COMPUTATIONAL SOFTWARE

FXRS: Fast X-Ray Spectrum-Simulator Theory and Software Implementation

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Abstract. We propose a simple, computationally efficient scheme for an X-ray spectrum simulator. The theoretical models describing the physical processes involved are employed in our Monte Carlo software in a coherent way, paving the way for straightforward future improvements. Our results compare satisfactorily to experimental results from literature and to results from dedicated simulation software. The simplicity, excellent statistical errors, and short execution time of our code recommend it for intensive use in X-ray generation simulations.

AMS subject classifications: 68U20, 65C05

Key words: Electron-matter interaction, X-ray generation, Monte Carlo simulation, interaction forcing, detection forcing.

Program Summary

Program title: FXRS: Fast X-Ray Spectrum-Simulator

Nature of problem: Simulation of X-Ray energy and angle-resolved emission spectra. Optionally, the deposited energy as a function of depth can be computed.

Programming language(s): Fortran 90

Computer platform: Any

Operating system: Any

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Compilers: gfortran

RAM: 4.5 MB

External routines/libraries: Xraylib, ELSEPA

Running time: The execution time for 10^5 injected electrons with energy of 20 keV is about 1 minute on an Intel Xeon X5650 processor (2.67 GHz).

Restrictions: The low-energy spectrum is not describable with the physics included in the present software.

Additional Comments: The software is very modular, and can be easily changed for research purposes.

1　Introduction

X-rays are widely used in various applications such as non-destructive structural analysis, imaging, microscopy and radiography, *etc*. In any application, especially in metrology measurement and diagnostic, performance of the technique-in-use strongly depends on the quality of X-ray beam. Understanding of the X-ray beam quality therefore plays an important role in interpretation of data, correction of artifacts as well as optimization of X-ray source design. The quality of X-ray beam varies from one to another depending on various parameters such as anode material, filtration, high voltage and focusing system. Experimentally investigation of how X-ray generation is correlated to the specifications of a given X-ray source would be difficult and time consuming, as well as not cost effective. This difficulty can be overcome by performing computer simulation of X-ray spectra.

A few codes are available as open source for X-ray generation simulation [1–3]. However, many of these codes are designed for a wide scope of application, and consequently grow in size and complexity. Hence, the user who is interested to implement new physical models, for example, faces a difficulty. Moreover, the other state-of-the-art general-purpose codes with coupled electron-photon transport like Geant4, PENELOPE, MCNPX [4–6] are generally computationally expensive. For this reason, we pursue here the goal to create FXRS (Fast X-Ray Simulator): a modular software simulating the emission of X-rays under electron impact, with allowance for more sophistication to be added, as future requirements of the users dictate. This way, we have access to all the variables that describe the interactions and to the way the output is generated. By employing interaction and detection forcing method, our code can deliver results with very good statistics in fast execution time.

Atomic units are used throughout this work, unless otherwise specified.

2　Monte Carlo method: Variance reduction techniques

Monte Carlo methods are a class of methods that simulate real-life processes by means of random sampling. In the case of the simulation of X-ray spectra, Monte Carlo method