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The Monte Carlo code MCSHAPE: Main features and recent developments

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ABSTRACT

MCSHAPE is a general purpose Monte Carlo code developed at the University of Bologna to simulate the diffusion of X- and gamma-ray photons with the special feature of describing the full evolution of the photon polarization state along the interactions with the target. The prevailing photon–matter interactions in the energy range 1–1000 keV, Compton and Rayleigh scattering and photoelectric effect, are considered. All the parameters that characterize the photon transport can be suitably defined: (i) the source intensity, (ii) its full polarization state as a function of energy, (iii) the number of collisions, and (iv) the energy interval and resolution of the simulation. It is possible to visualize the results for selected groups of interactions. MCSHAPE simulates the propagation in heterogeneous media of polarized photons (from synchrotron sources) or of partially polarized sources (from X-ray tubes). In this paper, the main features of MCSHAPE are illustrated with some examples and a comparison with experimental data.

1. Introduction

The increasing importance of the Monte Carlo (MC) method in X-ray imaging and X-ray fluorescence applications is testified by the growing number of publications on these subjects. The existing general purpose MC codes like for instance MCNP [1,2], EGSnrc [3], PENELOPE [4], and Geant4 [5,6] present some limitations for the description of certain applications. For this reason, in the last decades, many developers have realized ad hoc MC codes for specific tasks, such as X-ray imaging and spectroscopy (xrmc, [7,8]), energy-dispersive X-ray fluorescence (EDXRF) and quantification (XMI-MSIM [9–12]), X-ray tracing for instrumentation (McXTrace [13]), and confocal experiments [14].

Polarization is a fundamental property of the electromagnetic radiation that is widely exploited on synchrotron sources. However, it is usually disregarded or only partially considered in both, deterministic and MC codes. Many MC codes use an average-polarized description or considers only linearly polarized photons (i.e., EGS5 [15]). Both of these descriptions introduce an error, as it is demonstrated in Fernandez (1998) [16]. The polarization state has to be considered also when dealing with partially polarized sources, like X-ray tubes. In fact, as pointed out by Fernandez et al. (1993) [17], the polarization state changes as a consequence of the number and type of the interactions of the radiation with the medium. Therefore, unpolarized photons may become polarized as a consequence of the scattering. The effects of the polarization were firstly computed with deterministic methods in the works of Fernandez and Molinari [18] and Fernandez et al. [17]. The adopted transport model is derived from the so-called Boltzmann–Chandrasekhar "vector" transport equation [18,19]. The polarization state is described by means of the four components of the Stokes vector I (the intensity of the beam—the only parameter considered in the scalar transport models), Q, U and V, which have the dimension of intensities and contain all the physical information about the polarization state [20]. The analytical solution was used to analyze the influence of polarization on multiple scattering, but it is limited by the number of collisions that can be considered (up to three for selected interactions) and by the capability to describe only a plane geometry [17].

The MC code MCSHAPE [21] was developed at the University of Bologna to extend the results of the deterministic method to higher orders of collision and maintain a proper detailed description of the evolution of the polarization state of the radiation. MCSHAPE considers the prevailing photon–matter interactions in the energy range 1–1000 keV and is particularly appropriate for describing the multiple scattering terms which, overlapped, build up the whole spectrum. All the parameters that characterize the photon transport can be suitably defined: (i) the source intensity, (ii) its full polarization state as a function of energy, (iii) the number of collisions, and (iv) the energy interval and resolution of the simulation. Recently, PENELOPE has included the simulation of arbitrary polarized photons using the Stokes parameters [22], but the capability to give at the same time the energy dependence of the polarization degree (with all the four components of the Stokes vector) and the full spectrum of the scattered radiation

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remains a unique feature of MCSHAPE. The great attention devoted in MCSHAPE to the description of the scattering interactions is justified by the importance of the quantification of the scattering in different fields, such as for quantitative XRF analysis, for medical applications, for the determination of the nature of the matrix by means of the Compton to Rayleigh ratio, and for the study of density profiles.

Contributions from Compton and photo-electrons to the photon transport require the solution of the coupled photon–electron transport. These contributions have been recently characterized and stored as external databases for describing Inner-shell Impact Ionization (ISII) and bremsstrahlung in a photon transport code like MCSHAPE [23–25].

Some complementary codes have been developed at the University of Bologna to be used in combination with MCSHAPE. In particular

- XRAY_TUBE is a tool for the generation of X-ray spectra by means of the analytical models developed by Pella et al. [26,27] and by Ebel [28];
- MCInput is a graphical dedicated software to edit the input files necessary to run MCSHAPE;
- RESOLUTION [29,30] is a graphical tool which models the detector resolution function. RESOLUTION convolutes the energy deposited spectrum in the detector, computed by means of a deterministic or MC code, with the detector resolution function, giving as output a realistic measured spectrum;
- MCPPU (Monte Carlo Pulse Pile-Up) [31] is a Monte Carlo code, which corrects the experimental data for pileup effects.

This paper illustrates the main features of the code MCSHAPE. Simulations with the latest version of the code taking into account the detector response function and the energy resolution are compared with experimental data.

2. Outline of the model

MCSHAPE is based on a transport model derived from the so-called Boltzmann–Chandrasekhar 'vector' transport equation [18,19]. The complete description of the model can be found elsewhere [17,19,32,33]. This section reports a brief overview of the significant quantities computed in the code MCSHAPE.

Four parameters are necessary to completely describe a general beam of X-rays, which can be regarded as a mixture of elliptically polarized and unpolarized photons. The first one is the intensity of the beam, which is the only parameter considered in the so-called "scalar" treatment. The second parameter is the degree of polarization, i.e., the fraction of the beam which is elliptically polarized. The last two parameters are necessary to characterize the elliptically polarized fraction of the beam: the orientation of the polarization ellipse, i.e., the angle χ between the major axis of the ellipse and a fixed coordinate axis in the space, and the ellipticity, i.e., the ratio of the two axes of the ellipse (see Fig. 1). Since these four quantities are heterogeneous, with diverse nature and dimensions, it is convenient to use the equivalent set of parameters introduced by Stokes *I*, *Q*, *U*, and *V*, all having the dimension of intensities, which specify respectively the intensity, the degree of polarization, the orientation, and the ellipticity of the ellipse of polarization. The Stokes parameters are defined in term of the angles χ and β (related to the ellipticity) as follows [33]: $\vec{f} = [I, Q, U, V]$, with $Q = I \cos 2\beta \cos 2\chi$, $U = I \cos 2\beta \sin 2\chi$, and $V = I \sin 2\beta$In terms of the Stokes parameters, the degree of polarization is defined as

$$P = \frac{\left(Q^2 + U^2 + V^2\right)^{1/2}}{I} \quad [1]$$

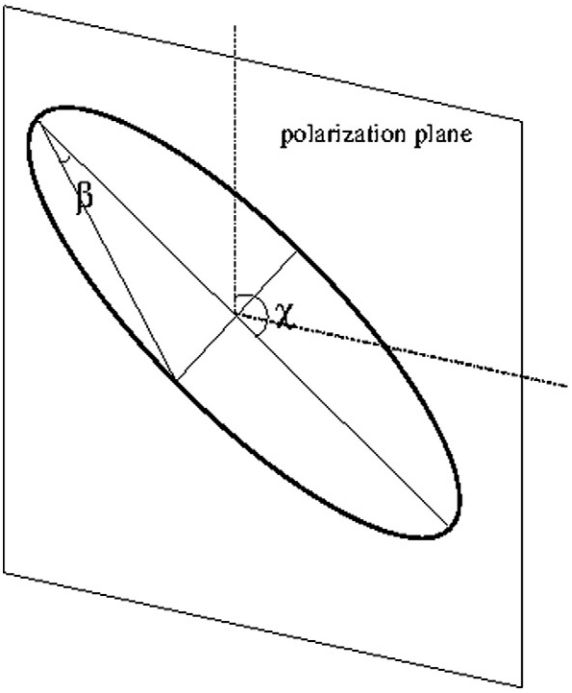

Fig. 1. Graphical representation of the ellipse of polarization.

Using the Stokes formalism, the Boltzmann–Chandrasekhar vector transport equation describing the vector flux $\vec{f}\left(\vec{r},\vec{\omega},\lambda\right)\, d\vec{\omega}\, d\lambda$ of polarized photons can be written as:

$$\vec{\omega}\cdot\nabla\vec{f}^{(S)}\left(\vec{r},\vec{\omega},\lambda\right) = -\mu\left(\vec{r},\lambda\right)\ \vec{f}^{(S)}\left(\vec{r},\vec{\omega},\lambda\right) + \int_0^{\infty} d\lambda' \int_{4\pi} d\omega'\ H^{(S)}\left(\vec{r},\vec{\omega},\lambda,\vec{\omega}',\lambda'\right)\ \vec{f}^{(S)}\left(\vec{r},\vec{\omega}',\lambda'\right) + \vec{S}^{(S)}\left(\vec{r},\vec{\omega},\lambda\right) \quad [2]$$

where $\vec{r}$, $\vec{\omega}$, and λ represent position, direction, and the wavelength of the photon, respectively. In Eq. (2),

$$H^{(S)}\left(\vec{r},\vec{\omega},\lambda,\vec{\omega}',\lambda'\right) = L^{(S)}(\pi-\psi)\ K^{(S)}\left(\vec{r},\vec{\omega},\lambda,\vec{\omega}',\lambda'\right)\ L^{(S)}\left(-\psi'\right) \quad [3]$$

is the kernel matrix in the meridian plane of reference; $K^{(S)}\left(\vec{r},\vec{\omega},\lambda,\vec{\omega}',\lambda'\right)$ is the scattering matrix in the scattering plane of reference; and $L^{(S)}$ the four-by-four rotation matrix that transforms the scattered flux from the scattering plane to the meridian plane of the reference. Primed magnitudes denote incidence. $\mu\left(\vec{r},\lambda\right)$ is the narrow-beam attenuation coefficient, which is independent of the state of polarization of the photons (assuming the matter is isotropic), and $\vec{S}^{(S)}\left(\vec{r},\vec{\omega},\lambda\right)$ is the source vector flux with components (S_I, S_Q, S_U, S_V).

It is worth noting that $H^{(S)}$ is non-diagonal, and therefore the interaction term introduces coupling between the components of the angular flux. As a consequence, it is not possible to solve separately the equation for the intensity without considering the other coupled equations. A formal demonstration of such impossibility has been given by Fernandez (1998) [16].