Simulation of Physical Phenomena Intervening in the Interaction of X Ray - Matter with Monte Carlo Method

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Abstract. The X-ray imaging techniques, such as radiography, radioscopy and tomography are used in various applications, particular in the medical field and material science. According to the material density, the geometry and applied energy, the beam X-rays can penetrate in material to analyze with a depth of several centimetres and bring information in depths among the defects of macroscopic and microscopic structures. The X-ray beam applications rest on total phenomena resulting from the elementary interactions which occur between the photons X and materials. Then it is necessary to know the physical phenomena which produced in the sources, in the object and the detection system. This paper studies by modelling, the phenomena resulting from the interaction photon X and material, by approximating a model which takes into account attenuation laws and the Monte Carlo method. We have developed a numerical model by analogy with the author's studies and an example of statistical simulation is presented for monochromatic beam of photons X and for a homogeneous finite and semi-infinite target SiO_2. We classified the various physical events which can occur, with a percentage of appearance. This calculation makes it possible to identify the event dominating; the other least probable processes (which we can call them minority phenomena) can bring other information during analysis of a microstructure and will be negligible in the case of an analysis of macrostructures. In general we can identify these phenomena by undesirable mechanisms which disturb the analysis.

1. Introduction

When a beam of X-ray penetrates in a medium a progressive disappearance of the photons lay down by the absorption capacity of medium. This reduction in the number of incident photons is due to their interactions with the atoms and the molecules and more particularly with the electrons of the atomic layers.

The elementary interaction between photons and electrons can give; the Compton effect, i.e. diffusion of the photon with energy loss and change wavelength; a simple diffusion, i.e. a photon deviated of it's trajectory without energy loss and without change wavelength; and finally the photoelectric effect i.e. a total absorption of the energy incident photon, the excited atom re-emits then two kinds of secondary radiations: electrons and X-rays of fluorescence whose wavelength does not have a relationship with the primary wavelength.

The effect energy absorption of the secondary electrons and the secondary photons contribute in the generation of the noises.

We have developed a numerical model using the Monte Carlo method and the attenuation coefficients according to the random physical events. For each effect, we associate to him an attenuation coefficient where we introduce a density of probability relating to the effect and the element constituting the target, therefore it make possible to follow the physicals events of the photons X during their interaction with the matter to be analyzed.

Macroscopically in the imaging systems, the formation of the image can be induced with percentages of appearance of theses effects and sometimes with a predominance of an effect compared to others and also accompanied with the noises effects.

Macroscopically, this mechanism is described by attenuation law [1], [2], [3], [4], based on the total attenuation coefficient.

The purpose of the work was the classification and identification of the effect dominating at homogeneous medium when it is penetrated by X-rays mono-energetic photons. The principal interactions used were the Compton effect and the photoelectric effect. The variation of the attenuation coefficient of photons X was approached according to energy.

2. Description of model

2.1 Basic physics

A photon can enter in interaction with an electron and more rarely with a core of the medium.

The cause of the interaction reside in the forces which are exerted at very short distance between the electromagnetic field associated to the photon and the electric field associated to the electron - or the core -. The image of a shock between material corpuscles is enough with interpretation to these events, the photon being regarded as a projectile of kinetic energy E. We work with low energy then the interaction with the core is negligible [3]. The principal interactions are the Compton effect and the photoelectric effect.

a) Compton effect

The interaction process of Compton effect takes place between the incident X-ray photon and the electron in the absorbing material. The photon transfers a portion of its energy to the electron (assumed to be initially at rest), which is then known as a recoil electron [3].

The Compton relations reveal that a photon cannot transfer all its energy to an insulated particle, there is thus always a diffused photon whose energy Es included between Es_{max} ("tangential" shock) and Es_{min} ("frontal" shock): in this last case, the diffused photon is returned "backwards ".
Indeed, energy T is in near total carried by the Compton electron in the form of kinetic energy; it is absorbed by the medium in the vicinity of the point where the interaction took place [4].

b) Simple diffusion

The incident photon absorptive by the atom was re-emitting with same initial energy E in an unspecified direction. This phenomenon is equivalent to a simple change of direction of the incident photon [4].

c) Photoelectric effect

In the photoelectric absorption process, a photon undergoes an interaction with an absorber atom in which the photon completely disappears [3].

In its place, a photoelectron is produced from one of the electron shells of the absorber atom with a kinetic energy given by the incident photon energy E minus the binding energy of the electron in its original shell W_j.
The photoelectric effect can take place with an electron of a layer *j*, only if $E \geq W_j$ [4].

The X-ray attenuation law [1], [3], [4], is the basis of our simulation. We write the classical relation which makes it possible to calculate the number of the photons which traverse without undergoing interaction at a thickness x [2]:

$$dN = -N(x)\mu_i(E)dx \tag{1}$$

In the standard law of attenuation, the coefficient attenuation total equal to the sum of the attenuation coefficients corresponds for each physicals effect to consider [3]:

$$\mu_i N dx = \sum_k \mu_k N dx \tag{2}$$

$\mu_i(E)$ is the sum of all the linear attenuation coefficients describing the various events types (Compton effect, photoelectric effect, …) induced by interaction of the incident photon of energy E with an atom '*i*' or a molecule '*i*'.

In this work we approached the variation of the attenuation coefficient of photons X according to energy, in a simple form using a curve of the experimental values [5], in the case of an oxide of silicon target ($SiO2$).

Approximately the coefficient of the Compton effect in the vicinity of energy E=100 KeV is written:

$$\mu_1 \approx C\rho \frac{1}{E} \tag{3}$$

C: Constant characteristic of the element constituting the target. ρ: Density.
The coefficient of the photoelectric effect is given by [2]:

$$\mu_2 \approx C_i \rho \frac{Z^3}{E^3} \tag{4}$$

C_i : constant representing values very different from a layer i with the other of a given element when $E=W_s, \ldots E=W_l$.

The preceding effects are introduced separately by considering their attenuation coefficients μ_1, μ_2 which are equivalent respectively to a probability so that a photon undergoes an interaction of the type Compton or photoelectric to the crossing of material '*i*'.

2.2 Basic numerical

The Monte Carlo simulation used in this paper is arguably the most accurate method to simulate the phenomenon radiation transport and the physics random process.
We consider the method step by step [6] and by analogy with this study we can proposed this following model.
And our study rests on two cases:
1. Case of a beam of photons X in a number of N_0 (or intensity I_0), monochromatic of energy E, falling on a homogeneous semi infinite medium.
2. Case of a monochromatic beam of photons X with energy E, falling on a finite homogeneous medium of width "a".

For a beam containing a population N_0 of photons the program makes it possible to follow the interactions type with the elements of the target. We take each photon individually and using pulling of the random numbers, we can identify the type of interaction with an element, by using the method step by step [6].

We repeat the process for the follow photons, until we reach the total number N_0. We carry out the statistics and classification of these events by making the same preceding stages more time than the number of pulling fixed in calculation (N_t).

In this simulation the square root of sample variance S has called error.
To be precise, the sample variance is more fundamentally defined as the average value of the squared deviation of each data point from the true mean value $\overline{N}$ [3].

$$S^2 = \frac{1}{N_t}\sum_{l=1}^{N_t}(N_l - \overline{N})^2 \qquad (5)$$

N_l: number of photons which undergoes the event physic process (Compton or photoelectric effects) with element material 'i' at the l^{th} number of pulling
$\overline{N}$: average number of photons which undergoes the event physic process.
N_t : the total number of pulling.

3. Results and discussion

The classification of the effects is made according to the percentage results of the photons computation. The following figures (1, 2, 3, 4) show the statistical of photons population undergoing the various physical events interactions which can occur.

We chose a small limited number of incident photons N_0=5000, for limited the execution time of the program which is implemented under MALAB.

The results of the population of incident photons sudden of the interaction with the oxygen' atoms and the silicon' atoms with different probabilities are obtained after a pulling randomly of one hundred blows and according to a Beta or Exponential probability laws.

The first results relate to a semi infinite homogeneous medium composed of SiO_2 is shown in figure (1, 2).

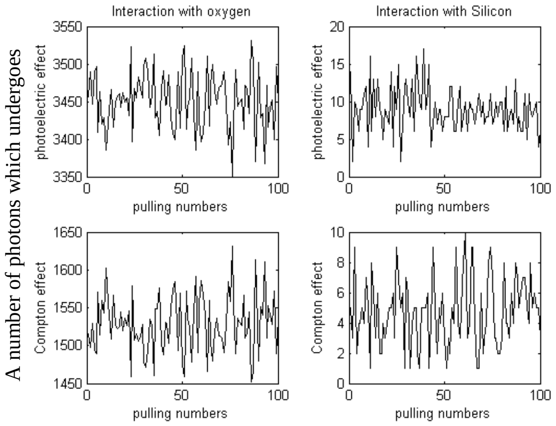

Figure 1: statistics of the physical processes induced by photons X of energy E=100KeV according to exponential probability law.
The photoelectric effect with O_2 =69.0140%
The photoelectric effect with Si =0.1796%
The Compton effect with O_2 =30.5864%
The Compton effect with Si =0.0944%
Simple diffusion =0%

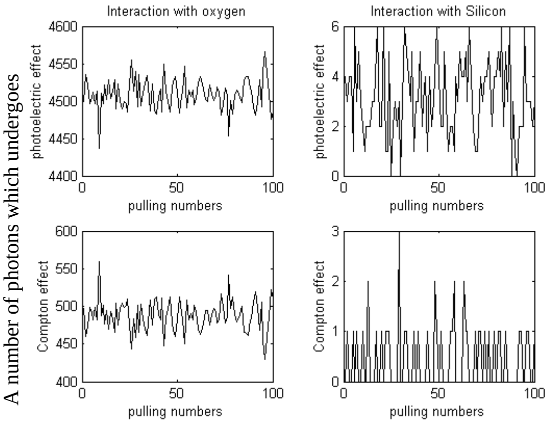

Figure 2 : statistics of the physical processes induced by photons X of energy E=100KeV according to Beta probability law.
The photoelectric effect with O_2 = 90.1798 %
The photoelectric effect with Si = 0.0628 %
The Compton effect with O_2 = 9.7484 %
The Compton effect with Si = 0.0090 %
Simple diffusion = 0 %

In the two cases of distributions we notice that the photoelectric effect is dominating, the classification remains the same but with a difference in percentage of appearance. This difference due to the change of the generation law of the random numbers. The simulation results show a weak pea of interaction probability with silicon and important probability with oxygen.

The following results relate to a homogeneous finished medium with thickness a = 0.5cm composed of SiO_2 is shown in figure (3, 4).

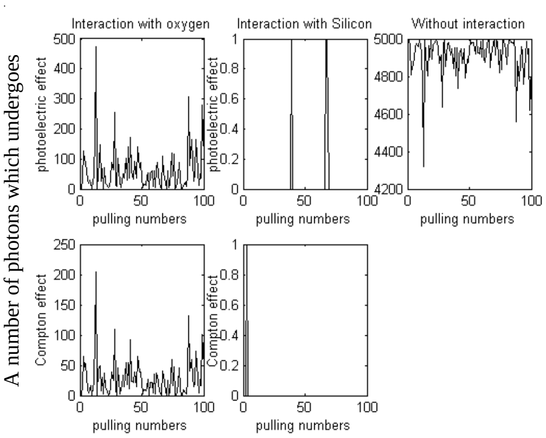

Figure 3 : statistics of the physical processes induced by photons X of energy E=100KeV according to exponential probability law in a medium of width a=0.5cm.
The photoelectric effect with O_2 = 1.2138 %
The photoelectric effect with Si = 6.0000e-004 %
The Compton effect with O_2 = 0.5496 %
The Compton effect with Si =2.0000e-004 %
Without interaction =98.2350 %

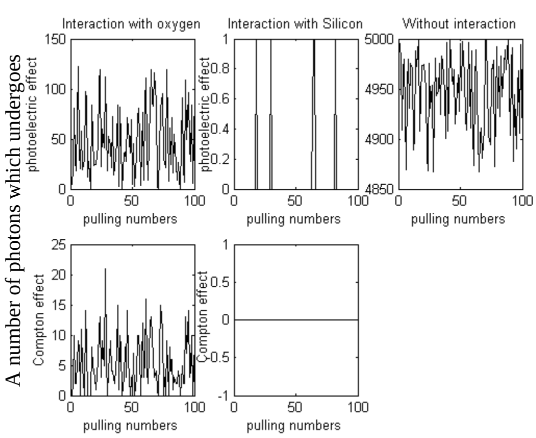

Figure 4 : statistics of the physical processes induced by photons X of energy E=100KeV according to Beta probability law in a medium of width a=0.5cm.
The photoelectric effect with O_2 =0.9660%
The photoelectric effect with Si =0.0010%
The Compton effect with O_2 =0.1092%
The Compton effect with Si =0
Without interaction = 98.9238%

As previously, we notice that in both cases of distributions the photoelectric effect is dominating for the small number of photons which have sudden interaction.

These results show that the greatest number of photons of the total population did not undergo an interaction and thus transmitted, therefore the thickness of the zone of interaction influences considerably on the results.

As long as the number of entries N_0 is reasonably large, the error decreases little for all effect, in the case of semi-infinite target, and has roughly the same variance for second case finite target

4. Conclusion

The proposed simulation makes possible to reveals and draws the effect predominance percentage compared to the other and makes evidence the dependence of the interaction with sample thickness. Our simulation treats only two effects quoted above and is limited to low energy.

In the case of x-rays analysis by transmission process the capture image is given by transmitted or attenuated beam and rests on the attenuation lows whose the effects photo-electric, simple diffusion and transmitted photons, participate to bring the information of the sample structure.

The particular application of the model for SiO2 structure, shows that the photons which have undergoes the photoelectric effect are dominant i.e. the beam is attenuated. The remainder of the photons which have undergoes the Compton effect are minority i.e. the part of beam will disperse in the sample whose generate a Compton electron, diffusion photons and others effects and contribute in generation of the noise which disturb the analysis and then called undesirable phenomena, but they will carry important information for others cases of x-rays analysis.

This work will be able to support the finer expressions of the attenuation coefficients drawn from the experiment to take account of other effects and to work with a very great range of energy.

References

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