Optical elements for hard X-ray radiation
Anette Jensen
copyright Anette Jensen

Published by:
Nano-Science Center
University of Copenhagen
Universitetsparken 5
2100 Copenhagen Ø
Denmark
Typeset with \LaTeX 2\epsilon
Abstract

This thesis describes the development and characterization of an optical element for the next-generation x-ray source the Compact Light Source (CLS). The CLS is a miniature synchrotron light source recently developed by the company Lyncean Technologies Inc. [1]. At present it is expected that this powerful x-ray machine will be installed at the University of Copenhagen during the year 2008. The development of the optical element is the result of a collaboration between the Nano-Science Center at the University of Copenhagen, the Danish National Space Center, the small Danish company JJ-XRAY A/S [2] and Lyncean Technologies Inc. The optical element is based upon two multi-layer mirrors positioned in a classic Kirkpatrick-Baez geometry. The curvature of the mirrors is not fixed, rather each mirror is mounted in a mirror bender which precisely controls the deflection of the mirror. Step by step this thesis describes and explains the development and the characterization of this optical element.

The characterization of the mirror bender performance is presented in the view of a combination of the Bernoulli-Euler beam theory and ray-tracing calculations. It is shown that the bender performance complies with the high expectations based upon these theoretical considerations. The multilayers and the substrates for these have been characterized by x-rays at three different x-ray experimental setups, all three at laboratory sources providing Cu $K\alpha$ radiation. The characterization thoroughly documents both the magnitude of the substrate figure error and the focusing performance of the optical element.

The multilayer mirrors are produced by DC magnetron sputtering at the Danish National Space Center. Until recently this facility has been optimized solely for the coating of mirrors with a radius of curvature in the range from 40 mm to 120 mm, mirrors which are used in the production of x-ray telescopes in collaboration with NASA. Here it is described how this sputtering facility has been qualified for the production of long (∼ 240 mm) flat mirrors suitable for optical elements for hard x-ray radiation.
Preface

This thesis is submitted as a partial fulfillment of the requirements for obtaining the Ph.D. degree from the University of Copenhagen, Denmark. The research reported has been conducted at the Danish National Space Center and the Nano-Science Center in the period from June 2003 to January 2007. The project has been supervised by Professor Jens Als-Nielsen and financed partly by a grant from the Nano-Science Center, partly by BIOXHIT. BIOXHIT stands for Biocrystallography (X) on a Highly Integrated Technology Platform for European Structural Genomics and is funded under the 6th Framework Programme of the European Commission (LSHG-CT-2003-503420).

The project would not have been possible without the help from numerous people that I would like to take the opportunity to thank here.

First of all, I would like to thank my supervisor Jens Als-Nielsen for recommending me for the Ph.D. grant and for helping me avoid many pitfalls during the project.

The production of the multi-layer mirrors would not have been possible without the help from Carsten P. Jensen and Finn E. Christensen at the Danish National Space Center. I would like to thank Finn and Carsten for a very good collaboration and for always being ready with their support and inspiration.

I thank my fellow Ph.D. student Christian Bjerg Mammen for a good collaboration in our different projects and for a good atmosphere in the office we have shared. Thanks are also due to all the people in the X-ray group for both providing a good atmosphere and inspiring discussions.

I thank Kaare Brandt Pedersen and Pia Redanz for invaluable scientific assistance, and Markus Vickery for helping me with various computer related problems. On the practical side, thanks are due to laboratory technicians Keld Theodor and Joan Momberg and secretaries Hanne Tulinius and Anette Uhl for their always kind assistance. Also thanks to Freddy Bruus at the workshop of Risø National Laboratory.

During the project, I have also received assistance and inspiration from a number of industry-employed people, and I would like to thank them for sparing some time for a project not directly related to their bottom line. In particular, I would like to thank Christian Bjerg Mammen and Henning Bro Pedersen from JJ X-RAY for invaluable help with the design and construction of the mirror benders. Further I would like to thank Ronald Ruth and Jeff Rifkin, President and Chief Scientist and Vice President, General Manager respectively of Lyncean Technologies, Inc. for
inspiration and good discussions regarding the development of the optical element for the Compact Light Source. Also a warm thank is due to Dr. Simon Cockerton, managing director of Crystal Scientific Ltd., for a fast delivery of the substrates and for helping us with the re-polishing of these after a fatal mistake.

I would also like to thank everyone at the Nano-Science Center and the Ørsted Laboratory, whose help has not been of technical nature, but who has in one way or another made HCØ a nice place to work and the years I have spent here very enjoyable.

Finally, I thank my family for all their support and patience.

Copenhagen, 18.04.2007

Anette Jensen
## Contents

1 Introduction ................................................................. 1
   1.1 The optical system .................................................. 1
   1.2 Constant \(d\)-spacing multi-layer mirrors - physics and design . 2
       1.2.1 The basic x-ray physics of multi-layer mirrors .............. 3
       1.2.2 The design of the first multi-layer mirrors for the Compact
             Light Source (CLS) optics .................................. 7
   1.3 Focusing by an elliptic curved mirror ............................ 11
       1.3.1 The circle approximation ................................... 13

2 The production of the multi-layer mirrors ............................ 17
   2.1 The planar magnetron sputtering facility at DNSC .............. 17
       2.1.1 The pressure of Ar in the sputtering chamber ............. 18
       2.1.2 The power applied to the magnetrons ....................... 20
       2.1.3 Calibration of the sample carrousel speed ............... 20
       2.1.4 Collimation of the sputtered particles .................... 20
       2.1.5 Longitudinal homogeneity of the bi-layer thickness ...... 24
       2.1.6 Erosion of the targets ..................................... 24
   2.2 Cleaning procedure for Si and glass substrates ................. 25

3 Collimation of the sputtered particles compatible with long flat sub-
   strates .................................................................. 27
   3.1 The honeycomb mesh collimation .................................. 27
   3.2 Relating the honeycomb collimation to the separator plate collimation ............................................ 29
   3.3 An estimate of the angular distribution of the particles ejected from
       the target .......................................................... 32
   3.4 Summary ............................................................... 35

4 The crystal bender ............................................................ 37
   4.1 Beam theory ........................................................... 37
       4.1.1 \(F_A = F_B\) ..................................................... 38
   4.2 Design of the bender ................................................. 39
   4.3 Characterization of the bender performance ...................... 41
       4.3.1 Derivation of the bending moments ......................... 44
   4.4 The focusing of the bent mirror compared with the focusing of an
       ellipse .............................................................. 46
   4.5 Calibration of the bender motor ................................... 47
4.6 Summary .................................................. 48

5 X-ray characterization of the substrates ................................... 51
  5.1 The Figure Error characterization .................................. 51
      5.1.1 The experimental setup .................................. 52
      5.1.2 Dispersive and non-dispersive geometry ............... 55
  5.2 The X-ray reflectivity measurements .............................. 59
      5.2.1 Specular X-ray reflectivity from a thick mirror ....... 59
      5.2.2 The experimental setup .................................. 60
  5.3 The experimental results of the X-ray characterization of the sub-
      strates ................................................................ 62
      5.3.1 The figure error characterization ......................... 62
      5.3.2 The specular reflectivity measurements ............... 64
      5.3.3 Summary .................................................. 65

6 Characterization of the multi-layer mirrors for the CLS optics ........ 69
  6.1 The multi-layer coating ........................................... 69
  6.2 Witness samples .................................................. 70
      6.2.1 The longitudinal homogeneity of the bi-layer thickness ... 70
      6.2.2 The specular reflectivity and the relative bandwidth of the
            first order Bragg reflection ................................ 71
  6.3 The X-ray characterization of the multi-layer mirrors for the CLS
      optics .................................................................. 72
      6.3.1 Understanding the performance of a focusing mirror: an
            example ......................................................... 73
      6.3.2 The experimental setups for the measurement of the specu-
            lar intensity reflectivity, the focussing performance and the
            bi-layer thickness gradient ................................. 74
  6.4 The experimental results of the X-ray characterization of the multi-
      layer mirrors for the CLS optics ................................. 76
      6.4.1 The specular intensity reflectivity and the relative bandwidth
            ................................................................. 76
      6.4.2 Measurement of the bi-layer thickness longitudinal gradient
            of mirrorI ....................................................... 77
      6.4.3 The focusing performance of mirrorI ...................... 78
      6.4.4 M=0.88 focusing of mirrorII .............................. 80
  6.5 Discussion .......................................................... 81
      6.5.1 Bandwidth and Bragg peak intensity reflectivity .......... 81
      6.5.2 The focusing performance .................................. 82
      6.5.3 The efficiency vs the magnification factor ............... 83

7 Conclusion .................................................................. 85

A Crystal bender solution .................................................. 91

B Exact determination of the bilayer thickness gradient and the mirror
  curvature .................................................................. 93
  B.1 Focusing by an elliptical mirror .................................. 93
B.2 Collimating by a parabolic curved mirror .......................... 95

C Computer code .................................................................. 97
  C.1 The ellipse calculations .................................................. 97
Chapter 1

Introduction

1.1 The optical system

The optical system is developed for the Compact Light Source [1] (the CLS). The system is a classic two-mirror setup first described by Kirkpatrick and Baez in 1948 [3]. Fig. 1.1 top show two figures taken from the original paper. To the left is shown the perpendicular arrangement of the two concave mirrors and to the right is shown a pattern produced by the two mirrors. The object was a screen with a mesh. In addition to the full image of the screen (upper left), two partial images,
each formed by one mirror and a large spot caused by the direct beam appear on
the film. Below is shown a drawing of the proposed optical system. The system is
designed by Keld Theodor, JJ-X-ray [2] and Jens Als-Nielsen and the dimensions
of the two mirrors are 240 mm by 37 mm. The mirrors are not provided with
a fixed curvature, rather each mirror is placed in a crystal bender, also designed
by JJ-X-ray. The crystal bender is motorized so the mirror curvature can be
changed to provide a focusing which is optimal for the experiment in question.
For increased flexibility of the focusing system each mirror can be coated with
up to three different stripes of multi-layer, say one stripe for 1:1 focusing, one
stripe for collimation and one stripe for demagnification of the source. To control
the direction of the focussed beam, the two mirrors are situated in an Euler
cradle. The results of a thorough characterization of the crystal bender are given
in Chapter 4 and the results of the characterization of the focusing performance
of the optics are given in Chapter 6.

1.2 Constant \( d \)-spacing multi-layer mirrors - physics
and design

The first multi-layer mirrors produced for the optical system are 1:1 focusing mir-
rors with a relative bandwidth of the same order of magnitude as the source,
that is of the order of 2\%(FWHM). 1:1 focusing mirrors are relatively simple to
produce and are therefore ideal for the purpose of testing the performance of the
crystal benders. As expected our experiments show that performance of the crys-
tal benders is very good (Chapter 4), so if the future experiments on the Compact
Light Source demands it, new and more complicated multi-layer structures will
be deposited on the substrates. By having multi-layers with different properties
on the same substrate the one optical element can serve different kinds of users.
If a relative bandwidth of 2\% is suitable for the experiment, the use of multi-layer
mirrors in the optical system instead of for example Si (111) crystals offers an
increase in the flux. This is simply because the relative bandwidth of the multi-
layer mirrors matches that of the source (\( \sim 2\%\text{FWHM} \)) in contrast to the Si(111)
reflection which has a relative bandwidth below 0.02\%. So even though the ef-
ciciency of each of the two multi-layers only amounts to 50\%, the flux available
at the sample position is more than 30 times larger than the flux which could be
delivered by two Si (111) reflections.

In [4] is reported on a multi-layer with 800 bilayers of thickness 27 Å comprised
of \( \text{Al}_2\text{O}_3 \) and \( \text{B}_4\text{C} \), see Fig. 1.2. The bandwidth of this multi-layer is as small as
0.22\%, but it is deposited on 30mm thick substrate in order to avoid the bending
of the substrate owing to the strain built into the multi-layer during deposition.
Since we need the thin (4 mm) substrates to be able to bend them into the desired
shape, such a multi-layer may not be an option for us.
A multi-layer mirror can be tailored to meet the bandwidth requirements of a given experiment. This can be utilized to increase the available flux as the following example indicates: a multi-layer mirror with a bandwidth of 0.22% has been reported to give sufficiently resolution for crystallography of medium sized proteins (with a unit cell volume of $480000 \text{Å}^3$) \cite{4}. By exchanging two Si(111) Bragg reflections with two 0.22% bandwidth multi-layers (assume the efficiency of each mirror is 50%), the flux can be increased by a factor of 5. For the experimentalist the flux increase means either better data, faster data collection or it makes data-collection from smaller crystals feasible. If the experiment does not require a particular small bandwidth the flux available for the experiment can be maximized by using multi-layer mirrors with bandwidths similar to that of the source, in this case 2%.

### 1.2.1 The basic x-ray physics of multi-layer mirrors

A thorough introduction to the physics of multi-layers can be found in for example \cite{5} and \cite{6}. The purpose of this section is merely to give an overview of the theory necessary to understand the considerations behind the design of the multi-layer mirrors for the optical system developed for the CLS. The actual design of the multi-layers is based upon optical constants computed from scattering factors available from \cite{7} and an exact recursive method developed by Parrat \cite{8}. The exact method is also thoroughly explained in \cite{6} and this treatment even includes a Matlab programme which calculates the intensity reflectivity curve of a multi-layer. Therefore, in this overview only the simple kinematic theory of the specular reflectivity is included.

For x-rays the refractive index deviate from unity by a number which is of the order of $-10^{-5}$. Since the refractive index is slightly less than one, there exists a critical angle for total reflection. The magnitude of the critical angle scales with the square-root of the electron-density of the material and the wavelength of the incident radiation. For Silicon at Cu $K\alpha_1$ radiation the critical angle is $\frac{1}{2\pi} \text{rad}=3.8 \text{ mrad}$ as shown with the red curve in Fig. 1.3. For glancing angles below the
critical angle the intensity reflectivity is close to 100%, but to utilize the total reflection in a focusing mirror would be impractical: assume that the incident beam has a height of 1 mm. As indicated by the upper x-axis of the view-graph a glancing angle equal to the critical angle for total reflection for Silicon corresponds to a footprint with a length of 260 mm. This means that if a naked Silicon surface is used for a focusing mirror, due to the small critical angle either the mirror must be very long or the efficiency very low. As shown in Fig. 1.3 the critical angle can be increased by coating the Silicon with a material with a larger electron-density, say Gold. However, even for the Gold-coated Silicon a glancing angle equal to the critical angle for total reflection implies a footprint with a length which is of the order of 100 times the height of the incident beam. A multi-layer comprised of a stack of alternating layers of for example Molybdenum and Silicon can be used to overcome the problem of extended footprints. If the thickness of each layer-type is constant through the stack, according to Bragg’s law the periodicity will give rise to Bragg reflections. As is also indicated in Fig. 1.3 the Bragg peak reflectivity is strongly dependent on the number of layers in the multi-layer stack. Below follows a summary of the basic x-ray-physics of multi-layers.

Fig. 1.4 left shows a sketch of a multi-layer seen from the side. It consists of \( N \) bi-layers comprised of material A and B. If there is no electron-density contrast between A and B, the stack is not recognized as a multi-layer by the x-rays. To calculate the reflectivity from this whole stack the strategy is the following: first the reflectivity of one bilayer is calculated. This is done by integrating over slabs of infinitesimal thickness \( \Delta \) each with an amplitude reflectivity which is proportional to the number of scattering centers in the ray path \( \rho_{A-B} \frac{\Delta}{\sin \alpha} \) and the scattering...
1.2 Constant $d$-spacing multi-layer mirrors - physics and design

Figure 1.4: 
Left: a sketch of a multi-layer seen from the side. The bilayer thickness is of thickness $d$ and is comprised of the fraction $(1 - \Gamma)$ of material A and the fraction $\Gamma$ of material B.
Right: intensity reflectivity curves calculated using Parrat’s exact recursive method [8]. See text for details.

amplitude of the electron, that is the Thomson scattering length $r_0$,

$$r_{\text{thin slab}} = r_0 \rho_{A-B} \frac{\Delta}{\sin \alpha} \frac{\lambda}{i}.$$  

Here $\alpha$ is the glancing angle, $\rho_{A-B}$ is the electron-density contrast and the factor $1/i$ expresses the phase-shift $\pi$ of the scattered rays. Only the appearance of the wavelength of the incident radiation $\lambda$ in the above expression is not as transparent. However, bearing in mind that the reflectivity is a dimensionless number and the wavelength is the only remaining characteristic length in the problem, it is clear that $\lambda$ must also enter into the expression. The bilayer amplitude reflectivity is then

$$r_1(Q) = \frac{r_{\text{thin slab}}}{\Delta} \int_{-\Gamma d/2}^{\Gamma d/2} e^{i Q z} \, dz$$  \hspace{1cm} (1.1)$$

where $Q = 2k \sin \alpha$ is the wave-vector transfer and the factor of $e^{i Q z}$ is the phase difference between rays reflected at different depths $z$ in the bilayer. The amplitude reflectivity of the whole multi-layer is calculated as the sum over all the $N$ bi-layers,

$$r_N(Q) = \sum_{\nu=0}^{N-1} r_1(Q) e^{i Q \nu d} e^{-\nu \beta}$$

$$= r_1(Q) \frac{1 - e^{i Q N d} e^{-N \beta}}{1 - e^{i Q d} e^{-\beta}}$$  \hspace{1cm} (1.2)$$

where $e^{i Q \nu d}$ is the phase difference and the absorption is included as the factor $e^{-\nu \beta}$. $\beta$ is the weighted average of the absorption coefficients,

$$\beta = \frac{2d}{\sin \alpha} \left( \frac{\mu_A \Gamma}{2} + \frac{\mu_B (1 - \Gamma)}{2} \right),$$
where the first factor is the total path-length of the incident and the reflected beam. The absorption coefficient $\mu$ refers to intensity so the amplitude absorption coefficient is $\mu/2$.

The intensity reflectivity is calculated as the absolute square of the amplitude reflectivity. From the above equations it is possible to understand the main features of the intensity reflectivity curves shown in Fig. 1.4 right. First consider the reflectivity of the multi-layer which consists of 10 bilayers comprised of Silicon and Molybdenum, that is the blue curve. Each bilayer has the thickness $d = 3$ nm. When $Q$ takes the value of an integer times $2\pi/d$ the denominator of Eq. 1.2 assumes a minimum, and this gives rise to the principal diffraction maxima. The smaller oscillations are due to minima of the numerator occurring for $Q$ equal to an integer times $2\pi/(Nd)$.

The grey curve shows the reflectivity for a similar multi-layer, but now with an infinite number of bilayers. By increasing the number of bilayers the reflectivity increases until a saturation is reached and the width of the Bragg peak decreases like $1/N$. The number of bilayers necessary to reach a saturation of the reflectivity can be estimated from the Bragg peak reflectivity from one bilayer (here $\Gamma = 0.5$ and the absorption is not taken into account):

$$|r_1(Q_B)| = \frac{2\rho_{A-B} r_0 d^2}{\pi}. \quad (1.3)$$

With $r_0 = 2.82 \cdot 10^{-5}$ Å, $d = 30$ Å and $\rho_{A-B} = 2\text{Å}^{-3}$ the reflectivity of one bilayer is of the order 3%. The amplitude of the incident radiation will be diminished to $(1 - r_1)^N$ after the penetration of $N$ bilayers. In this example only 10% of the incident radiation is left after the penetration of 75 bilayers. Adding more layers to the multi-layer stack will thus only have very little effect on the Bragg peak reflectivity.

So far, it has for simplicity been assumed that the interfaces between the layers are perfectly sharp and perfectly smooth. In the real world the interfaces are characterized by having both roughness and inter-diffusion which is the mixing of the two materials at the interface. Both of these two different deviations from perfection diminish the specular reflectivity from each layer by an attenuation factor analogous to the static Debye-Waller factor. From a specular measurement of the intensity reflectivity the interfaces can therefore only be characterized in terms of a combination $\sigma$ of the roughness $\sigma_r$ and the inter-diffuseness $\sigma_d$,

$$\sigma = \sqrt{\sigma_r^2 + \sigma_d^2}.$$

As described in for example [9][10], a far more detailed characterization of the interfaces can be obtained from a non-specular measurement of the intensity reflectivity. Non-specular data can be analyzed in order to reconstruct the correlation function of the interface profile and it is thus possible to distinguish the roughness from the inter-diffuseness. The nature of the imperfections of the interfaces is both dependent on the combination of materials in the multi-layer [11] and the conditions under which the multi-layer was produced. For the magnetron sputtering at the Danish National Space Center (DNSC) the latter includes the Ar
From the above considerations the fundamentals of constant \( d \)-spacing multi-layer mirror design can be understood: a large bandwidth mirror consists of materials with a high electron density contrast, since then a few number of bi-layers are necessary in order to obtain saturation of the Bragg peak. A small bandwidth mirror is comprised of many layers with either a lower electron density contrast or a small (\( \sim 15 \) Å) bilayer thickness \[12\][13]. Fig. 1.5 compares the electron-density contrast of different material combinations.

**Figure 1.5:** The electron-density contrast for different material combinations. The small (0.22%) bandwidth mirror reported on in [4] is comprised of 800 bilayers of \( \text{Al}_2\text{O}_3 \) and \( \text{B}_4\text{C} \). The mirrors for the CLS optics consist of 75 bilayers comprised of \( \text{WC} \) and \( \text{SiC} \), a material combination with an intermediate electron density contrast. These mirrors have a bandwidth of the order 2%.

### 1.2.2 The design of the first multi-layer mirrors for the Compact Light Source (CLS) optics

The multi-layer mirrors for the Compact Light Source (CLS) optics are produced using the magnetron sputtering facility at the Danish National Space Center. The production is done in close collaboration with Researcher Carsten P. Jensen (Ph. D.) and Senior Scientist Finn E. Christensen (Ph. D.). The first mirrors for the CLS optics are 1:1 focusing mirrors with a bandwidth of the order of 2%. 1:1 focusing mirrors are relatively simple to produce for the following reason: in 1:1 focusing the curvature of the mirror is such that the glancing angle \( \alpha \) of the incident beam is approximately the same along the length of the mirror (Sec. 1.3). This means that the optimal reflectivity of the mirror is obtained if the bilayer
thickness \( d = \frac{\lambda}{2 \sin \alpha} \) also is constant along the length of the mirror, and this is more straight-forward to obtain than some specific longitudinal gradient of the bilayer thickness.

**Characteristics of the CLS relevant for the design of optics**

The Compact Light Source is tunable in energy in the range from 7 keV to 30 keV and the relative bandwidth is of the order 2%. The beam divergence \( \sigma_S \) (FWHM) is energy-dependent,

\[
\sigma_S (\text{mrad}) = 4 \sqrt{\frac{13.8}{E(\text{keV})}}.
\]

The source is circular with a diameter of 50 \( \mu \text{m} \) (FWHM). The optics will be positioned at the distance \( p = 1.5 \) m from the source.

**The derivation of the optimal multi-layer parameters**

The aim of the optics is to provide a 1:1 focusing of the whole bandwidth of the CLS. In the design process there are four parameters to decide upon:

1. the material combination,
2. the bilayer thickness \( d \),
3. the fraction of material with high electron-density \( \Gamma \) and
4. the number of bilayers.

In order to reflect the whole bandwidth of the CLS, the relative bandwidth of the multi-layer Bragg peak is required to be at least 2%. As described in Sec. 1.2.1 a relative bandwidth of this magnitude and a high peak reflectivity can be obtained by choosing a material combination with a large electron-density contrast. At the Danish National Space Center (DNSC) at the time of the production the following materials were readily at hand: Mo, C, Si, SiC, W, and WC. Fig. 1.5 shows that a combination of two of the latter four materials results in the highest electron-density contrast. Of these four combinations the material combination [WC/SiC] is known to form bilayers with the lowest interface roughness and the smallest degree of inter-diffusion [11]. Therefore the multi-layer mirrors for the CLS optics will be comprised of WC and SiC.

Given energy of the incident radiation, the bilayer thickness and the fraction of WC in the multi-layer an efficient intensity reflectivity \( R_{\text{eff}} \) can be derived by taking into account

1. the Bragg peak intensity reflectivity \( R_{\text{Bragg}} \)
2. the bandwidth of the Bragg reflection compared to the bandwidth of the source
3. the fraction \( F_{\text{foot}} \) of the footprint which falls inside the mirror,
so

\[ R_{\text{eff}} = R_{\text{Bragg}} \frac{(\Delta E/E)_{\text{mirror}}}{(\Delta E/E)_{\text{source}}} F_{\text{foot}}, \]  

(1.5)

if the bandwidth of the source exceeds the bandwidth of the mirror. If this is not the case the efficiency is simply

\[ R_{\text{eff}} = R_{\text{Bragg}} F_{\text{foot}}. \]

$F_{\text{foot}}$ is a factor $0 < F_{\text{foot}} < 1$ which assumes the value 1 if the whole footprint is reflected from the mirror and is less than 1 otherwise. The CLS source is circular so the shape of the footprint is approximately elliptic. Had the source been squarish with the divergence $\sigma_S$, $F_{\text{foot}}$ would simply assume the value

\[ F_{\text{foot}} = \frac{L_M}{p \sigma_S / \sin \alpha} \quad \text{where} \quad p \sigma_S / \sin \alpha > L_M, \]  

(1.6)

when the mirror of length $L_M$ is positioned the distance $p$ from the source and the glancing angle is $\alpha$. $p \sigma_S$ is the height of the beam denoted by $h$ in Fig. 1.3. Fig. 1.6A is a top-view sketch of the mirror of length $L_M$ and the footprint in the case of a circular source. The length of the footprint exceeds the length of the mirror, so only the heavy colored area of the footprint is reflected from the mirror. In this case $F_{\text{foot}}$ is the ratio between the area of the heavy colored region and the area of the whole ellipse. Fig. 1.6B is obtained from A by a scaling of the horizontal axis (the $x$-axis in B) by the factor $\sin \alpha$. Then it is straightforward to calculate $F_{\text{foot}},$

\[
F_{\text{foot}} = \frac{\int_0^{L_M} \sin \alpha/2 \sqrt{(p \sigma_S/2)^2 - x^2} \, dx}{\int_0^{p \sigma_S/2} \sqrt{(p \sigma_S/2)^2 - x^2} \, dx} = \frac{\pi}{4} \int_0^{x_0} \sqrt{1 - x^2} \, dx = \frac{1}{2} \left( x_0 \sqrt{1 - x_0^2} + \arcsin x_0 \right),
\]

(1.7)

**Figure 1.6:** A and B: illustration for the derivation of $F_{\text{foot}}$ (Eq. 1.7) in the case of a circular source. See text. **Right:** The energy and $x_0$ dependence of the footprint efficiency $F_{\text{foot}}$ for a bi-layer thickness of $d=3\text{nm}$ and a source–mirror distance of $p = 1.5 \text{ m}$. $F_{\text{foot}}$ is shown in the case of a circular source (the full line) and in the case of a rectangular source (the dashed line). The black circle marks the footprint efficiency at Cu $K\alpha$ radiation $E = 8.05 \text{ keV}$. At this energy $F_{\text{foot}}^{\text{circ}} = 0.69$ and $F_{\text{foot}}^{\text{rect}} = 0.57$.
where \( x_0 = L_M \sin \alpha / (p \sigma_S) \) is the ratio between the length of the mirror and the length of the footprint. The view-graph to the right in Fig. 1.6 compares the expressions Eq. 1.6 and Eq. 1.7 for the footprint efficiency.

\( R_{\text{eff}} \) (Eq. 1.5) has been calculated for multi-layers with bi-layer thicknesses in the range 20–40 Å. To ensure that the Bragg peak intensity reflectivity is saturated, in the calculations the number of bi-layers has been chosen to \( N = 300 \).

The lower part of Fig. 1.7 shows three contour plots vs. the energy of the incident radiation (\( E \)) and the fraction of WC in the multi-layer (\( \Gamma \)). Plot A shows the Bragg peak intensity reflectivity, plot B shows the relative bandwidth of the Bragg peak and plot C shows the efficient intensity reflectivity as defined in Eq. 1.5. The three upper plots of Fig. 1.7 show cuts through the contour plots at \( \Gamma = 0.44 \). The results shown are derived from calculations based on Parratt’s exact recursive method [8]. In plot A the existence of the W L3 absorption edge at \( E_{W L3} = 10.21 \text{ keV} \) displays itself as an abrupt decrease in the Bragg peak intensity reflectivity. Plot B shows that in general the bandwidth increases with increasing WC content: an increase of the fraction of WC implies an increase of the absorption per bilayer. This means that the incident radiation will be diminished after penetration of fewer bi-layers and this causes a broadening of the Bragg peak. For a fixed value of the fraction \( \Gamma \) of WC, at the W L3 edge the bandwidth decreases abruptly. This is caused by the decrease at the L3 edge of the amplitude reflectivity from each bilayer, so more bi-layers are penetrated by the incident radiation. As defined in Eq. 1.5 the efficiency of the mirror is calculated as the product of the data shown in plot A with B and the footprint efficiency shown in Fig. 1.6 right. The efficiency for \( d = 3 \text{ nm} \) is shown in plot C.

Calculations similar to those shown in Fig. 1.7 have been performed for a wide range of bilayer thicknesses. The variation of the maximum mirror efficiency (Eq. 1.5) with the bilayer thickness is shown in Fig. 1.8 left for an incident radiation of \( E = 8.5 \text{ keV} \) and different bandwidths of the source. For a source with \( \sigma_S = 2\% \) the optimal bilayer thickness is 31 Å. With an assumed interface rms roughness of 3 Å the mirror efficiency is 51%. Fig. 1.8 right shows the variation of the efficiency with the energy of the incident radiation. Due to the W L3 absorption edge at 10.2 keV the efficiency decreases abruptly to a semi-constant level of only 35% for energies above the absorption edge. The maximal efficiency of the mirrors is in the energy range 6–10 keV.

### Table 1.1: The parameters for the multi-layer mirrors for the CLS optics optimized for an x-ray energy in the range 6–10 keV and a source bandwidth of 2%. \( \Gamma \) is the fraction of WC in the multi-layer.

<table>
<thead>
<tr>
<th>material combination</th>
<th>( N )</th>
<th>rms roughness (Å)</th>
<th>( d ) (Å)</th>
<th>( \Gamma )</th>
<th>( E ) (keV)</th>
<th>efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>[WC/ScC]</td>
<td>75</td>
<td>3</td>
<td>31</td>
<td>0.44</td>
<td>6–10</td>
<td>( \sim 0.50 )</td>
</tr>
</tbody>
</table>
1.3 Focusing by an elliptic curved mirror

A beam of X-rays can be focused by a mirror with an elliptical curvature. The focal property of an ellipse is so, that any ray coming from one focal point will be reflected through the other focal point. Consider now, as in Fig. 1.9, an elliptical
curved mirror of length \( L \). The mirror is positioned at the distance \( p \) from the source and at distance \( q \) from the image point. The glancing angle of the central ray is \( \alpha_0 \), whereas the glancing angle away from the midpoint is denoted \( \alpha \). The magnitude of \( \alpha \) is a function of the coordinates \((x, y)\) of the mirror. If the mirror is a multi-layer mirror, it is crucial that the mirror is designed so that Bragg’s law is satisfied along the whole length of the mirror, that is the bilayer thickness should vary according to

\[
d(x, y) = \frac{\lambda}{2 \sin \alpha(x, y)}.
\]

By taking into account Snell’s law \( \cos \alpha = n \cos \alpha' \), where \( n \) is the refractive index, the effects of refraction can be included and the bilayer thickness is then given by

\[
d(x, y) = \frac{\lambda}{2 \sin \alpha(x, y)} \frac{1}{\sqrt{1 - \frac{2\delta}{\sin^2 \alpha(x, y)}}},
\]  

(1.8)

where \( \delta \) is the bilayer weighted real part of the refractive index [5].

In App. B it is shown that for each set of parameters \((p, q, \alpha_0)\), there exists one unique set of ellipse parameters \((a, b)\). These ellipse parameters determines the function \( \alpha(x, y) \) from which the optimal bilayer thickness variation can be calculated, see Fig. 1.10. The exact equations are very useful for computer calculations.

In App. C is given the Matlab function which is used to generate the data and illustration shown in Fig. 1.10. If what is needed is merely an estimate of for example the necessary bilayer thickness gradient for a given magnification factor the exact equations are not very convenient. For the purpose of quick estimates, the approach described in Sec. 1.3.1 is more useful.
1.3 Focusing by an elliptic curved mirror

The standard equation of the ellipse is
\[ \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1. \tag{1.9} \]

The focal length \( f \) is related to the distance \( p (q) \) to the source (image) through the general equation of optics,
\[ \frac{1}{p} + \frac{1}{q} = \frac{1}{f}. \tag{1.10} \]

For a magnification factor close to 1 and for small glancing angles \( b = a \sin \alpha_0 \) and \( p \approx q \approx a \). In this case the focal length \( f = a/2 \). In the neighborhood of \( x = 0 \), the ellipse may be is approximated by a circle. The radius of that circle is

Figure 1.10: For the top illustration, \( p = 1.5 \text{ m}, M = 0.5, 1, 2, \alpha_0 = 30^\circ \) and the length of the mirror is 0.4 m. This value of \( \alpha_0 \) is not realistic for a multi-layer mirror, but it is convenient for the purpose of illustration. Bottom: To the left is shown the variation of the glancing angle along the length of the mirror when \( \alpha_0 = 1.45^\circ \) and the length of the mirror is 0.24 m. This value of \( \alpha_0 \) corresponds to a bilayer thickness of approximately 30 Å at 8.05 keV. Notice that for \( M < 1 \), the end of the mirror with the largest bilayer thickness should be closest to the source. For \( M = 1 \) the bilayer gradient is negligible. To the right is shown that the deflection of the mirror decreases with increasing magnification factor.

1.3.1 The circle approximation

The standard equation of the ellipse is
\[ \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1. \tag{1.9} \]

The focal length \( f \) is related to the distance \( p (q) \) to the source (image) through the general equation of optics,
\[ \frac{1}{p} + \frac{1}{q} = \frac{1}{f}. \tag{1.10} \]
found by requiring that the derivatives \( \frac{dy}{dx} \) of the circle \( x^2 + y^2 = R^2 \) and the ellipse Eq. 1.9 are equal. The radius \( R \) is related to the semi-major axis and the semi-minor axis by

\[
R = \frac{a^2}{b} = \frac{a}{\sin \alpha_0} \approx \frac{a}{\alpha_0} . \tag{1.11}
\]

The equation of optics can then be rewritten as

\[
\frac{1}{p} + \frac{1}{q} = \frac{M + 1}{pM} = \frac{2}{R\alpha_0} , \tag{1.12}
\]

where \( M = q/p \) is the magnification factor.

Figure 1.11: The circle approximation. The ideal elliptic shape of the mirror is approximated by a circular arc. The radius of the circle is \( R \).

Figure 1.11 shows the variation of the glancing angles \( \alpha(x) \) across the mirror of length \( L \) in the circle approximation. The glancing angle of the central ray is \( \alpha_0 \), the distance from the source to the mirror is \( p \) and the radius of the mirror curvature is \( R \). Assume first that the mirror is flat. Then the distance \( AB \) can be expressed by the difference between \( \alpha_0 \) and \( \alpha(x) \),

\[
AB = (\alpha(x) - \alpha_0)p = x\alpha(x) ,
\]

so the glancing angle varies with \( x \) as

\[
\alpha(x) = \alpha_0 \frac{p}{p + x} \approx \alpha_0 \left( 1 - \frac{x}{p} \right) \quad \text{for} \quad x \ll p .
\]

When the curvature of the mirror is included, the result for the glancing angles is

\[
\alpha(x) = \alpha_0 \left( 1 - \frac{x}{p} \right) + \frac{x}{R} . \tag{1.13}
\]

Using Eq. 1.12, the linear gradient of the glancing angles is

\[
\frac{\Delta \alpha}{\alpha_0} = \frac{L}{2} \left( \frac{1}{q} - \frac{1}{p} \right) .
\]
When the glancing angle is small, the linear bilayer thickness gradient is

$$\frac{\Delta d}{d_0} = -\frac{\Delta \alpha}{\alpha_0} = L \left( \frac{1}{p} - \frac{1}{q} \right).$$

(1.14)

Figure 1.12 compares the above result for the linear gradient with the linear gradient which can be calculated from Eq. B.1. In the large view-graph, the full lines indicate the exact bilayer thickness variation for different magnification factors. In each case, a linear gradient is derived from the linear fits indicated by the dashed lines. The derived linear gradients are marked by circles in the small inset, which shows the variation of the linear gradient with the magnification factor for $p = 1.5\,m$ and for $p = 15\,m$. The results from the circle-approximation, Eq. 1.14, are marked by the red dashed line while the blue lines are the results from the linear fits to the exact calculations. In the shown examples the two different approaches give the same result.

For the elliptical mirror, the energy dependence of the longitudinal gradient of the bilayer thickness is negligible as shown in Fig. 1.13.

Figure 1.12: The bilayer thickness variation along the length of a 240 mm long mirror. The dashed lines are linear fits to the exact results calculated by Eq. B.1. The small inset compares the linear gradients obtained by the circle approximation Eq. 1.14 (dashed red lines) with the results from the linear fits (blue lines). The two approaches gives nearly identical results.
Figure 1.13: In accordance with Eq. 1.14 the required longitudinal gradient of the $d$-spacing is very close to be independent of the energy. Here, $L = 400$ mm, $p = 1.5$ m and the central bilayer thickness is $d_0 = 21 \text{ Å}$. The full line shows the exact results obtained from the equations Eq. B.1, Eq. B.4, Eq. B.5 and Eq. B.6. The results obtained by using the approximations Eq. B.7 and Eq. B.8 together with Eq. B.1 and Eq. B.4 are shown with the dots.
Chapter 2

The production of the multi-layer mirrors

The multi-layer coatings for the Compact Light Source (CLS) optics are produced at the Danish National Space Center (DNSC). A complete and thoroughly description of the planar magnetron sputtering facility at DNSC is given in [14]. Therefore in this chapter is only given a brief description of the sputtering facility and an outline of the production procedure.

2.1 The planar magnetron sputtering facility at DNSC

Sputtering is a method of depositing thin films of either a metal or an insulator onto a substrate. Fig. 2.1 is a cartoon illustrating the principles behind magnetron sputtering. A description of the physics and plasma technology relevant to sputter deposition can be found in [16].

Figure 2.2 shows a photograph of the inside of the magnetron sputtering chamber at the Danish National Space Center and a top-view sketch of the coating geometry. The substrates are mounted vertically on the mounting plates of the big sample carrousel so the coating geometry is cylindrical. Normally the chamber is used for making multi-layer mirrors for x-ray telescopes [14], and therefore it is very convenient that the chamber is geared for mass production: there are 16 mounting plates in the chamber, each is 600 mm tall and 150 mm wide. Fig. 2.3 shows a photograph of a x-ray telescope. The DC magnetron sources (the targets) are located inside the sample carrousel. When the front of the magnetron source faces the sample carrousel (‘open position’) material is deposited onto the substrates passing by. The magnetron sources can be rotated by $\pm 160^\circ$ from the open position so the sputtered material is deposited onto the screen behind the magnetron source (‘closed position’) rather than onto the substrates. During the coating the targets remain stationary and the thickness of the deposited layers are then controlled by the speed of the sample carrousel, see Sec. 2.1.3 given the values of the following parameters:
Figure 2.1: A cartoon from [15] illustrating the principles behind magnetron sputtering. The following is cited from [15]: "The sputtering takes place in an evacuated chamber in which Argon is introduced at a low pressure (3 mTorr/4e-6 bar). Inside the chamber the Argon gas is ionized. The chamber contains the substrate and the target of the film material to be sputtered. The target is maintained at a negative potential relative to the positively charged Argon ions. The positive ions are accelerated towards the negative charge, striking the target with sufficient force to remove material. Since the chamber is maintained at a vacuum, the liberated material settles on everything in the chamber, and of course also on the substrate. Plasma confinement on the target surface is achieved by locating a permanent magnetic structure behind the target surface."

1. the pressure of Ar in the sputtering chamber (see Sec. 2.1.1),
2. the power applied to the magnetrons (see Sec. 2.1.2),
3. the degree of collimation of the sputtered material (see Sec. 2.1.4) and
4. the distance between the target and the substrates (see Sec. 2.1.5).

2.1.1 The pressure of Ar in the sputtering chamber

The multi-layers described in this thesis are comprised of the materials WC and SiC. Experiments reported on in [14] indicate that for the sputtering of W and Si at the DNSC facility the optimal Ar pressure is about 3 mTorr (0.4 Pa). When it comes to the sputtering process the properties of Si/W and SiC/WC are similar, so the results from [14] applies equally well to the sputtering of WC and SiC. The pressure of Ar pressure in the sputtering chamber influences

1. the coating rate,
2. the stability of the plasma in front of the magnetrons,
3. the interfacial roughness of the layers comprising the multi-layer.
Figure 2.2: Left: the sputtering chamber seen from above. At the time the picture was taken there were two vertical 500 mm targets in the chamber. At present there is room for four targets but only three targets are in operation. Right: a top-view sketch of the coating geometry. See text.

To some extent there will be some scattering of the sputtered material on the Ar ions. Tab. 2.1 compares the masses of Ar, Si and W. Since the mass of a W atom is more than 4 times that of an Ar ion the path of a W atom will not be severely affected by a collision with an Ar ion. The mass of a Si atom amounts to only 70% of the Ar ion-mass, so the paths of the Si atoms from the target to the substrate are more likely to be affected by the scattering on the Ar ions. Therefore the coating rate of Si is severely affected by the Ar pressure: a lowering of the Ar pressure from 6 mTorr to 2.5 mTorr increases the Si coating rate by more than 50%.

An Ar pressure higher than the optimal (3 mTorr (0.4 Pa)) will lead to an increase of the rms interfacial roughness while a lowering of the Ar pressure will decrease the interfacial roughness only marginally. Experimental results reported on in Sec. 2.1.4 indicate that the scattering of SiC influences the interfacial roughness. The Ar pressure also affects the stability of the plasma: if the plasma ‘dies’ because of arcing it will not self-ignite if the Ar pressure is lower than about 3 mTorr.

<table>
<thead>
<tr>
<th>Z</th>
<th>M (g/mole)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>18</td>
</tr>
<tr>
<td>Si</td>
<td>14</td>
</tr>
<tr>
<td>W</td>
<td>74</td>
</tr>
</tbody>
</table>
2.1.2 The power applied to the magnetrons

For magnetron sputtering, the coating rate of SiC is lower than that of WC. Therefore two of the targets are used for the sputtering of SiC and only one target is used for WC. The ratio between the thickness of one WC layer and the total thickness of one bilayer is denoted by $\Gamma$. The value of $\Gamma$ is controlled by adjusting the power applied to the magnetrons. In Sec. 1.2.2 it is shown that for the CLS multi-layers the optimal value of $\Gamma$ is 0.44 corresponding to a WC content in the multi-layer of 44%.

2.1.3 Calibration of the sample carrousel speed

For a given coating rate (determined by the power applied to the magnetrons, the Ar pressure and the degree of collimation of the sputtered material) the thickness of the deposited layers is dependent on only the speed $v$ of the sample carrousel, i.e. the exposure time is proportional to $1/v$. The design of the sputtering facility allows us to produce up to 8 multi-layer mirrors with different bilayer thicknesses in one run. The acceleration and deceleration of the sample carrousel then takes place when the empty sample mounting plates are located in front of the target. As shown in Fig. 2.4 the bilayer thickness $d$ is proportional to one over the speed of the carrousel. The coating rate is experimentally determined as the slope of a linear fit of $d$ to $1/v$.

2.1.4 Collimation of the sputtered particles

Until recently the magnetron sputtering facility at DNSC has primarily been used for the production of multilayer mirrors for x-ray telescopes. These multilayer
2.1 The planar magnetron sputtering facility at DNSC

Figure 2.4: Top: Results from the measurements of the x-ray specular intensity reflectivity from two of the four calibration samples (samples si2133 and si2134). The measurements were conducted at DNSC and the experimental setup is described in Chapter 5. The measured data are indicated by red dots while blue curves are the best IMD [17] fits. The magnitudes of the bilayer thickness, $\Gamma$ and the rms roughness $\sigma$ have been derived from the fits. The lower plot shows that the bilayer thickness (the d-spacing) is inversely proportional to the speed of the sample carrousel. The power applied to the magnetrons was 900 W for SiC and 450 W for WC.

mirrors are curved as shown in Fig. 2.5 left. Experiments have shown that in order to minimize the interface roughness it is necessary to collimate the sputtered particles, see Fig. 2.6. For the curved mirrors the collimation is provided by the separator plates and the view-graph to the right shows that optimally the opening angle of the separator plates should not exceed say 50$^\circ$. Note that the top-view sketch to the left shows that the opening angle of the chimneys is also about 50$^\circ$. The geometry of the sputtering chamber limits the width of the separator plates to 62 mm, so for $\beta = 50^\circ$ the maximum space between the separator plates is D=147 mm. This in turn limits the length of the substrates in the vertical direction and the cylindrical coating geometry limits the dimensions of the substrates in the horizontal direction.

Regarding the quality of the multilayer coating, in addition to the rms roughness there is another important issue: the homogeneity of the bilayer thickness measured along the length of the mirror. The magnetron sputtering with the
The production of the multi-layer mirrors

Figure 2.5: Pictures from [14].

Left: a side view of the sample mounting plate with four curved mirrors for the HEFT telescope. Between the mirrors are mounted five separator plates to provide a collimation of the particles incident on the substrate. Here the distance between the separator plates is $D = 80$ mm and the width of the plates is $S = 50$ mm.

Right: one of the magnetrons seen in the "open" position. The target is 500 mm tall and 38 mm wide. Due to inhomogeneities in the magnets of the magnetrons and their finite length the coating rate varies with up to 20% over 350 mm measured along the length of the sample mounting plates. The role of the masks mounted on each magnetron is to compensate for the variation of the coating rate: with the masks the variation of the coating rate is below 5% over 350 mm. This result is obtained from multilayers produced without any separator plates. See text.

Separator plate collimation has resulted in curved mirrors for x-ray telescopes of an excellent quality, both when it comes to roughness and bilayer thickness homogeneity. However, several attempts to obtain flat mirrors with a homogeneous bilayer thickness (as required for the Compact Light Source (CLS) optics) with the separator plate collimation failed completely due to unwanted shadowing effects from the separator plates (as explained in the caption of Fig. 2.6). With the masks shown in Fig. 2.5 the bilayer thickness of the flat mirrors varied with up to 15% over 50 mm, and many re-designs of the masks did only make things worse. If a flat substrate is coated without any collimation the bilayer thickness is
2.1 The planar magnetron sputtering facility at DNSC

Figure 2.6: Left: a top-view sketch of the coating geometry. Middle: a side view sketch of the coating geometry. The target is standing vertical and the arrows symbolize the particles ejected from the target on their way to the substrate shown to the right. The horizontal lines indicate the separator plates which provide the collimation and prevent the material symbolized with the red arrows from reaching the substrate. The separator plates induce a strong variation of the coating rate along the length of the substrate (referred to in the text as the shadowing effect): experiments with $D = 140$ mm and $S = 50$ mm have shown that 50 mm from the center of the substrate (that is towards the ends of the substrate close to the separator plates), the coating rate has decreased with 15%. For clarity, in this side-view sketch the chimney around the target has been left out. The dimensions of the sputtering chamber (see the top-viev sketch to the left) limits the maximum width of the separator plates to $S = 475$ mm-365 mm-48 mm=62 mm.

Right: the rms roughness (of multi-layers comprised of 10 bilayers of WC/SiC) vs the opening angle $\beta = \arctan(D/(2S))$. The rms roughness is determined by measurements of the specular x-ray intensity reflectivity. The substrates are commercially available Si wafers with a rms roughness of about 2.75 Å. From this view-graph one could be deceived to believe that a further increase of the collimation will suppress the rms roughness completely. However, other experiments (see Chapter 3) indicate that a further increase of the collimation will not suppress the rms roughness further.

homogeneous within 5% over 350 mm. However, the homogeneity is only obtained at the expense of the low rms roughness: with no collimation the rms roughness increases with about 50%, see Fig. 2.6 right.

The multilayer mirrors for the CLS optics must be homogenous (or have a linear gradient of a few percent) over at least 180 mm. Further it is important to keep the roughness of the multilayer as low as possible in order to obtain a maximum intensity reflectivity of the first order Bragg peak. As indicated by the viewgraph of Fig. 2.6 the collimation is an essential part of the setup in the sputtering chamber. Chapter 3 describes a new kind of collimation of the sputtered material developed at DNSC. With these new collimators installed, the sputtering facility at DNSC is qualified for the production of long ($\sim 200$ mm) flat mirrors with a low roughness and a homogeneous bilayer thickness.
2.1.5 Longitudinal homogeneity of the bi-layer thickness

Due to scattering of the sputtered particles on the Ar ions, the coating rate decreases with increasing distance from the target. This implies that if the substrate is not vertical during the deposition, the bilayer will vary along the length of the substrate. At the time of the production of the multilayer mirrors for the CLS optics the construction of the sample mounting plates did not allow us to have full control of vertical alignment of the substrates. The blue data points of Fig. 2.7 show the variation of the bilayer thickness as function of the position of a nominally vertical substrate in the sputtering chamber. The green data points show the variation of the bilayer thickness for a substrate which is inclined by nominally 1.8°.

![Figure 2.7: The variation of the bilayer thickness vs the vertical position in the sputtering chamber. See text.](image)

The construction of the sample mounting plates has now been improved so it is possible to fully control the vertical alignment of the substrates in the sputtering chamber. The data shown in Fig. 2.7 suggest that the variation of the coating rate with the distance from the target can be utilized in the production of multilayer mirrors with specific linear gradients.

2.1.6 Erosion of the targets

During the magnetron sputtering, material is ejected from the targets and in this way an erosion process takes place. The degree of erosion depends on

1. the coating time
2. the power applied to the magnetrons
3. the sputtering gas pressure

It is well known [18] that the coating rate is affected by the erosion of the targets. Dependent on the duration of the multi-layer coating, the erosion may induce an
2.2 Cleaning procedure for Si and glass substrates

Before coating the substrates are cleaned by the following steps:
1. Soap-water at 60°C, 15 minutes in ultrasound
2. Rinsing in Millipore water
3. Acetone, room temperature, 15 minutes in ultrasound
4. Ethanol, room temperature
5. Rinsing in Millipore water
6. Blow dry with Nitrogen

For glass substrates the soap-water is a mixture of 280 mL DeContam in 14 L Millipore water. If this type of soap is used for the cleaning of Si substrates the surface roughness is dramatically increased due to an etching of the surface. For Si substrates the soap-water should be a mixture of detergent and 14 L Millipore water.
Chapter 3

Collimation of the sputtered particles compatible with long flat substrates

In Sec. 2.1.4 it was shown that the rms roughness of multilayers produced by magnetron sputtering at the Danish National Space Center (DNSC) can be decreased by collimating the sputtered particles. It was also explained that with the optimal degree of separator plate collimation it is not possible to deposit multilayers on long (> 177 mm) flat substrates. Further an unwanted shadowing effect of the separator plate collimators induces a variation of the bilayer thickness of up to 15% over 50 mm. This chapter describes how these problems are solved. At the magnetron sputtering facility at DNSC it is now possible to produce homogeneous multilayers with a length of up to ~ 200 mm. The homogeneity of the bilayer thickness is described in Sec. 2.1.5.

3.1 The honeycomb mesh collimation

By providing the collimation by mounting a mesh between the target and the substrate, the length of the substrate is not limited in any way by the collimator, see Fig. 3.1 top. Further the honeycomb mesh collimation does not induce the unwanted shadowing effect which is associated with the separator plate collimation (explained in the caption of Fig. 2.6). Therefore the homogeneity of the coating rate along the length of the substrate is not affected by the honeycomb mesh collimation.

The degree of collimation is dependent on the cell ”diameter” and the mesh thickness. Given these two mesh parameters the area visible through the mesh and the solid angle spanned by the mesh can be calculated, see Fig. 3.1 Bottom, left and middle and Tab. 3.1. Fig. 3.1 bottom, right shows the rms roughness of [W/Si] multilayers (not [WC/SiC] as in Fig. 2.6) produced with different degrees of collimation. The data show that the collimation provided by mesh of types 1–4 results in multilayer mirrors with an acceptable low rms roughness. The data also show
Collimation of the sputtered particles compatible with long flat substrates

Figure 3.1: The honeycomb mesh collimation qualifies the magnetron sputtering facility at DNSC for the coating of long (up to ~ 200 mm) homogeneous multilayer mirrors with a low rms roughness.

Top: sketch of the honeycomb mesh and a side view of the coating geometry.

Bottom, left and middle: the transparency of the honeycomb mesh is dependent on the both the cell diameter and the mesh thickness. Here is shown two views from one point (0,0) at the target towards the sample carrousel when the mesh is mounted 48 mm from the target. The view shown to the left is limited by the mesh only. The other view is in the horizontal direction limited by the chimney which is 80 mm wide.

Bottom, right: the rms roughness of multilayers comprised of 10 bilayers of W/Si, the dashed red line is a guide to the eye. The multilayers has been produced with different degrees of collimation provided by honeycomb mesh of types 1–6, see Tab. 3.1. The number next to each data point refer to the mesh type in Tab. 3.1 and the grey dashed line indicates the rms roughness of a [W/Si] multilayer mirror produced with no collimation at all. The rms roughness has been determined by measurements of the specular x-ray intensity reflectivity. The substrates are commercially available Si wafers with a rms roughness of about 2.75 Å. The blue and the green point indicates the rms roughness of multilayers produced with 10 mm thick mesh with cell diameters of 6.4 mm and 9.6 mm respectively as collimators. The lower x-axis indicates the transparency of the mesh quantified as the total area of the colored region shown in the views to the left. \( \theta_{\text{MAX}} \) at the upper x-axis is defined as follows: 99% of the particles which reaches the substrate has been ejected from the target with a polar angle smaller \( \theta_{\text{MAX}} \). See also Sec. 3.2.
that an increase of the collimation beyond that provided by mesh type 4 will not affect the rms roughness noteworthy. In order not to decrease the coating rate needlessly the collimation provided by mesh type 4 is chosen for the coating of the CLS mirrors.

When using a Si wafer with a rms roughness of 2.75 Å as substrate, a [W/Si] multilayer produced without collimation of the sputtered particles has a rms roughness about 5 Å. It has now been documented that the magnetron sputtering with the honeycomb collimation results in multilayers with a rms roughness which is considerably lower than this. In Sec. 3.2 the effect of the honeycomb collimation is related to that of the separator plate collimation. The results regarding the homogeneity of the bilayer thickness along the length of the mirror are included in Sec. 2.1.5.

## 3.2 Relating the honeycomb collimation to the separator plate collimation

The experimental results given in the sections 2.1.4 and 3.1 document that two different types of collimation give similar results regarding the rms roughness of multilayers produced by magnetron sputtering at DNSC. In this section the two methods are related and thereby we get one step closer to an understanding of why the collimation works. It is shown that the one of the conditions for obtaining low roughness multilayers is that the limiting angles $\beta$ (defined in Fig. 2.6) and $\theta_{\text{MAX}}$ (defined in Fig. 3.1) do not exceed $\sim 50^\circ$. This section explains how the values of $\theta_{\text{MAX}}$ at the upper x-axis of Fig. 3.1 bottom, right are determined.

As illustrated by the side-view sketch Fig. 3.1 top, right, particles ejected from the target at angles exceeding a certain limit $\theta_{\text{MAX}}$ will most likely not reach the substrate, rather they are caught by the mesh. A more precise definition of $\theta_{\text{MAX}}$ is the following: 99% of the particles which reach the substrate have been ejected from the target with a polar angle $\theta$ smaller than $\theta_{\text{MAX}}$. For each mesh the value of $\theta_{\text{MAX}}$ is determined from the angular distribution of particles $I(\theta)$ incident on

<table>
<thead>
<tr>
<th>mesh type</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>mesh thickness (mm)</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>cell diameter (mm)</td>
<td>6.4</td>
<td>9.6</td>
<td>12.8</td>
<td>6.4</td>
<td>9.6</td>
<td>12.8</td>
</tr>
<tr>
<td>solid angle (st. rad.)</td>
<td>0.32</td>
<td>0.61</td>
<td>0.88</td>
<td>0.92</td>
<td>1.4</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Table 3.1: The solid angle spanned by the honeycomb mesh calculated according to Eq. 3.2. The mesh is mounted the distance $L_H = 48$ mm from the target. The data shown in Fig. 3.1 indicate that magnetron sputtering at DNSC with a collimation provided by the mesh types 1–4 results in [W/Si] multilayers with a rms roughness below 3.75 Å (The substrates are commercially available Si wafers with a rms roughness of about 2.75 Å).
the substrate,

$$0.99 = \sum_{\theta=\theta_{\text{MAX}}}^{\theta=0} \frac{I(\theta)}{I_{\text{tot}}} \quad \text{where} \quad I_{\text{tot}} = \sum_{\theta} I(\theta). \quad (3.1)$$

In the following the angular distribution of particles incident on the substrate $I(\theta)$ is estimated from a simple model which neglects the scattering of the particles on i.e. the Ar ions. This means that the particles ejected from the target are assumed to follow a linear path to the substrate. Further, the model does not consider the effects of re-sputtering and backscattering from the surface of the substrate.

Assume naively that in the sputtering process, particles are ejected from the target with equal probability $P(\theta)$ for all angles $\theta$, that is

$$P(\theta) = C,$$

where $C$ is a constant. Then the total number of particles transmitted through the mesh is directly proportional to the total solid angle $\Phi_{\text{tot}}$ spanned by that mesh.

For the calculation of $\Phi_{\text{tot}}$ a coordinate-system oriented as shown in Fig. 3.2 is defined. Further it is convenient to define a function $T(x, y, L_H)$ which describes the transparency of a given mesh which is placed the distance $L_H$ from the target. This function assumes the value 1 if the mesh is transparent (corresponding to the green areas of Fig. 3.2) and 0 otherwise (corresponding to the black areas of Fig. 3.2). With these definitions at hand the solid angle $\Phi_{\text{tot}}$ can be calculated as

$$\Phi_{\text{tot}} = \sum_{(x,y)} T(x, y) \frac{\Delta x \Delta y}{(L_H / \cos \theta)^2}, \quad (3.2)$$

where

$$\theta = \arccos \left( \frac{L_H}{\sqrt{x^2 + y^2 + L_H^2}} \right)$$

is the polar angle from the $z$-axis which is perpendicular to the target (and the mesh) and $\Delta x \Delta y$ is an infinitesimal area element.
3.2 Relating the honeycomb collimation to the separator plate collimation

However, to obtain the distribution of particles incident on the substrate vs the angle \( \theta \) it is more useful to calculate the solid angle in the following way:

the points \((x, y)\) of a circle with the center at \((0, 0)\) are sharing the same polar angle \( \theta \), i.e. the dashed circle of Fig. 3.2 corresponds to the polar angle \( \theta_0 = \arccos \left( \frac{L}{H} / \sqrt{R_0^2 + L^2} \right) \). The number of particles ejected from the point \((0, 0)\) at the target which are incident on the substrate with the angle \( \theta_0 \) is then proportional to \( \Phi(\theta_0) \) where

\[
\Phi(\theta_0) = \sum_{(x,y)/\sqrt{x^2+y^2}=R_0} T(x, y) \frac{\Delta x \Delta y}{(L_H / \cos \theta_0)^2},
\]

and the total solid angle is calculated as

\[
\Phi_{\text{tot}} = \sum_{\theta} \Phi(\theta).
\]

Figure 3.3: Left: the number of sputtered particles transmitted through the mesh vs the polar angle \( \theta \) calculated according to Eq. 3.5. The green and blue curves are calculated assuming that \( P(\theta) = C \) while the grey curves are calculated with a more realistic model for \( P(\theta) \) described by Eq. 3.7 with \( \alpha = 1.15 \). This model is explained in Sec. 3.3. The red regions mark the range of angles which is excluded by the separator plate collimation.

Right: the rms roughness of [W/Si] multilayers produced by magnetron sputtering with collimation of the sputtered particles. The number next to each data point indicates which mesh type provided the collimation (see Tab. 3.1). The thick dashed line indicates the rms roughness of a [W/Si] multilayer produced without any collimation and \( \theta_{\text{MAX}} \) is for each mesh type determined according to Eq. 3.1. See also Tab. 3.2.

The substrates for the multilayers are commercially available Si wafers with a rms roughness about 2.75 Å.

The number of particles per time \( I(\theta) \) transmitted through the mesh vs the polar angle \( \theta \) averaged over the target is then proportional to

\[
I(\theta) \propto P(\theta) \langle \Phi(\theta) \rangle_{\text{target}}.
\]
Note that $\Phi(\theta)$ is defined with a point of origin at $(0,0)$. Since not only this point but all points $(x,y)$ of the target contribute with ejected particles, $I(\theta)$ is calculated as an average over all points of the target. From this function the value of $\theta_{\text{MAX}}$ can be determined from Eq. 3.1. The blue and green curves of Fig. 3.3 left show the function $I(\theta)$ calculated with the assumption $P(\theta) = C$. $I(\theta)$ calculated for the mesh types 1–4 and mesh types 5–6 are shown as the green and blue curves respectively. Of the six curves only the blue ones have tails inside the red areas which indicate the range $\theta > 51^\circ$. Fig. 3.3 right shows that a collimation with the mesh types 5–6 result in multilayers with a relatively large rms roughness compared to that obtained with the mesh types 1–4.

Until now it has for simplicity been assumed that an equal number of particles is ejected from the target at all polar angles, that is $P(\theta) = C$. The calculations within this simple model indicate that for the mesh of types 1–4 the value of $\theta_{\text{MAX}}$ does not exceed $\sim 50^\circ$. The data presented here show that a collimation of the sputtered particles with these four mesh types results in multilayers with a low rms roughness compared to that obtained with mesh types 5–6. These results are consistent with the results of the separator plate collimation (Fig. 2.5): with this type of collimation, the lowest rms is obtained if the opening angle $\beta$ is less than $50^\circ$.

In Sec. 3.3 it is shown that the assumption of a more realistic model [18] for $P(\theta)$ does not change this result noteworthy.

### 3.3 An estimate of the angular distribution of the particles ejected from the target

As described in Chapter 2 at the sputtering facility of DNSC the thickness of the bilayers is controlled by the speed of the sample carrousel and in Sec. 2.1.3 it is shown that the bilayer thickness $d$ equals the coating rate over the carrousel speed. Since it is possible in one run to produce up to 8 multilayer samples with different bilayer thicknesses, it is a simple task to determine the coating rate experimentally. Fig. 3.4 left shows that the bilayer thickness is proportional to $1/v$ (i.e. the exposure time). The coating rate for each of the 6 honeycomb mesh has been determined as the constant of proportionality. Not surprisingly there is a different coating rate associated with each mesh, that is a collimation with a more transparent mesh results in a bigger coating rate. The collimation with the most transparent mesh (type 6) reduces the coating rate to approximately 50% of the coating rate when there is no collimation at all.

Fig. 3.4 right shows the coating rate vs the solid angle of exposure $\Phi_{\text{tot}}$. The coating rate is proportional to

$$\sum_{\theta} I(\theta),$$

(3.6)

with $I(\theta)$ is defined as in Eq. 3.5,

$$I(\theta) \propto P(\theta) \langle \Phi(\theta) \rangle_{\text{target}}.$$
3.3 An estimate of the angular distribution of the particles ejected from the target

This means that if the angular distribution of particles ejected from the target could be described by \( P(\theta) = C \) as assumed in Sec. 3.2, the coating rate would be directly proportional to \( \Phi_{\text{tot}} \). The dashed line shows a linear fit to the data points. The position of the data point representing the coating rate associated with the most transparent mesh (that is type 6) deviates from this line, and this points towards that the simple model \( P(\theta) = C \) is not sufficient to describe the angular distribution of particles ejected from the target. In [18] and [19] is suggested a more realistic model for the angular distribution \( P(\alpha, \theta) \) of particles ejected from the target,

\[
P(\alpha, \theta) = \frac{2 \cos \alpha}{\alpha^2 + (1 - \alpha^2) \cos^2 \theta}.
\] 

Here \( \theta \) is (as in Sec. 3.2) the polar angle and the value of the parameter \( \alpha \) determines the angular width of \( P(\alpha, \theta) \), see Fig. 3.5. Ideally the angular distribution of of particles ejected each target should be considered independently. However, following the approach adopted in [18], here is considered an efficient angular distribution of the two materials (W and Si) together. In [18] a value of \( \alpha = 1 \) is estimated for the material combination Mo/Si.

Fig. 3.6 left shows a plot of the transparency function \( T \) multiplied by the angular distribution \( P(\alpha = 1, \theta) \) of particles ejected from the target. \( T \) is defined in Sec. 3.2 and \( \theta = \arccos \left( \frac{L_H}{\sqrt{x^2 + y^2 + L_H^2}} \right) \). The color indicates the weight from the flux distribution function: the dark red corresponds to \( P \approx 1 \) and the green corresponds to \( P \approx 0.5 \). The black squares of Fig. 3.6 middle show the coating rate vs the spanned solid angle \( \Phi_{\text{tot}} \) and the red circles show coating rate vs \( \sum_\theta \Phi(\theta) P(\alpha, \theta) \) with \( \alpha = 1.15 \). The dashed lines are linear fits \( y \) to the data.
Collimation of the sputtered particles compatible with long flat substrates

Figure 3.5: The angular distribution $P(\alpha, \theta)$ of particles ejected from a point on the target (Eq. 3.7). The insets show a top view of the target during sputtering. The length of the vector with the direction specified by $\theta$ is a measure of the amount of material ejected in that direction. In both cases shown the intensity of ejected particles is strongest in the forward direction towards the substrate and decreases with increasing angle $\theta$.

Figure 3.6: Left: a view from the point (0,0) at the target towards the substrate through a honeycomb mesh. See text. Middle: the coating rate increases with the total solid angle. See text. Right: the goodness of the linear fits (GOF) of the coating rate to $\sum_\theta \Phi(\theta) P(\alpha, \theta)$ vs the parameter $\alpha$. The dashed line indicates GOF for $P(\theta) = C$. The red circle marks the maximum of GOF corresponding to the value $\alpha = 1.15$.

points $Y$ and Fig. 3.6 right compares the goodness of the fits (GOF) defined as

$$GOF = 1 - \frac{\sum_i (Y_i - y_i)^2}{\sum_i (Y_i - \langle Y \rangle)^2}. \quad (3.8)$$

Here $(Y_i - y_i)$ is the deviation of one data point $Y_i$ from the fit $y_i$ and $(Y_i - \langle Y \rangle)$ is the deviation of one data point from a horizontal line through mean value of all the data points. The solid line indicates GOF vs the parameter $\alpha$ and the dashed line indicates the goodness of the linear fit to the coating rate vs $\Phi_{tot}$. The best fit is obtained with $\alpha = 1.15$. 
Table 3.2 compares the values of $\theta_{\text{MAX}}$ calculated with the two different models for the angular distribution of particles ejected from the target, namely $P(\theta) = C$ and $P(\theta)$ defined by Eq. 3.7 with $\alpha = 1.15$. As expected from Fig. 3.3 the two different models for $P(\theta)$ give similar results for $\theta_{\text{MAX}}$.

**Table 3.2:** The collimation of the sputtered particles with mesh of types 1–4 gives similar results regarding the rms roughness of the multilayer. The values of $\theta_{\text{MAX}}$ have been calculated assuming that the honeycomb mesh is mounted 48 mm from the target.

<table>
<thead>
<tr>
<th>mesh type</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>mesh thickness (mm)</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>cell diameter (mm)</td>
<td>6.4</td>
<td>9.6</td>
<td>12.8</td>
<td>6.4</td>
<td>9.6</td>
<td>12.8</td>
</tr>
<tr>
<td>$\theta_{\text{MAX}}$ ($^\circ$), $P(\theta) = C$</td>
<td>31</td>
<td>41</td>
<td>48</td>
<td>49</td>
<td>58</td>
<td>64</td>
</tr>
<tr>
<td>$\theta_{\text{MAX}}$ ($^\circ$), $P(\theta)$ defined by Eq. 3.7, $\alpha = 1.15$</td>
<td>31</td>
<td>41</td>
<td>48</td>
<td>48</td>
<td>57</td>
<td>62</td>
</tr>
</tbody>
</table>

### 3.4 Summary

At the sputtering facility of DNSC it has been shown that the collimation of the sputtered particles plays an important role in the production of W/Si and WC/SiC multilayers with low rms roughness. Two methods of collimation have been presented, they are referred to as the separator plate collimation and the honeycomb mesh collimation respectively. The data and calculations presented in this chapter indicate that provided the collimators exclude material ejected from the target with polar angles exceeding $\sim 50^\circ$ the two methods of collimation give similar results regarding the rms roughness.

The results indicate that when it comes to [W/Si] and [WC/SiC] multilayers, there is a strong experimental evidence that the rms interface roughness can be minimized by excluding material ejected from the target with polar angles greater than approximately $50^\circ$.

The data presented here indicate that the interface width of the bilayers comprising the multilayer increases as the polar angle of ejection from the target exceeds $\sim 50^\circ$. A study of the nature of the real roughness vs the inter-diffusion of multilayers produced with the different collimation modes may reveal the cause of the observed rms roughness increase. The relative magnitudes of the real roughness and the inter-diffusion can be derived from measurements of the both the specular and off-specular x-ray intensity reflectivity. From the off-specular data the correlation function of the interface roughness profile can be reconstructed. [9][10].

One may speculate if the increase of the roughness is caused by the formation of a nanometric rippled surface pattern, strongly resembling the macroscopic ripples observed for example on a sandy beach. Such patterns are known to be produced by ion-beam sputtering erosion of amorphous targets at off-normal incidence [20]. If this is the case I would expect the magnitude of the real roughness (rather than the degree of inter-diffusion) to increase with the decreasing degree of collimation.
It would be interesting to correlate an analysis of the off-specular and specular x-ray intensity reflectivity with AFM/STM measurements.
Chapter 4

The crystal bender

4.1 Beam theory

Figure 4.1(1) shows a side view sketch of the mirror placed in the bender. The mirror is supported at points separated by the distance $L_M + l$, and by applying suitable forces $F_A$ and $F_B$ at points separated by the distance $L_M$, the mirror can be bent elastically. The shape of the centroidal axis of the mirror $y(x)$ is then described by the differential equation \[22\]

$$EI \frac{d^2 y}{dx^2} = M(x),$$

(4.1)

where $M(x)$ is the bending moment, $E$ is the modulus of elasticity (Young’s modulus) and $I$ is the second moment of the cross-sectional area. For a mirror of width $b$ and thickness $h$,

$$I = \frac{bh^3}{12}.$$  

(4.2)

For the geometry shown, the bending moment varies with $x$ as [23][22]

$$M(x) = \begin{cases} 0 & \text{for } -\frac{L}{2} < x < -\frac{L_M + l}{2} \\ \frac{M_A}{l} \left(2x + L_M + l\right) & \text{for } -\frac{L_M + l}{2} < x < -\frac{L_M}{2} \\ \frac{M_B - M_A}{L_M} x + \frac{M_B + M_A}{2} & \text{for } -\frac{L_M}{2} < x < L_M \\ -\frac{M_B}{l} \left(2x - L_M - l\right) & \text{for } \frac{L_M}{2} < x < \frac{L_M + l}{2} \\ 0 & \text{for } \frac{L_M + l}{2} < x < \frac{L}{2}. \end{cases}$$

(4.3)

Eq. 4.1 is solved by imposing the boundary conditions that both $y(x)$ and $dy/dx$ are continuous functions and $y(-((L_M + l)/2)) = y((L_M + l)/2) = 0$, that is at the points of support. The solution is given in Eq. A.1 and Eq. A.2.

In addition to the curvature along the length of the mirror, the bending moment induce another deformation. This deformation is perpendicular to the length axis.
and is called anticlastic deformation. However, when the ratio between the width and the length of the mirror is small, this deformation is negligible and therefore it will not be treated here. In [21] the anticlastic deformation is treated in detail.

4.1.1 $F_A = F_B$

In this section it is assumed that the forces $F_A$ and $F_B$ applied to the mirror are equal, so the bending moment is constant in the region between the applied forces. The constant bending moment deforms the mirror into the shape of a parabola, see Eq. 4.1. The linear behavior of the bending moment near the ends of the mirror gives rise to a shape which is described by a 3rd order polynomial. Outside the outer support where there is no bending moment, the ends of the mirror are straight with the slope of the 3rd order polynomial.

The elastic deflection of the mirror is linear in the applied force. The following expressions for the deflection are derived from Eq. A.1 and Eq. A.2. In the parabolic region of length $L_M$, see Fig. 4.2, the deflection is

$$\text{def}_{L_M} = (F_A + F_B) \frac{L_M^2}{32EI}, \quad (4.4)$$
4.2 Design of the bender

The mirror bender is designed and produced by JJ-X-ray. The dimensions of the

\[ L_{M} + l \]

while the deflection of the central \( L_M + l \) part of the mirror is given by

\[ \text{def}_{L_M+l} = \left(1 + \frac{6L_M l + 2l^2}{3L_M^2}\right) \text{def}_{L_M}. \]  

(4.5)

In Sec. 4.4 it is shown that only the parabolic part of the mirror works well as a focusing device. For the purpose of e.g. determining the distance from the mirror to the focus point Eq. 4.4 is useful. The deflection of the mirror measured with a gauge head is in accordance with Eq. 4.5.

4.2 Design of the bender

The mirror bender is designed and produced by JJ-X-ray. The dimensions of the

\[ L_M \]

The width of the mirror allows for deposition of up to three stripes of different multi-layers. See Tab. 4.1 for values of \( b', b'', L_M \) and \( l \).

Si (100) substrates are \( h = 4 \text{ mm}, b = 37 \text{ mm} \) and \( L = 240 \text{ mm} \). On the same substrate we have the possibility of depositing up to three different multi-layers, for example one for 1:1 focusing, one for collimation and one for magnification of the beam as shown in Fig. 4.3. As shown in the sketch the transverse distance \( b'' \) between the points of force transfer is different from the transverse distance \( b' \) between the points of support. The reason for this is the following: in [21] it has
been shown by a Finite Element Analysis that the anticlastic deformation can be diminished by shifting the transverse position positions of supports relative to the transverse positions of force transfer. See [21] for details.

Each multi-layer will have different requirements for the curvature of the mirror, and therefore the bender must be provided with a motor which can adjust the deflection of the mirror to a given value. Fig. 4.4 top shows a drawing of the mirror bender. The bending force is transferred to the mirror by the arms which are separated by the distance $L_M$. The magnitude of the bending force is controlled by the motor which drives an eccentric wheel, see Fig. 4.4 bottom. This drawing shows a cut through the center of the mirror bender. The arms are connected to the plate which contains a weak link. When the eccentric wheel is rotated by the motor, the plate is deflected symmetrically around the weak link. The deflection of the plate pulls the force arms downwards and in this way force is transferred to the mirror.

**Figure 4.4:** Drawings of the mirror bender by Henning Bro Pedersen, JJ X-ray A/S. 
*Top:* the mirror in the mirror bender. *Bottom:* a cut through the center of the mirror bender shows that the motor drives an eccentric wheel. See text.
The fundamental design of the bender can be described by Fig. 4.1, but to reduce the risk of breaking the substrate, the force is transferred to the substrate at four points instead of only two. Before the final bender was produced, preliminary experiments were conducted using a dummy bender and glass plates, see Fig. 4.5. In the experiment, the deflection of two glass plates of different thickness were measured for different applied forces, see Fig. 4.6. The sets of data show that Young’s modulus for the glass plates is of the order of 70 GPa, in agreement with tabulated values. The dummy bender was loaded with up to 31.9 kg without leaving signs of destruction on the glass plates. The real Si substrates have a Young’s modulus of approximately 170 GPa, and since the deflection is proportional to $1/E$ they are harder to bend than the glass used in the experiment. Therefore, to be absolutely sure that the bender will not break the Si substrate, the final bender geometry was changed in order to obtain a larger ratio between the deflection and the applied force, see Tab. 4.1 and Tab. 4.2.

<table>
<thead>
<tr>
<th>Table 4.1:</th>
<th>The data for the dummy and the final bender. Here $F = F_A + F_B$.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$ b'$</td>
</tr>
<tr>
<td>dummy bender</td>
<td>33.0</td>
</tr>
<tr>
<td>final bender</td>
<td>33.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 4.2:</th>
<th>The data for the Si substrates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$h$</td>
</tr>
<tr>
<td>final bender</td>
<td>4</td>
</tr>
</tbody>
</table>

4.3 Characterization of the bender performance

The ideal shape of a focusing mirror is an arc of an ellipse. To obtain this ideal shape, the width of the mirror must vary like [21]

$$w(x) = \frac{12((M_A + M_B)/2 - (M_A - M_B)x/L_M)}{h^3 E b a (a^2 - x^2)^{-3/2}},$$ (4.6)

where $a$ and $b$ are the semimajor and semiminor axis of the ellipse. For 1:1 focusing with $p = 1.5$ m and a glancing angle of 1.448°, the variation of the width with the length of the mirror is shown in Fig. 4.7. The average width of the mirror is 37.06 mm, and the mirror is 0.19 mm wider at the center than it is at the ends, so the deviation from a rectangular shape is negligible. In Sec. 4.4 it is shown that if the force is applied symmetrically ($F_A = F_B$) to a rectangular mirror, for 1:1 focusing the figure error is less than 1 $\mu$rad. If, for some reason,
Figure 4.5: Top: The disassembled dummy bender with a glass plate placed in the bottom part. The distance $L_M + l$ between the outer supports is 235 mm. The force is applied at the points separated by $L_M = 195$ mm.

Middle: The assembled dummy bender. The force is transferred by the 4 'legs' so space is left for a measuring device such as a gauge head.

Bottom: The conduction of the experiment. The dummy bender was loaded with either water or lead (up to approximately 32 kg). The deflection $\text{def}_{L_M+l}$ of the glass plate was measured with a gauge head. Christian B. Mammen (to the right) from the company JJ X-ray assisted in the experiment.
4.3 Characterization of the bender performance

Figure 4.6: The deflection of glass has been measured with a gauge head vs the applied force. The error-bars are of the same size as the data-points. The dimensions of the two glass plates used in the experiment were \( b = 37 \) mm, \( L = 240 \) mm and \( h = 3 \) mm and 4 mm respectively. The measured deflection is proportional to the ratio of the applied force and Young’s modulus: \( \text{def}_{L,M+l} C = \frac{F}{E} \) where \( C = \frac{96 f}{3 L_{MM}^{2} + 6 L_{MM} L^{2} + 2 L^{4}} \), see Eq. 4.5. The measured data indicate that Young’s modulus for the glass plates is about 70 GPa which is in agreement with tabulated values for glass.

Figure 4.7: The variation of the width of the substrate for 1:1 focusing calculated using Eq. 4.6 with \( p = 1.5 \) m, \( \alpha_0 = 1.448^{\circ} \), \( F_A = F_B = 18.9 \) N and the final bender geometry from Tab. 4.1.

Figure 4.8: The Zeiss coordinate measuring machine. At Risoe National Laboratory the machine is operated in a room with controlled climate at 20\(^{\circ}\)C.
the force is distributed asymmetrically, the focusing performance of the mirror will be affected. In Sec. 4.3.1 the bending moments $M_A$ and $M_B$ are derived from measured data-sets, and it is shown that the design of the final bender may induce a small difference between the forces applied to the mirror. Ray-tracing calculations presented in Sec. 4.4 show that if the asymmetry in the force distribution is less than 10%, the figure error is less than 20 $\mu$rad.

### 4.3.1 Derivation of the bending moments

**Figure 4.9:** Top, left: As explained in Sec. 4.2 the deflection of the mirror is controlled by the position of an eccentric wheel which may be driven by a motor. The data points show the measured profile of the bent Si dummy-mirror along the mirror length for one position of the eccentric wheel (in the figure this position is called the 'bender position'). By fitting Eq. A.1 to the data points, the values for $F_A$ and $F_B$ have been derived. The curve shows the result of the fit, and the blue part of the curve indicates the region of length $L_M$. The data have been offset so $y(-L_M/2) = 0$. The mirror profile has been measured for 16 different bender positions.

Top, right: The deflection $\text{def}\_L_M$ vs. the bender positions. The point marked by a square corresponds to the mirror profile shown to the left.

Bottom, left: The estimator for the variance $s^2$ vs. the bender position. The circles show the variance for fits of Eq. A.1 to the measured data with the constraint that $F_A = F_B$. The squares show the result of fitting with $F_A \neq F_B$. The points marked by red squares correspond to the mirror profile shown above to the left.

Bottom, right: The values for $F_A$ and $F_B$ derived from the mirror profiles. The points marked by red squares correspond to the mirror profile shown above to the left.

A unpolished piece of Si with the same dimensions as the real substrate was placed
4.3 Characterization of the bender performance

in the bender. For different bender positions, the mirror profile along the length axis was measured by Freddy Bruus at Risoe National Laboratory using a Zeiss Prismo Vast 3D CNC coordinate measuring machine, see Figures. 4.8 and 4.9 Top, left. By fitting Eq. A.1 to the measured data, values for $F_A$ and $F_B$ are derived from the measured data in the following way: the shape of the mirror is linear in the bending moments, so Eq. A.1 can be recast in the form

$$y = \frac{1}{EI} (g_A(x, L_M, l) M_A + g_B(x, L_M, l) M_B), \quad (4.7)$$

where $g_A$ and $g_B$ are functions of the known quantities $x$, $L_M$ and $l$. For each bender position, a set of $N$ data points $[(x_1, Y_1), (x_2, Y_2), \ldots, (x_N, Y_N)]$ have been measured. By denoting

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_N \end{pmatrix} \quad \text{and} \quad \mathbf{g} = \frac{1}{EI} \begin{pmatrix} g_A(x_1, L_M, l) & g_B(x_1, L_M, l) \\ g_A(x_2, L_M, l) & g_B(x_2, L_M, l) \\ \vdots & \vdots \\ g_A(x_N, L_M, l) & g_B(x_N, L_M, l) \end{pmatrix}, \quad (4.8)$$

the $N$ equations 4.7 can be written in the compact form

$$\mathbf{Y} = \mathbf{g} \mathbf{M} \quad \text{where} \quad \mathbf{M} = \begin{pmatrix} M_A \\ M_B \end{pmatrix}. \quad (4.9)$$

The only unknown in the above equation are the bending moments $M_A$ and $M_B$, and these are the estimated by [24][25][26]

$$\begin{pmatrix} M_A \\ M_B \end{pmatrix} = \mathbf{g}^+ \mathbf{Y}, \quad (4.10)$$

where $\mathbf{g}^+$ is the Moore-Penrose pseudoinverse of the matrix $\mathbf{g}$. The results of the mirror profile measurements are summarized in Fig. 4.9. The variance in the error between the $N$ measured data points $Y_i$ and the points $y_i$ of the fitted curve is estimated by [27]

$$s^2 = \frac{\sum_{i=1}^{n} (Y_i - y_i)^2}{n - 2}. \quad (4.11)$$

Fig. 4.9 Bottom, left shows that the variance for fitting with $F_A \neq F_B$ is significantly smaller than fitting with $F_A = F_B$. Fig. 4.9 Bottom, right shows the relation between $F_A$ and $F_B$ derived from the 16 sets of data,

$$F_B = 1.05 F_A + 4.19 \text{ N}.$$ 

This difference between $F_A$ and $F_B$ is certainly larger than expected from the design of the mirror bender. The constant term of 4.19 N is most likely caused by a mistake during the mounting of the dummy substrate in the mirror bender. As is shown in Sec. 4.4 an asymmetry of this magnitude will give rise to a huge figure error of the order of 30 $\mu$rad.
4.4 The focusing of the bent mirror compared with the focusing of an ellipse

When rays emitted from the point source $S$ are reflected in a elliptic mirror, they...
are focussed in the point \((c,0)\) as described in Sec. 1.3 and shown in Fig. 4.10, top, left. If the curvature of the mirror deviate from the ideal elliptic shape, at \(x = c\) the reflected rays will be distributed around \(y = 0\) as indicated by the red shaded area. The distribution of the intensity depends on the variation of the figure error \(\Delta \alpha\) along the length of the mirror. To the right is shown the variation of \(\Delta \alpha\) calculated for 1:1 focusing with the force applied symmetrically to the mirror. The dashed part of the curve indicates that the figure error increases significantly towards the ends of the mirror, where the mirror shape is described by a third order polynomial. The shape of the central parabolic region is very close to the ideal elliptic shape, and the figure error is smaller than 1 \(\mu\)rad. To the left in Fig. 4.10 middle and bottom is shown the variation of the figure error for two different force distributions, and here only the central region of the mirror is taken into account, that is the region of length \(L_M = 185\) mm. The histograms in the middle show the intensity distribution vs figure error, and the colors refer to the left view-graphs. To the right is shown the accumulated intensity vs figure error. In Fig. 4.11 it is shown that the 5\% difference between \(F_A\) and \(F_B\) corresponds to an effective figure error of approximately 4.7 \(\mu\)rad. The plot of the accumulated intensity shows that 63\% of the intensity is reflected with a figure error of less than 4.7 \(\mu\)rad, a value which corresponds to the effective figure error. If \(F_B = (1+x) F_A\),

![Figure 4.11](image)

**Figure 4.11:** 1:1 focusing of a source with fwhm = 50\(\mu\)m \((p = 1.5\) m). In the calculation \(F_A = 18.4\) N and \(F_B = 1.05\) \(F_A\). The contours show the levels 0.01, 0.1, 0.5, 0.9 and 0.99. The inset shows a cut through the focus at the position marked by the circle. The small asymmetry in the force distribution leads to a broadening of the focus to 64\(\mu\)m corresponding to a figure error of approximately 4.7 \(\mu\)rad.

the effective figure error is linear in \(x\) as shown in Fig. 4.12.

## 4.5 Calibration of the bender motor

The deflection of the mirror vs bender motor position has been measured with a TESA GT30 multi-angle gauge head. By Eq. 4.5 and Tab. 4.1 the measured
The effective figure error vs $x$ for the case where $F_B = (1 + x) F_A$.

The maximum deflection of the mirror is of the order of 200 $\mu$m. For a source–mirror distance of $p = 1.5$ m and a glancing angle $\alpha \approx 1.4^\circ$ this corresponds to a minimum magnification factor of 0.2, see Fig. 4.14.

### 4.6 Summary

The shape of the bent mirror has been calculated. When the force from the bender is applied symmetrically to the mirror the central region of length $L_M = 185$ mm has the shape of a parabola. The deviation of this shape from the ideal elliptic shape is very small: the figure error is below 1 $\mu$rad. The curvature of the ends of the mirror is very far from the ideal elliptic shape, so even though the full length of the mirror is 240 mm, only the central region of length 185 mm takes part in the focusing of the incident beam.

With the present design of the bender it is possible to obtain a maximal deflection of 200 $\mu$m of the mirror. For a glancing angle of 1.45° this corresponds to a magnification factor as small as 0.2. Assume that the purpose of the optical system is to deliver either a collimated beam or an image of the source characterized by a magnification factor $M > 0.5$. Then the efficiency of the mirror can be increased by a small change of the bender-design: for $M > 0.5$ the required deflection of the mirror is considerably smaller than the 200 $\mu$m and therefore the distance $L_M$ between the points of force–transfer can safely be increased. With the present design of the bender only 77% of the mirror can be used for the focusing of the incident beam. An increase of $L_M$ will lead to an increase the efficient area of the mirror.
4.6 Summary

Figure 4.13: The squares and circles show the deflection of the mirror vs the motor position B1 of bender measured with a TESA GT30 multi-angle gauge head. The dashed line is a linear fit to the circular data-points corresponding to bender positions in the interval from -22 to 48. One unit of B1 position corresponds to 300 motor-steps. This means that the deflection can be adjusted with a precision which is better than 0.01 µm.

Figure 4.14: The deflection vs. the radius of curvature of the central part of the mirror has been calculated and is shown here as the dashed red curve. The full blue curve shows the magnification factor vs. the radius of curvature as calculated by Eq. 1.12.

The measurements of the dummy mirror profile vs the bender motor position showed that the force from the bender was transferred asymmetrically to the mirror. An asymmetry in the force transfer of this magnitude will give rise to an unacceptable large figure error of the order of 30 µrad. However, the X-ray characterization of the focusing performance of the CLS mirror in the bender (Chapter 6) shows that the total figure error (including the figure error from both the substrate and the bender) is below 20 µrad. The conclusion is that the observed asymmetry is most likely inherited from the mounting of the dummy mirror in the bender. Therefore it is important to emphasize that great care must be taken when the mirror is mounted in the mirror bender.
Chapter 5

X-ray characterization of the substrates

The figure error and surface roughness of the substrates have been characterized by using two different x-ray experimental setups at the Danish National Space Center. The first two sections of this chapter explains in detail the design of the experimental setups. The results of the characterization are given in the last section.

5.1 The Figure Error characterization

As described in chapter 4, a perfectly flat rectangular substrate can be deformed to have a nearly perfect elliptic curvature, simply by bending it. However, a real substrate is rarely perfectly flat, rather the surface may consist of 1) facets and/or 2) be provided with some fixed curvature inherited from the polishing process. When the substrate is coated with a multi-layer mirror, the facets will of course remain on the surface and influence the focusing performance as shown in Fig. 5.1. If the source has the height \( h \) and the mirror is positioned at the distance \( p \) from the source, then ideally the figure error should not exceed say \( h/(10p) \). If \( h = 50 \, \mu m \) and \( p = 1.5 \, m \) as is the case for the Compact Light Source, then a conservative limit for figure error is 3.3 \( \mu \text{rad} \) or 0.7”. Whether the focusing performance will be affected by the fixed curvature depends on the shape of the substrate profile, i.e. the virgin curvature before the substrate is coated with a multi-layer and put into the mirror bender. If the fixed curvature can be

![Figure 5.1: The blue ray was reflected from a facet which had a figure error of \( h/(4p) \)](image)
approximated by say an arc of a circle, it is likely that the mirror bender is able to force the substrate into the wanted shape. If the shape is more complicated, say $S$-like, the focusing performance of the mirror will most likely be affected.

For the mirror optics we have purchased two Si substrates from the company Crystal Scientific [28]. The substrates are polished on both sides. Below is explained how we have measured the figure error and mapped out the unstressed shape of the substrates.

5.1.1 The experimental setup

The experimental set-up for figure error measurements at the Danish National Space Center (DNSC) is shown schematically in Fig. 5.2 top and is first described in [29]. The scattering plane is horizontal and the approximate dimensions of the X-ray source is 1 mm wide and 1 mm high. The X-ray generator is a rotating Cu anode machine, typically running at 30 kV and 100 mA. The divergence of the beam incident on the monochromator is defined by slits 1 and 2 to 2.78 mrad, a number which is much larger than the angular bandwidth $\Delta \theta = \Delta E \tan \theta / E = 0.11$ mrad of the Cu $K\alpha_1$ line [30]. A slit (#6) positioned after the monochromator (#5) excludes the Cu $K\alpha_2$ line from the beam and defines the size of the footprint on the sample (#7). Using a position sensitive detector the horizontal alignment of this slit can be done in a simple way. During the experiments the maximum width of this slit is 0.5 mm and the glancing angle is $0.15^\circ$, that is below the critical angle for total reflection for Si ($\alpha_c = 0.22^\circ$). To keep the scattering plane horizontal, the substrate must be carefully aligned vertically. The substrate can therefore be rotated around an axis which is parallel to the substrate surface. The direction of the X-rays scattered by the sample is determined by the analyzer crystal. Details on the monochromator and the analyzer are given in the following section. The difference between the dispersive and non-dispersive scattering geometries is explained in Sec. 5.1.2. The position of the footprint on the sample is controlled by the translation of the sample by motor $a$.

The monochromator and the analyzer

The monochromator and the analyzer are identical channel-cut perfect Si(220) crystals, allowing for 5 reflections, see Fig. 5.2, top right. The channel-cut crystals improve the resolution of the non-dispersive setup for figure error characterization compared to the same setup with single reflection crystals as is explained below. If the reflectivity curve of a single crystal is denoted $R$, then the reflectivity curve of a channel-cut crystal with $m$ reflections is $R^m$ [31]. To calculate the reflectivity curve for a perfect crystal it is necessary to apply the theory of dynamical diffraction [32], a theory which allows for multiple scattering effects. When the beam penetrates the perfect crystal, a small fraction is reflected into the exit beam at each atomic plane. This implies that only a finite number of crystal planes will contribute to the Bragg scattering, and therefore the reflectivity curve will
5.1 The Figure Error characterization

Experimental setup at DNSC. All distances are in mm.

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>X-ray source</td>
<td>5,8 Monochromator, analysator: 5 x Si (220) reflections</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Slit 1 (1mm[h]x2mm[v])</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Evacuated tube</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Slit 2 (2mm[h]x2mm[v])</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Monochromator</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Slit 3 (0.5mm[h]x2mm[v])</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Sample</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Analysator</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Evacuated tube</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Linear position sensitive detector</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Dispersive

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>ma = 0 (mm)</td>
<td>mb = 815tan(2·mf) (mm)</td>
</tr>
<tr>
<td>md = 2·mf (mdeg)</td>
<td>mf = 150 (mdeg)</td>
</tr>
<tr>
<td>mh = -2·mf (”)</td>
<td></td>
</tr>
</tbody>
</table>

Non-dispersive

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>mb = 0 (mm)</td>
<td>mc = -(180° - 2θh) (mdeg)</td>
</tr>
<tr>
<td>md = 4θh (mdeg)</td>
<td>mh = 0 (”)</td>
</tr>
</tbody>
</table>

Figure 5.2: The setup for figure error measurements at DNSC. The motors are named ma, mb, mc, md, mf and mh. The motor-positions corresponding to each geometry are listed to the right.

have a finite width, that is the Darwin width. Due to refraction the center of a Bragg reflection does not fall on the Bragg angle $\theta = \arcsin(\lambda/(2 \cdot d))$, rather it
is displaced towards higher angles. For Cu $K\alpha_1$ radiation the Si(220) reflection this displacement amounts to 20.7 $\mu$rad (4.26”), and the angular Darwin width is 23.1 $\mu$rad (4.77”). Fig. 5.3 shows the calculated reflectivity curves for $m = 1$ and $m = 5$ reflections on logarithmic scale, and clearly the tails of the $R^5$ curve are reduced compared with the tails of $R$. Had the reflectivity curves been shown on a linear scale it would be clear that the width of the $R^5$ curve is somewhat smaller than the Darwin width of the single reflection. The primary improvement of the resolution is due to the reduction of the tails.

![Reflectivity curves](image)

**Figure 5.3:** Reflectivities from Si(111) and Si(220) for $m=1$ and $m=5$ at $E = 8.04778$keV calculated using the theory of dynamical diffraction [32]. Full lines correspond to (111) reflections, dashed lines correspond to (220) reflections. For completeness the reflectivity curves have been calculated in three cases: *Left:* The polarization is perpendicular to the scattering plane. *Middle:* Unpolarized source. *Right:* The polarization is in the scattering plane.

The logarithmic scale is chosen on order to show that the tails of the $m = 5$ reflectivity curves are enormously reduced compared to the $m = 1$ curves. The width of the reflectivity curve is dependent on the polarization. The most narrow curve is found for the horizontal scattering plane of a synchrotron (that is $\parallel$ to the polarization) and the widest curve is for the vertical scattering plane of a synchrotron (that is $\perp$ to the polarization). The width of the curve for the unpolarized source is approximately the mean-value of the widths for the $\parallel$ and $\perp$ polarization [33].

**The detector**

The detector is position sensitive with 2000 channels within 100 mm (horizontal). In the figure error measurements the reflection from the analyzer crystal is registered within only 200 channels of the detector. The detector software allows one to define an 'electronic detector slit', and therefore the position sensitive detector is convenient. For the figure error measurements the electronic slit is set so only the channels relevant for the data collection are in use, and this gives a great reduction of the background level. When running the rotating anode at 40 kV, 100 mA, for 200 channels the total background is as low as of the order of 0.1 count/s. This is to be compared with the peak intensity which is typical 700 counts/s.
5.1.2 Dispersive and non-dispersive geometry

In this section is explained the difference between the dispersive and the non-dispersive geometry of an experimental setup. Scanning the analyzer in a dispersive setup yields information about the wavelength distribution in the incident beam. In the non-dispersive setup an analyzer scan will give no such information, instead the direction of the scattered beam can be determined rather accurately. For the figure error characterization it is therefore crucial that the geometry is non-dispersive. The difference between the dispersive and non-dispersive geometries is quite transparent in the situation where only two crystals (the monochromator and the analyzer) are under consideration. If a mirror or a crystal is placed between the two crystals, the system becomes somewhat more complicated and one needs to do a more careful analysis. One possible source of confusion is that what is a non-dispersive setup for two crystals and a mirror becomes a dispersive setup if the mirror is replaced by a Bragg-reflecting sample. In the following is explained why.

Two identical crystals

Suppose there is no sample in the experiment, only the monochromator and the analyzer as shown in the two lower windows of Fig. 5.2. The situation can in both cases be analyzed in a simple way by the graphic method proposed in 1937 by J. W. M. DuMond [34].

First consider the case where two identical crystals are aligned anti-parallel as in Fig. 5.4 top. Two rays with different wavelengths $\lambda$ and $\lambda + \Delta \lambda$ are incident on crystal A. $\Delta \theta_A$ is related to $\lambda$ and $\Delta \lambda$ according to Bragg's law,

$$\Delta \theta_A = \frac{\Delta \lambda}{\lambda} \tan \theta_A,$$

(5.1)

where $\theta_A$ is the Bragg angle. The two rays are Bragg reflected from crystal A and the angle between the rays remains $\Delta \theta_A$. When the angle $\omega$ between the two crystals equals $2\theta_A$, the ray of wavelength $\lambda$ falls on crystal B with the Bragg angle $\theta_A = \theta_B$. The other ray, which fell on crystal A with the angle $\theta_A + \Delta \theta_A$ will now fall on crystal B with the angle $\theta_B - \Delta \theta_A$, that is an increase of the angle $\theta_A$ corresponds to a decrease of the angle $\theta_B$ of equal magnitude. Therefore, in order to reflect the ray with wavelength $\lambda + \Delta \lambda$ crystal B must be rotated the amount $2\Delta \theta_A$ counter-clockwise. In other words, a scan of crystal B will have the angular width $2\Delta \theta_A$ determined by the bandwidth of the incident beam (provided that the Darwin width of the crystal is much smaller than $\tan \theta \Delta \lambda / \lambda$), and therefore this geometry is dispersive.

In the middle of Fig. 5.4 is shown the graphic method of analysis. The black (blue) curve is a plot of the Bragg equation for crystal A (B). The two curves are identical, but since the geometry implies that $\theta_B = \omega - \theta_A$ their $\theta$ coordinates are mutually reversed and displaced by $\omega$. To the right is zoomed in on the DuMond diagram and it is indicated that the angular width of the curves is determined by the Darwin width of the crystal. The available wavelength band $\Delta \lambda$ is marked as
Figure 5.4: A graphic analysis of the non-dispersive and dispersive geometries for two identical crystal (see text). Bandwidth data for Cu $K\alpha$ lines and Darwin widths for the Si(220) reflection are given in Tab. 5.1.

The intersection of the two Bragg curves at the point marked by the green circle corresponds to situation where the green ray is Bragg reflected by both crystals. The red circle on curve A corresponds to the ray of wavelength $\lambda + \Delta\lambda$ which is Bragg reflected in crystal A. Since this point does not belong to curve B, this wavelength is not reflected by crystal B for this particular value of $\omega$. Suppose now that $\omega$ is changed as it is in a scan of crystal B. In the diagram this corresponds to a horizontal sliding of the curve B. In order to make the two curves intersect at the red point curve B must be translated by the angle $2\Delta\theta_A$, and the conclusion
is identical to the one we arrived at above.

Table 5.1: Data for the Si (220) Bragg reflections and bandwidths of Cu $K\alpha_1$ and $K\alpha_2$. $\omega_0^{\text{FWHM}}$ is the angular Darwin width of the Si(220) reflection and $\Delta \theta_0$ is the amount that the center of the reflectivity curve is deviated from the Bragg angle $\theta_B$. These values have been calculated according to [32] and [6] p. 185. $\Delta \theta = \tan \theta_B \frac{\Delta E}{E}$ is the angular bandwidth. Bandwidth data is from [30].

<table>
<thead>
<tr>
<th></th>
<th>$E$ (keV)</th>
<th>$\Delta E/E$</th>
<th>$\Delta \theta$ (&quot;)</th>
<th>$\theta_B$ (&quot;)</th>
<th>$\Delta \theta_0$ (&quot;)</th>
<th>$\omega_0^{\text{FWHM}}$ (&quot;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu $K\alpha_1$</td>
<td>8.04778</td>
<td>2.62 $\cdot$ 10$^{-4}$</td>
<td>23.7</td>
<td>23.651</td>
<td>4.26</td>
<td>4.77</td>
</tr>
<tr>
<td>Cu $K\alpha_2$</td>
<td>8.02783</td>
<td>2.70 $\cdot$ 10$^{-4}$</td>
<td>24.5</td>
<td>23.713</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The case of two successive reflections when the two identical crystals are aligned parallel is shown in Fig. 5.4 bottom. In this situation an increase in the angle $\theta_A$ corresponds to an increase of the angle $\theta_B$ of equal amount. Therefore, in the DuMond diagram the Bragg curves are superposed with their $\theta$ axis increasing in the same direction. In the DuMond diagram shown to the right, the curves have been displaced from the position corresponding to complete parallelism so they can be distinguished from each other. The result of scanning crystal B is the convolution of the Darwin curves of crystal A and B. Thus no information on the wavelength band can be derived from an analyzer scan in the non-dispersive geometry if the two crystals have the same $d$-spacing.

Two identical crystals and a mirror

Figure 5.5 shows the dispersive and non-dispersive scattering geometry for two identical crystals with a mirror positioned between them. The glancing angle on the mirror is below the critical angle for the wavelength $\lambda$, so the whole wavelength band is total reflected. The grey dotted lines outline the situations from Fig. 5.4 without the mirror. The position of crystal B is then given by the reflection of the dotted outline in the thick grey line parallel to the mirror. If the mirror is perfectly flat, the angular width of an analyzer scan in the non-dispersive geometry is the convolution of the Darwin curves of crystals A and B. Thus the limit for resolution of the figure error measurement is defined by the Darwin widths of the analyzer and the monochromator.

Two identical crystals and a Bragg reflecting sample

Figure 5.6 shows the dispersive and non-dispersive scattering geometry for two identical crystals with a Bragg reflecting sample positioned between them. The full lines indicate the paths of the rays with wavelengths $\lambda$ and $\lambda + \Delta \lambda$. The dashed lines indicate the positions of the monochromator (M), the sample (S)
and the analyzer (A). For each reflecting element two positions are shown, one for each wavelength $\lambda$ and $\lambda + \Delta \lambda$. The rays are reflected from the monochromator with the angle $\theta_1$ and $\theta_1 + \Delta \theta_1$ where $\Delta \theta_1 = \tan \theta_1 \Delta \lambda / \lambda$. It is worth noting that the crystals and the sample in the non-dispersive geometry of Fig. 5.6 are arranged in the same way as they are in the dispersive set-up of Fig. 5.5. The big difference between the two setups is that now the sample is Bragg reflecting: the ray of wavelength $\lambda$ is reflected from the sample with the Bragg angle $\theta_2$. In order to reflect the ray of wavelength $\lambda + \Delta \lambda$, the sample must be rotated by the amount

$$\Delta \theta_1 - \Delta \theta_2 = \frac{\Delta \lambda}{\lambda} (\tan \theta_1 - \tan \theta_2)$$

clockwise (for $\theta_1 > \theta_2$). The angle between the rays so reflected from the sample is then

$$\left( \theta_2 + \Delta \theta_1 - 2(\Delta \theta_1 - \Delta \theta_2) \right) - \theta_2 = 2 \Delta \theta_2 - \Delta \theta_1 .$$

Assume that the analyzer is in the position to reflect the ray of wavelength $\lambda$ with the angle $\theta_1$. Then in order to reflect the other ray of wavelength $\lambda + \Delta \lambda$ the analyzer must be rotated by the amount $x$ so the glancing angle of this ray is $\theta_1 + \Delta \theta_1$,

$$\theta_1 - (2 \Delta \theta_2 - \Delta \theta_1) + x = \theta_1 + \Delta \theta_1 \Rightarrow x = 2 \Delta \theta_2 .$$

This means that, provided that the sample is fixed, the width of an analyzer scan is independent on the wavelength content of the incident beam.

The two dispersive setups of Fig. 5.6 can be explained with similar arguments.
5.2 The X-ray reflectivity measurements

5.2.1 Specular X-ray reflectivity from a thick mirror

The theory of X-ray reflectivity is explained in great detail in for example [6]. This section will therefore only give an outline which is necessary to understand

Figure 5.6: The dispersive and non-dispersive geometry for two identical crystals A,B and a Bragg reflecting sample. The non-dispersive and the dispersive (b) setup is also described in [35].
the interpretation of the measured data.

The reflection and transmission of X-rays in a perfectly flat sharp interface is described by the Fresnel equations

\[
\begin{align*}
    r_F &= \frac{\alpha - \alpha'}{\alpha + \alpha'} \\
    t_F &= \frac{\alpha - \alpha'}{2\alpha},
\end{align*}
\]

where \(\alpha\) is the glancing angle and \(\alpha'\) is the angle between the interface and the transmitted ray. \(\alpha'\) is related to the refractive index and the glancing angle through Snell’s law,

\[\cos \alpha = n \cos \alpha'.\]

The intensity reflectivity \(R_F\) (transmittivity) is calculated as the absolute square of the complex amplitude reflectivity (transmittivity). If the interface is perfectly sharp but possess a rms roughness \(\sigma_r\), the specular intensity reflectivity will be diminished so

\[R = R_F e^{-Q^2 \sigma_r^2}.\]

If the density profile of the interface can be described by the error-function

\[f(z) = \text{erf}\left(\frac{z}{\sqrt{2} \sigma_d}\right)\]

where \(\sigma_d\) is a measure of the width of the graded region, the specular intensity reflectivity can be expressed as

\[R = R_F e^{-Q^2 \sigma^2} \quad \text{where} \quad \sigma = \sqrt{\sigma_r^2 + \sigma_d^2}.\]

The conclusion is that in a specular measurement of the reflectivity it is not possible to distinguish the roughness from the diffuseness.

### 5.2.2 The experimental setup

The experimental set-up for reflectometry at the Danish National Space Center (DNSC) is shown schematically in Fig. 5.2. The scattering plane is horizontal and the approximate dimensions of the X-ray source is 0.1 mm wide and 10 mm high. The X-ray generator is a rotating Cu anode machine, typically running at 40 kV and 150 mA. The setup is designed to deliver a high flux of the \(K\alpha_1\) line at the sample, and in the following is explained how.

The in-plane divergence of the beam incident on the monochromator is limited to \(\alpha_{S2} = 489 \mu\text{rad}(1.68'')\) by slit 2. After the monochromator, the in-plane divergence \(\alpha_M\) is limited by the angular Darwin width of 242 \(\mu\text{rad}(50'')\) of the monochromator and the angular bandwidth of 115 \(\mu\text{rad}(23.7'')\) of the Cu \(K\alpha_1\) line,

\[\alpha_M = \sqrt{(242 \mu\text{rad})^2 + (115 \mu\text{rad})^2} = 268 \mu\text{rad}(55.4'').\]
5.2 The X-ray reflectivity measurements

![Diagram of X-ray setup](image)

1. X-ray source
2. Slit 1 (0.2mm[h] x 15mm[v])
3. Evacuated tube
4. Slit 2 (0.2mm[h] x 15mm[v])
5. Monochromator
6. Aluminum filters
7. Slit 3 (0.2mm[h] x 15mm[v])
8. Sample
9. Evacuated tube
10. Linear detector

**Figure 5.7:** The experimental setup for fast reflectometry at DNSC. See text for details.

see also the next section on the monochromator and Tab. 5.2. The divergence allowed by slit 3 is $\alpha_{S3} = 259 \mu\text{rad}(53.4^\circ)$. Since $\alpha_{S2} > \alpha_M \approx \alpha_{S3}$ the flux of the $K\alpha_1$ line is determined by the monochromator crystal and is not limited by slits.

The Ge (111) Bragg angles for the Cu $K\alpha_1$ and $K\alpha_2$ lines is separated by $611 \mu\text{rad}(2.1')$. Since this number is approximately the double of the angular acceptance of the monochromator, the $K\alpha_2$ line can be excluded from the beam incident on the sample.

The same setup is also used for transverse (off-specular) reflectivity measurements. For these measurements it is relevant that the resolution of the detector matches the divergence of beam incident on the sample. The detector position resolution is 0.3 mm which over the sample–detector distance corresponds to a divergence of $303 \mu\text{rad}(1.04')$, a number which is close to the value of the divergence defined by the monochromator.

**The monochromator**

For the reflectometry it is desirable at the same time to have a high monochromatic flux and a narrow beam at the sample, and the monochromator is designed to meet these requirements. The intensity reflectivity decreases like $(\alpha_c/(2\alpha))^4$ so a high flux is necessary in order to have acceptable counting times at glancing angles much larger than the critical angle for total reflection $\alpha_c$. Further, a simple and accurate determination of $\alpha_c$ requires that the length of the footprint of the beam on the sample do not exceed the sample length. At glancing angle $\alpha$ the length of the footprint of a beam of width $w$ is $w/\sin \alpha$. This means that at the
critical angle for for example Si ($\alpha_c = \frac{1}{260}$ rad) the length of the footprint is $260w$, so therefore a narrow beam is advantageous.

The monochromator is an asymmetrically channel-cut Ge crystal with an asymmetry angle of $\alpha = 11.25^\circ \pm 0.1^\circ$ between the (111) crystal planes and the surface, see Fig. 5.7. The asymmetry angle increases the Darwin width relative to that of an symmetric crystal by a factor $1/\sqrt{b}$ where

$$b = \frac{\sin(\theta_B - \alpha)}{\sin(\theta_B + \alpha)}.$$  

With the values from Tab. 5.2 the Darwin width of the monochromator is $243 \mu$rad($50.03^\circ$). The non-dispersive arrangement of the two reflections of the monochromator crystal preserves both the direction and the width of the incident beam. Had there only been one reflection the beam would be expanded by a factor $1/b = 10.09$.

### Table 5.2: Data for the Ge (111) Bragg reflections and bandwidths of Cu $K\alpha_1$ and $K\alpha_2$. $\omega_0^{\text{FWHM}}$ is the angular Darwin width of the Ge(111) reflection and $\Delta\theta_0$ is the amount that the center of the reflectivity curve is deviated from the Bragg angle $\theta_B$. These values have been calculated according to [32] and [6] p. 185. $\Delta\theta = \tan\theta_B \Delta E/E$ is the angular bandwidth. Bandwidth data is from [30].

<table>
<thead>
<tr>
<th></th>
<th>$E$ (keV)</th>
<th>$\Delta E/E$</th>
<th>$\Delta\theta$ (&quot;)</th>
<th>$\theta_B$ (&quot;)</th>
<th>$\Delta\theta_0$ (&quot;)</th>
<th>$\omega_0^{\text{FWHM}}$ (&quot;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu $K\alpha_1$</td>
<td>8.04778</td>
<td>2.62 $\cdot$ 10$^{-4}$</td>
<td>23.7</td>
<td>13.639</td>
<td>13.09</td>
<td>15.75</td>
</tr>
<tr>
<td>Cu $K\alpha_2$</td>
<td>8.02783</td>
<td>2.70 $\cdot$ 10$^{-4}$</td>
<td>24.5</td>
<td>13.674</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The detector

The detector is identical to the detector for the figure error measurements.

### 5.3 The experimental results of the X-ray characterization of the substrates

#### 5.3.1 The figure error characterization

As explained above, the resolution of the figure error measurement is limited by the width of the analyzer scan of the direct beam in the non-dispersive geometry. The angular Darwin width of a single Si(220) reflection is $23.13 \mu$rad($4.77^\circ$), and the width of the convolution of two $m = 5$ Si(220) reflections is $20.4 \mu$rad($4.1^\circ$) as shown in Fig. 5.8. The same view-graph shows the data points from an analyzer scan. Slit 3 is $0.3 \text{mm}[h] \times 2 \text{mm}[v]$ corresponding top a footprint of length $115 \text{mm}$,
5.3 The experimental results of the X-ray characterization of the substrates

Figure 5.8: An analyzer scan of the direct beam in non-dispersive geometry. The blue dashed line is the convolution of 2 m=5 Si(220) reflections.

Figure 5.9: An analyzer scan of the direct beam in non-dispersive geometry (circles) shown together with an analyzer scan of the reflection from a reference glass plate.

see also the sketch of the experimental setup in Fig. 5.2. The agreement between the calculated and the measured result is acceptable: the width of the analyzer scan is 21.3 µrad(4.4°).

Figure 5.9 shows the result of an analyzer scan of the beam reflected from a reference glass plate with the same slit-settings as in Fig. 5.8. The glancing angle is α = 0.15°(540")°, so the real peak position is 2α = 0.30°(1080")°, however in the graph the analyzer position axis has been off-set so the data readily can be compared with the analyzer scan of the direct beam. Had the glass plate been perfectly flat the data-points could not be distinguished from the analyzer scan of the direct beam in the non-dispersive geometry. However, the measured curve is wider than the scan of the direct beam, and the reason for the broadening can only be figure error. The measured width (26.7 µrad(5.5"°)) corresponds to a figure error of $\sqrt{(26.7 \, \mu\text{rad})^2 - (21.3 \, \mu\text{rad})^2}/2 = 8.0 \, \mu\text{rad}(1.7")$.

The position of the footprint on the substrate is controlled by a translation of the substrate along an axis perpendicular to the direct beam. This translation makes it possible to a) map out the variation of the figure error along the length of the substrate and b) to distinguish between the figure error due to long range curvature and that due to smaller facets/roughness on the surface. The curvature of the substrate can be derived from the position of the analyzer scan of the beam reflected from the substrate, while the width of the scan gives the information on the population of facets/roughness. As pointed out in Sec. 5.1.1 the scattering plane is horizontal, and it is therefore of great importance that the substrate is aligned vertical during the figure error characterization. A motor enables a rotation of the substrate around an axis which is parallel to the substrate surface. The figure error mapping is repeated for different positions of this motor, see Fig. 5.10 left. The view-graph shows the widths of the analyzer scans for 8 different motor positions. In general the widths decreases for motor positions 1–4, remain
Figure 5.10: The width of the slit 3 is 0.05 mm. The glancing angle is $0.15^\circ$ ($540''$), so the length of the footprint is 19 mm. Left: the width of analyzer scans vs the footprint center position on the substrate. Right: the peak position vs the footprint center position.

on the same level for positions 4–6 and increases again for positions 6–8. From these data it follows that the substrate is (very close to) vertical with the motor at position 5. To the right is shown the variation of the peak positions along the length of the mirror, and from this information the long range shape (that is the curvature) of the substrate can be derived. The shown variation corresponds to a radius of curvature of approximately 3.6 km.

Fig. 5.11 shows the results of the figure error characterization of the double-polished substrates for two different lengths of footprint, 4 mm and 19 mm. The different footprint sizes give nearly identical results and this indicates that the facets are of a length scale below 4 mm. The shapes of the substrates correspond to radii of curvature in the range 2–4 km. This is about a 100 times the radius of curvature necessary to obtain a 1:1 focusing so the fixed curvature of the substrate is therefore not likely noteworthy to affect the focusing performance of the final optics. The figure error due to facets is in the range 10–25 $\mu$rad. Assume that a 1:1 focusing mirror with a figure error in this range is positioned 1.5 m away from a 50 $\mu$m source. Due to the figure error the image of the 50 $\mu$m wide source will be smeared out to have the magnitude in the range 80–125 $\mu$m.

5.3.2 The specular reflectivity measurements

The left view-graphs of Figures 5.12 show the results of the reflectometry of substrate #1 and #2. The full lines indicate the Fresnel reflectivity multiplied by the ‘Debye-Waller factor’ $\exp\left(-Q^2 \sigma^2\right)$, where $Q$ is the wave-vector transfer and $\sigma$ is the rms roughness. The magnitude of $\sigma$ is in the range from 4.2 Å to 6.4 Å. The right sides of Figures 5.12 show the specular reflectivity data divided by the Fresnel reflectivity. Since

$$R = R_F e^{-Q^2 \sigma^2},$$
the points ln \( R/R_F \) will fall on a straight line if plotted vs \( Q^2 \), and the slope of that line is \( -\sigma^2 \). Only the data points which are significantly above the background level are used in the data analysis. The results of the fits are shown as full lines. The \( Q^2 \)-range covered by one line indicates the range where the measured data is significantly above the background level.

5.3.3 Summary

The figure error due to facets on the surface reduce the quality of the substrates relative to what is optimal for high-performance X-ray optics. In general the figure error is in the range 10–25 \( \mu \)rad, that is to be compared with the optimal value of a maximum figure error of 3.3 \( \mu \)rad. Flat 1 of substrate #1 is of the lowest quality regarding figure error.

The purpose of the figure error characterization was to clarify whether the focusing performance of the mirrors to be produced would be affected by substrate surface imperfections. The scatter-data show that the main contribution to the substantial figure error is due to facets rather than micro-roughness. Therefore the data-analysis is entirely focussed on the width of the analyzer scans which is related to the population of facets rather than the detailed behavior of the wings of the scans which is related to the micro-roughness. As is described in detail in [36] a surface correlation function can be fitted to the high resolution scattering data in order to derive a detailed information on the micro-roughness.

The surface roughness of substrate #1 is below 5 Å while that of substrate #2 is below 7 Å. The surface roughness of the substrates is acceptable and is not likely noteworthy to affect the Bragg peak intensity of the WC/SiC multi-layer which will be deposited on the substrates.
Figure 5.11: The results of the figure error characterization of two double-side polished substrates. To the left is shown the figure error due to facets on the substrate surface, to the right is shown the shape of the substrates. The shape of the substrates is derived from the angular positions of the analyzer scans, see also Fig. 5.10 right. Note that the required deflection for 1:1 focusing is about 100 $\mu$m.
5.3 The experimental results of the X-ray characterization of the substrates

![Graphs showing reflectivity measurements of substrates #1 and #2.](image)

**Figure 5.12:** The data from reflectivity measurements of the substrates. The value of the rms roughness $\sigma$ has been derived from the linear fits shown to the right.
Chapter 6

Characterization of the multi-layer mirrors for the CLS optics

This chapter describes the characterization of the two mirrors for the CLS optics. The characterization includes

1. an outline of the coating procedure
2. mirrorI and mirrorII: measurement of the specular intensity reflectivity
3. mirrorI: measurement of the longitudinal bi-layer thickness gradient
4. mirrorI: measurements of the width of the focus-line for a wide range of magnification factors and two different source sizes

The two mirrors are produced in the same batch and can therefore be considered nearly identical. This is confirmed by the measurements if the specular intensity reflectivity. For both mirrors at Cu $K_{\alpha}$ radiation the specular intensity reflectivity of the first order Bragg peak is approximately 60% and the Bragg angle is $\alpha_0 \approx 1.46^\circ$. As expected from the mirror design (Sec. 1.2.2), the bandwidth of the mirrors exceeds the bandwidth of the CLS source. As described in Sec. 1.2.2 the total efficiency of the mirrors is strongly dependent on the fraction of the footprint which falls on the mirror. Assuming that the optics is positioned $p = 1.5$ m from the source and the divergence of the source is $\sigma_S = 5.2$ mrad (fwhm) the efficiency of one mirror is estimated by Eq. 1.5,

$$R_{\text{eff},1} = 0.6 \frac{\int_0^{L_M \sin \alpha/2} \sqrt{(p \sigma_S/2)^2 - x^2} \, dx}{\int_0^{p \sigma_S/2} \sqrt{(p \sigma_S/2)^2 - x^2} \, dx} = 0.41.$$ 

The efficiency of the CLS optics with two mirrors is $R_{\text{eff},1}^2$.

6.1 The multi-layer coating

The two multi-layer mirrors for the CLS optics are produced at the magnetron sputtering facility at the Danish National Space Center. Descriptions of the sput-
tering facility, the calibration of the bi-layer thickness and the general multi-layer production procedure are given in Chapter 2. During the multi-layer coating the sputtered material passes through a collimator before it reaches the substrate. The purpose of the collimation is to minimize the surface roughness of the layers, see Chapters 2 and 3 for details.

As described in Sec. 1.2.2 the multi-layers are comprised of WC (40%) and SiC (60%) and the bi-layer thickness $\sim 31$ Å is optimized for an x-ray energy in the range 6–10 keV and a source relative bandwidth of 2%. The amplitude reflectivity of one such bilayer is about 3%, see Eq. 1.3. In Sec. 1.2.1 it is shown that when the amplitude reflectivity is 3% 75 bi-layers is enough to obtain a saturation of the Bragg peak intensity reflectivity. The characterization of the substrates is described in Chapter 5. The collimation of the sputtered material was provided by honeycomb meshes with cell diameters of 6.4 mm and thickness 5 mm. During the sputtering of the multi-layer the coating rate decreases due to wear of the targets, see Chapter 2. To estimate the decrease of the coating rate the calibration of the speed of the sample carrousel included

1. calibration run 1 with 5 samples with 10[WC/SiC] (that is 10 bi-layers consisting of WC and SiC) and different bi-layer thicknesses,

2. one test-coating of a witness sample with 75[WC/SiC] (6 hours),

3. calibration 2 run with 5 samples with 10[WC/SiC] and different bi-layer thicknesses.

In Chapter 2 it is explained how the coating rate is derived from the samples produced in the calibration runs. As expected from Sec. 2.1.6 the coating rate derived from calibration run 2 is smaller than the coating rate derived from calibration run 1. This indicates that the thickness of the first deposited bilayer of the witness sample with 75[WC/SiC] is larger than the thickness of the last deposited bilayer, see Sec. 6.2.

### 6.2 Witness samples

The witness samples are produced prior to the CLS mirrors. Two types of witness samples are produced: one set of samples for the documentation of the longitudinal homogeneity of the bilayer thickness and one sample with a coating similar to the proposed coating for the CLS mirrors. The substrates for the witness samples are commercially available Si wafers with a rms roughness in the range 2.5–2.75 Å.

#### 6.2.1 The longitudinal homogeneity of the bi-layer thickness

The substrate holders in the sputtering chamber are presently being improved in order to gain a better control of the longitudinal homogeneity. At the time the mirrors for the CLS optics were produced the bi-layer thickness variation
could be approximated by a linear gradient of the order of 1–4% over 180 mm. As is described in Sec. 2.1.5 at that time the exact magnitude of the longitudinal gradient was dependent on the actual mounting of the substrates in the sputtering chamber. Fig. 6.1 shows the variation of the bi-layer thickness with vertical the

![Graph showing the variation of bi-layer thickness with vertical position.]

**Figure 6.1:** The variation of the bi-layer thickness vs the vertical position of the substrate in the sputtering chamber. The bi-layer thickness was determined by measurements of the specular intensity reflectivity at DNSC. The experimental setup is described in Sec. 5.2.2.

sample position in the sputtering chamber. In the sputtering chamber the each target material is comprised of two individual pieces. The two pieces are joined at the position corresponding to the height 330 mm. At this height is observed an abrupt increase of the bilayer thickness. It is therefore likely that the increase in bilayer thickness is caused by small differences between the two pieces of material comprising the target. The dashed line is a linear fit to the data points marked by blue circles.

**6.2.2 The specular reflectivity and the relative bandwidth of the first order Bragg reflection**

![Graphs showing the intensity reflectivity.]

**Figure 6.2:** The intensity reflectivity of the test-coating. See text.

Figure 6.2 shows the intensity reflectivity from the test-coating of 75[WC/SiC] measured at DNSC. The experimental setup is described in Sec. 5.2.2. To the left
is shown the data on a semi-logarithmic scale and to the right is zoomed in at the first order Bragg reflection and the data is on a linear scale. On the linear scale it is clear that the peak reflectivity is approximately 0.65 and the width of the peak is 49.6 mdeg. Since the divergence of the beam incident on the sample is 14.8 mdeg (259 µrad) the measured width of the peak corresponds to a bandwidth of
\[
\frac{\Delta E}{E} = \frac{\pi}{180} \sqrt{0.0496^2 - 0.0148^2} \tan 1.479 = 3.2\%.
\]
The measured bandwidth is considerably larger than \(\Delta E/E = 2.2\%\) which is expected from calculations using Parratt’s exact recursive method [8][6]. A broadening of the Bragg peak of this order of magnitude may be caused by a variation of the bi-layer thickness through the multi-layer stack. The results of the calibration runs 1 and 2 give evidence for this hypothesis: the data from the two calibration runs indicate that the coating rate decreases by approximately 3.5% during the 6 hours it takes to produce the 75[WC/SiC] witness sample. Therefore, as a first approximation the bi-layer thickness can be assumed to follow a linear depth gradient of 3.5%. Tab. 6.1 compares the calculated bandwidths and first order Bragg peak intensity reflectivities with the measured results. From these calculations it is clear that a linear depth gradient of -3.5 % cannot account completely for the observed broadening of the Bragg peak. Further studies aiming at a more complete understanding of the observed Bragg peak broadening are presently being conducted at DNSC.

As a cautious attempt to reduce the bandwidth and increase the peak intensity reflectivity, the CLS optics were coated with a depth gradient of -1.5%.

**Table 6.1:** Comparison of calculated and measured bandwidths and peak reflectivities at \(E = 8.05\) keV. The substrate for the test-coating is a commercially available Si wafer with a rms roughness in the range 2.5–2.75 Å. It has been shown [11] that the WC/SiC interface rms roughness is in the same range as the rms roughness of the substrate.

<table>
<thead>
<tr>
<th></th>
<th>(N)</th>
<th>(d) (Å)</th>
<th>(\sigma_{\text{sub}}) (Å)</th>
<th>(\sigma_{\text{ML}}) (Å)</th>
<th>peak (R)</th>
<th>(\Delta E/E) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>calc (0% depth grading)</td>
<td>75</td>
<td>30.8</td>
<td>2.75</td>
<td>2.8</td>
<td>0.74</td>
<td>2.2</td>
</tr>
<tr>
<td>calc (3.5% depth grading)</td>
<td>75</td>
<td>30.8</td>
<td>2.75</td>
<td>2.8</td>
<td>0.70</td>
<td>2.8</td>
</tr>
<tr>
<td>calc (5% depth grading)</td>
<td>75</td>
<td>30.8</td>
<td>2.75</td>
<td>2.8</td>
<td>0.65</td>
<td>2.9</td>
</tr>
<tr>
<td>measured</td>
<td>75</td>
<td>30.8</td>
<td>2.75</td>
<td>2.8</td>
<td>0.65</td>
<td>3.2</td>
</tr>
</tbody>
</table>

### 6.3 The X-ray characterization of the multi-layer mirrors for the CLS optics

For a perfectly focusing mirror without figure error the width of the focus line is given by the product of size of the source with the magnification factor \(M\). \(M\) is the ratio between the distances from the mirror to the focus \((q)\) and from the source to the mirror \((p)\),

\[
\text{fwhm}_{\text{focus}} = M \cdot \text{fwhm}_{\text{source}}, \quad \text{where} \quad M = \frac{q}{p}.
\]
As described in Sec. 1.3 for a given longitudinal bi-layer thickness gradient there is a magnification factor \( M_0 = q/p \) for which the intensity reflected from the mirror (the efficiency) assumes a maximum. In the following it is shown that if the bandwidth of the mirror is small (0.3\%) the efficiency decreases abruptly when \( M \neq M_0 \). If the bandwidth is much larger than this, say 3\% as is the case for the CLS mirrors, the efficiency is nearly constant in a wider range around \( M_0 \). For \( M_0 = 0.8 \) the efficiency is above 80\% for 0.6 < \( M \) < 1.4. The function of the example given in this section is twofold:

1. it illustrates the difference between the efficiency vs \( M \) for narrow and wider bandwidth mirrors,

2. it explains the strategy behind the characterization of the focusing performance of mirror I for the CLS optics.

### 6.3.1 Understanding the performance of a focusing mirror: an example

Assume that a (flat) mirror has a longitudinal bi-layer thickness gradient corresponding to \( M_0 = 0.8 \). The bi-layer thickness \( d \) is so that at wavelength \( \lambda \) the Bragg angle at the mirror center is \( \alpha_0 = \arcsin (\lambda/2/d) = 1.45^\circ \). As shown in Fig. 6.3 left the Bragg angle decreases towards the source and increases towards the focus point. The width of the Bragg reflection is 5 mdeg corresponding to a bandwidth of 0.3\% (10 times smaller than the bandwidth of the CLS optics).

The top of Fig. 6.3 left shows the mirror when it is placed in a mirror bender. The mirror is curved so at each point the glancing angle equals the Bragg angle. This means that each point \( x \) of the mirror gives a maximum contribution \( R(x) \) to the total reflected intensity,

\[
R_{\text{total}} = \sum_x R(x). \tag{6.1}
\]

In the figure, three of the contributions \( R(x) \) are marked by the yellow squares. When the position of the mirror is fixed relative to the source, a given curvature of the mirror corresponds to a given variation of the glancing angles along the length of the mirror. The yellow dashed line in Fig. 6.3 middle shows the variation of the glancing angles for the curvature corresponding to \( M = 0.8 \). The circular points show magnitude of the Bragg angle for three points of the mirror, and as assumed these points lie on the dashed yellow line. The green band and the bars indicate the width of the Bragg reflections.

The black dashed line in Fig. 6.3 middle indicates the variation of the glancing angles for a different curvature of the mirror corresponding to \( M = 0.85 \). At one point, namely at the mirror center, the glancing angle equals the Bragg angle and the contribution to \( R_{\text{total}} \) from this point is maximal. However, since only a small fraction of the line is within the green band which marks the fwhm (0.005\°) of the Bragg peaks, the total reflected intensity from the mirror must be far from maximum. To the left three of the contributions to the total intensity are marked...
74 Characterization of the multi-layer mirrors for the CLS optics

by the circles. Fig. 6.3 right shows the total reflected intensity $R_{\text{total}}$ (Eq. 6.1) vs the magnification factor. The yellow square marks the maximum of $R_{\text{total}}$ (at $M = 0.8$) and the circle marks $R_{\text{total}}$ calculated for $M = 0.85$. If the mirror (by mistake) is rotated by 180° the variation of the total reflected intensity follows the dashed curve. The green curve shows the variation of $R_{\text{total}}$ with the magnification factor if the bandwidth is 3%, the bi-layer thickness has a longitudinal linear gradient of 1.4% and the glancing angle is 1.45°. The curve shows that the efficiency of a multi-layer mirror with a bandwidth of this magnitude is above 80% of the maximum for a broad range of magnification factors $0.6 < M < 1.1$. This is in sharp contrast to the efficiency of a narrow bandwidth multi-layer.

Figure 6.3: A calculated example to illustrate how the total reflected intensity (the efficiency) of a mirror can be estimated given the longitudinal gradient of the bi-layer thickness and the bandwidth of the mirror. The view-graph to the right compares the efficiency vs the magnification factor of two multi-layer mirrors with relative bandwidths of the first order Bragg reflection of 3 % and 0.3 %. See text.

6.3.2 The experimental setups for the measurement of the specular intensity reflectivity, the focussing performance and the bi-layer thickness gradient

The experimental setup at the H. C. Ørsted Institute (HCO) used for the characterization of the focusing performance of mirror I for the CLS optics is shown schematically in Fig. 6.4. The setup is designed so it is possible to imitate the CLS regarding the source size and the divergence of the beam. The scattering plane is horizontal and the approximate dimensions of the X-ray source is 450 µm wide and 360 µm high, see the lower part of Fig. 6.4. The source is a Cu X-ray tube typically running at 20kV, 20mA. The spectrum from the source is comprised of the discrete Cu $K\alpha$ and $K\beta$ lines superimposed on the continuous bremsstrahlung radiation. A 2 mm pinhole (#2) positioned 570 mm from the source limits the divergence of the beam to 3.5 mrad. A Ni filter (#3)
can be inserted in the beam to suppress the Cu Kβ radiation. The input slit (#4) is located 220 mm from the mirror center. The mirror can be aligned vertically by a chi-circle and rotated around a vertical axis which goes through the mirror center. The detector is a Cyberstar point detector with an opening of 30 mm. The transverse position of the detector is controlled by a motor and the detector opening can be limited by a 0.05 mm detector slit (#6).

The CLS source is circular and has a diameter of 50 µm. To imitate the CLS source a 50 µm pinhole can be inserted 7 cm from the source.

**Experimental setup for the measurement of the bi-layer thickness gradient**

The distance from the source to the mirror was $p = 1.2$ m and the distance from the source to the input slit was 0.7 m. The width of the input slit (#4) was 0.2 mm so the beam divergence was limited to 0.20 mrad. With a glancing angle $\alpha$ of approximately $1.45^\circ$ (corresponding to the Bragg angle for the first order reflection) the width of the input slit corresponds to a footprint of length 8 mm. The position of the footprint on the mirror is controlled by a simultaneous translation of the input slit and the source. The Bragg angle is determined by
rotating the mirror around a vertical axis which goes through the center of the mirror. Since the rotation axis of the mirror is fixed, the position $x$ of the footprint is not absolutely constant during a measurement of the Bragg angle (except when the footprint is at the mirror center). As shown in Fig. 6.5 by rotating the mirror the amount $\delta \alpha$ the footprint moves by $\delta x$ where

$$\delta x = x \left( 1 - \frac{\sin \alpha}{\sin (\pi - \alpha - \delta \alpha)} \right).$$

However, since the width of the Bragg reflections is of the order of 50 mdeg and the length of the mirror is 240 mm the maximum movement of the footprint during a measurement is $\pm 2$ mm. The bi-layer thickness gradient is of the order of 1–4% over 180 mm, so the movement of the footprint during the measurement can safely be neglected.

The distance from the mirror to the detector is 0.7 m and the opening of the detector is 30 mm corresponding to an angular acceptance of $2.46^\circ$. Since the angular acceptance is much larger than two times the width of the Bragg reflection it is not necessary to move the detector during the measurements.

![Figure 6.5: Top-view sketch of a beam of X-rays incident on a (vertical) mirror. The red line indicates the X-ray beam and the blue full line indicates the mirror. When the glancing angle is $\alpha$ the beam is incident so the footprint center is at the distance $x$ from the mirror center. By rotating the mirror by the amount $\delta \alpha$ the footprint center moves to the position $x - \delta x$. See text.](image-url)

The specular intensity reflectivity has been measured at the Danish National Space Center. The experimental setup for these measurements is described in Sec. 5.2.2.

### 6.4 The experimental results of the X-ray characterization of the multi-layer mirrors for the CLS optics

#### 6.4.1 The specular intensity reflectivity and the relative bandwidth

The measured specular intensity reflectivities of the mirrors I and II for the CLS optics are shown in Fig. 6.6. The blue curves are calculated using Parratt’s exact recursive method with the parameters given in Tab. 6.2. To the right is shown
The experimental results of the X-ray characterization of the multi-layer mirrors for the CLS optics

![Graphs showing intensity reflectivity of mirrors I and II](image)

**Figure 6.6:** The intensity reflectivity of the mirrors I and II for the CLS optics. The identical blue curves are calculated using Parratt’s exact recursive method with the parameters given in Tab. 6.2.

The first order Bragg reflection on a linear scale. The bandwidth is approximately 2.9% for mirrorI and 2.6% for mirrorII. For both mirrors the intensity reflectivity of the first order Bragg peak is 0.6.

<table>
<thead>
<tr>
<th>$N$</th>
<th>material combination</th>
<th>$d$ (Å)</th>
<th>$\sigma_{\text{sub}}$ (Å)</th>
<th>$\sigma_{\text{ML}}$ (Å)</th>
<th>$E$ (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>75</td>
<td>[WC/SiC]</td>
<td>31.5</td>
<td>4.5</td>
<td>3.0</td>
<td>8.0478</td>
</tr>
</tbody>
</table>

**Table 6.2:** Parameters used for the calculation of the blue reflectivity curves shown in Fig. 6.6.

### 6.4.2 Measurement of the bi-layer thickness longitudinal gradient of mirrorI

The bi-layer thickness gradient has been determined by measuring the angular position of the first order Bragg reflection with the beam incident at different positions along the mirror. Fig. 6.7 shows two measurements of the first order Bragg reflection: one with a Ni filter inserted in the beam and one without the Ni filter and the suppression of the Cu $K\beta$ radiation is evident. The widths and angular positions of the first order Bragg reflections shown in Fig. 6.8 are derived.
from measurements with the Ni filter inserted in the beam. The observed variation of the angular positions is caused by a variation of the bi-layer thickness. The variation can be approximated by a linear gradient of the bi-layer thickness of 1.4%.

### 6.4.3 The focusing performance of mirror I

At the time the characterization of the mirrors took place we had only one mirror bender available. Therefore only one of the two mirrors has been thoroughly characterized regarding the focusing performance. However, since the two mirrors have nearly identical reflecting properties and similar figure error the focusing performance can be assumed to be similar. The bender for mirror II was ready a couple of months after the characterization of mirror I, see Sec. 6.4.4.

The focusing performance of mirror I has been measured for two different source sizes:

1. the full size of the source, that is 450 µm (wide) by 360 µm (high),
2. a 50 µm circular source defined by a pinhole.

For both source sizes the width of the focus line has been determined by scanning the transverse position of the detector. In case 1 the width of the detector slit was 170 µm and in case 2 the width was 50 µm. For a given set of source—mirror distance $p$ and mirror—detector slit distance $q$ the purpose of the measurements was to determine

1. the optimal deflection of the mirror,
2. the optimal glancing angle,
6.4 The experimental results of the X-ray characterization of the multi-layer mirrors for the CLS optics

3. the width of the focus line,

4. the integrated intensity of the focus line.

Given the position of the mirror relative to the source and relative to the detector slit there are only two parameters left to consider: 1) the bender motor position B1 and 2) the glancing angle OM1. For each set \((p, q)\) the width of the focus line was measured as function of these two parameters. Fig. 6.9 shows a contour-plot of the peak intensity vs these two parameters.

![Contour-plot of peak intensity vs B1 position and OM1](image)

**Figure 6.9:** A contour-plot of the peak intensity vs the bender motor position and the glancing angle. The data was measured using the full source size. The black circles mark the data-points and the white circle mark the point of maximum integrated intensity.

Fig. 6.10 shows the results of the characterization using the full source (top) and the source defined by the 50 \(\mu m\) pinhole (bottom). The view-graphs to the left shows the width (black squares) and the integrated intensity of the focus line vs the magnification factor \(M = q/p\). The integrated intensity has been corrected for the transmission in air. The dashed black lines are linear fits to the measured widths of the focus lines whereas the red full lines are guides to the eye. The view-graphs to the right shows the optimal deflection (red squares) and glancing angle (white circles) vs \(M\). The black lines are guides to the eye and the red lines are calculated as

\[
def_{LM} = R \left( 1 - \cos \frac{L_M}{2R} \right),
\]

where \(R\) is the optimal radius of curvature,

\[
R = 2 \frac{1}{\alpha_0 \frac{1}{p} + \frac{1}{q}}.
\]

and \(\alpha_0\) is the glancing angle at the middle of the mirror. The above equations are explained in Sec. 1.3.1.
Figure 6.10: The results of the characterization of the focusing performance of mirror I. See text.

Figure 6.11: Mirror II focusing at $M = 0.88$. Left: a contour plot of the peak intensity vs the bender motor position and glancing angle. The data points are marked by circles and the white circle marks the optimal bender motor position and glancing angle. Right: a detector scan of the focus-line at the optimal bender motor position and glancing angle.

6.4.4 M=0.88 focusing of mirror II

The bender for mirror II was constructed a couple of months after the ending of the characterization of mirror I and only one month before the finishing of this
thesis. Therefore a full characterization of the focusing performance of mirrorII has not been conducted. Fig. 6.11 shows the results of the characterization of the $M = 0.88$ focusing of mirrorII with a source size of 50 µm. At the optimal bender motor position and glancing angle the measured width of the focus-line is (97 µm). The width of the detector slit was 50 µm so the measured width corresponds to an intrinsic width of 83 µm.

6.5 Discussion

6.5.1 Bandwidth and Bragg peak intensity reflectivity

The measured relative bandwidth of the first order Bragg reflection is larger than expected from the theory and the peak specular intensity reflectivity is smaller. One contribution to the peak broadening is identified and can be compensated for in the future production of multi-layers:
during the 6 hours it takes to sputter the 75 bilayers of the multi-layer the coating rate decreases by approximately 3%, and this leads directly to a decrease of the bilayer thickness of the same magnitude, corresponding to a positive bilayer thickness depth gradient. A depth gradient of the bilayer thickness leads to both a broadening of the multi-layer Bragg peaks and a decrease of the peak specular intensity reflectivity. The decrease of the coating rate is caused by the continuous erosion of the targets and can be compensated for: as explained in Chapter 2 the bilayer thickness is controlled by the speed of the sample carrousel relative to the targets. By slowing down the carrousel speed during the sputtering the bilayer thickness can be kept constant throughout the coating process. However, this method requires a thorough knowledge about exactly how much the coating decreases rate as function of the elapsed coating time and further studies are necessary in order to solve the problem completely.

| Table 6.3: Comparison of the calculated and the measured bandwidths and peak reflectivities at $E = 8.05$ keV. |
|-----------------|-------|-------|-------|-------|-------|-------|
|                 | $N$   | $d$ (Å) | $\sigma_{\text{sub}}$ (Å) | $\sigma_{\text{ML}}$ (Å) | peak $R$ | $\Delta E/E$ (%) |
| calc (0% depth grading) | 75    | 31.5   | 5.9   | 3     | 0.73   | 2.2   |
| calc (2% depth grading)  | 75    | 31.5   | 5.9   | 3     | 0.72   | 2.3   |
| calc (3% depth grading)  | 75    | 31.5   | 5.9   | 3     | 0.70   | 2.6   |
| calc (6% depth grading)  | 75    | 31.5   | 5.9   | 3     | 0.60   | 3.1   |
| measured             | 75    | 31.5   | 5.9   | 3     | 0.60   | 2.6   |

By comparing the measured relative bandwidths and Bragg peak specular intensity reflectivities with the calculated values tabulated in Tab. 6.3 it is clear that the depth gradient of the bi-layer thickness cannot fully explain the observed peak broadening. Taking only the first order peak into account, at a first glance the relative bandwidth can be explained by a linear depth gradient of the order of 3%. However, a comparison of the complete specular intensity reflectivity data-set with
the calculated reflectivity with a 3% depth gradient shows that the measured specular intensity of the 4th order Bragg reflection is one order of magnitude above the calculated reflectivity, see Fig. 6.12. Therefore further studies are necessary in order to gain a full control of the bandwidth of the multi-layers to be produced in the future.

![Figure 6.12: The red curve shows the measured specular intensity reflectivity of mirrorII. The blue curve is calculated using Parratt’s exact recursive method. The bilayer thickness gradient is 3%, the remaining parameters for the calculation are given in Tab. 6.3](image)

### 6.5.2 The focusing performance

For a perfect mirror without any figure error the width of the focus line is given by the product of the source size and the magnification factor,

\[
\text{fwhm}_{\text{focus}} = M \cdot \text{fwhm}_{\text{source}}, \quad \text{where} \quad M = q/p.
\] (6.2)

The width of the focus-line has been measured vs the magnification factor for two different source sizes, \(\sim 450 \, \mu m\) and \(50 \, \mu m\). As expected from Eq. 6.2 the width of the focus-line is directly proportional to the magnification factor, and the constant of proportionality is the apparent source size. The influence of the figure error on the focusing performance is clearly seen in the data measured with the 50 \(\mu m\) source. With the mirror positioned the distance \(p = 1.43 \, m\) from the 50 \(\mu m\) source the measured apparent source size is \(\text{fwhm}_{\text{source}}^{\text{apparent}} = 100 \, \mu m\). The total figure error can be estimated to about 30 \(\mu rad\) by

\[
\sqrt{(\text{fwhm}_{\text{source}}^{\text{apparent}})^2 - (\text{fwhm}_{\text{source}})^2} / 2p.
\]

This magnitude of the figure error is in accordance with the results of the characterization of the substrates and the characterization of the performance of the bender.
Figure 6.13: *Left:* the angular position (MIDP) and fwhm of the first order Bragg reflection of mirror I vs the position of the footprint center. The variation of the angular position corresponds approximately to a longitudinal linear bilayer thickness gradient of 1.4% over 180 mm.

*Right:* comparison of the measured and calculated efficiency vs the magnification factor. See text.

### 6.5.3 The efficiency vs the magnification factor

The mirror efficiency vs $M$ has its maximum about $M = 1$. As expected from the example given in Sec. 6.3.1 the mirror efficiency is above 80% of its maximal value for $0.6 < M < 1.5$. Unfortunately the space available in the laboratory did not allow the measurement of the efficiency for $M > 1.5$. Fig. 6.13 *right* compares the measured efficiency with the calculated efficiency. The blue, the green and the red curves are calculated estimates of the efficiency. The shown calculations are based upon the principles explained in Sec. 6.3.1 but now the information on the actual bilayer thickness variation (Fig. 6.13 *left*) is included in the calculations.

The blue and green curves assumes that the glancing angle at the mirror center $\alpha_0$ is the same for all magnification factors. However, as is shown in Fig. 6.10 *left* this is not the case. The dashed red curve is calculated with the assumption that the glancing angle at the mirror center varies with the magnification factor according to the full black line in Fig. 6.10 *left*. 
Chapter 7

Conclusion

The purpose of this project has been to develop and characterize a focusing element for the Compact Light Source (CLS), a miniature synchrotron light source developed by Lyncean Technologies Inc. [1]. At present it is expected that the Compact Light Source will be installed at the University of Copenhagen during the year 2008 and that this new machine will serve users from many different fields of science, i.e. physics, (bio-)nano-science, medicine, chemistry, geology, . . . . The focusing element has been designed with the expectations about the arrival of many different users – with many different requirements to the experimental set-up – in mind. This means that we have made an effort to make the optical element both a flexible and a user-friendly tool.

The optical element is based upon two multi-layer mirrors positioned in a classic Kirkpatrick-Baez geometry. The focusing properties of the element depend on the nature of the multilayer coatings and the magnitude of the mirror curvature. For each mirror the magnitude of the curvature is controlled by a motorized mirror bender developed in close collaboration with the Danish company JJ-XRAY [2]. At present only one stripe of multilayer designed for 1:1 focusing ($M = 1$) is deposited on the middle of each substrate. However, since the deflection of each mirror can be closely controlled by the motorized bender, the efficiency of the mirrors is above 80% of its maximum value for magnification factors $M$ in the range $0.6 < M < 1.5$. In addition to the multilayer stripes already deposited on the substrates, the substrate dimensions and the design of the mirror benders allow us in the future to deposit and utilize two other stripes of multilayer on each substrate. With three stripes of multilayers on each substrate combined with the flexibility offered by the mirror bender, the optical element can comply with the demands of a great many different experiments.

With the present design of the mirror benders, the 4 mm thick Si substrate can be bent to a radius of curvature in the range from 20 m to 70 m and the deflection of the substrate can be adjusted with a precision which is better than 0.01 $\mu$m. The profile shape of the bent substrate is well described by the Bernoulli-Euler beam theory. It has been shown that the central part of the mirror has the shape of a parabola, a shape which does not deviate noteworthy from the ellipsoid shape which is ideal for $M \sim 1$ focusing: the figure error is below 1 $\mu$rad. The
characterization of the bender performance indicated that a correct mounting of the mirror in the mirror bender is essential to obtain the nearly perfect shape of the mirror profile.

The multilayer coatings for the CLS optics are produced at the sputtering facility of the Danish National Space Center. Until recently the sputtering facility has primarily been utilized in a collaboration with NASA on the mass production of curved multilayer mirrors for X-ray telescopes. These mirrors have a radius of curvature ranging from 40 mm to 120 mm.

During this project one of the major challenges has been to qualify the sputtering facility to the production of longer (240 mm) flat mirrors with a homogeneous bilayer thickness and a low rms interface roughness. The keystone of this qualification was the development of a new kind of collimation of the sputtered particles. Further we have developed the principles behind a simple method to produce multilayer mirrors with a bilayer thickness gradient along the length of the mirror.

The calculations presented here regarding the collimation of the sputtered particles strongly motivate further work on this subject. We have observed a dramatically increase of the interface width with a decreasing degree of collimation of the sputtered particles. A combined AFM/STM and x-ray study of both single- and multi-layer samples may reveal the mechanism behind the observed growth of the interface width. An obvious path to follow would be to measure and analyze both the specular and the off-specular x-ray intensity reflectivity and in this way derive the relative magnitudes of the diffuseness and the real roughness. Further, the correlation function of the of the interface roughness profile can be reconstructed from the off-specular x-ray intensity reflectivity. A correlation of the results of a AFM/STM study with the information from the roughness correlation function may lead to a thorough understanding of the nature of the interface width.
Bibliography


[23] Pia Redanz. Private communication.


Appendix A

Crystal bender solution

The solution to the differential equation Eq. 4.1 is solved by imposing the boundary conditions that both \( y(x) \) and \( dy/dx \) are continuous functions and \( y((-L_M + l)/2) = y((L_M + l)/2) = 0 \), that is at the points of support. The full solution is

\[
\begin{align*}
\frac{dy_1}{dx} &= \frac{1}{EI} \left( \frac{M_A (x^2 + (L_M + l) x)}{l} + C_{11} \right) \\
y_1 &= \frac{1}{EI} \left( \frac{M_A (x^3 + (L_M + l) x^2)}{2} + C_{11} x + C_{12} \right) \\
\frac{dy_2}{dx} &= \frac{1}{EI} \left( \frac{(M_B - M_A) x^2}{2 L_M} + \frac{(M_B + M_A) x}{2} + C_{21} \right) \\
y_2 &= \frac{1}{EI} \left( \frac{(M_B - M_A) x^3}{6 L_M} + \frac{(M_B + M_A) x^2}{4} + C_{21} x + C_{22} \right) \\
\frac{dy_3}{dx} &= \frac{1}{EI} \left( \frac{M_B (-x^2 + (L_M + l) x)}{l} + C_{31} \right) \\
y_3 &= \frac{1}{EI} \left( \frac{M_B (-x^3 + (L_M + l) x^2)}{2 l} + C_{31} x + C_{32} \right)
\end{align*}
\]

(A.1)

where the the constants are

\[
\begin{align*}
C_{31} &= \frac{-l^2 M_B + l^2 M_A + 2 M_A L_M l - 2 L_M l M_B - 3 M_B L_M^2}{12 l} \\
C_{32} &= \frac{-3 M_B L_M l^2 + 2 M_A L_M l^2 + 2 L_M^2 l M_A + L_M^2 l M_B - M_B L_M^3 + M_B l^3 + M_A l^3}{24 l} \\
C_{21} &= \frac{-M_A L_M^2 - \frac{L_M l M_B}{8} - \frac{M_A L_M l}{8} - \frac{M_B L_M^3}{16} - \frac{l^2 M_B}{24} - \frac{l^2 M_A}{24}}{24 l} \\
C_{12} &= \frac{-3 M_B L_M l^2 + 2 M_A L_M l^2 + L_M^2 l M_A + 2 L_M^2 l M_B + M_B l^3 + M_A l^3 - M_A L_M^3}{24 l} \\
C_{22} &= \frac{-M_B L_M}{24} + \frac{M_A L_M}{24} - \frac{M_B l}{12} + \frac{l M_A}{12} \\
C_{11} &= \frac{3 M_A L_M^2 - l^2 M_B + l^2 M_A + 2 M_A L_M l - 2 L_M l M_B}{12 l}.
\end{align*}
\]

(A.2)

For the actual benders the values of \( L_M \) and \( l \) is given in Tab. 4.1.
Appendix B

Exact determination of the bilayer thickness gradient and the mirror curvature

B.1 Focusing by an elliptical mirror

The coordinates \((x, y)\) of the ellipse (Fig. B.1) are described by the equations
\[
x = a \cos t \quad \text{and} \quad y = b \sin t.
\]
The coordinates of the unit tangent vector \(T(t) = [x_T(t), y_T(t)]\) of the ellipse so parameterized are
\[
x_T(t) = \frac{-a \sin t}{\sqrt{(b \cos t)^2 + (a \sin t)^2}} \quad \text{and} \quad y_T(t) = \frac{b \cos t}{\sqrt{(b \cos t)^2 + (a \sin t)^2}}.
\]
The foci of the ellipse are at \((\pm c, 0)\) where \(c = \sqrt{a^2 - b^2}\). The source is located at the focus \((-c, 0)\) and the image is at the point \((c, 0)\). The vector from the source to the point \((x(t), y(t))\) at the ellipse is
\[
R(t) = \left[ \begin{array}{c} x(t) + c \\ y(t) \end{array} \right]
\]
From the dot product of \(R(t)\) and \(T(t)\),
\[
R(t) \cdot T(t) = R(t)T(t) \cos \alpha = (x(t)+c)x_T(t) + y(t)y_T(t) = \frac{-c^2 \cos t \sin t - ac \sin t}{\sqrt{(b \cos t)^2 + (a \sin t)^2}},
\]
the cosine of the glancing angle \(\alpha\) is derived,
\[
\cos \alpha = \frac{-c \sin t}{\sqrt{a^2 - c^2 \cos^2 t}}. \quad \text{(B.1)}
\]
Below the parameters \(a\) and \(c\) are determined in terms of \(p, q\) and \(\alpha_0\). When \(a\) and \(c\) are fixed, the optimal longitudinal bilayer gradient can be calculated from Eq. B.1.
In the case of 1:1 focusing (that is $q = p$), the determination of $a$ and $b$ is trivial, since then $a = p$ and $b = a \sin \alpha_0$. In the following is shown how to determine $a$ and $b$ uniquely and exactly from the source—mirror distance, the energy and the multi-layer $d$-spacing in general, where the magnification factor $M = q/p$ may be different from 1. In the end it is shown that the expressions simplifies significantly when $b \ll a$, which is the case when the glancing angle is of the order of $1^\circ$.

Assume that the central ray is incident at the $x$-coordinate $x_0 = a \cos t_0$. Then the distances $p$ and $q$ can be expressed in terms of $\cos t_0$ by

$$p = \sqrt{(a \cos t_0 + c)^2 + (b \sin t_0)^2} \quad \text{and} \quad q = \sqrt{(a \cos t_0 - c)^2 + (b \sin t_0)^2}.$$  

The above equations can be solved for $\cos t_0$ to yield

$$\cos t_0 = \frac{-a + p}{c} = \frac{a - q}{c}, \quad (B.2)$$

from which an expression for $\cos t_0$ is obtained in terms of the magnification factor,

$$\cos t_0 = \frac{(1 - M) a}{(1 + M) c}. \quad (B.3)$$

The next step is to eliminate the apparent dependency of $\cos t_0$ on $a$ and $b$. To do so, insert in Eq. B.3 the following expression for $c$ obtained from Eq. B.1,

$$c = \frac{a \cos \alpha_0}{\sqrt{1 - \cos^2 t_0 + \cos^2 \alpha_0 \cos^2 t_0}}, \quad (B.4)$$

to yield

$$\cos t_0 = \frac{1 - M}{\sqrt{1 - 2M + M^2 + 4M \cos \alpha_0^2}}. \quad (B.5)$$
The equations Eq. B.2 and Eq. B.4 fix the parameter $a$ in terms of $t_0$ and $\alpha_0$,

$$a = \frac{p \sqrt{1 - \cos^2 t_0 + \cos^2 \alpha_0 \cos^2 \alpha_0 \cos^2 t_0}}{\cos t_0 \cos \alpha_0 + \sqrt{1 - \cos^2 t_0 + \cos^2 \alpha_0 \cos^2 \alpha_0 \cos^2 t_0}}. \quad (B.6)$$

The equations Eq. B.4, Eq. B.5 and Eq. B.6 determines the shape of an elliptical mirror for a given choice of source—mirror distance, energy, magnification factor and multi-layer bilayer thickness.

**The case $b \ll a$**

When $b \ll a$, or equivalently $c \approx a$ the following approximations are valid:

$$\cos t_0 \approx \frac{1 - M}{1 + M} \quad \text{and} \quad p \approx a(1 + \cos t_0) \approx a \left(1 + \frac{1 - M}{1 + M}\right) = \frac{2a}{1 + M}, \quad (B.7)$$

from which we get

$$a \approx (1 + M) \frac{p}{2}. \quad (B.8)$$

### B.2 Collimating by a parabolic curved mirror

The coordinates $(x, y)$ of the parabola is described by the equations

$$x = a t^2 \quad \text{and} \quad y = 2at.$$

The unit tangent vector $T(t) = [x_T(t), y_T(t)]$ of the parabola so parameterized is

$$x_T(t) = \frac{t}{\sqrt{1 + t^2}} \quad \text{and} \quad y_T(t) = \frac{1}{\sqrt{1 + t^2}}.$$
The source $S$ is located at the focus of the parabola $(a, 0)$. The vector from $S$ to the point $(x(t), y(t))$ of the parabola is

$$R(t) = \begin{bmatrix} x(t) - a \\ y(t) \end{bmatrix}$$

From the dot product of $R(t)$ and $T(t)$ we derive the cosine of $\alpha$,

$$\cos \alpha = \frac{t}{\sqrt{1 + t^2}}. \quad (B.9)$$

**Parabolic mirror design: determination of the parabola parameters**

Assume that the central ray is incident at the $x$-coordinate $x_0 = a t_0^2$. Then the source—mirror distance $p$ can be expressed in terms of $t_0$ by

$$p = a(a t_0^2 + 1) \quad \text{which implies} \quad a = \frac{p}{1 + t_0^2}.$$  

From Eq. B.9 we get $t_0$ in terms of the glancing angle $\alpha_0$,

$$t_0 = \frac{\cos \alpha_0}{\sqrt{1 - \cos^2 \alpha_0}}. \quad (B.10)$$

These two equations determine $a$,

$$a = p \sin^2 \alpha_0. \quad (B.11)$$

The magnitude of the longitudinal gradient is independent of the energy:

$$\frac{\Delta d}{d_0} = \sqrt{1 + \frac{L}{2p}} - \sqrt{1 - \frac{L}{2p}} \quad (B.12)$$
Appendix C

Computer code

C.1 The ellipse calculations

Below follows the Matlab function used for the ellipse calculations in Sec. 1.3:

```matlab
function [x, y, X, Ang, def, xC, yC, a, b, c] = EllipseDeflection(L, M, p, alphaC);
% Input
% L The mirror length (m)
% M The magnification factor q/p
% p The source-mirror distance (m)
% alphaC The grazing angle [°]

t = -pi; 0.0001:pi;
ccst0 = (1 - M) / sqrt(1 - M^2);
a = p * sqrt(1 - ccst0^2 + (cos(alphaC)^2) / (ccst0^2 + (cos(alphaC)^2)));
ccsatpha = -c * sin(t) / sqrt((a - c)^2 + (c * cos(t))^2);
alpha = acos(ccsatpha);
b = sqrt(a^2 - c^2);
x = a * cos(t); y = b * sin(t);

% Calculation of the deflection:
x1 = x(ind(1)); y1 = y(ind(1));
x2 = x(ind(length(ind))); y2 = y(ind(length(ind)));
A = (x2^2 - x1^2) / (y2^2 - y1^2);
Ahat = [-A(2) A(1)];
Tp = (y2 - y1 + y2 - y1) * x2 - x1 / (y2 - y1) / ((x2 - x1)^2 + (y2 - y1)^2);
T = (x2 - x1) * Tp / (x2 - x1);
def = norm(Tp * Ahat) / pi;
```

97