FACULDADE DE
CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA
Departamento de Física

Doctoral Program– 2020
Thesis Project

Title: Analysis and simulation of X-ray spectroscopy for fundamental physics and applications

Objectives

Precise atomic parameters related with x-ray interactions with matter, often known as fundamental parameters, are need for a broad spectrum of applications, ranging from medical applications to environmental control. Nowadays, it is well known by the atomic physics community of a lack of reliable values of these parameters, either by having low uncertainties, or incomplete data sets. This constitutes a limitation to x-ray based technologies.

To improve this present status, a high-precision double crystal spectrometer (DCS) is being constructed at the LIBPhys, which allows X-ray energy measurements to be performed without external calibration, setting a high standard in X-ray metrology. The use of a DCS will ensure measurements of line energies and shapes, with accuracies of a few parts per million, in the soft X-ray regime, where most fundamental parameter databases are severely incomplete. Its high-energy resolution will also allow the characterization of rare earths geological samples with the goal of developing standard reference materials for X-ray fluorescence (XRF).

To accomplish this goal, it is necessary a full characterization, not only of the DCS, but also of the processes of X-ray interaction with matter, in conjunction with an accurate theoretical analysis of the X-ray fluorescence This allows an accurate determination of chemical and Auger shifts.

The high precision of this spectrometer is directly linked to the double Bragg diffraction at the two crystals arranged in a series configuration that allows only a narrow region of energies to reach the detector. In order to optimize precision and study possible systematic effects it is necessary to perform Monte-Carlo simulations of the spectrometer.
In the context of the present thesis, the first task will be making the necessary modifications of the custom-made Monte-Carlo code developed by the group [1], by including the necessary geometry changes, as well as including an arbitrary X – ray input.

This arbitrary X-ray input constitutes the x rays excited by the sample, as any XRF technique. It is a simple and fast technique that enables multielemental analysis of a variety of materials, from liquids to metals. The Geant4 Monte Carlo simulation

package will be employed for retrieving accurate X-ray excitation by the sample [2].

Additionally, the intensities of the fluorescence lines produced by the Geant4 code will be attested with state-of-the-art atomic structure calculations and further corrected [3]. While understanding the fluorescence process theoretically from first principles, the process of quantum interference between paths can be investigated, which might give insightful and unexpected physics to be explored.

In conclusion, this thesis will pave the way for an optimal simulation of the DCS that will provide accurate data analysis of future measurements.

Framework

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Venue

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References

[1] http://link.aps.org/doi/10.1103/PhysRevLett.109.043005
[2] http://www.sciencedirect.com/science/article/pii/S0584854716302476
[3] https://journals.aps.org/pra/abstract/10.1103/PhysRevA.92.022507