The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
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MONTE CARLO SIMULATION OF X-RAY THANSMISSION THROUGH MONO-CAPILLARIES

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ABSTRACT

The x-ray transmission property of capillary tubes is the basis of capillary x-ray optic designs. Based on the theory of x-ray transmission through capillaries, a detailed Monte Carlo method is suggested in this paper. An associated corresponding computer program is worked out. It can deal with the surface roughness/waviness effects of x-ray reflection on non-perfect surface. For a given model, the transmission efficiencies of capillary tube versus diameters and curvature radius are calculated. The distributions of x-ray intensity on the reception plane are presented. The calculated results agree well with the experimental results.

Key Words: x-ray capillary tube, transmission property, Monte Carlo method, simulation

1 INTRODUCTION

Capillary x-ray lens (Kumakhov lens) is composed of tiny glass capillary tubes which guide x-ray by total external reflections from the inside surface of the hollow tubes. Its ability to focus and control x-rays is now been employed by various scientific applications, such as material analysis, microelectronics manufacture, x-ray astronomy and medical image. Because each lens contains hundreds or thousands of precisely shaped and located hollow channels, it is desirable to assess the feasibility of a variety of capillary geometries for a new application without physically constructing the lens. The performance of capillaries is influenced by a number of factors, such as the composition of the capillary material, the status of x-ray source, the dimensions and actual shape of the capillary, as well as the surface roughness/waviness of the reflecting surface. Therefore, it is essential to estimate the transmission property of tubes or mono-capillaries by theoretical simulation for x-ray optics design.

Three models, non-acceleration of gravity model (J. B. Ullrich *et al.* 2000), beam dispersed model (B. Z Chen *et al.* 1993) and rays tracing model (L. Vincze *et al.* 1998) had been used for calculation of x-ray transmission through capillary tubes. The non-acceleration of gravity model treats the x-ray transmission in meridional space of capillary, and can only give an approximate result. The beams dispersed model requires that the x-ray must be parallel, and it only accounts for the roughness effect of specular reflection. In this paper, a ray tracing model using Monte Carlo method is adopted. It ha s the advantage of dealing with various x-ray sources, simulating x-ray reflection on rough surface, and getting statistic. An associated computer program is worked out according to this method. The effects of capillary bending and internal surface roughness/waviness are treated effectively in the program.

2 THEORY OF CAPILLARY

2.1 Reflection

Capillary x-ray optics relies on reflection of x-ray on the inner surfaces of the hollow capillary tubes. The refractive index of glass for x-ray is slightly less than one, and the refractive index of air inside tubes is almost unity. Total internal reflection occurs only for those x-rays that strike tubes at angles large than the critical angle.

The refractive index of glass for x rays can be written as

$$n = 1 - \delta - i\beta \tag{1}$$

where δ is the refractive index decrement, β is proportional to absorption of glass. The relation between δ , β and the factor of scattering $f = f_1 + i \bullet f_2$ is

$$\delta = \frac{r_e \lambda^2 N f_1}{2\pi} = \frac{e^2 \lambda^2 N f_1}{2\pi m_e c^2} \tag{2}$$

$$\beta = \frac{r_e \lambda^2 N f_2}{2\pi} = \frac{e^2 \lambda^2 N f_2}{2\pi m_e c^2} \tag{3}$$

where r_e is the classical radius of electron, λ is x-ray wavelength, N is the density of free electron in the glass, and m_e is the electron mass.

The reflectivity on perfect surface can be given by Fresnel's formula (R. H. Pantell *et al.* 1978)

$$\overline{R}(\theta) = \begin{cases} 1 - \dfrac{4\beta}{\theta_c^2 \sqrt{(\theta_c/\theta)^2 - 1}} & 0 \le \dfrac{\theta}{\theta_c} < 1 - 2\gamma^2 \\ 0 & 1 - 2\gamma^2 \le \dfrac{\theta}{\theta_c} \end{cases} \tag{4}$$

where θ_c is the maximum angle with which an x-ray can strike the capillary wall and still be reflected, i.e. critical angle, θ is the incident angle, $\gamma = \beta / \delta << 1$. An expression using Snell's law for the critical angle is

$$\theta_c = \sqrt{2(n-1)} = \sqrt{2\delta} \tag{5}$$

2.2 Surface roughness modeling

For an actual capillary tube, its inner surface could not be perfect smooth. The reflectivity of x-ray for the rough surface can be calculated from the relation (R. H. Pantell *et al.* 1978),

$$\tilde{R}(\theta) = \overline{R}(\theta)\exp[-(\frac{4\pi\sigma\sin\theta}{\lambda})^2] \tag{6}$$

where σ is the rms (root of the means square) surface roughness parameter.

An obvious shortcoming of the above model is that it accounts for the attenuation of the beam reflected in the specular direction only. The diffuse scattering of x-ray at the rough surface is neglected. This means that the actual intensity loss from the reflected photon as a result of the above roughness correction is overestimated.

In order to include the above mentioned diffuse scattering at rough surface, a model described by Kimball *et al.* (Y. W. Tan *et al.* 1995) has been used. The total reflectivity R is given as the sum of the specular and diffuse reflectivity coefficient (R_S and R_D),

$$R = R_S + R_D \tag{7}$$

As shown in Fig.1, in case of specular component, the angle of reflection is equal to the angle of incident, while the diffuse scatterd component will emerge with an angle θ'.

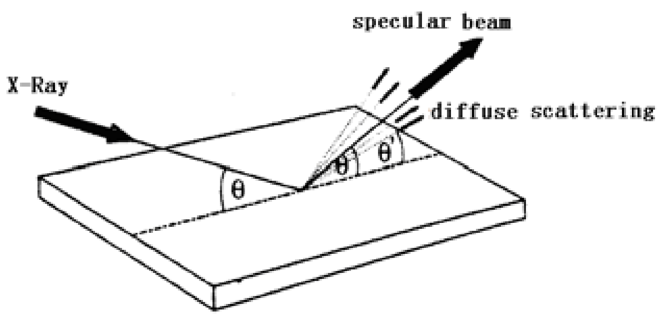

Figure 1. Schematic description of the reflection geometry from a rough surface

The specular reflectivity can by expressed in terms of the dimensionless parameters: $\tau = \theta/\theta_c$, $\varphi = s/P$, and $B = \sigma/D$ in the following form:

$$R_S = R_0 - 4\tau B^2[\sqrt{r_A}\cos(\xi_A/2) - \sqrt{r_B}\sin(\xi_B/2)] \tag{8}$$

with

$$r_A = \sqrt{(1/\varphi)^2 + \tau^4}\ ,\ r_B = \sqrt{(1/\varphi)^2 + (1-\tau^2)^2}\ ,$$

$$\tan(\xi_A) = 1/(\varphi \cdot \tau^2),\ \tan(\xi_B) = 1/[\varphi(1-\tau^2)].$$

In the expression above, s is the roughness correlation length, $D = c/\omega_p$ is the glancing angle penetration depth and $P = 2D/\theta_c$ is the approximate distance the ray travels in the glass while being reflected, ω_p is the plasma frequency of electrons in the glass.

Note that in this model the rough surface is characterized by two parameters, i.e., by the rms surface height deviation relative to the mean height, σ, and by the correlation length of the roughness, s. The latter is related to the rate of height changes along the material surface.

The diffuse scattering coefficient R_d is characterized using its differential form:

$$\frac{dR_D}{d\tau'} = \tau\tau'^2 B^2 \frac{8}{\pi}\left(\frac{\varphi}{1+\varphi^2(\tau^2-\tau'^2)^2}\right) \tag{9}$$

where $\tau' = \theta'/\theta_c$ is the dimensionless parameter of the diffuse scattering angle, in the range of 0~1. Therefore, R_D may be written as

$$R_D = \int_0^1 \tau\tau'^2 B \frac{8}{\pi}\left(\frac{\varphi}{1+\varphi^2(\tau^2-\tau'^2)^2}\right) d\tau' \tag{10}$$

The total reflectivity R can be obtained from Eqs. (8) and (10). The diffuse scattering angle may be randomly sampled by the cumulative distribution function,

$$F(\tau) = \frac{1}{R_D}\int_0^{\tau}\left(\frac{dR_d}{d\tau'}\right) d\tau' \tag{11}$$

3 MONTE CARLO SIMULATION

3.1 Outline of the simulation

The transmission of x-ray in capillary tubes may be regarded as two processes. One is that x-rays are reflected by inner surface of tubes. The change of x-rays' direction and intensity through reflection are expressed in this process. Another is the transmission process of x-rays between capillary walls. The track of x-ray is almost near straight line because the radius of guide is much larger than the wavelength of x-ray. The transmission process of x-ray in a tube is shown in Fig. 2, in which l_1 is the distance between x-ray source and entrance of capillary, l_2 is the distance between exit end of the tube and the detecting plane (Σ), R is the radius of capillary curvature, d is the inner diameter of capillary.

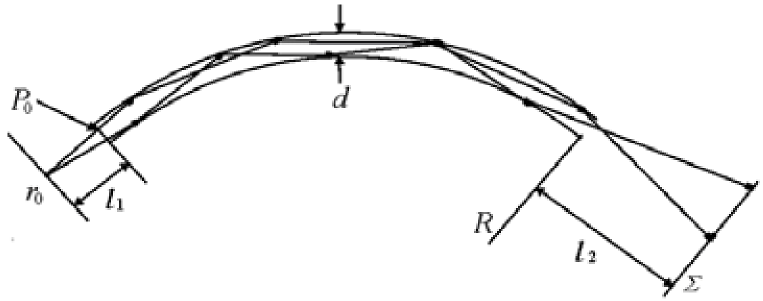

Figure 2. Transmission of X-Ray in a curved capillary

The whole process can be simulated by Monte Carlo methods. The detail method is given as follow.

First, the coordinate, direction and energy of initial simulation photons are determined. Initial coordinates $\mathbf{r_0}$ are selected according to the spatial distribution of the source, while the initial direction is chosen on the basis of the source's angular distribution. For an isotropic source, the probability of x-ray entering the capillary tube is very low due to small radius of capillary tube. In order to increase the sampling efficiency, the directions of initial photons should be bias sampled. On the plane of capillary entrance, an intersection point $\mathbf{P_0}$ is generated by uniformly sampled. The direction of x-ray $\mathbf{\Omega_0}$ was determined by $\mathbf{r_0}$ and $\mathbf{P_0}$. Then the probability W of initial photons entering the tube can be calculated. So, the intensity of photons entering tube can be given by the form $I = I_0 \cdot W$, where I_0 is the x-ray source intensity. Using the bias sample method, every initial sampled photon can enter the capillary tube.

The next step is the determination of the location where a reflection of a sampled photon occurs. If the direction of a photon would not satisfy the reflection condition, the photon should not be simulated, and another photon should be sampled. Otherwise, the intensity and direction of the simulated photon after the reflection is then updated by the reflection theory of roughness surface described in the previous section. The probabilities of specular and diffuse are calculated respectively according to formulas (8) and (10). Depending on the relative magnitudes of these probabilities, a random choice is then made between the two processes. In the case of the specular component, the angle of reflection is simply chosen as $\theta' = \theta$. For the diffuse scattering component, the angle of reflection θ' is selected by using the cumulative distribution function of equation (11). The above procedure is repeated until the photon either escapes from the device or exceeds the critical angle.

The last, the statistics including the transmission efficiency, the intensity distribution on the detection plane of x-rays passing through the capillary tube are given. The transmission efficiency η is given by the form: $\eta = I_{out} / I_{in}$, where I_{out} is the intensity of x-ray entering capillary, I_{out} is the intensity of x-ray escaping from capillary. The average transmission efficiency is given as

$$\overline{\eta} = \frac{\sum_{m=1}^{K} \eta_m}{K} \tag{12}$$

where η_m is the transmission efficiency of any sampled photon, and K is the number of sampling photons. The calculation precision is judged by the relative error ε, which is written as

$$\varepsilon = S_{\bar{\eta}} \Big/ \bar{\eta} \tag{13}$$

$$S_{\bar{\eta}}^2 = \frac{1}{K}\left[\overline{\eta^2} - (\bar{\eta})^2\right] = \frac{1}{K}\left[\sum_{m=1}^{K}\eta_m^2 \Big/ K - \left(\sum_{m=1}^{K}\eta_m \Big/ K\right)^2\right] \tag{14}$$

A corresponding computer program is worked out to simulate above processes. The flow chart of the program is shown in Fig.3.

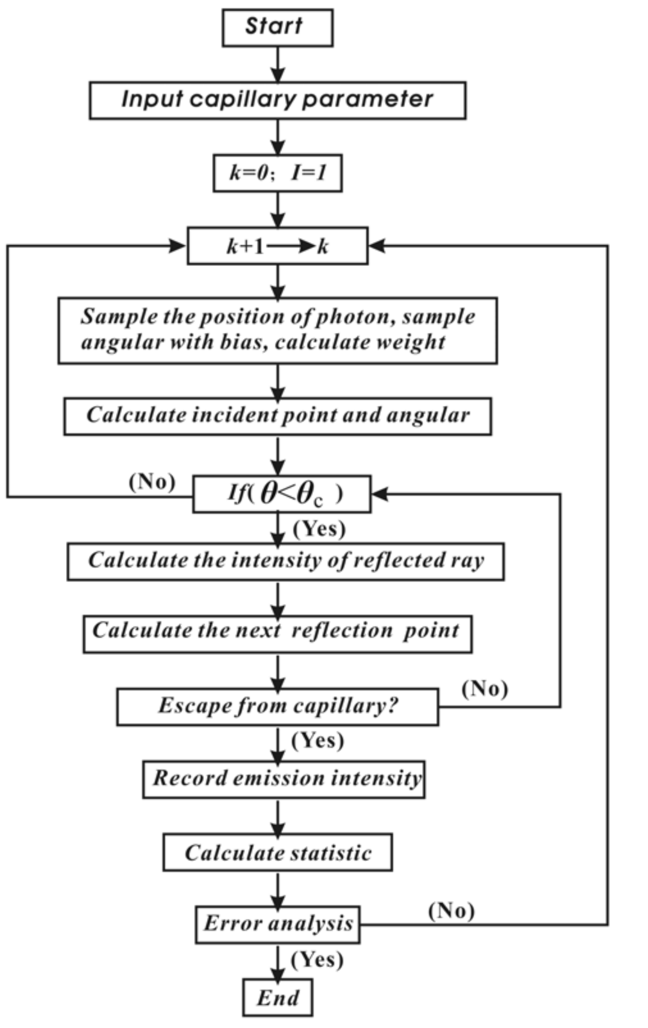

Figure 3. Flow chart of the program

3.2 Examples and Results

In order to verify the method described above, the transmission efficiency of a simple straight cylinder capillary guide for 8keV x-ray was calculated for comparing with experiment. The capillary guide at the distance of 50mm from the x-ray source with the length is of 550mm and the surface roughness of 2nm was used in the calculation. The critical angle and parameter γ , obtained from Eqs.(2), (3) and (5), are 0.0041rad and 0.0076. Taking different diameters, we calculate the transmission efficiencies using the program. The calculation and the experiment results (Y. W. Tan *et al.* 1995) are shown in Fig.4. It shows that the results obtained in this paper agree well with the experimental results.

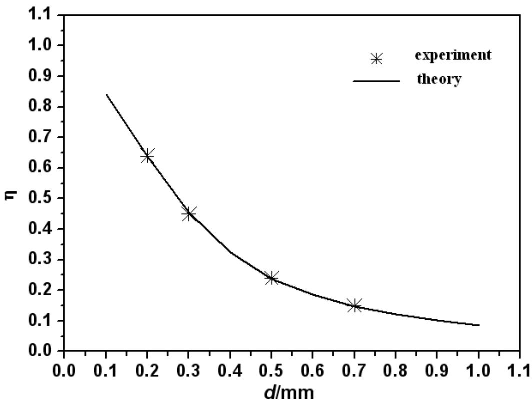

Figure 4. Transmission efficiency versus diameter

For a curved capillary tube, the transmission character is related to its curvature radius. The transmission efficiencies of curved capillary tubes versus curvature radius for 8keV x-ray is studied. In the calculation, we assume that $l_1 = 50mm$, $L = 550mm$, $d = 0.3mm$, and the surface roughness $\sigma = 2nm$. Table I lists the calculation results of transmission efficiency for various curved capillaries. It shows that the transmission efficiencies increase as the curvature radius. When the curvature radius of curved capillary approaches infinity, the transmission efficiency of curved capillary tends to that of straight capillary.

Table I. Transmission efficiency of x-ray through various curved capillaries

R/m	50	100	150	1500	(straight)
η	0.296	0.412	0.437	0.452	0.456

In the above calculation, we only consider the specular reflection on roughness surface. The effect of diffuse scatter has been taken into account in the calculation. When we assume the curvature radius of 150m and the correlation length of the roughness with 0.001, the transmission efficiency is 0.441. It is slightly larger than the result listed in the table I. This accords with the theoretical analysis in the previous section.

The distribution of x-ray intensity on the reception plane, which has a distance of 100mm from the capillary exit end, is shown in Fig. 5.

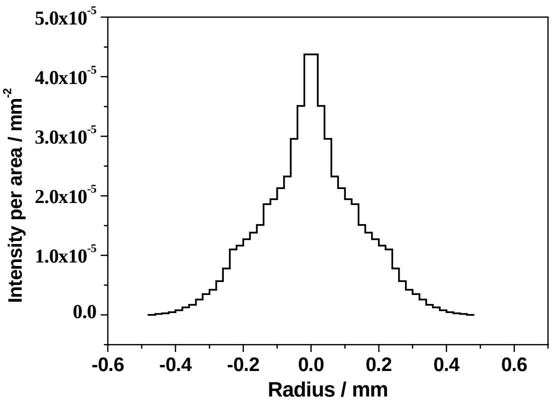

Figure 5. Distributions of x-ray intensity on the reception plane

4 CONCLUSION

Using the Monte Carlo simulation described in the paper, the transmission of x-rays in capillary is simulated, and the simulation methods not limited by the direction of x-ray and the source position. And the surface roughness is carefully taken into account. The property of x-rays through capillary guides is simulated using our program. The calculation results agree well with the experiment. The program can be used to simulate the transmission of x-ray in arbitrary capillary tube. And the simulation method can be extended to simulate the transmission of x-ray through assemble capillaries.

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