MCSHAPE: A MONTE CARLO CODE FOR SIMULATION OF POLARIZED PHOTON TRANSPORT

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ABSTRACT

MCSHAPE, a new Monte Carlo code based on the recent analytical solution of the vector transport equations in plane geometry including polarization effects, was developed to provide a proper description of the polarization state evolution of photons through multiple scattering collisions. The code considers a detailed description of the prevailing interactions in the X-ray regime (Rayleigh and Compton scattering, and photoelectric effect) and infinite/finite thickness multi-component homogeneous target. As a result, MCSHAPE can give the final state of polarization for each collision number. Good agreement with both deterministic calculation and experimental data was obtained for excitation with unpolarized and linearly polarized sources.

INTRODUCTION

It is possible to trace back the atomic properties of a material by studying the secondary radiation generated by the interactions between a source of X-rays and its atoms. One of these properties is the polarization state of the interacting photons which changes as a consequence of the number and type of the undergone interactions. The effect of the polarization state on the intensity spectrum is mainly important when the incident beam is partially or totally polarized. MCSHAPE is a Monte Carlo code developed to describe the diffusion of X-rays into a sample taking into account their full state of polarization. The mathematical model is deduced in the frame of transport theory, using the Boltzmann equation for photons.

There are different degrees of approximation to describe the diffusion of photons in the matter. A first approximation consists in the use of the so called ‘scalar’ model in which we assume that the photons interacting with a sample cannot modify an average polarization state. Under this condition, the transport of photons is analogous to that of neutrons, i.e. they are considered as neutral ‘particles’. In this case, photon interactions are described using average polarized differential cross-sections. This is the model adopted in the widely used standard versions of the Monte Carlo codes MCNP and EGS4. A higher level of detail can be reached by introducing the so called ‘vector’ transport equation (Chandrasekhar 1950; Fernandez and Molinari 1993). Such a model describes properly the transport of photons with an arbitrary state of polarization. The code MCSHAPE has been written following this second
approach, so it can simulate the full state of polarization of the photons at any given position, wavelength and solid angle.

**THEORY**

To describe the evolution of the state of polarization of the photons, we need four parameters. The first is the *intensity of the beam*, the only quantity considered in scalar transport models. Then, it is important to analyse the fraction of polarized X-rays: the *degree of polarization*. In fact, at each space point and for a given wavelength and direction of propagation, the most general beam of X-rays can be regarded as a mixture of elliptically polarized and unpolarized X-rays. The remaining two parameters are necessary to describe the ellipse associated with the polarized component: the *orientation of the ellipse* of polarization (the angle between the major axis of the ellipse and a fixed coordinate axis in the space) and the *ellipticity* (the ratio of the two axis of the ellipse).

![Diagram](image)

**Fig. 1** - Graphical representation of the electric field vector for a polarized beam: a)definition of the scattering plane; b)definition of the polarization plane.
To follow the evolution of these four quantities, the code MCSHAPE uses the parameters I, Q, U, and V, having the dimension of an intensity, introduced by Stokes. These quantities are defined as:

\[ Q = I \cos 2\beta \cos 2\chi \]

\[ U = I \cos 2\beta \sin 2\chi \]

\[ V = I \sin 2\beta \]

in terms of the rotation angle \( \chi \) referred to the scattering plane, and of the angle \( \beta \) whose tangent is equal to the ellipticity. The degree of polarization of a partially polarized beam is usually expressed as:

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

The prevailing interactions in the X-ray regime (1-100 keV) are displayed in fig. 2. MCSHAPE neglects the possibility of photon production by scattered electrons. Scattered electrons feedback new photons into the photon interaction cycle and, therefore, the full transport problem should be solved with two coupled systems of transport equations, one for polarized photons and one for polarized electrons. However, our model, which neglects these electron interactions, is an excellent approximation when the probability for bremsstrahlung is low. So, the code simulates Compton and Rayleigh scattering and photoelectric effect with emission of characteristic photons. Moreover, for Compton scattering, Doppler broadening is considered.

Fig. 2 – Prevailing interactions in the X-ray regime.
OUTLINE OF THE PROGRAM

Starting from the scalar code SHAPE, a first version of the program was written in Pascal in 1995. Then, two new codes were developed using FORTRAN: MCSHAPE0 follows up to four collisions of the photons in the target, using analog calculation, and MCSHAPE1, in which there is no limit in the number of the collisions considered. In fig. 3, a benchmark between MCSHAPE0 and MCSHAPE1 shows the equivalent answer for 4 collisions.

Fig. 3 - Benchmarking MCSHAPE0 and MCSHAPE1. The target is aluminium, the source is unpolarized and the scattering angle is 90º. Both codes perform four collisions. The similarity of both results ensures the proper answer of the N-collision code MCSHAPE1.

Fig. 4 – Geometry of the backscattering model used by MCSHAPE.
In our model, we assume that photons interact only within the target, i.e. those photons escaping towards the surrounding empty space or air may suffer absorption but never return back to the target. In fact, this is a good model to represent the behaviour of radiation in two media of different density, the one in the sample being much greater than the density in the half-space outside the target. The geometry of MCSHAPE backscattering model is shown in fig. 4. For the selection of the scattering angle, the code operates as follows: for every collision, the final polar angle is sampled from the scalar differential cross-section for the event (isotropic for the photoelectric effect, anisotropic for Compton and Rayleigh scattering). The azimuthal angle in the local centre of mass reference system is sampled uniformly.

RESULTS AND DISCUSSION

Fig. 5 shows a comparison between MCSHAPE and the scalar MC version, based on a scalar representation of the photon transport model. MCSHAPE gives a greater contribution mainly due to the double Compton collision. Such a behaviour is not due to statistical phenomena but to the interaction between the different Stokes parameters which increases the value of the intensity. In fact, the vector transport model represents a system of four coupled equations that cannot be uncoupled with mathematical techniques (Fernandez, 1998).

![Graph showing comparison between MCSHAPE and scalar MC version](image-url)
CONCLUSIONS

The model adopted has two open problems. The first one regards coherence (Fernandez 1995): the vector transport equation behaves linearly only for an incoherent source (Pomraning 1973), i.e. when there is not a prevailing phase at the source beam. Coherent radiation is not considered yet in the transport models used to study X-ray diffusion.

The second problem regards variance reduction. Actually, the variance reduction on the angular variables is performed using the average kernel, while the Stokes components Q, U, and V are computed using weights. As a result, we use a mixed method in which only the first component of the Stokes parameters, the intensity I, is optimised.

Our future work will be oriented in two directions. First, we want to split the program in two independent parts: one for the acquisition of the input and the construction of the cumulative distributions for Compton and Rayleigh scattering; the second in which the real Monte Carlo simulation is performed.

Then, we have planned to perform more detailed tests to compare the results of MCSHAPE with experimental data, especially for excitation with polarized sources (we have obtained good agreement with laboratory experiments for unpolarized sources).

Moreover, a web site (URL http://shape.ing.unibo.it) is being created to illustrate the main characteristics of MCSHAPE and other related deterministic codes.

REFERENCES


