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Simulation of Direct Transport of X-Ray Photons Using the General Purpose Monte Carlo Code MCSHAPE: Main Features and Recent Developments

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MCSHAPE [1] is a general purpose Monte Carlo code developed at the University of Bologna to simulate the multiple scattering of the prevailing photon-matter interactions in the energy range 1-1000 keV, including a detailed evolution of the polarization state of the radiation. MCSHAPE is particularly appropriate for describing the multiple scattering terms which, overlapped, build up the whole x-ray spectrum. All the aspects that characterize the computed multiple-scattering contributions can be suitably defined: (i) the intensity term, (ii) the full polarization state as a function of energy, (iii) the number of collisions, and (iv) the involved processes. MCSHAPE3D, the 3D extension of the code [2], simulates the propagation of photons in complex heterogeneous media originating from either polarized or unpolarized sources and, therefore, represents a valuable tool for the simulation of scanning XRF experiments, XRF tomography and for the interpretation of the experimental results of any technique involving photon-matter interactions requiring a 3D description of the experiment.

The influence of the detector is considered by means of a two stage procedure [3]. In the first stage, MCSHAPE computes the diffusion of the incoming photons into the detector. In the second stage, the broadening and the energy resolution (which depends specifically on the detection mechanism) and the influence of the electronics (pulse-pile up) are included by means of the independent codes MCPPU [4] and RESOLUTION [5], respectively.

It is well known that the most accurate description of the radiation field in X-ray spectrometry requires the modelling of coupled photon-electron transport, because Compton scattering and photoelectric effect give both photons and electrons as secondary particles. Photon transport codes usually neglect electron contributions since the solution of the coupled problem is time consuming. Nevertheless, secondary electrons contribute to the photon field through electron-photon conversion mechanisms like bremsstrahlung (which produces a continuous photon spectrum) and inner-shell impact ionization (ISII) (which modifies the intensity of the characteristic lines). The approach adopted recently by Fernandez et al. [6] allows to introduce a new photon kernel comprising the correction due to ISII. The new kernel is suitable to be adopted in photon transport codes with a minimal effort. The study of the bremsstrahlung contribution is under development [7].

Simulations with the latest version of the code taking into account the detector response function and the energy resolution are compared with experimental data.

References

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