FINDING THE OPTIMUM BERYLLIUM LENS COMBINATION:

BEYOND THE SIMPLE THIN LENS APPROXIMATION

DESY Summer Student Programme 2010 Report

By Rima Al-Khuzheyri

Supervisor: Michael Sprung

September 7, 2010

DESY, Hamburg, Germany

TABLE OF CONTENTS

Motivation

A new synchrotron Petra III has just started operation in Hamburg. Since the synchrotron is the brightest in the world, the coherent portion of its beam is larger than anywhere else. When studying samples with X-rays, one may find that it is necessary to use as much of the coherent flux as possible. The transverse coherent length is given by:

$$\xi = \lambda \frac{s2s}{G}, \tag{1}$$

where λ is the X-ray wavelength, $s2s$ is the source to sample distance and G is the source size. In our case the vertical coherence length $\xi_v \approx 10^{-4}$ m, and the horizontal - $\xi_h \approx 10^{-5}$ m, the coherence volume can also be calculated.

For coherent scattering experiments it is necessary to resolve the speckles on the detector. The speckle size is given by:

$$s = \lambda \frac{d}{p\_s} \approx \begin{cases} 10^{-5} \text{ m for the PI-LCX detector} \\ 10^{-6} \text{ m for the Pilatus detector} \end{cases}, \tag{2}$$

where d is the distance from the detector to the sample (5 m is our case), and p_s is the pixel size (20 μm and 172 μm respectively). Formula (2) can be used to determine the maximum pinhole size before the sample.

It turns out that the coherent volume is much larger than the pinhole size (see Table 1), so in order to solve this problem, it is necessary to focus the beam.

Table 1.

	Maximum pinhole size, $[m^2]$	Coherence volume, $[m^2]$
PI-LCX	10^{-10}	10^{-9}
Pilatus	10^{-12}	

The contradiction between the maximum pinhole size and the coherent volume at the coherence beamline P10 at PETRA III.

There are multiple ways of focusing X-rays: by using curved mirrors, multilayers, single and multiple capillaries, and diffracting lenses [3]. Parabolic refractive X-ray lenses are a relatively new optical system element that is used to focus X-rays in the 5 keV to 120 keV range. These lenses are compact and easy to use, and that is the reason such a system was chosen to be used on the coherence beamline at P10 at the new synchrotron PETRA III.

In order to achieve a focal length of the order of a meter, many lenses have to be aligned in a row. In our case in particular, lenses of different radii are available and are assembled into stacks. Therefore, the length of the lens system is quite large (about 30 cm), and it is not possible to use the thin lens approximation to calculate the parameters of the lens system as a whole. This paper describes the work done to create a programme that calculates the parameters of a parabolic X-ray lens system beyond the thin lens approximation.

THEORY

Introduction

The index of refraction for X-rays in condensed matter can be written as follows:

$$n = 1 - \delta + i\beta, \tag{3}$$

where δ is the refractive decrement of the order of 10^{-6}:

$$\delta = \frac{N_a}{2\pi} r_0 \lambda^2 \rho \left(\frac{Z}{A}\right), \tag{4}$$

where N_a is Avogadro's number, r_0 is the classical electron radius, λ is the photon wavelength, ρ is the density of the lens material, Z is the atomic number of the lens material, and A is the atomic mass of the lens material and the absorption coefficient:

$$\beta = \frac{\lambda\mu}{4\pi} \tag{5}$$

is characterised by the linear absorption coefficient μ. Both δ and β are energy dependent, which is the cause of a large number of complications [1].

X-rays in condensed matter have weak refraction (the real part of n is very close to one) and strong absorption. For this reason for a long time focusing lenses for X-rays were considered to be impossible to create. However, refraction of X-rays is not quite zero, and absorption is not quite infinite, so it is possible to create such a lens [1]. The first such lenses where created at Aachen University and made of beryllium, boron, aluminium and silicon [2].

Refractive X-ray lenses

Since the real part of n is less than one, a focusing lens would have a concave form rather that a convex one, as is the case for visible light. The first type of refractive X-ray lenses had cylinder and crossed-cylinder symmetry [3]. A system of such lenses was basically a row of holes with 1 mm diameter, drilled in a block of aluminium [2]. The focal length was about a metre, and focal spot size was several micrometres long. The material between the holes absorbed the beam [3]. In order to get such a short focal distance the radius of curvature R of the holes had to be small – 1 mm or less [1]. In the thin lens approximation the focal length for such a system would be equal to

$$f = \frac{R}{2N\delta}, \tag{6}$$

where N is the number of lenses in the system [1].

Due to the fact that in order to focus the beam a large number of holes had to be drilled in a row, such a system is called a compound refractive lens (CRL), see Figure 1 [3].

Because of absorption, the absorption region d (see Figure 1) has to be kept small (in our case $d = 30$ μm), and the number of lenses – limited.

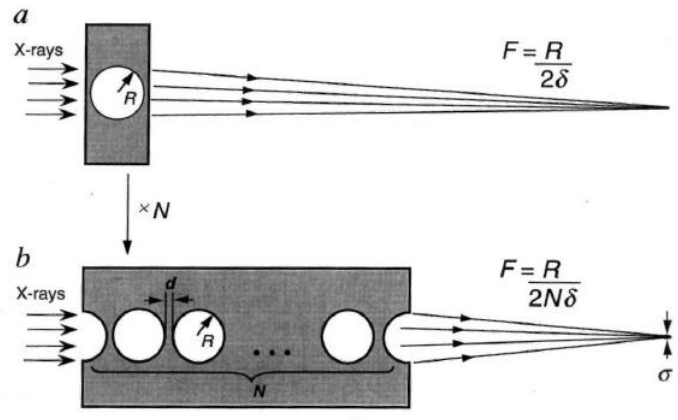

Figure 1.

A diagram showing how the CRL with a spherical profile focuses X-ray: a, simple concave lens – a cylindrical hole in the material; b, a CRL consisting of N cylindrical holes placed close together in a row along the optical axis. In the second case the focal length is N times shorter than in the case with only one lens. R is the radius of the holes, d is the distance between the holes, λ is the X-ray wavelength, and F is the focal distance for the lens system, assuming that the falling beam is parallel. Figure from [6].

However, these cylindrical lenses were found to have strong spherical aberration. This problem was solved when new lenses were introduced. They are different from the old ones in that they have a parabolic profile and rotational symmetry around the optical axis, focus in both directions and have no spherical aberration due to their parabolic nature, see Figure 2 [3]. For parabolic lenses R in the formula for the focal length is the radius of curvature at the tip of the parabola (see Figures 3 and 4) [4]. The length of the parabolic CRL system is equal to the following:

$$L_p = N\left(\frac{R_0^2}{R} + d\right), \tag{7}$$

where $2R_0$ is a parameter that can be chosen independently of the radius of curvature R (which is not the case for lenses with a spherical profile), and d is the thickness of the lens between two closest points of adjacent parabolas, see Figure 5 [4]. $2R_0$ determines the point where transmission falls by $1/e$ times.

Today the fabrication technique had improved enough that it is possible to create parabolic refractive lenses with different radii of curvature.

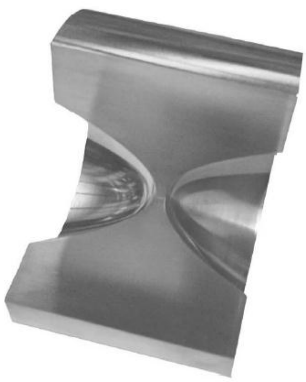

Figure 2.

A model of a parabolic refractive lens. One quadrant of the lens has been removed in order to show the lens profile. Figure from [1].

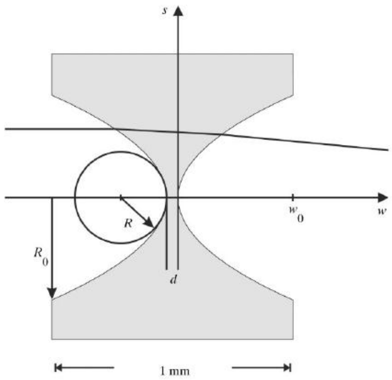

Figure 3.

A schematic diagram showing the principles of X-ray focusing by a single lens with a parabolic profile. R is the radius of curvature and $2R_0$ is the aperture. Figure from [3].

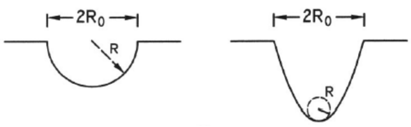

Figure 4.

Cross-section of a spherical refractive lens and a parabolic one. R is the radius of curvature and $2R_0$ is the aperture. Figure from [1].

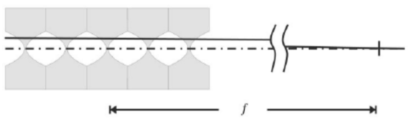

Figure 5.

A schematic diagram showing the principles of X-ray focusing by a row of individual lenses with a parabolic profile stacked together to form a CRL. f is the focal length. Figure from [3].

Transmission and gain of refractive X-ray lenses

The gain of a CRL is defined as the ratio of the intensity in the focal spot to the intensity behind a pinhole of the size of the focal spot without a lens [2]. The gain of a lens system depends strongly on the choice of the lens material [2]. In order to reach a high gain, materials with a small mass absorption coefficient μ/ρ must be chosen [2]. This coefficient is proportional to Z^3/E^3, where Z is the atomic number and E is the photon energy, so only low Z materials must be used for creating high-gain CRLs [2]. Even for hard X-rays only materials of light elements such as lithium, beryllium, boron, carbon, and aluminium can be used to create focusing X-ray lenses [1]. Moreover, homogeneous materials are preferred because small angle scattering must be minimized [2].

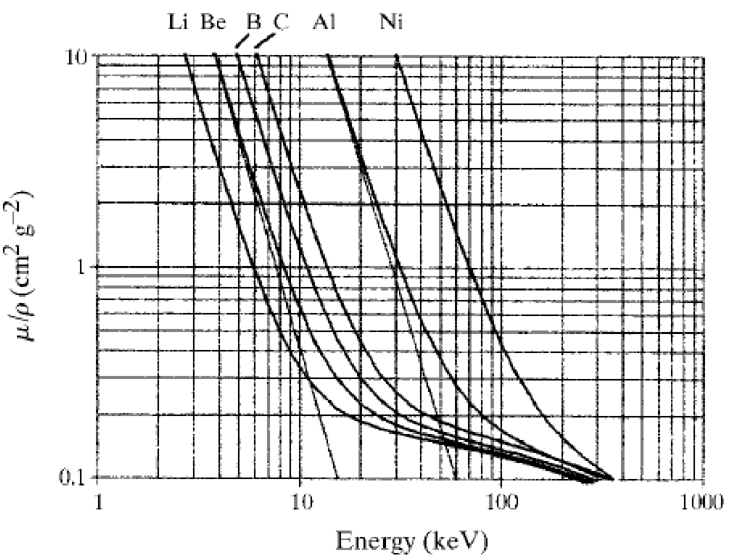

Figure 6.

The mass absorption coefficient μ/ρ for lithium, beryllium, boron, carbon, and nickel. The photoabsorption coefficient τ/ρ is shown for beryllium and aluminium. Figure from [3].

The photoabsorption of a lens system increases proportionally with Z^3 so again, only low Z materials should be used for lens creation. Another effect that can contribute to the mass absorption coefficient at high photon energies for light elements is the Compton scattering [4]. Photons that are Compton scattered do not take part in the formation of the image, thus this effect limits the effectiveness of the X-ray lenses. Moreover, the Compton scattered photons form a background image in the detector that lessens the signal-to-background ratio for the lens image [2]. Figure 6 shows the mass absorption and the photoabsorption coefficients for some common elements.

The transmission of a CRL with a parabolic profile and rotational symmetry is

$$T_p = \frac{1}{a_p}\left[1 - exp\left(-a_p\right)\right]exp(-\mu N d), \tag{8}$$

where

$$a_p = \frac{\mu N R_0^2}{R}, \tag{9}$$

and the gain is given by

$$g_p = \frac{4R_0^2 T_p}{h_v h_h}, \tag{10}$$

where h_v and h_h is the horizontal and vertical image size [4].

At first glance lithium appears to be the best material to use for the creation of CRLs, but it turns out that it is highly reactive and oxidizes easily, and is therefore quite difficult to handle. While both beryllium and aluminum are used for the creation of parabolic lenses, beryllium is considered to be best for focusing X-rays with energies between 10 and 40 keV because of its low atomic number (Z=4), as opposed to aluminum (Z=13) [2]. The imaging properties of beryllium lenses are considered to be far better than the imaging properties of aluminum lenses. Experiments have shown that not only is the transmission increased in the case of beryllium lenses, but also the effective aperture, which determines the diffraction limit. This leads to an increase of the lateral resolution and of the field of view. In addition, beryllium lenses are found to be more transparent than aluminum for lower X-ray energies, and therefore can be used for focusing X-rays at energies as low as 2 keV [5].

THE PROGRAMME

Project objective

The project consisted of finding the optimum beryllium lens combination for the coherence beamline at P10 at the new synchrotron PETRA III. The beamline offers a focusing device based on sets of parabolic beryllium lenses to optimize the coherent flux at the sample position. This work describes how the ideal lens combination is found based on two parameters: X-ray energy and the distance between the lens and the sample.

Description of the lens system

The proposed lens system (see Figure 7) consists of eight stacks of one to eight beryllium lenses each. Each of the eight stacks can be removed from the lens system independently of the others. The stacks are positioned in the order of increasing strength with the weakest stack closest to the source of the beam (see Table 2). The lens system is an (almost) binary system. One has to keep in mind that the lenses are achromatic, because δ is a function of the wavelength. That means that the program can calculate the best lens combination for only one energy at a time, because if the energy changes, the focal spot moves.

Table 2.

Stack number	Number of lenses	$R, * 10^{-6}$ m
1	8	50
2	4	50
3	2	50
4	1	50
5	2	200
6	1	200
7	1	500
8	1	1000

The proposed lens system for the coherence beamline P10 at PETRA III.

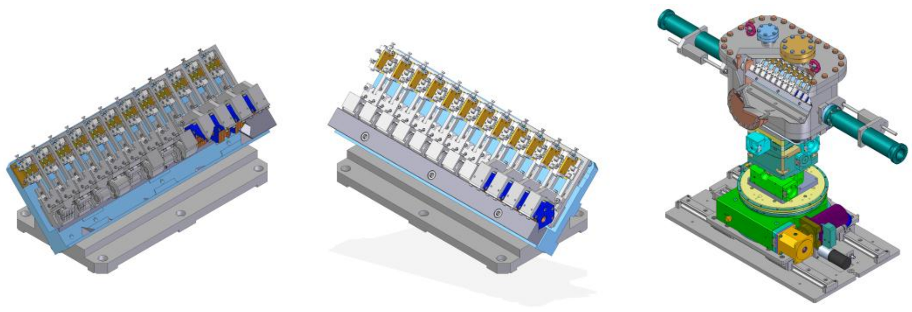

Figure 7.

The proposed lens system for the coherence beamline P10 at PETRA III, from the right and from the left, and a mechanism for aligning the lens system.

Description of the programme

The input of the program is the X-ray energy and the desired distance from the center of the lens system to the sample, for example:

[a, b, c, d, e, f, g] = P10_lens_final(8.000,2.219)

The X-ray energy for the beamline can change from 3,500 keV to 23,500 keV. The fixed parameters for the P10 beamline at PETRA III are the horizontal (one of two possible ones) G_h and vertical G_v source size. The program can import the index of refraction data from Be_IoR.mat file and the attenuation lengths from Be_AL.mat for a certain number of fixed energies, and interpolate this data for the input energy.

There are 255 possible lens combinations for each energy that the program has to check to find the best one. The number of the combination written in binary code backwards shows which stacks are present: a zero means that the stack is removed from the system, and a one – that the stack is present in the system. The number on the left corresponds to the weakest lens stack that is closest to the source.

The parameters of each separate stack are calculated in the thin lens approximation. The focal length is equal to:

$$f_0 = \frac{R}{2N\delta_{Be}}. \tag{11}$$

This formula does not take into account that each separate lens is not infinitely thin, so it is necessary to correct this formula for thickness:

$$f_0^* = \frac{1}{\sqrt{f_0 L}\left[sin\left(\sqrt{\frac{L}{f_0}}\right)\right]}, \tag{12}$$

where L is the total thickness of all lenses in the stack, and is equal to:

$$L = F_0 * N, \tag{13}$$

where F_0 is the thickness of a single lens ($F_0 = 1{,}6$ mm in our case), and N is the number of lenses in the stack.

When more than one stack is present in the lens system, the thin lens approximation cannot be used for the whole lens system at once, because the stacks of lenses are located quite far apart from each other, which complicates the calculations somewhat. The written program uses the calculated focal length for the first used stack and the source to stack distance to calculate the location of the image of the first stack, which is used as the source for the second stack.

The program considers the opening of the lenses to be equal to the vertical coherence length if it is less than $500 * 10^{-6}$ m, and $500 * 10^{-6}$ m if it is greater.

The distance g from the source to the lens is a known value and can be used to calculate the image distance b:

$$\frac{1}{b} = \frac{1}{f_0^*} - \frac{1}{g}. \tag{14}$$

The horizontal B_h and vertical B_h sizes of the focal spot can be calculated with the following formulas:

$$B_{h,v} = \frac{G_{h,v} * b}{g}. \tag{15}$$

The image distance b cannot be equal to the input image distance b_{goal} for any one lens combination because the number and the strength of lenses is limited. The program uses the parameter $dist$ to evaluate how good each lens combination is:

$$dist = b_{goal} - b. \tag{16}$$

The lens system can be moved 15 cm in the direction closer and further away from the source, so if the absolute value of $dist$ is more than 15 cm, it would be impossible to arrange the system so that the sample would be in the focal spot. Such lens combinations cannot be used, and are ignored by the program.

At this point the program has a certain number of lens combinations that fulfill the image distance criteria. For instance, for the energy $e_{goal} = 8.000$ keV and the desired image distance $b_{goal} = 2.219$ m, the program choses five combinations: 35, 36, 37, 38, and 39. For the properties of these lens combinations see Table 3.

Table 3.

j	*inout*	*dist*, [m]	*num_lens*	*b*, [m]	*Bv*, $*10^{-7}$ [m]	*Bh*, $*10^{-6}$ [m]
35	11000100	-0.1132	3	2.2405	3.7044	8.6856
36	00100100	-0.0107	2	2.1380	3.5367	8.2924
37	10100100	0.0372	3	2.0901	3.4620	8.1174
38	01100100	0.0831	3	2.0441	3.3886	7.9453
39	11100100	0.1271	4	2.0001	3.3201	7.7845

The uncorrected parameters of the lens combinations chosen by the program for $e_{goal} = 8.000$ keV and the desired image distance $b_{goal} = 2.219$ m. Here j is the number of the lens combination, *inout* is j written in binary code backwards, *dist* is the difference between the desired image distance and the calculated image distance, *num_lens* is the number of stacks in the system, *b* is the image distance, and *Bv* and *Bh* are the vertical and horizontal focal spot size.

Next, the program repeats the above calculations with only one difference: the initial source to lens distance for the first stack is corrected for the parameter $dist$. Afterwards the transmission and the gain are calculated using the formulas (8), (9), and (10). The distance corrected parameters of the energy $e_{goal} = 8.000$ keV and the desired image distance $b_{goal} = 2.219$ m can be seen on Table 4. Notice that $dist$ in the second table is much smaller than the corresponding value in the first. This is a direct consequence and the reason for the distance correction procedure.

Table 4.

j	*dist_corr*, $*10^{-5}$ [m]	*b_corr*, [m]	*Bv_corr*, $*10^{-7}$ [m]	*Bh_corr*, $*10^{-6}$ [m]	*Tp*, %	*Gp*, $*10^4$
35	-7.8201	2.2406	3.7094	8.6974	76.1978	5.9046
36	-0.69141	2.1380	3.5372	8.2935	75.8107	6.4607
37	2.2411	2.0900	3.4605	8.1137	74.8651	6.6659
38	4.7922	2.0441	3.3853	7.9374	74.4244	6.9244
39	7.0333	2.0000	3.3150	7.7727	73.4961	7.1310

The distance corrected parameters of the lens combinations chosen by the program for $e_{goal} = 8.000$ keV and the desired image distance $b_{goal} = 2.219$ m. Here *j* is the number of the lens combination, *dist_corr* is the corrected difference between the desired image distance and the calculated image distance, *b_corr* is the image distance, *Bv_corr* and *Bh_corr* are the vertical and horizontal focal spot size, *Tp* is the transmission of the CRL, and *Gp* is the gain.

The next step in the program is choosing the best of the remaining lens combinations. To do this the program compares the number of lenses, the transmission, and the gain of all remaining lens combinations. The program output are the following parameters: the number describing the best lens combination j *(a)*, the binary representation of the number j written backwards $inout$ *(b)*, the distance correction $dist$ *(c)*, the vertical and horizontal focal spot sizes Bv *(d)* and Bh *(e)*, the transmission T_p *(f)* and the gain G_p *(g)* of the CRL. An example of the program output for $e_{goal} = 8.000$ keV and the desired image distance $b_{goal} = 2.219$ m is the following:

```
a =
   36

b =
   0   0   1   0   0   1   0   0

c =
-6.9141e-006
```

d =

3.5372e-007

e =

8.2935e-006

f =

75.8107

g =

6.4607e+004

The results calculated by the program for desired image distance $b_{goal} = 2.219$ m and various energies of X-rays are presented in Table 5.

Table 5.

E, keV	a	b	c, $*10^{-5}$ [m]	d, $*10^{-7}$ [m]	e, $*10^{-6}$ [m]	f, %	g, $*10^{4}$
3.5	7	11100000	-6.7472	3.8085	8.9297	43.6333	3.2075
4.5	-	-	-	-	-	-	-
5.5	16	00001000	-8.7738	3.7551	8.8044	69.4802	5.2539
6.5	24	00011000	2.3365	3.4959	8.1968	70.1227	6.1177
7.5	32	00000100	8.3447	3.4823	8.1649	74.9953	6.5941
8.5	40	00010100	-2.9325	3.5981	8.4365	76.7152	6.3180
9.5	48	00001100	-9.6083	3.7488	8.7897	79.4304	6.0265
10.5	64	00000010	1.8597	3.4122	8.0006	79.0168	7.2360
11.5	80	00001010	6.4492	3.2813	7.6935	78.4633	7.7704
12.5	88	00011010	-1.8835	3.5427	8.3066	79.4463	6.7492
13.5	104	00010110	-0.071526	3.4901	8.1832	78.9007	6.9066
14.5	128	00000001	5.7101	3.2493	7.6185	77.7273	7.8498
15.5	144	00001001	4.2439	3.3140	7.7703	78.1603	7.1373
16.5	160	00000101	2.1458	3.3831	7.9323	79.6705	6.1606
17.5	176	00001101	-0.52452	3.4695	8.1348	80.9173	5.2888
18.5	192	00000011	-3.9101	3.5472	8.3169	81.9852	4.5872
19.5	224	00000111	2.5988	3.3755	7.9145	81.6411	4.5402
20.5	240	00001111	-1.2159	3.4911	8.1854	82.5202	3.8820
21.5	252	00111111	-8.2016	3.6703	8.6056	83.3118	3.2237
22.5	-	-	-	-	-	-	-
23.5	-	-	-	-	-	-	-

The program output for the desired image distance $b_{goal} = 2.219$ m and X-rays energies from 3.5 keV to 23.5 keV, a is the number describing the best lens combination j, b is the binary representation of the number j written backwards $inout$, c is the distance correction $dist$, d is the vertical and e is the horizontal focal spot sizes $(Bv$ and $Bh)$, f is the transmission T_p and g is the gain G_p of the CRL.

One can see from Table 5 that for 4,5 keV, 22,5 keV, and 23,5 keV the combination of the set energy and the desired image distance is such, that the focal spot is too far away from the sample for all lens combinations, so the program cannot choose an optimal one.

SUMMARY

The written program can be used to determine the best lens combination for focusing the coherent flux at the P10 beamline at PETRA III in order to resolve the speckles, which can be useful for coherent scattering experiments.

ACKNOWLEDGEMENTS

I would like to thank my supervisor Michael Sprung for his patience and advice that helped me to complete this project.

REFERENCES

[1] Lengeler B, Schroer C G, Benner B, Gerhardus A, Gunzler T F, Kuhlmann M, Meyer J and Zimprich C 2002 *J. Synchrotron Rad.* **9** 119-124

[2] Lengeler B, Schroer C G, Kuhlmann M, Benner B, Gunzler T F, Kurapova O, Zontone F, Snigirev A and Snigireva I 2005 *J. Phys. D:Appl. Phys.* **38** A218-A222

[3] Lengeler B, Schroer C G, Tummler J, Benner B, Richwin M, Snigirev A, Snigireva I and Drakopoulos M 1999 *J. Synchrotron Rad.* **6** 1153-1167

[4] Lengeler B, Tummler J, Snigirev A, Snigireva I and Raven C 1998 *J. Appl. Phys.* **84**(11) 5855-5861

[5] Schroer C G, Kuhlmann M, Lengeler B, Gunzler T F, Kurapova O, Benner B, Rau C, Simionovici A S, Snigirev A A and Snigireva I 2002 *Design and Microfabrication of Novel X-Ray Optics* ed D C Mancini (Bellingham, WA: SPIE) *Proc. SPIE* **4783** 10-18

[6] Snigirev A, Kohn V, Snigireva I and Lengeler B 1996 *Nature (London)* **384** 49