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Nuclear Instruments and Methods in Physics Research B 243 (2006) 223–226

NIM B
Beam Interactions with Materials & Atoms

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The X-ray distribution after a focussing polycapillary – a shadow simulation

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Received 23 May 2005
Available online 8 September 2005

Abstract

The X-ray propagation in a focusing polycapillary (X-ray focusing lens) was simulated with the ray-tracing program SHADOW. The X-ray intensity distribution after the polycapillary was investigated for the relative source-optics positions.

PACS: 41.50.Th; 42.15.Eg; 42.81.Wg

Keywords: Computer simulation; Ray-tracing; SHADOW; Polycapillary X-ray lens; Focusing

1. Introduction

Polycapillary X-ray optics has been developed for more than one decade and became more practical and commercially available in recent years [1–3]. In a previous study [4], we have reported the simulation results on polycapillaries having cylindrical and polynomial profiles. The simulation was done with the ray-tracing program SHADOW developed by the Center for Nano Technology of University of Wisconsin – Madison (UW-CNTech) [5–7].

In this study, with the same method, we will report the simulation results for a focusing polycapillary. Fig. 1 shows the longitudinal and perpendicular cross-section views of this focusing polycapillary. All simulations were done for a point X-ray source emitting 30 keV photons and for the silicon dioxide capillaries with a perfect smooth inner surface (assume roughness = 0). Two lakhs random rays emitted from the X-ray source were used in most simulation. Fig. 2 illustrates the arrangement used in simulating the focusing optics. The X-ray source is placed on point S with the distance to the optics entrance as $\boldsymbol{d}_\mathrm{s}$ (mm). The angle distribution of the X-ray source is *CONICAL* with the cone internal half aperture of θ (radian). The beams will propagate toward the $-Z$ direction through the entrance of lens at the X–Y plate with $z = 0$. The X-ray image will be taken at the point I with the distance $\boldsymbol{d}_\mathrm{i}$ from the exit of polycapillary.

The focusing polycapillary investigated in this simulation is composed of 91 straight tubes packed together in a Wigner–Seitz cell algorithm (see Fig. 1). A family of polynomials that track the centerline and the change in radius specifies the array of tubes (channels). The equations determine the position and the profile of these tubes are as follows:

$$(X - C_i g(z))^2 + (Y - C_j g(z))^2 = (r_0 f(z))^2 = R^2, \quad (1)$$

$$f(z) = a\_fz + b\_fz^2 + 1, \quad (2)$$

$$g(z) = a\_gz + b\_gz^2 + 1, \quad (3)$$

where C_i, C_j are center coordinates of each tube at the X–Y plane (at $z = 0$) that locates the entrance of lens. r_0 is the entrance radius of each tube. The function $f(z)$ specifies variation of r_0 along the beam moving direction. The

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doi:10.1016/j.nimb.2005.07.209

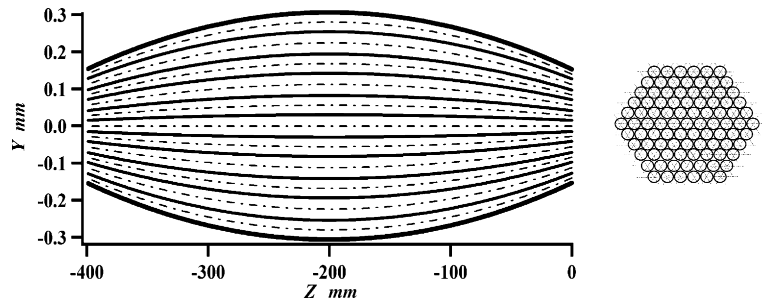

Fig. 1. The longitudinal and perpendicular cross-section views of a focusing lens. It shows the centerline (dotted lines) and wall (solid lines) of each channel.

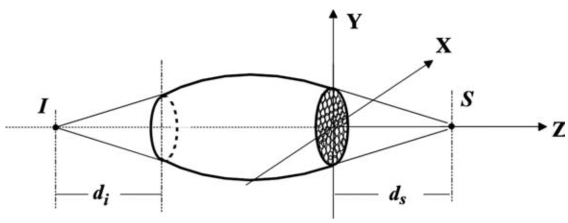

Fig. 2. Layout of polycapillary lens and X-ray source in simulation with SHADOW.

function $g(z)$ specifies how does the centerline of tube change. Table 1 gives an example of parameters used in simulation of the polycapillary. L is the length of lens, R_{max} is the maximum radius of lens. The unit for all lengths used in this simulation is mm.

2. X-ray image and beam intensity distribution

SHADOW can simulate the X-ray image or beam density (intensity) distribution at any position along the X-ray pathway – before, inside and after the polycapillary. The most interested is the X-ray images after the optics. These images reveal the collimation function of the polycapillary and the factors that influence this function. Figs. 3–5 present the X-ray images at immediate exit, 83 mm and 5000 mm away from exit of the focusing lens respectively. The 83 mm approximates the "focal point" of the polycapillary specified by parameters shown in Table 1. All curves in Fig. 2 will meet at $z = 82.8427$ and $z = -482.8427$. These z values were obtained by taking $g(z) = 0$ in Eq. (3). $z = 82.8427$ is the focal point at source side, and $z = -482.8427$ is the focal point at image side.

At $\boldsymbol{d}_i = 0$, the fine structure of hexagonally arranged channels can be seen obviously. In *Kumakhov method 1*, Wigner–Seitz cell algorithm is used for unlimited number of tube lattice. The number of tubes that build the polycapillary are selected either by restricted illumination area of X-ray beams or by a screen arranged before the entrance. A round screen is used in this simulation because the hexagonal screen is not available in SHADOW. Tubes just on edge of the round screen produced the "halo" around outer loop of lens shown in Fig. 3. On right side of Figs. 3–5 are images that demonstrate the beam intensity distribution in three dimensions. These 3D images were created by MATLAB from exported "scatter data" of SHADOW. The vertical coordinate is the beam density (beam numbers at certain area). The beam density was counted within a 0.008×0.008 mm square that we call as the box. The 3D image at $\boldsymbol{d}_i = 0$ mm (Fig. 3) clearly shows many high intensity tips on exit of each tube. When imaging plane is being moved further away from lens exit, beams from each channel are mixing up and the "fine structure" disappeared.

At $\boldsymbol{d}_i = 83$ mm, X-ray image became to a well-focused round with very high density at its center. In order to show the details of the tip, the counting box used here is 0.002×0.002. This clearly demonstrates the capability of "focusing" X-ray beams by this polycapillary.

With further increase of distance from lens exit, the focusing peak disappears and X-ray image expands significantly to a large round. At $\boldsymbol{d}_i = 5000$ mm, the diameter of image become larger than 15 mm with more flat intensity distribution as shown in Fig. 6.

Fig. 6 shows the 2D plots of beam density distribution for $\boldsymbol{d}_i = 0$, 83 and 5000 mm. These 2D plots were produced from extracting data at $y = 0$ in corresponding 3D plots in Figs. 3–5 and normalized to box $= 0.008 \times 0.008$. The background (the beam intensity without polycapillaries at same distance) is also calculated by SHADOW and is shown as the dotted lines in three plots for comparison.

A ratio ρ is defined in this simulation as the "gain" of focusing polycapillary. For example, at $\boldsymbol{d}_i = 83$ on $X = 0$, beam intensity is 6000 (with lens) and 3 (without lens), thus

Table 1
Parameters used in simulation

Shape	Function	L, mm	R_{max}, mm	r_0, mm	a_g	b_g	a_f	b_f
Barrel	Focusing	400	0.3	0.015	−0.01	−0.000025	−0.01	−0.000025