Design options for multilayer mirrors for higher harmonics suppression

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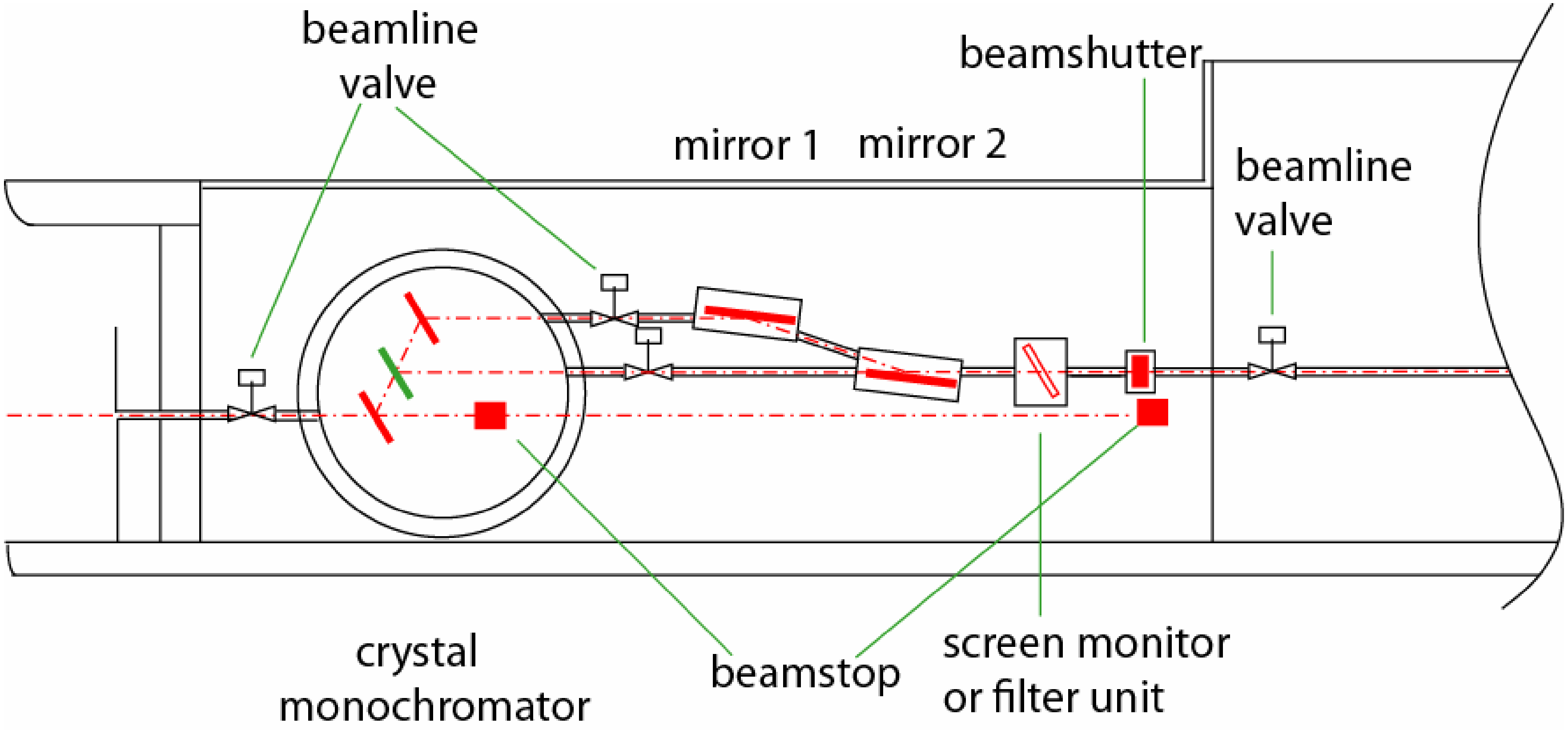
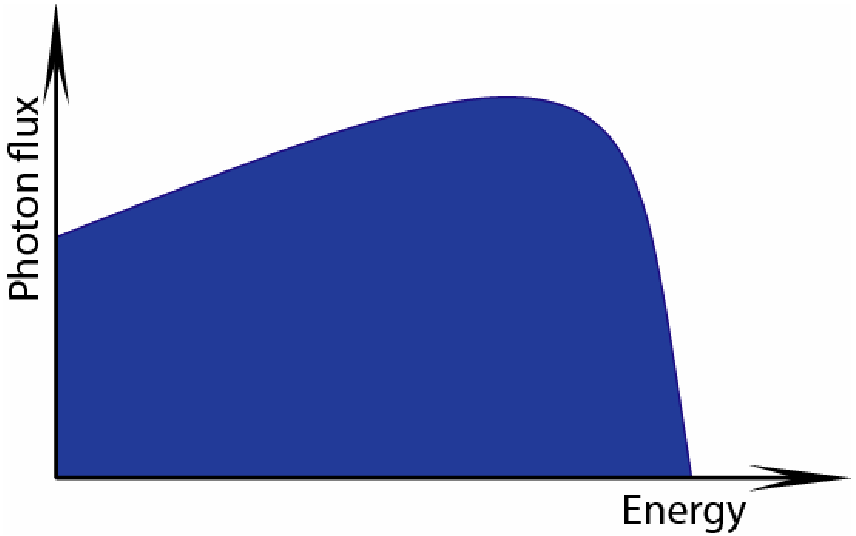
High resolution beamline at PETRA III:



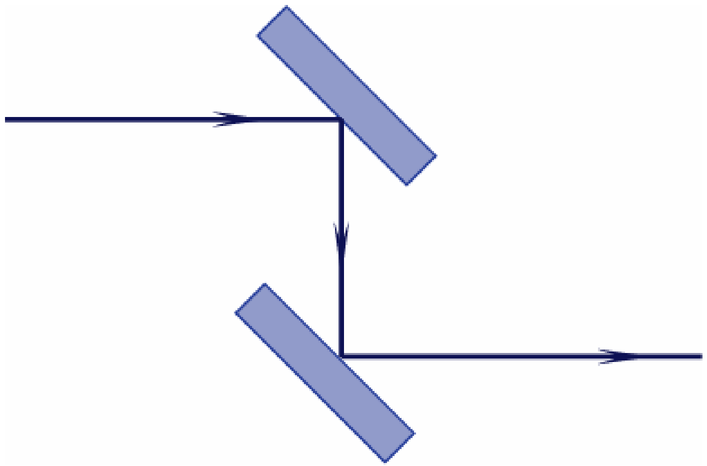
1. Suggest materials for mirror coating for higher harmonics suppression
2. Suggest how to move mirrors while tuning angles

What are higher order harmonics?

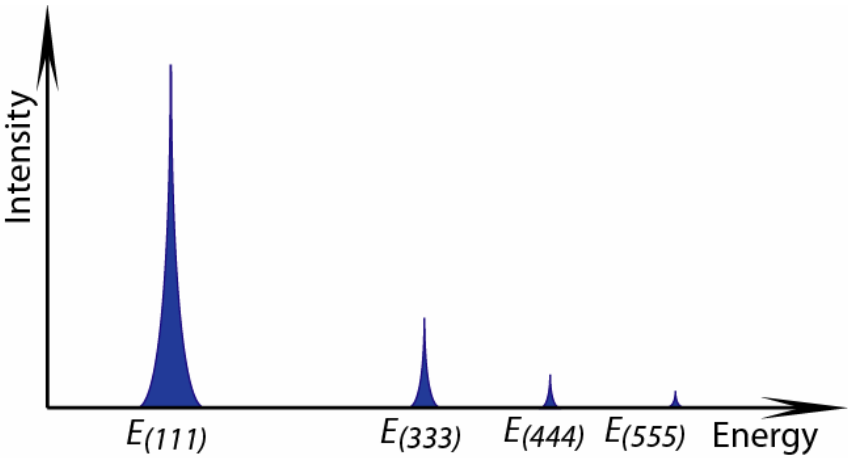
Primary beam spectrum:



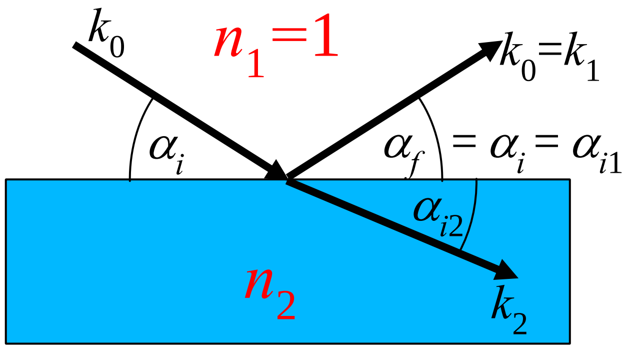
Double crystal Si(111) monochromator:
Two silicon single crystals oriented
to give Bragg reflection from (111) plane



In reflected beam also reflections from (333), (444), (555), *etc.* planes are presented:



Cutting higher harmonics by X-ray critical angle mirrors



For X-rays refractive index $n = 1 - \delta + i\beta$

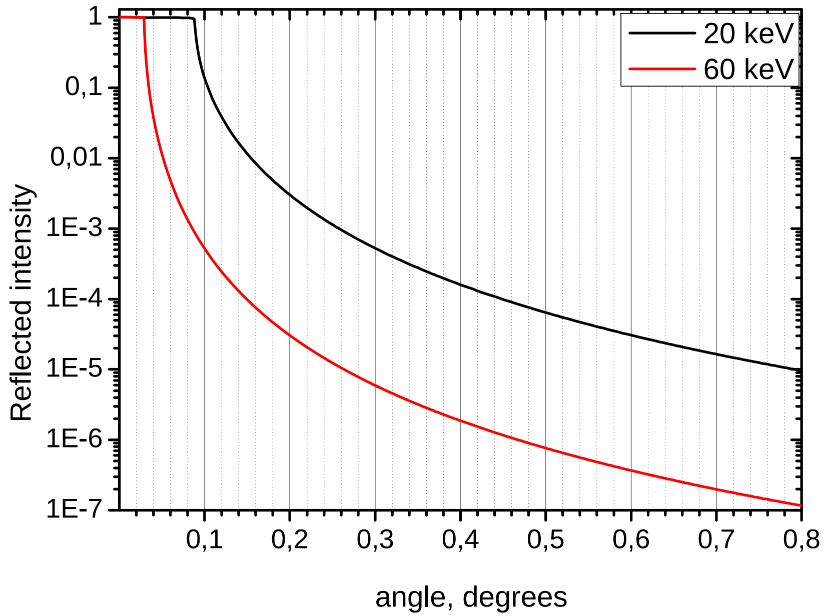
where $\delta \propto \lambda^2 \rho_e$ and $\beta \propto \lambda^2 \rho_e$

Mean value of the refractive index: n<1

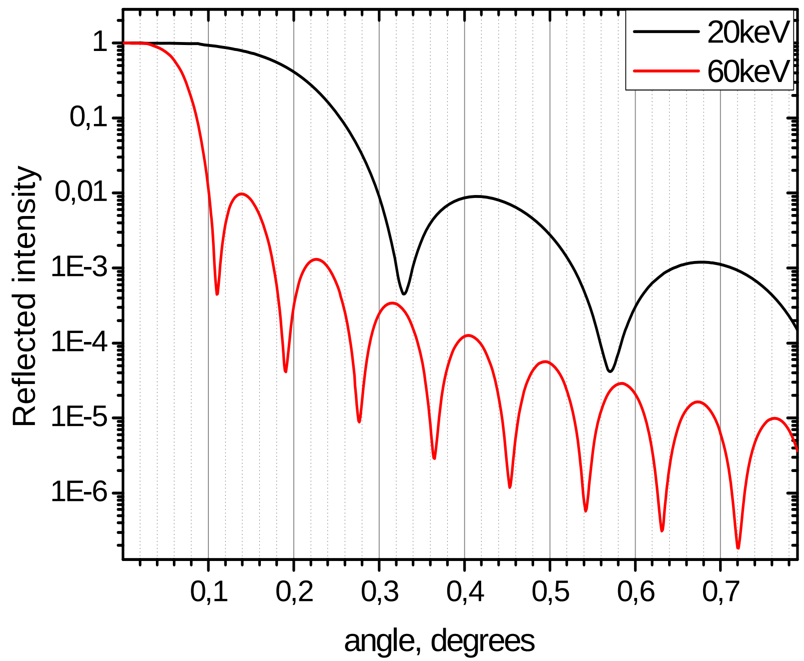
⇒total external reflection

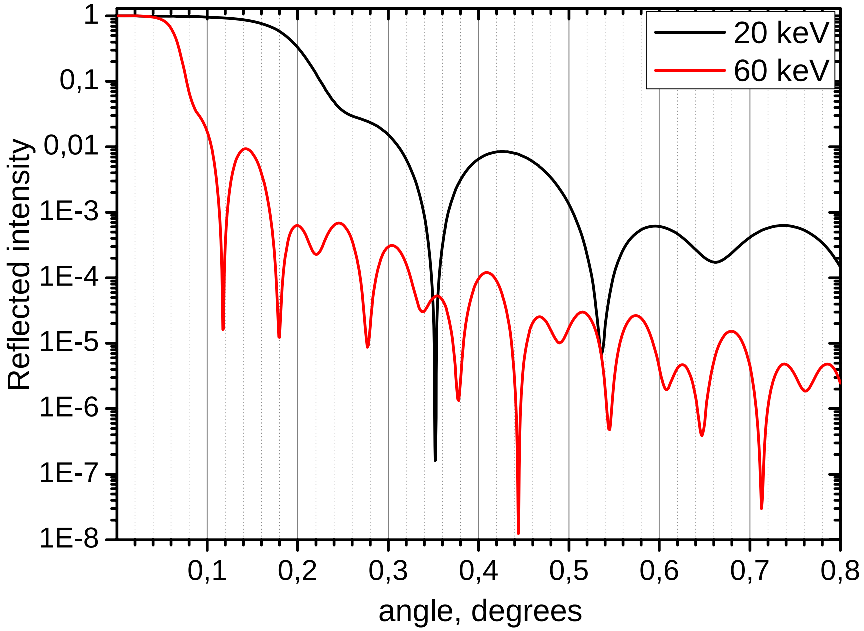
⇒critical angle $\alpha_c \approx \sqrt{2\delta}$

Silicon mirror: very small α_c= 0,09°



Silicon mirror coated with Rh: α_c= 1,30°





Reflectivity of layer systems can be calculated using Parratt recursive algorithm:

$$I(a_i) = \left| X_j \right|^2$$

$$X_j = \exp(-2ik_{z,j} z_j) \frac{r_{j,j+1} + X_{j+1} \exp(2ik_{z,j+1} z_j)}{1 + r_{j,j+1} X_{j+1} \exp(2ik_{z,j+1} z_j)}$$

$$k_{z,j} = \frac{4\pi}{\lambda} \sin \alpha_i \sqrt{n_j^2 - \cos^2 a_i}$$

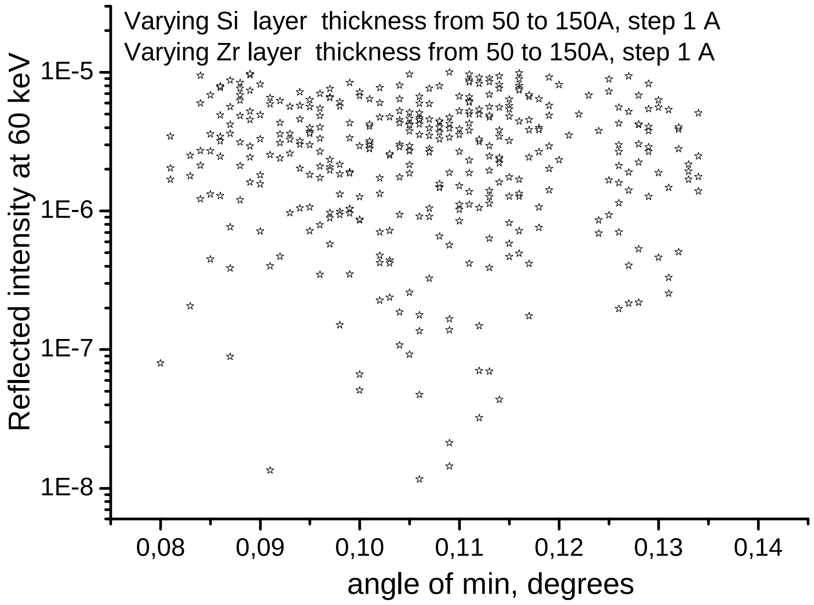
$$r_{j,j+1} = \frac{k_{z,j} - k_{z,j+1}}{k_{z,j} + k_{z,j+1}}$$

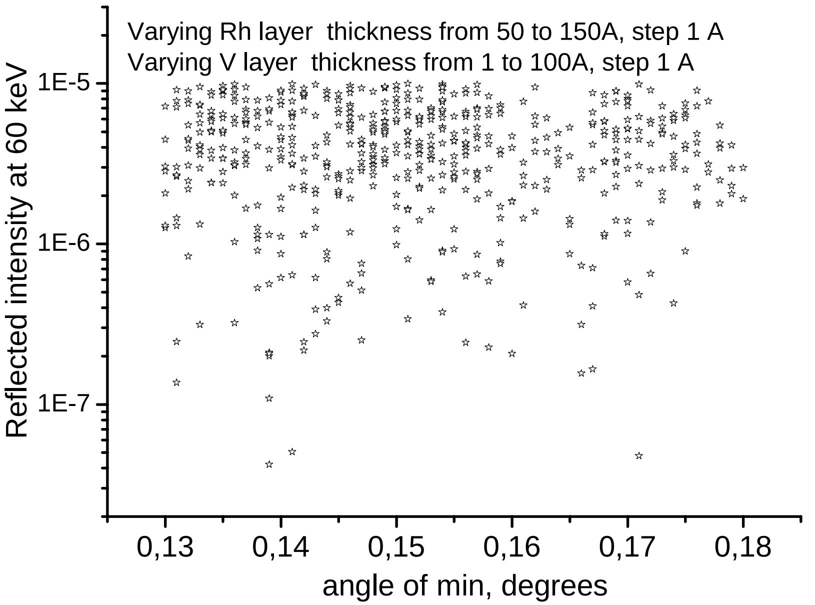
Reqirements:

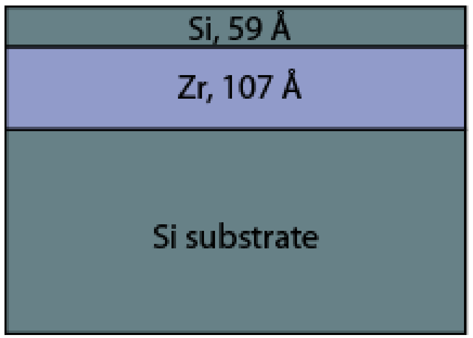
- Chemical and mechanical stability of layer materials
- Positions of absorption edges
- Ability to prepare very smooth layers
- Maximal density contrast

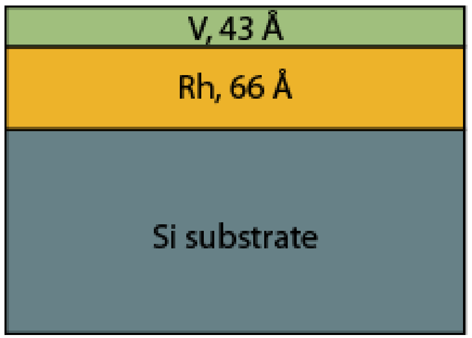
- Si on Zr layer on Si substrate for 5-20 keV region
- V on Rh layer on Si substrate for 20-30 keV region

Optimal combination for layer thicknesses:

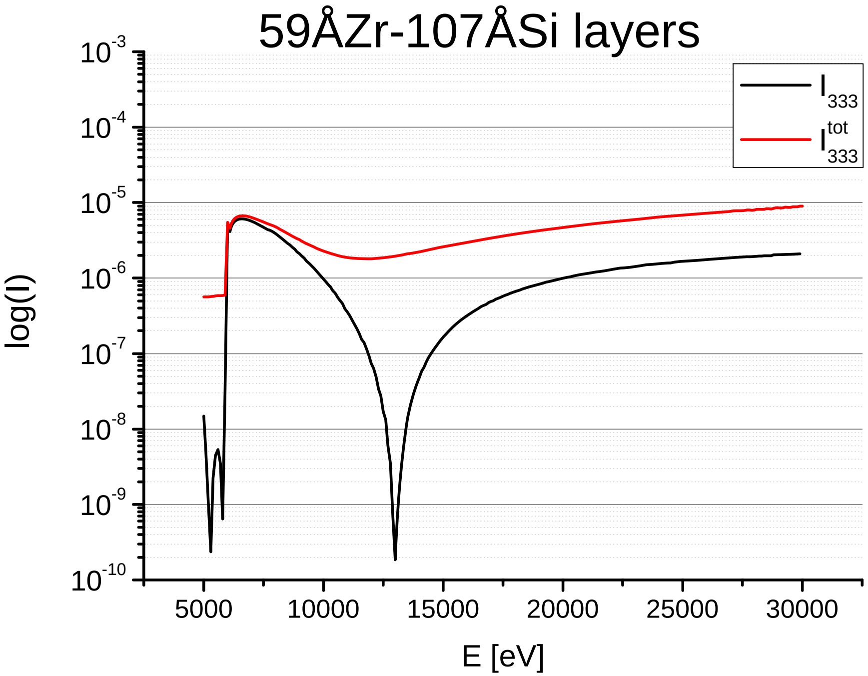


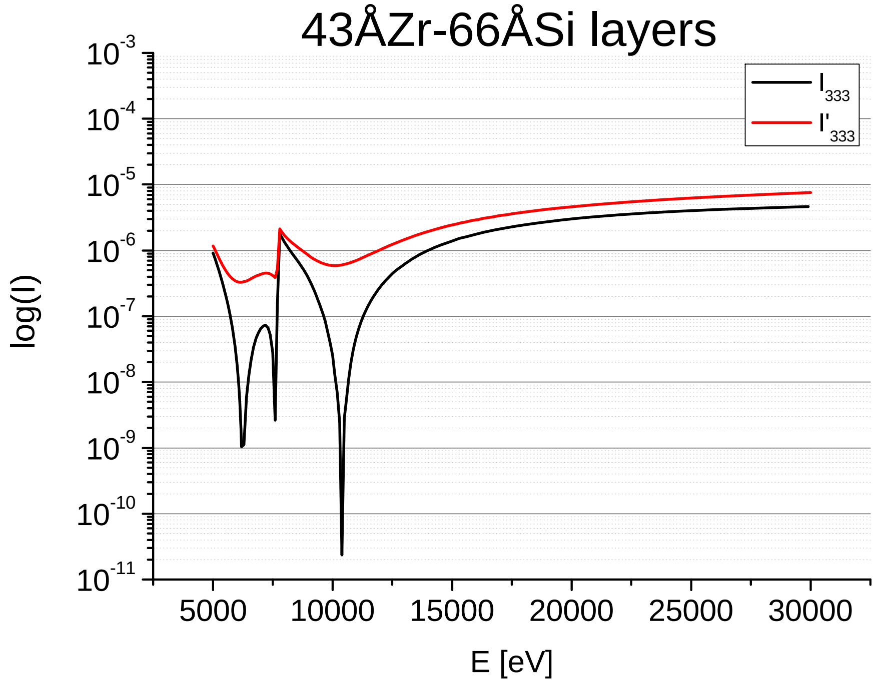






Calculation of higher harmonics suppression





Influence of the beam divergence

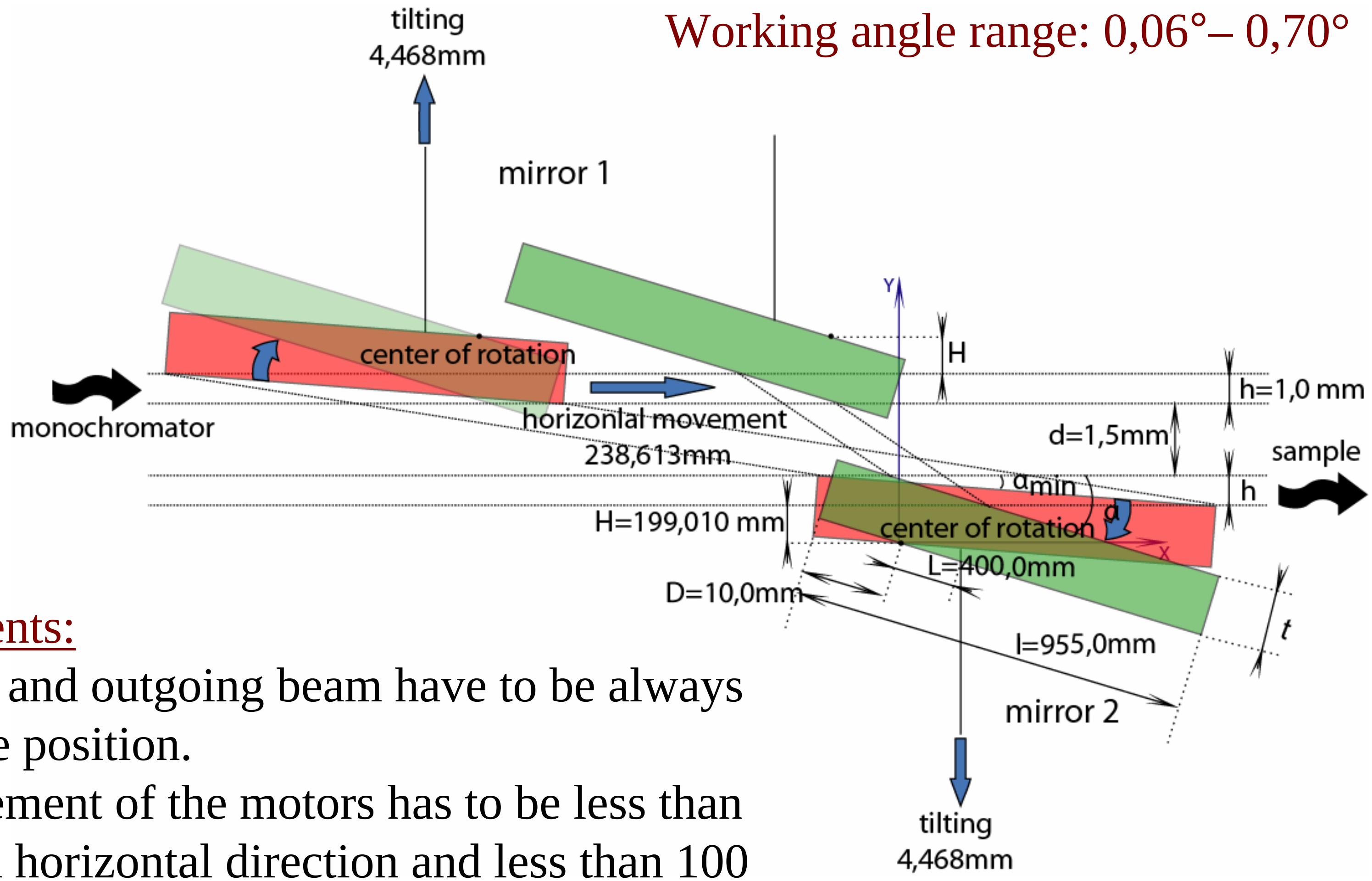
$$I_{333}^{tot} = I_{333}(a^*)$$

$$D(\varphi, \sigma_{Ty'}) = \frac{1}{\sqrt{2\pi}\sigma_{Ty'}} \exp\left[-\frac{1}{2} \left(\frac{\varphi}{\sigma_{Ty'}} \right)^2 \right]$$

$$I_{333}^{tot} = \int_0^{\frac{\pi}{2}} I_{333}(\alpha) D(\alpha - \alpha^*) d\alpha$$

Layout and movements of the mirrors

Working angle range: 0,06°– 0,70°



Requirements:

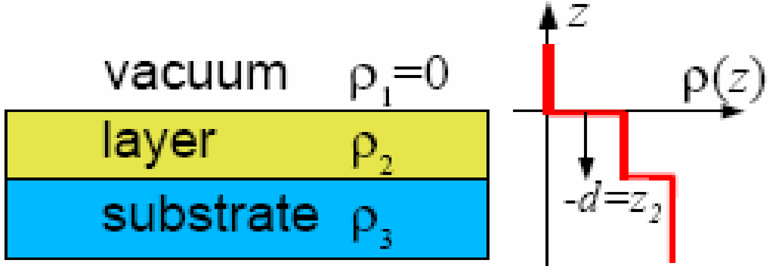
- Incoming and outgoing beam have to be always at the same position.
- The movement of the motors has to be less than 300 mm in horizontal direction and less than 100 mm in vertical direction.
- Geometry has to be safe and have hardware and software limits in order to prevent mirror crash if motors are run wrongly

Conclusions

- Two layer systems, Rh-V and Zr-Si deposited to silicon substrate can be used as filters for higher harmonics and provides the calculated suppression to 10^{-10}.
- The geometry for 2 parallel plain mirrors was suggested. This geometry provides constant position of incoming and outgoing beam and does not allow mirror crash in working angle range.

Thank you for attention!

single smooth layer with thickness d



Density profile:

$$\rho(z) = \frac{\Delta\rho_1}{2}[1 - \Theta(z)] + \frac{\Delta\rho_2}{2}[1 - \Theta(z+d)]$$

Derivative of $\rho(z)$:

$$\frac{d\rho}{dz} \propto \Delta\rho_1 \delta(z) + \Delta\rho_2 \cdot \delta(z+d)$$

with: $\Delta\rho_1 = \rho_2 - \rho_1$
$\Delta\rho_2 = \rho_3 - \rho_2$

$$I(q_z) \propto \frac{1}{q_z^4} \left| \int \frac{d\rho(z)}{dz} \exp(iq_z z)\, dz \right|^2 = \frac{1}{q_z^4} \left| \int [\Delta\rho_1 \delta(z) + \Delta\rho_2 \delta(z+d)] \exp(iq_z z)\, dz \right|^2$$

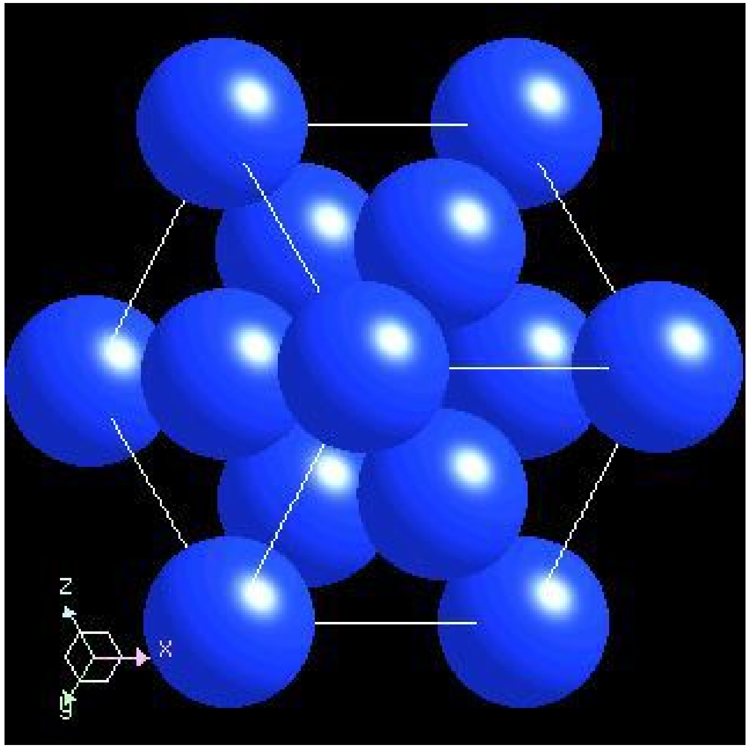
$$= \frac{1}{q_z^4} \left| \Delta\rho_1 + \Delta\rho_2 \exp(iq_z d) \right|^2 = \frac{1}{q_z^4} [\Delta\rho_1 + \Delta\rho_2 \exp(iq_z d)] \cdot [\Delta\rho_1 + \Delta\rho_2 \exp(-iq_z d)]$$

$$= \frac{1}{q_z^4} (\Delta\rho_1^2 + \Delta\rho_2^2 + \Delta\rho_1 \Delta\rho_2 [\exp(iq_z d) + \exp(-iq_z d)])$$

$$= \frac{1}{q_z^4} [\Delta\rho_1^2 + \Delta\rho_2^2 + 2\Delta\rho_1 \Delta\rho_2 \cos(q_z d)]$$

oscillating function

Silicon structure:



$$I = \left| S_f \right|^2$$

$$S_f = f_{at}(Q)(e^{iaQ(0,0,0)} + e^{iaQ(1/2,1/2,0)} +$$
$$+ e^{iaQ(1/2,0,1/2)} + e^{iaQ(0,1/2,1/2)} +$$
$$+ e^{iaQ(3/4,3/4,3/4)} + e^{iaQ(1/4,1/4,3/4)} +$$
$$+ e^{iaQ(1/4,3/4,1/4)} + e^{iaQ(3/4,1/4,1/4)}$$

Bragg peak allowed for :

1) h,k,l are odd
2) (h,k,l) are all even and (h+k+l) is divideable by 4

a(0,0,0)
a(0,1/2,1/2)
a(1/2,0,1/2)
a(1/2,1/2,0)
a(3/4,3/4,3/4)
a(1/4,1/4,3/4)
a(1/4,3/4,1/4)
a(3/4,1/4,1/4)