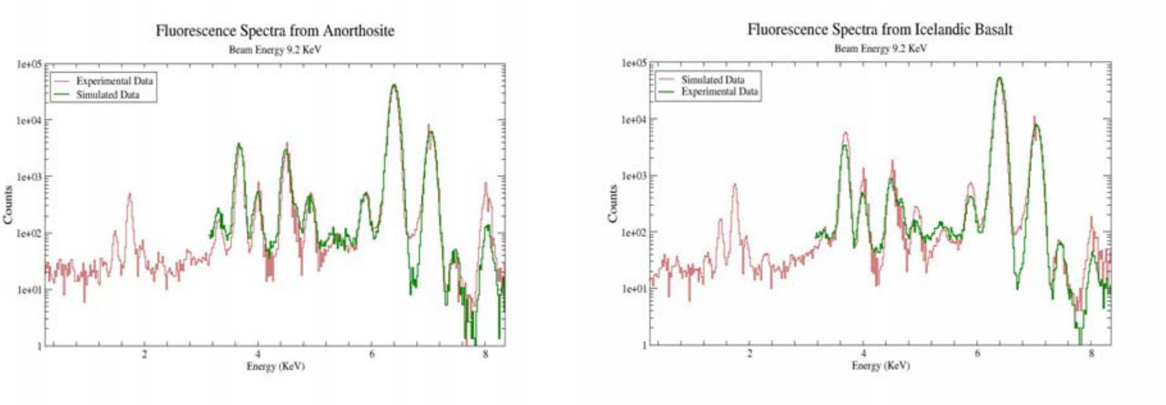

Figure 5: Simulated and experimental spectra comparison fro two different rock samples

Geant4 based simulations to reproduce X-ray fluorescence emission in complex materials, in particular rock samples. At the present time most of the data takings of the test beam were simulated, producing a database of simulated X-ray spectra of planetary surfaces analogues, figure 5 shows some of them. For the low-energy part of the spectra comparisons are not provided since the detector behavior is not well known in the energy range below 3 keV. However, a qualitative analysis shows a good agreement for energies greater than 3 keV.

At the present time a project of creating a database of simulated X-ray spectra from planetary surface analogues is going on; this database will be useful as a reference for planetary missions studies.

4 REFERENCES

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