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Technical notes

13.1 micrometers hard X-ray focusing by a new type monocapillary X-ray optic designed for common laboratory X-ray source

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ABSTRACT

A new type of monocapillary X-ray optic, called 'two bounces monocapillary X-ray optics' (TBMXO), is proposed for generating a small focal spot with high power-density gain for micro X-ray analysis, using a common laboratory X-ray source. TBMXO is consists of two parts: an ellipsoidal part and a tapered part. Before experimental testing, the TBMXO was simulated by the ray tracing method in MATLAB. The simulated results predicted that the proposed TBMXO would produce a smaller focal spot with higher power-density gain than the ellipsoidal monocapillary X-ray optic (EMXO). In the experiment, the TBMXO performance was tested by both an optical device and a Cu target X-ray tube with focal spot of 100 μm. The results indicated that the TBMXO had a slope error of 57.6 μrad and a 13.1 μm focal spot and a 1360 gain in power density were obtained.

1. Introduction

Capillary X-ray optics utilizing external total reflection (Kumakhov lens) is a type of X-ray regulation device whose main function is to focus the X-ray beam emitted from an X-ray tube or synchrotron X-ray source into a spot [1]. Capillary X-ray optics has many applications in micro X-ray analysis, including micro X-ray fluorescence (MXRF), confocal micro X-ray fluorescence (CMXRF), micro X-ray diffraction (MXRD), confocal micro X-ray diffraction (CMXRD), and micro X-ray absorption for fine structures (MXAFS) [2–6]. The common feature of these technologies is that they take advantage of the small focal spot and high gain of the capillary X-ray optics. Therefore, to decrease analysis time and acquire more information about a sample, a capillary X-ray optic with smaller focal spot and higher gain is beneficial in X-ray analysis. For instance, Sun et al. (2014) [7] determined the grain size of polycrystalline materials with CMXRD based on polycapillary X-ray optics. In their study, the focal spot size was a significant factor in determining the limit of detection of the technology used. Ohzawa et al. (2004) [8] employed high-intensity monocapillary X-ray optics with a 10 μm focal spot in an analytical X-ray microscope and compared the performance with that of a commercially available polycapillary tube. Yamamoto et al. (1988) [9] simultaneously used parabolic monocapillary X-ray optics to produce a focal spot of 5.7 μm with diffraction X-rays for observing local reactions and residual stresses, and X-ray fluorescence for analyzing least-amount-of-impurity elements in micro-regions during ultra-large-scale integration processing at temperatures of 900 °C or higher.

Capillary X-ray optics commonly used to focus the X-rays from synchrotron or X-ray tube sources are of two main types: polycapillary X-ray optics and monocapillary X-ray optics. Typical polycapillaries create beam sizes of tens of micrometers. Commonly in practice, monocapillary X-ray optics produce a smaller focal spot than polycapillary methods. Monocapillary X-ray optics could divide into three types according to there shape: paraboloidal monocapillary X-ray optics (PMXO), ellipsoidal monocapillary X-ray optics (EMXO) and tapered monocapillary X-ray optics (TMXO). For example, Bilderback et al. (1994) [10] condensed hard X-ray beams to ultra-small dimensions using a TMXO at the Cornell High Energy Synchrotron Source (CHESS), providing a spatial resolution of 50 nm for characterizing materials. Snigirev et al. (2007) [11] obtained a focal spot measuring about 250 nm using two-step focusing consisting of an EMXO and a Fresnel zone plate. A focus better than 18 μm diameter full-width-half-maximum (FWHM) 3 cm from the capillary tip was produced for protein crystallography by a single-bounce capillary with 12 keV X-rays from the CHESS D1 station

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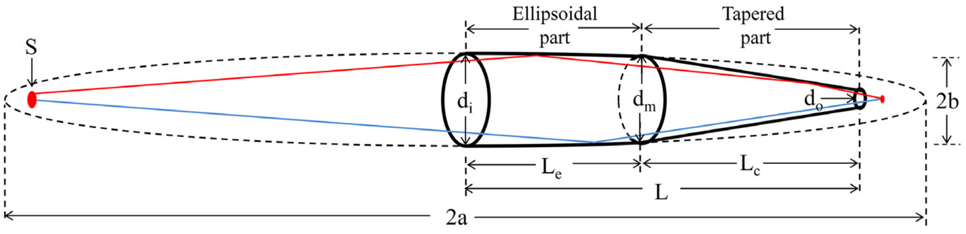

Fig. 1. Schematic of proposed TBMXO. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Design parameters of proposed TBMXO.

Parameters	a	b	L	L_e	L_c	d_i	d_o	d_m	D
Value (mm)	250	0.5	249	150	99	1	0.02	0.8	1.6

hard-bend dipole magnet [12]. Therefore, monocapillary X-ray optics with micro-focal spot is suitable for micro X-ray analysis.

Monocapillary X-ray optics is commonly combined with a synchrotron or micro-focal X-ray tube source [13,14]. However, it can be difficult to get beam time at a synchrotron facility. Similarly, micro-focal X-ray tubes are more expensive and also less powerful than common X-ray tubes. Therefore, a type of X-ray optics with small focal spot flexibly coupled with a common laboratory X-ray tube is needed for general laboratory micro X-ray analysis. To solve this problem, in this study a new type of monocapillary X-ray optics with several micrometers focal spot for use with a general laboratory X-ray tube source is proposed.

2. Configuration of the proposed TBMXO

The shape of the proposed TBMXO (Fig. 1) comprises two parts: an ellipsoidal part and a tapered part. The ellipsoidal part is identical to an EMXO. In the ideal situation, the blue line in Fig. 1 represents the path of X-rays emitted from the X-ray source passing through the ellipsoidal part and focused at the focal spot. The spot size of the X-ray source and imperfections in the optic result in deviation of the photon propagation path from the ideal path, shown by the red line in Fig. 1 [15]. In the proposed TBMXO, the tapered section re-condenses partially disordered X-rays at the tip. In this way, the TBMXO produces a smaller focal spot and higher intensity gain than the EMXO when used with a common large-focus X-ray tube.

Parameters a and b in Table 1 are the major and minor semi-axes of the ellipsoidal part, respectively; d_i, d_o are the entrance and exit diameters, respectively; d_m is the diameter at the junction of the ellipsoidal part and tapered part; L is the total length of the TBMXO; and L_e, L_c are the lengths of the ellipsoidal part and tapered part, respectively. D is the working distance which is the distance between the downstream end of the optic and the focal spot.

3. Simulating the TBMXO by ray-tracing method

Before testing, the operation of the TBMXO was simulated in MATLAB using a ray-tracing method [16]. Previous studies have indicated that the reflection of an X-ray dose occurs if the incidence angle of the X-ray is less than a critical angle θ_c, which depends on the X-ray energy and the material of the capillary. In general, θ_c (mrad) is given by:

$$\theta_c = \frac{20.3\sqrt{\rho}}{E_k}, \tag{1}$$

where ρ is the density of the reflector material (g/cm^3) and E_k is the photon energy (keV). In this study, the capillary was made of silicate glass of approximate density 2.4–2.6 g/cm^3; therefore:

$$\theta_c = \frac{30}{E_k}. \tag{2}$$

Table 2
Comparison of performances of TBMXO and EMXO for X-ray tubes with different focal size.

Parameter	Optic	50 μm	100 μm	150 μm	200 μm
Focal spot diameter (μm)	TBMXO	10.7	11.3	16.2	19.6
	EMXO	21.9	41.7	60.5	80.8
Gain	TBMXO	6650	2130	1010	518
	EMXO	3200	932	400	240
Transmission efficiency	TBMXO	80.1%	46.9%	26.3%	16.5%
	EMXO	100%	100%	100%	100%

The transmission efficiency (η) of X-ray beams through a capillary is given by:

$$\eta = \frac{I_o}{I_i}, \tag{3}$$

where I_o is the flux of exiting X-ray beams and I_i is the flux of X-ray beams entering the capillary. In the simulation, all incident X-rays were controlled by the source and the entrance of the capillary. The flux of exit beams included only the pass-through beams. Numerical integration was used to calculate I_o and I_i.

The gain (G) of capillary power density is defined as:

$$G = \frac{I_{with}}{I_{without}}, \tag{4}$$

where I_{with} and $I_{without}$ are the X-ray flux with and without capillary, respectively. Generally, we chose a pin-hole with diameter equal to the focal spot of the capillary to calculate the power density gain.

The parameters of the TBMXO in Table 1 were used in the simulation. The X-ray tube was a Cu target with a focal spot of 100 μm. Fig. 2, which shows the simulated profile of the TBMXO in operation, reveals the transmission process of the internal X-ray reflection in the optics. X-rays emitted from the source are firstly focused by the ellipsoidal part of the TBMXO, and further compressed at the tip of the tapered part. The 3D and 2D images of the simulated intensity distribution 1.6 mm from the exit of the TBMXO are shown in Fig. 3. To reveal the effect of the tapered part of the TBMXO, an EMXO with the same parameters as the ellipsoidal part of the TBMXO was simulated. Fig. 4 shows the simulated intensity distribution in the focus of the TBMXO (black line) and EMXO (red line). After Gaussian fitting, the focal spot sizes of the TBMXO and EMXO were 11.3 μm and 42.2 μm, respectively. The gain (G) in power density was 2130 for the TBMXO and 932 for the EMXO. The transmission efficiency (η) of the EMXO was taken to be 100%, since the initial condition in the simulation was that X-rays are totally reflected if the incident rays satisfy the total internal reflection condition for ideal optics. The value of η for the TBMXO was 46.9%.

Table 2 shows the performances of the TBMXO and EMXO on X-ray tubes with different focal spots. The focal spot of both types increased with increasing X-ray tube focal spot, but the EMXO was affected more than the TBMXO. The gain in power density of both decreased with