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X-RAY REFRACTION 3D-SIMULATION SOFTWARE: FIRST APPROACH

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Abstract

In this work preliminary results on simulation of X-ray propagation in media characterized by low index of both refraction and absorption. First approach has proved the feasibility of typical Math code application for the analysis of X-ray imaging measurements performed by means of high-flux and low-divergent beams shaped by polycapillary half lens.

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1 – INTRODUCTION

The X-ray radiography technique is a new approach to investigate both the fluid dynamics and the structure of liquid jets that allows us to overcome the limits of very-dense multi-scattering conditions verified by means of laser or visible light-source based techniques. However, this technique is characterized by its limits, which refer to the low X-ray refraction index and low X-ray absorption of the materials under investigation. Moreover, besides mentioned difficulties, it is rather problematic to manage complex sources and detectors typically used at running experiments.

In this work we would like to pursue a numerical simulation approach jointly to experimental tests based on the use of conventional laboratory sources in various combinations with polycapillary optical elements. The aim is to built up an open simulation code where both characteristics and nature of the radiation sources, structure and geometry of the samples, and, finally, detectors can be varied enabling in such a way to test a wide possibility of investigating conditions and choose the most effective.

As a starting condition 3D-simulation software, reproducing soft X-ray absorption by a static sample, has been developed. The source produces a parallel (or quasi parallel) X-ray beams. The optical path is in the vacuum and develops from the radiation source to the sample in a spherical geometry and successfully to the detector. The phase shift and intensity loss of the X-rays reaching the detector are very light due to the low value of deflection (δ) and absorption (β) parameter values (see definition below in text). Absorption percentage of 10^{-4} and phase shift around 10^{-15} radians have been calculated by the simulation. First elaboration results to check new software are shown in Figure 1.

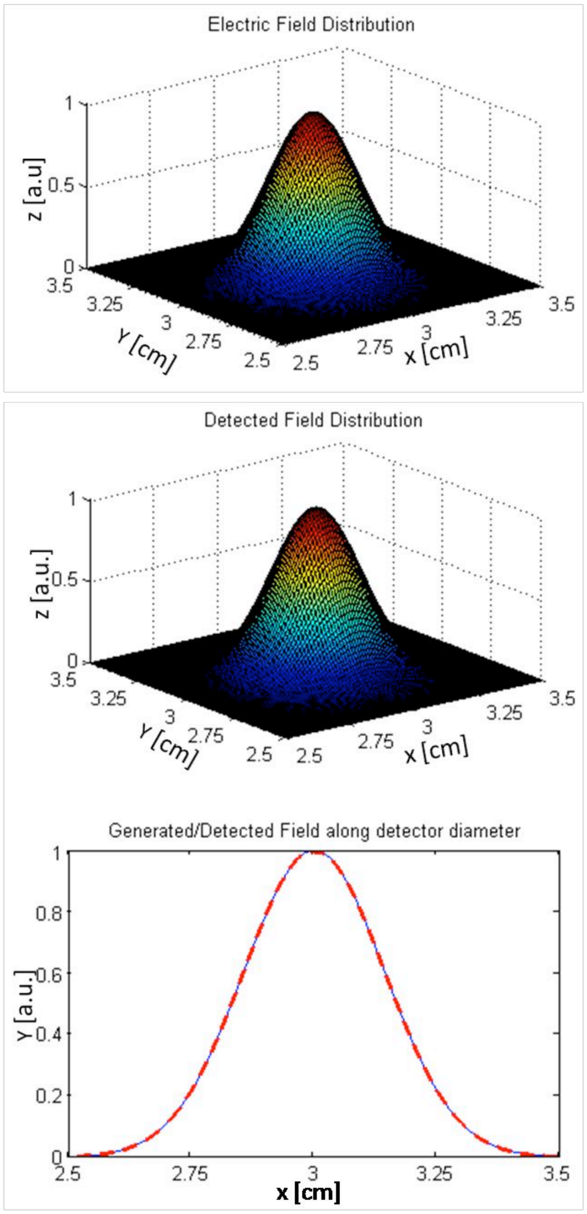

FIG 1 - a) Generated Beam; **b)** Detected Beam; **c)** Generated and Detected Fields median cross section

2 – SOURCE

The source geometry is represented by a circular spot. It is possible to select its position and size by the determination of the radius as well as coordinates of the centre. A normalized Gaussian distribution is generated by the formula:

$$p(x,y) = e^{-\frac{(x-\mu_x)^2+(y-\mu_y)^2}{2\sigma^2}} \quad , \qquad (1)$$

obtained modifying the classical Gaussian distribution equation:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad , \qquad (2)$$

where μ_x and μ_y are the independent variable values (but expected), or the distribution centre, and σ is the variance. The last one has been optimized to obtain a beam shape as realistic as possible, and it is automatically recalculated by the software at every change of the source diameter in order to preserve the distribution profile. The maximum value in relation to the source centre assumed by the distribution, $\sqrt{2\pi\sigma^2}$, is missing in the used formula and it is adapted for the 3D use.

This general description of the field distribution is transformed in energy setting but normalized to its maximum energy value.

The refraction index coefficients δ and β (normally characterizing the sample media) depend on the energy of the source and this dependence is taken into account according to the following well known relation:

$$n(\omega) = 1 - \delta + i\beta = 1 - \frac{n_a r_e \lambda^2}{2\pi}(f_1^0 - i f_2^0) \quad , \qquad (3)$$

where $f_1^0(\omega)$ and $f_2^0(\omega)$ are the atomic scattering factors and are function of propagating media and wave pulsation ω; n_a and r_e are the atomic density and the electron radius, respectively. In the code they are collected in a database as the Energy function.

The beam generated by the source can be assumed as parallel or quasi-parallel plane waves. In the last case a 3D-Gaussian distribution is adopted, setting zero radians for the expected value, while the maximum divergence angle is set at the boundary.

The electric field E of the propagating X-wave changes in the space according to the formula:

$$\vec{E}(\vec{r},t) = \vec{E}_0 e^{-i(\omega t - \vec{k}\cdot\vec{r})} \quad , \qquad (4)$$

where

$$k = \frac{\omega}{c}(1 - \delta + i\beta) \qquad (5)$$

Substituting the Eq.(5) in (4), we get

$$\vec{E}(\vec{r},t) = \vec{E}_0 e^{-i(\omega t - r/c)} e^{-i(2\pi\delta/\lambda)r} e^{-(2\pi\beta/\lambda)r} \quad , \qquad (6)$$

where the first exponential factor represents the vacuum propagation part, while the second is the phase shift; and the third corresponds to the wave intensity decay due to the absorption.

It is possible to estimate both modulus and phase in each point compatibly with the accuracy rate used. However, these values are estimated at the initial, final and medium sample-interface positions in order to speed up the software.

3 – SAMPLES AND SAMPLE-MEDIA INTERFACE

The simulation code has been structured in order to foresee different nature of the investigating samples and the transmitting media. In fact, it is possible to specify the chemical formula of medium as well as that of the samples to evaluate the refraction index and its coefficients. In this case the medium is set as a vacuum by default (n=1). The sample has been simulated as a single sphere or a collection of spheres with the possibility to define the center and the diameter of each one.

A specific subroutine generating random groups of samples of a defined shape is under development to simulate drops of different shapes or clouds of droplets (for instance, conical-like shapes for injected fuel sprays).

The propagating X-ray from the source impacts the sample with a wavelength vector k forming the angle with the normal to sample surface depending on the incident point. The code evaluates the refracted vector and point out direction inside the sample according the Snell's law. A 3D equation system is applied and the emerging wavelength vector k' of the refracted wave direction gives the new impact point at the sample/medium surface. A new incident angle respect to the normal to the surface is established and a new 3D equation system gives the direction of the emerging wave from the droplet. The direction of the last k'' vector enables to calculate the intersection with the detector plane giving the diffraction figure of the incident X-ray on the interposed sample.

3 – DETECTOR

Field distribution at detector place is evaluated. The detector is simulated by circular spot but no spatial limits have been posed. Diameter and centre position are defined by the user. All the field components estimated at the detector plane, which are out of the spot, are rejected.

4 – RESULTS

Absorption and phase-shift have been evaluated by running the software.
Here is reported a simple case concerning a parallel beam (cross-section diameter of 10 mm), which impacts against a spherical sample (diameter of 30 mm). The outgoing beam is collected by the detector, which characterized by the same source dimensions.

TABLE1- The field values at y corresponding to the source diameter section. E_0 is the source signal, E_{ms} is the signal at medium-sample interface; E_{sm} is the signal at sample-medium interface; E_f is the signal at detector;

x	E_0	E_{ms}	E_{sm}	E_f
2.7	0.11024626772842	0.11024626772842	0.11022072848879	0.11022072848879
2.9	0.78270349845259	0.78270349845259	0.78252136819129	0.78252136819129
3.0	1.0	1.0	0.99976717682014	0.99976717682014

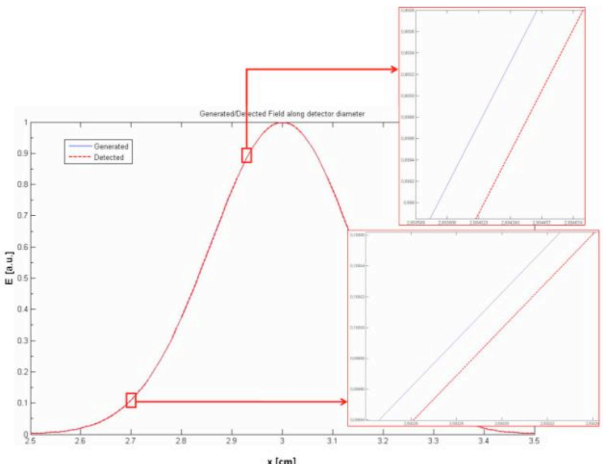

FIG 2 - Comparison between generated and detected fields on the source y diameter plane.

In our simulations we have aligned the source, sample and detector. The selected medium is the vacuum (n=1) while the sample has the following refraction coefficients: $\delta = 3.4129 \cdot 10^{-14}$ and $\beta = 6.1234 \cdot 10^{-15}$.

The initial electric field distribution is normalized and the waves are supposed to have the same polarization at start.

Figure 2 shows generated and detected distribution section at plane source diameter and parallel to y-z one. The signals are apparently overlapped, because of electric field absorption weakness that is typical for X-rays. A signal decreasing factor of 10^{-3} has been estimated. Table 1 reports signal values recorded at different points of the optical path and different distances from the detector centre, which matches the same distances from the sample centre, since the source, sample and detector are aligned. While E_0 (generated field) matches E_{ms} (field value at medium-sample interface), E_{sm} (field at sample-medium interface) matches E_f (signal at detector). It is expected since selected medium is vacuum and waves cross it without absorption or phase-shift phenomena.

Figures 3 and 4 represent the ratio and difference between the detected and generated signal

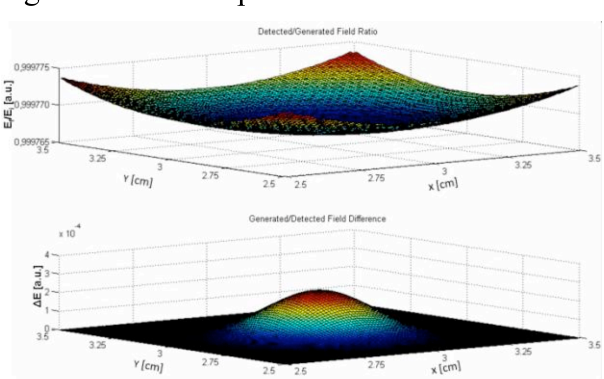

FIG 3 - a) 3D Detected/Generated Field Ratio; b) 3D Difference between Generated and Detected field

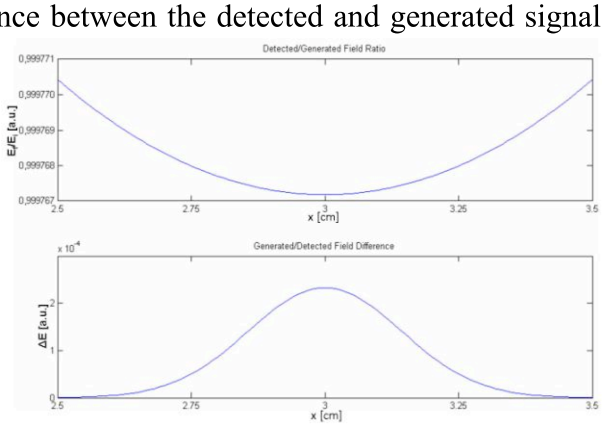

FIG 4 - a) Detected/Generated Field Ratio; b) Difference between Generated and Detected field

in 2D and 3D, respectively. Less is the distance from centre, greater is the beam path across the sample and stronger results for the absorption of the incident radiation. The estimated phase-shifts related have magnitude of 10^{-15} radians; the precision rate of the software doesn't allow to keep in account so slight angle difference in the generation of wave unit vectors.

A simulation software reproducing X-ray absorption by static sample has been developed. First results highlight a coherent estimation of the wave decay. An improvement is requested to evaluate phase shift more exactly because of its low magnitude.

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