Geometry calculations for the monochromator and double mirror system for the Materials Science upgrade

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Abstract

A step-by-step account is presented describing the calculations for the new monochromator/mirror configuration for the upgrade of the Materials Science beamline of the Swiss Light Source.

OVERVIEW

The upgrade of the Materials Science beamline involves replacing the present wiggler with a cryogenically-cooled permanent-magnet undulator (period 14 mm, called 'U14'). This also requires the x-ray optics to be changed. The new optics consist of a double-crystal monochromator (to be manufactured by Cinel, Padova) and downstream from this a double-mirror system manufactured by PSI. The beamline will provide photons between 5 keV and 40 keV. The lower energy limit of 5 keV might not be achievable, depending on possible collision problems between X1 and X2. However, it is important that we can access at least the Mn K-edge marginally above 6.5 keV. A schematic of the optics is given in Fig. 1.

The first Si(111) crystal X1 is cryogenically cooled using liquid nitrogen, while the second Si-crystal X2 is at room temperature and can be sagittally bent to achieve horizontal focussing of the beam. Because the two crystals are at different temperatures ($\Delta T \approx 200$ K), they also have marginally different Bragg angles, due to the thermal contraction of silicon in X1.

In order to maintain a constant height (+20 mm relative to the incoming beam) and horizontality of the beam after it exits the mirror chamber for all photon energies, the second crystal must be translated both vertically (y) and horizontally (z), while the first mirror M1 must be translated vertically. In addition, the mirror angles depend on the photon energy, and are adjusted to minimize harmonic content. Both mirrors have three regions: bare silicon, Rh-coating, and Pt-coating. The first mirror is kept flat, while the second mirror M2 can be bent to provide vertical focussing.

THE DIFFERENCE IN BRAGG ANGLES BETWEEN X1 AND X2

The thermal expansion coefficient of silicon changes almost linearly between 11 and 300 K such that

$$\frac{\Delta l}{l} = -2.55 \times 10^{-4} \tag{1}$$

as one cools from 300 to 100 K.

We let the Bragg angle at 300 K be θ for the room-temperature X2, and that for the same photon energy for X1 be $\theta + \delta$. From Bragg's law

$$d[1 - (\Delta l/l)] \sin(\theta + \delta) = d \sin\theta. \tag{2}$$

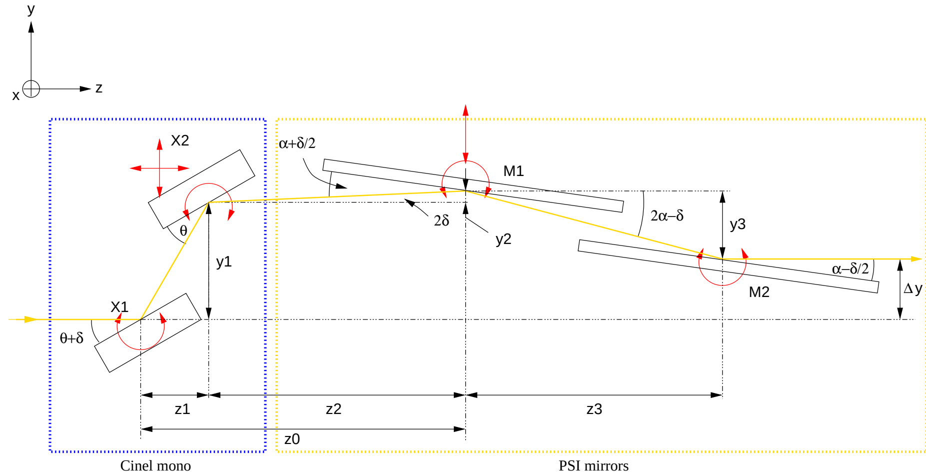

FIG. 1: Schematic figure of the optics setup. Movements required of each of the four components (X1, X2, M1, and M2) when changing the energy are shown with red arrows. Movements required for adjustment purposes are not shown. After exiting the mirror chamber, the x-ray beam has a vertical offset of +20 mm.

But $\sin(A+B) = \sin A \cos B + \cos A \sin B$ and hence

$$[1-(\Delta l/l)](\sin\theta\cos\delta + \cos\theta\sin\delta) = \sin\theta. \tag{3}$$

But $\delta \ll 1$ and hence $\cos\delta \approx 1$ and $\sin\delta \approx \delta$, so that

$$[1-(\Delta l/l)](\sin\theta + \cos\theta\delta) = \sin\theta, \tag{4}$$

$$\Rightarrow \sin\theta - (\Delta l/l)\sin\theta + \delta\cos\theta - \delta\cos\theta(\Delta l/l) = \sin\theta, \tag{5}$$

$$\Rightarrow \delta = (\Delta l/l)\tan\theta = 2.55\times 10^{-4}\tan\theta \tag{6}$$

in radians.

The consequence of this is that the beam is tilted upwards by an angle 2δ after X2 (see Fig. 1). This is compensated by tilting the first mirror to an angle of $\alpha+\delta/2$ relative to the beam and the second mirror to $\alpha-\delta/2$, so that the exiting beam is again horizontal. Note that $\delta/2\alpha \sim 0.01$ and hence this readjustment has no significant effect on the reflectivity of the mirrors.

MIRROR DENSITIES

The critical angle for total external reflection, α_c, is inversely proportional to the photon energy, and is proportional to the square-root of the electron density. The actual densities of the Rh- and Pt-coatings are marginally less than for bulk material, and are 12.0 g/cm^3 (96.8 % dense, 3.142 e/Å^3)

and 20.3 g/cm^3 (94.9 % dense, 4.86 e/Å^3), respectively. We want to tilt the mirrors to close to the critical angle in order to suppress the harmonic components as much as possible. However, we should avoid getting to close to α_c, as we begin to lose the reflectivity. We therefore chose a value of 85 % of the critical angle. We express this set angle in convenient units as

$$\alpha_{\mathrm{set}} = \frac{1.80863\sqrt{\rho}}{E}, \tag{7}$$

where α_{set} is in degrees, ρ is in e/Å^3, and the photon energy E is in keV. This yields

$$\alpha_{\mathrm{set}}^{\mathrm{Si}} = \frac{1.5078}{E}; \tag{8}$$

$$\alpha_{\mathrm{set}}^{\mathrm{Rh}} = \frac{3.2059}{E}; \tag{9}$$

$$\alpha_{\mathrm{set}}^{\mathrm{Pt}} = \frac{3.9872}{E}. \tag{10}$$

CALCULATING THE CRYSTAL AND MIRROR ANGLES AND POSITIONS

Referring back to Fig. 1, we see there are some constants to the proposed geometry. These are

- The vertical offset of the beam $\Delta y = y1 + y2 - y3 = +20$ mm
- The horizontal distance between the centers of M1 and M2, $z3 = 700$ mm
- The horizontal distance between the centers of X1 and M1, $z0 = z1 + z2 = 1350$ mm

This last constant $z0$ is provisional, and might be changed according to the space requirements of other components.

We now determine expressions for the positions and angles of the four optical components.

First, the Bragg angle of X2 is simply

$$\theta = \arcsin\left(\frac{1.977066}{E\,[\mathrm{keV}]}\right). \tag{11}$$

From Fig. 1,

$$\frac{y1}{z1} = \tan(2\theta + 2\delta), \tag{12}$$

$$\frac{y2}{z2} = \frac{y2}{z0 - z1} = \tan 2\delta, \tag{13}$$

$$\frac{y3}{z3} = \tan(2\alpha - \delta). \tag{14}$$

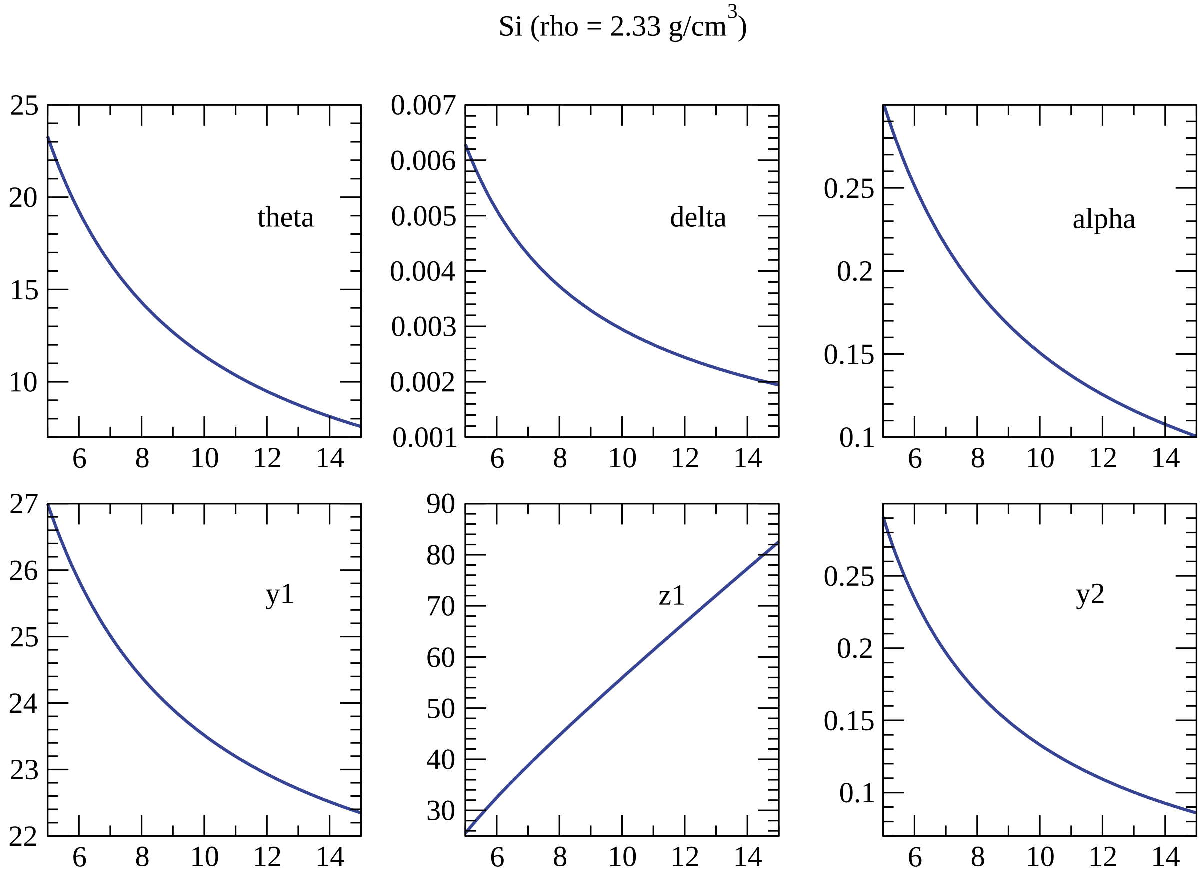

FIG. 2: Optics geometry when using the Si-stripe of the mirrors. The energy region of interest is 5 to 10 keV.

Remembering that $\Delta y = y1 + y2 - y3$, we immediately obtain

$$\begin{aligned}
\Delta y &= z1\tan(2\theta+2\delta) + (z0 - z1)\tan 2\delta - z3\tan(2\alpha-\delta) && (15)\\
&= z1\left[\tan(2\theta+2\delta) - \tan 2\delta\right] + z0\tan 2\delta - z3\tan(2\alpha-\delta) && (16)\\
\Rightarrow z1 &= \frac{\Delta y - z0\tan 2\delta + z3\tan(2\alpha-\delta)}{\left[\tan(2\theta+2\delta)-\tan 2\delta\right]}. && (17)
\end{aligned}$$

From this, we directly obtain $z2 = z0 - z1$, from which $y1$, $y2$, and $y3$ follow.

The crystal and mirror positions as a function of photon energy for the three mirror coatings are given in Figs. 2 to 4 with the coating densities given above, a beam offset of +20 mm, $z0 =$ 1350 mm, and $z3 = 700$ mm. I have also written a small MATLAB program for calculating these values for different setups.

Within the energy regions of interest, one can establish the rquired range of movements of the different movements. These are given in the table below.

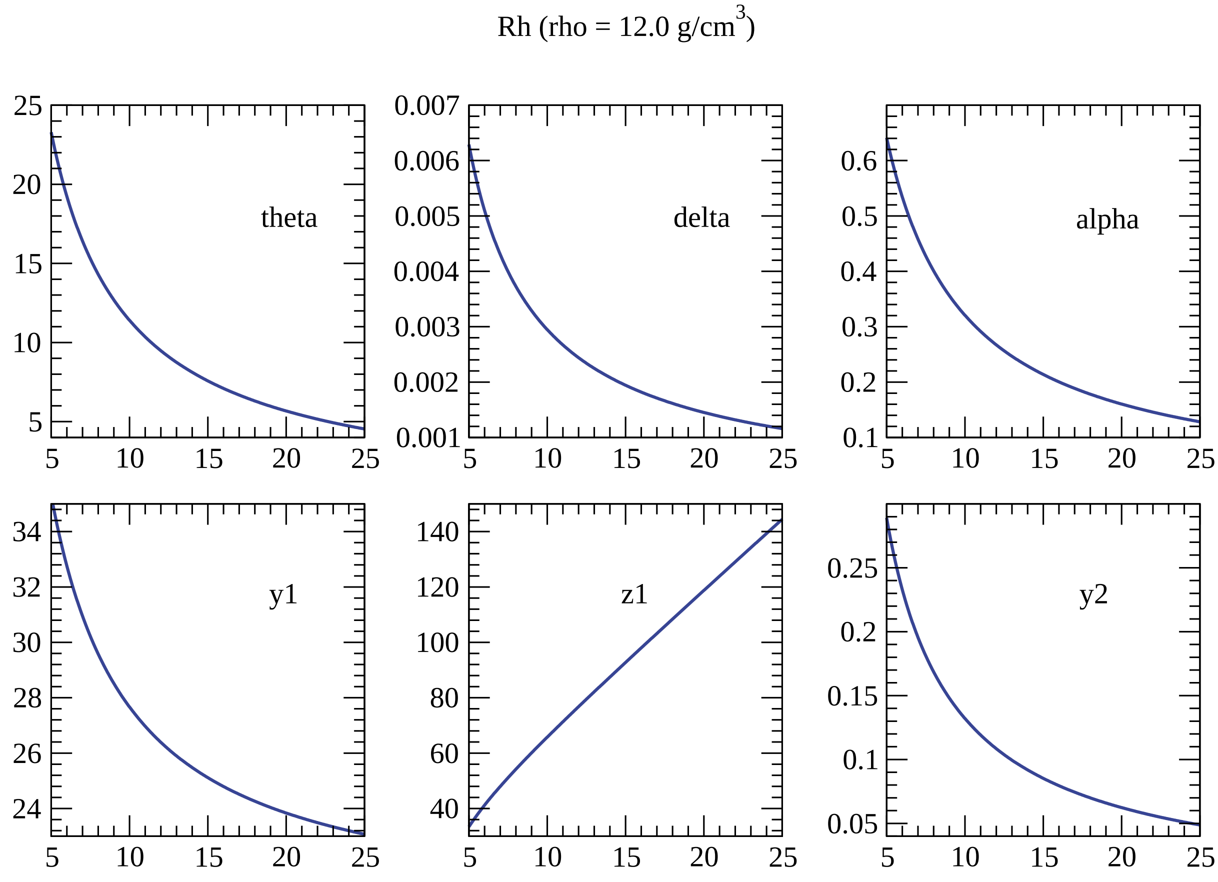

FIG. 3: Optics geometry when using the Rh-stripe of the mirrors. The energy region of interest is 5 to 20 keV.

Movement	Range
θ [degrees]	0 – 24
δ [degrees]	0 – 0.007
α [degrees]	0 – 0.7
$y1$ [mm]	20 – 35
$z1$ [mm]	25 – 225
$y2$ [mm]	0 – 0.3

TABLE I: Range of motions of the optics.

Of particular importance in the above table are the ranges for $theta$, $y1$, and $z1$ as these must be considered in the Cinel design. The reason for having a minimum angle for θ of 0 degrees is for alignment purposes and to allow the beam to pass uninterrupted when in pink beam mode. The

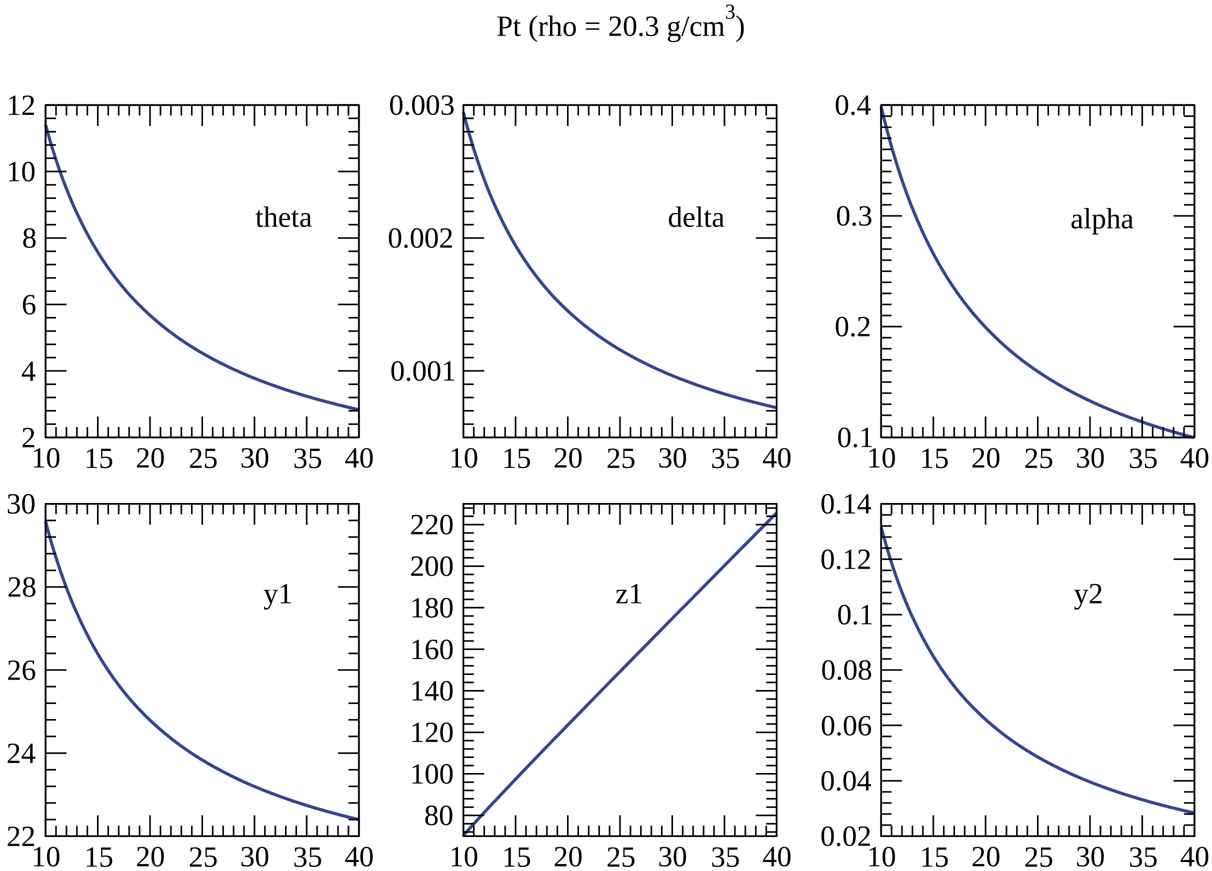

FIG. 4: Optics geometry when using the Pt-stripe of the mirrors. The energy region of interest is 10 to 40 keV.

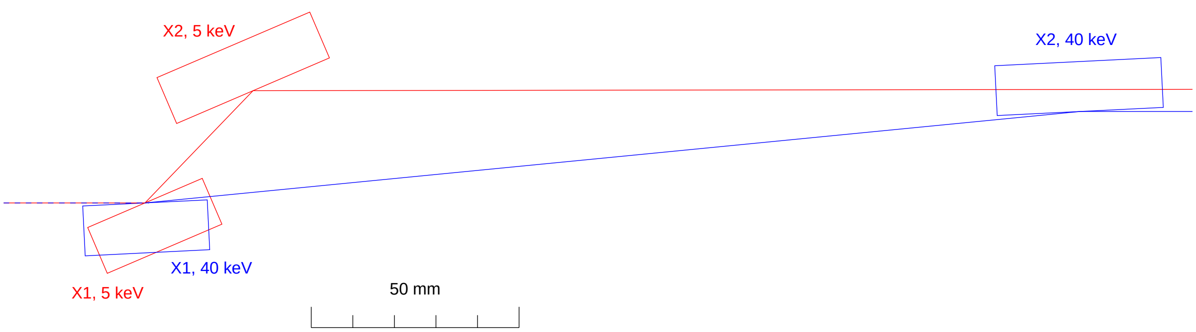

FIG. 5: The positions of X1 and X2 at 5 and 40 keV, using the Si and Pt-stripes on the mirrors, respectively.

positions at the lowest (5 keV, using Si reflection on the mirrors) and highest (40 keV, using Pt) are given in Fig. 5.

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