

# F7030 Rentgenový rozptyl na tenkých vrstvách

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PřF MU

Prezentace k přednášce  
Numerické simulace  
Příklady experimentů  
Vybrané vztahy

# Syllabus

1. Experimentální technika: zdroje, vznik rtg záření, goniometry, optické prvky (monochromátory, kolimátory, zrcadla, fokusační optika), detektory. Základní experimenty: polykrystalové a monokrystalové metody, mapování reciprokého prostoru
2. Kinematická teorie rozptylu: úvod do teorie rozptylu, rozptyl na elektronu, izolovaném atomu, krystal, strukturní a geometrický faktor, omezená velikost krystalu
3. Difrakce na polykrystalech I: strukturní faktor, velikost krystalitu (Scherrerova formule), vliv deformace na polohy a šířky difrakčních maxim, zbytková napětí, kvantifikace fázového složení (vnitřní normál)
4. Polykrystaly II: Full profile fitting; Textury, ODF (orientation distribution function); Debyeův vztah, PDF (pair distribution function).
5. SAXS: teoretický popis, řídké roztoky – Guinierův a Porodův vztah, uspořádané částice – long range a short-range order
6. Dokonalé, téměř dokonalé krystaly, epitaxní vrstvy: Kinematická teorie na monokrystalu a epitaxní vrstvě – polohy difrakcí, truncation rod, deformace v epitaxní vrstvě, relaxace. Mozaikový krystal
7. Dynamická teorie rtg reflexe: Jednovlnná aproximace – hloubka vniku, reflexe na hladkém rozhraní, multivrstvy (formalismus přenosové matice), TRXRF
8. Dynamická teorie rtg difrakce: Dvojevlnná aproximace: případ Bragg a Laue, Borrmannův jev, stojatá vlna, GID, epitaxní vrstvy
9. Semikinematická teorie I: DWBA, Rozptyl na drsných rozhraních – popis drsného rozhraní, příklady: fraktálové rozhraní, dvouúrovňové, vicinální, spekulární odraz a nespekulární rozptyl, drsné multivrstvy
10. Semikinematická teorie II: GISAXS na částicích na povrchu a uvnitř vzorku, Difuzní rozptyl na defektech v krystalu v okolí difrakce
11. Experimentální rozlišení Experimentální rozlišení v reciprokém prostoru: analyzer streak, detector streak, monochromator streak, DuMondovy grafy, disperzní a nedisperzní uspořádání, koherenční šířka a délka
12. Další rentgenové metody: Fluorescenční spektroskopie, absorpční spektroskopie – XAFS, XMCD.

# Optické prvky

- Rtg optika
  - Krystaly, monochromátory, kolimátory
  - Zrcadla, multivrstvy, mřížky
  - Fokuzální optika

Nezbytná pro zajištění požadovaných vlastností svazku elmag záření.

- spektrální vlastnosti (monochromaticnost)
- velikost svazku - úhlová i prostorová (rozměr, divergence)

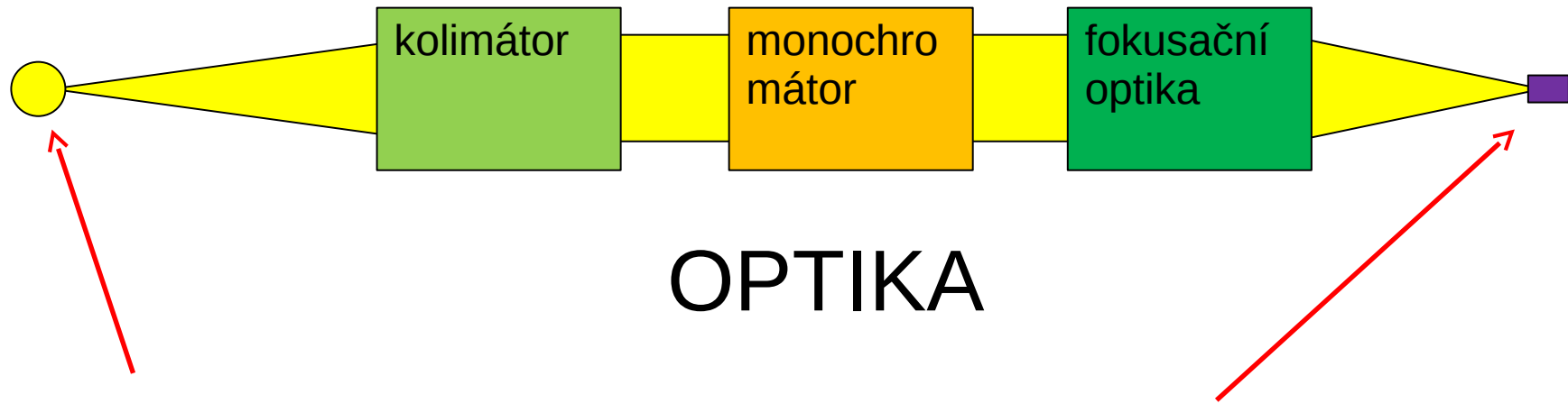
Co je na rtg optice jiné oproti zobrazování běžným světlem?

Index lomu materiálů - má v rtg úplně jiné vlastnosti než ve VIS.

Vlastnosti zrcadel, čoček, mřížek pro rtg se podstatně liší od těch

jak je známe pro viditelné světlo.

# Optické prvky



## Zdroj

Spektrum –  $\Delta E/E$   
Emitance (velikost  $\times$  divergence)  
Stupeň prostorové koherence  
Briliance  
Polarizace – lineární, kruhová, eliptická

## Vzorek

Velikost svazku  
Divergence svazku  
Tok intensity  
Časová koherence  $\Delta E/E$   
Prostorová koherence  
Polarizace

šterbiny, filtry, okna, zrcadla, děliče svazků. Monochromátory, fázové destičky, čočky, mřížky, difrakční elementy

# Optické prvky

Refrakční čočky



Zrcadla



Vlnovody



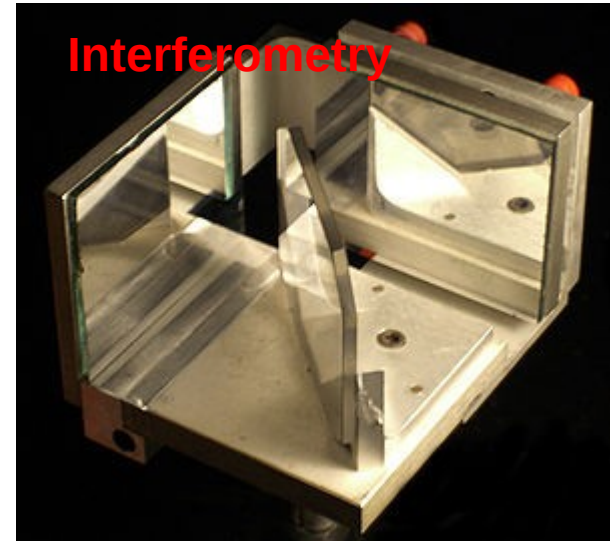
Fresnelovy čočky



Filtry



Interferometry



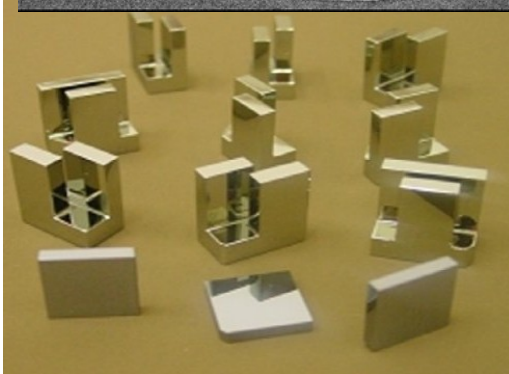
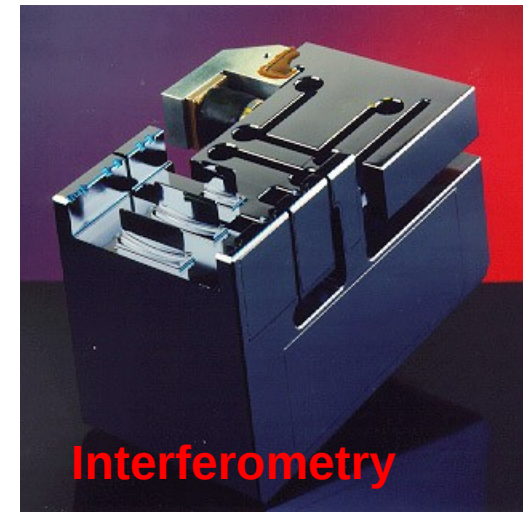
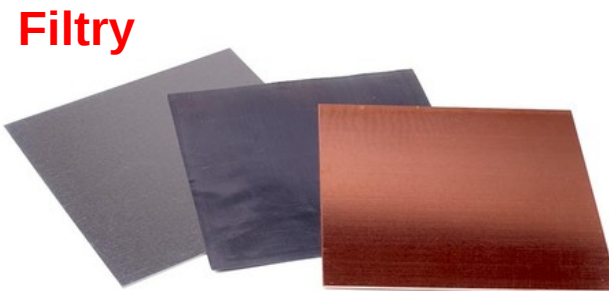
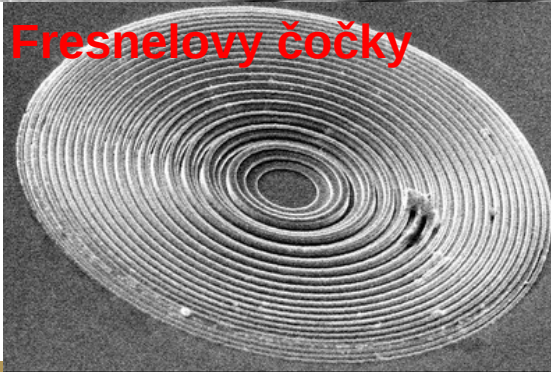
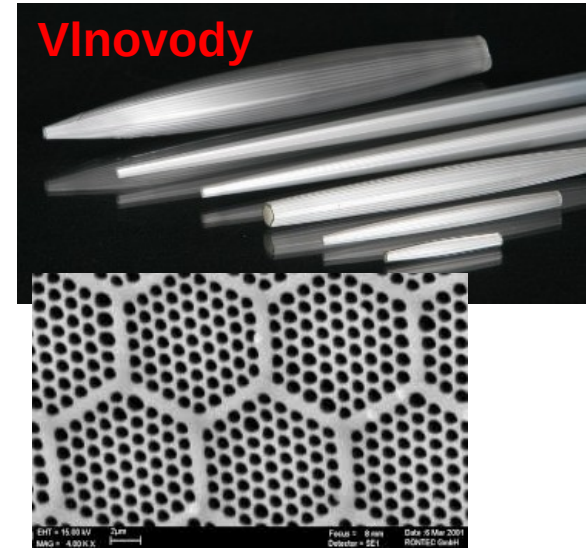
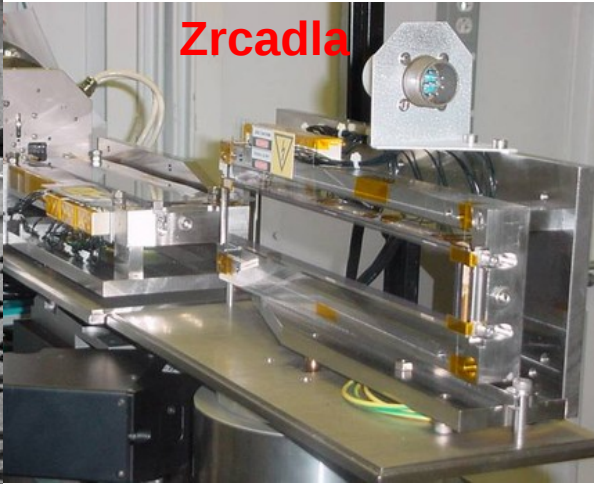
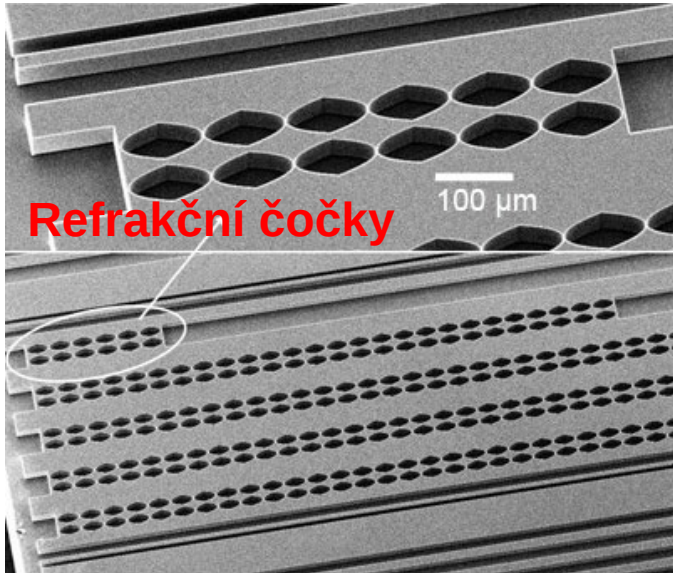
Difrakční optika



Polarizátory

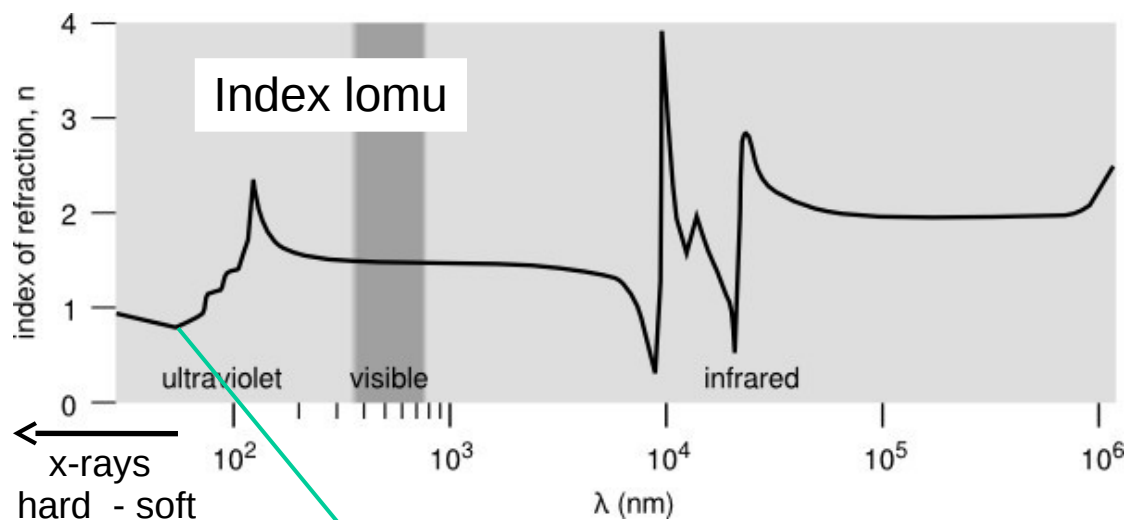


# Optické prvky



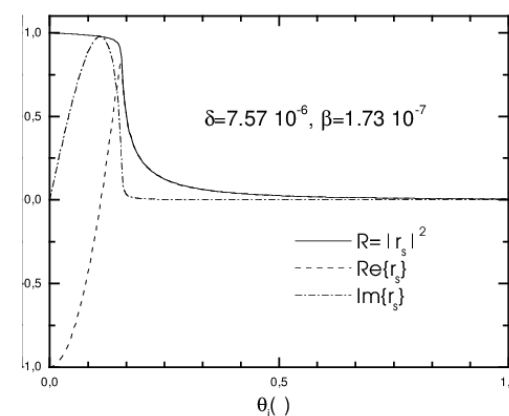
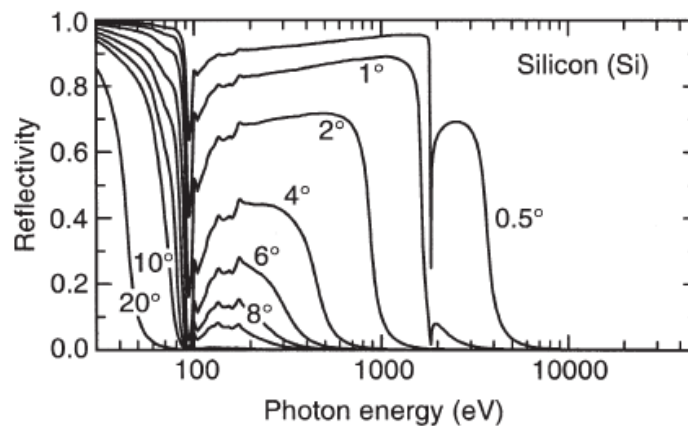
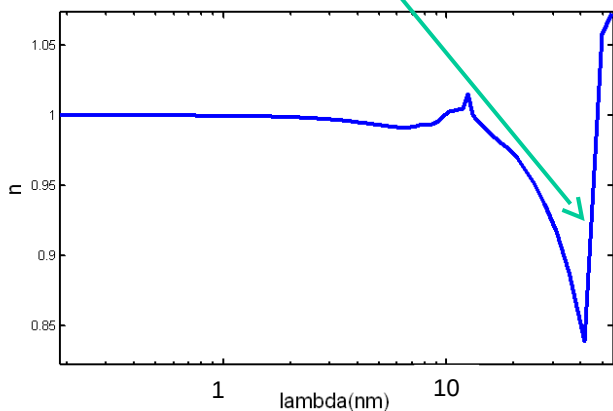
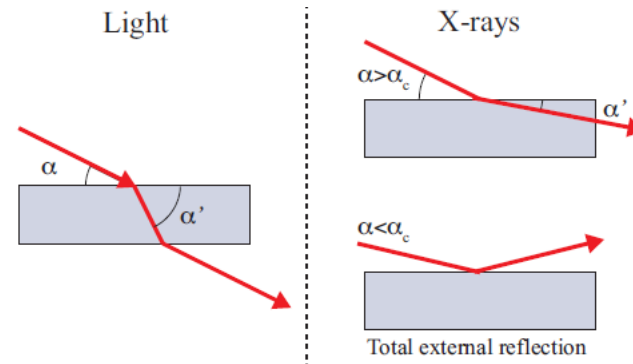
+Polarizátory

# Optické prvky



$$n = 1 - \delta - i\beta;$$

$$\delta, \beta \ll 1$$

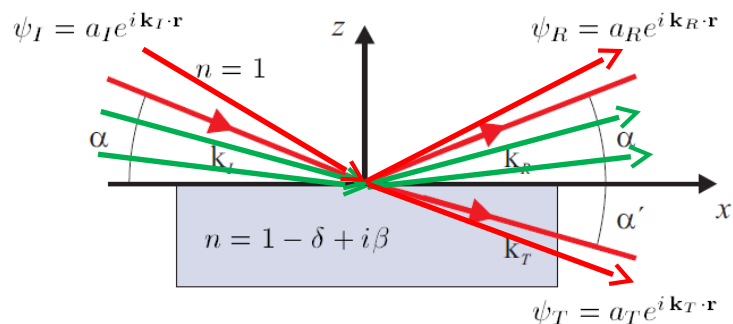


Odrazivost Si zrcadla pro různé úhly dopady a energie.

Totální odraz nastává pro velmi malé úhly  $\alpha < \alpha_c$

**Je obtížné vyrobit klasická zrcadla pro rtg záření nebo dokonce čochky!**

# Optické prvky



$$n \equiv 1 - \frac{2\pi\rho_{at}r_0}{k^2} \{f^0(0) + f' + i f''\}$$

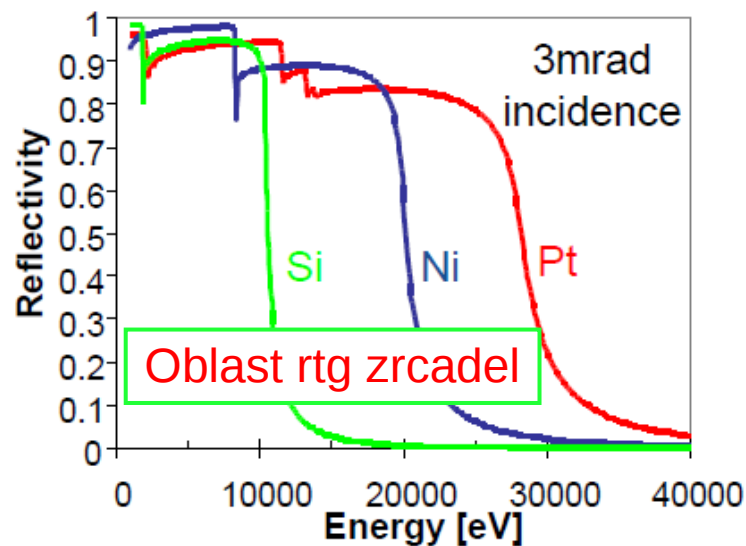
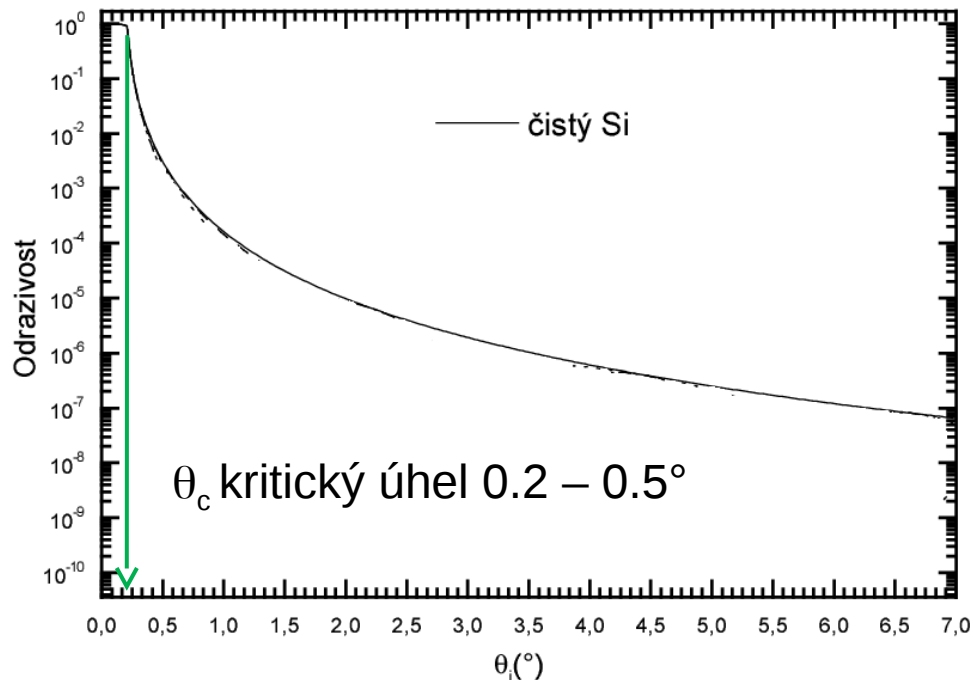
$$\theta_c \approx \sqrt{2\delta} \propto \lambda \sqrt{Z}$$

$$R = |r^2| = (\theta - \theta') / (\theta + \theta')$$

Použití:

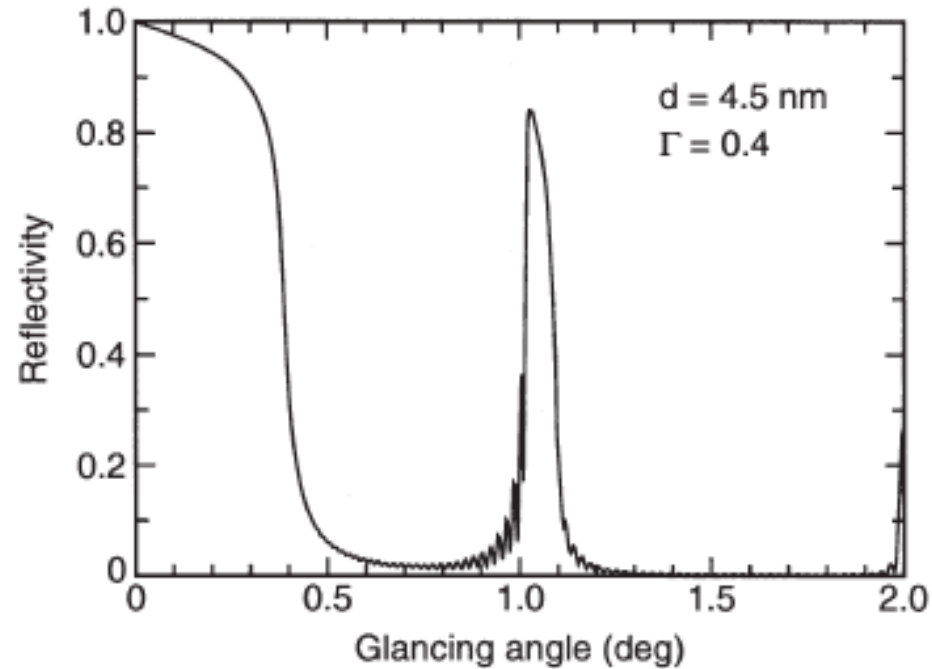
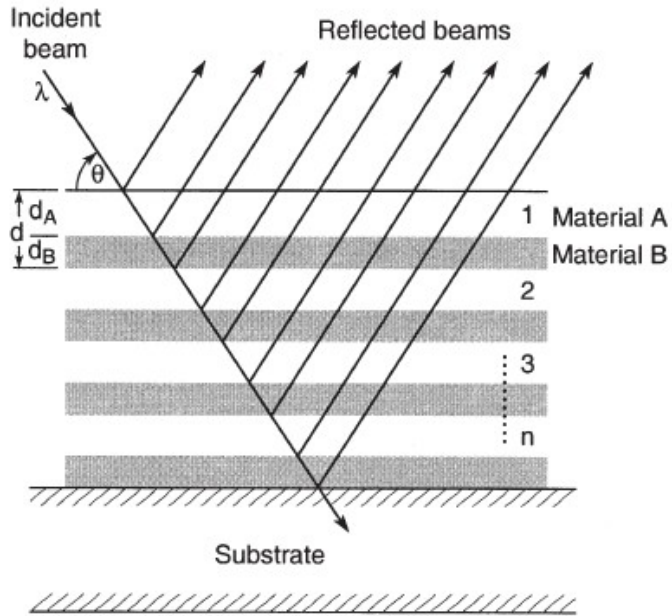
Zrcadla pod tečným úhlem

Kapiláry a vlnovody





# Optické prvky



$$Q_j = \sqrt{Q^2 - 8k^2\delta_j + i 8k^2\beta_j} \quad \text{Parratův rekurentní formalismus}$$

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}} \quad r'_{N,\infty} = \frac{Q_N - Q_\infty}{Q_N + Q_\infty}$$

$$r_{N-1,N} = \frac{r'_{N-1,N} + r'_{N,\infty} p_N^2}{1 + r'_{N-1,N} r'_{N,\infty} p_N^2}$$

Pro konstrukci zrcadel lze využít  
**1. Braggovo maximum** v odrazivosti multivrstvy  
 - výhoda: vyšší úhel dopadu

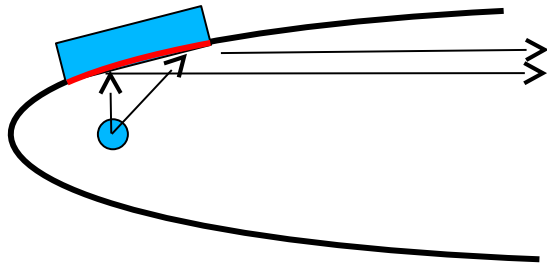
# Optické prvky

## Zrcadla s gradovanými multivrstvami

Slouží jako rtg zrcadla pro fokusaci nebo kolimaci rtg záření.

Mohou fungovat i jako monochromátory.

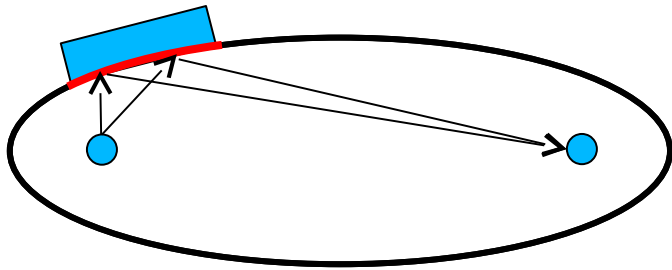
### Parabolické gradované zrcadlo s multivrstvou



Goebelovo parabolické zrcadlo



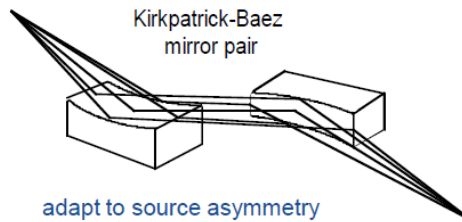
### Eliptické gradované zrcadlo s multivrstvou



U synchrotronu, kdy je zdroj bodový

Je možné zrcadlo vyrábět v toroidálním tvaru

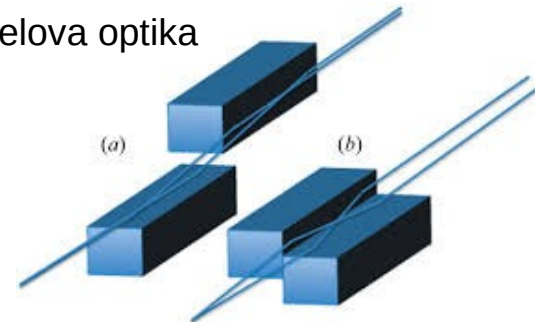
Nebo kombinovat 2 zrcadla kolmé na sebe -levnější



adapt to source asymmetry

- apertures
- demagnification

### Montelova optika



# Optické prvky

Hlavní funkce rtg zrcadel:

**Ohyb** – regulace polohy a směru svazku

**Filtr výkonu** – regulace intensity změnou úhlu dopadu u žádoucích experimentů

**Tvaruje spektrum** – odstraňuje vyšší frekvence (vyšší harmonické z undulátoru), geometricky lze nastavovat energiové okno.

**Fokusace** – u wigglerů a bending mag. jsou prohnutá zrcadla (sfér. cyl. toroid.) pro mikrosundu či mikroskopii: zmenšení zdroje, (elipt., zkřížená KB ...)

**Kolimace** – parabolická zrcadla: úhlová divergence zdroje odpovídá akceptanci.

Lze aplikovat i pro ohýbání krystalů

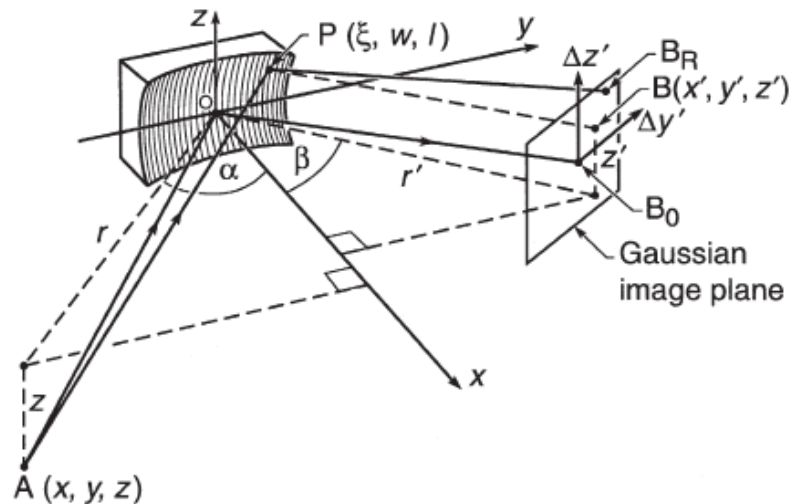


Fig. 4-7. Focusing properties notation.

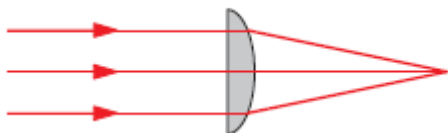


# Optické prvky

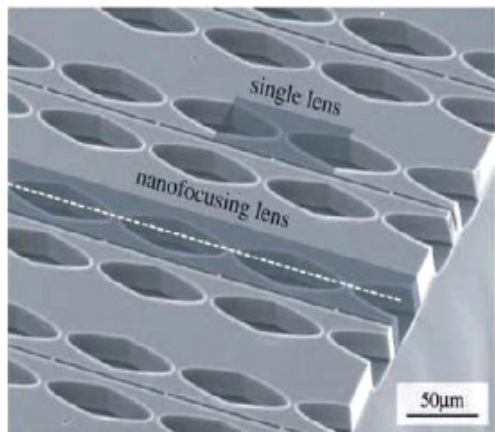
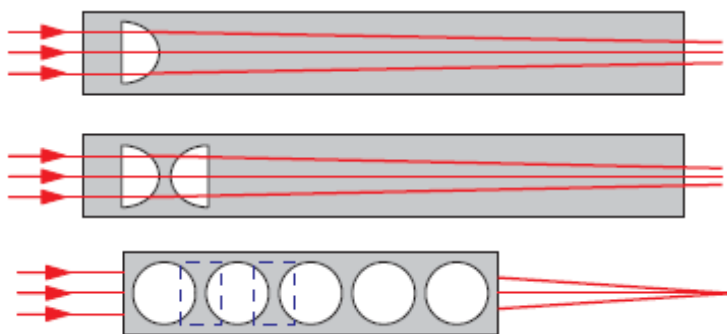
## Fokusační optika

### Refrakční čočky

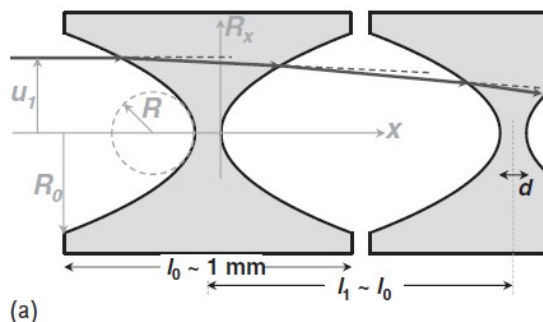
viditelné světlo



rtg záření

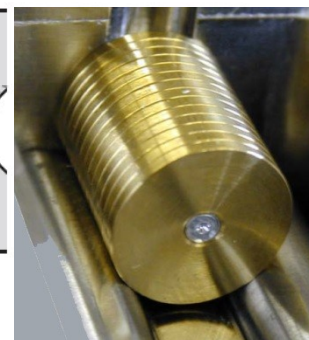
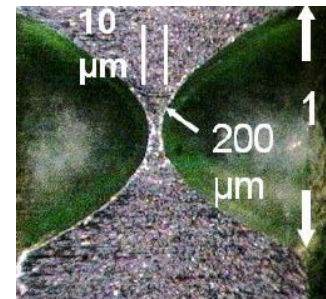


Parabolické čočky



(a)

Figure 3.5 (a) Illustration of a single parabolic lens used for X-ray focusing (adapted from an image in [77]). The X-ray beam path is schematically shown by the arrows. Typical



dimensions of the lens (apex radius of curvature  $R$ , thickness of the lens at the apex  $d$ , geometrical aperture  $2R_0$ , length of a lens  $l_0$ ) are also shown; (b) a stack of several lenses.

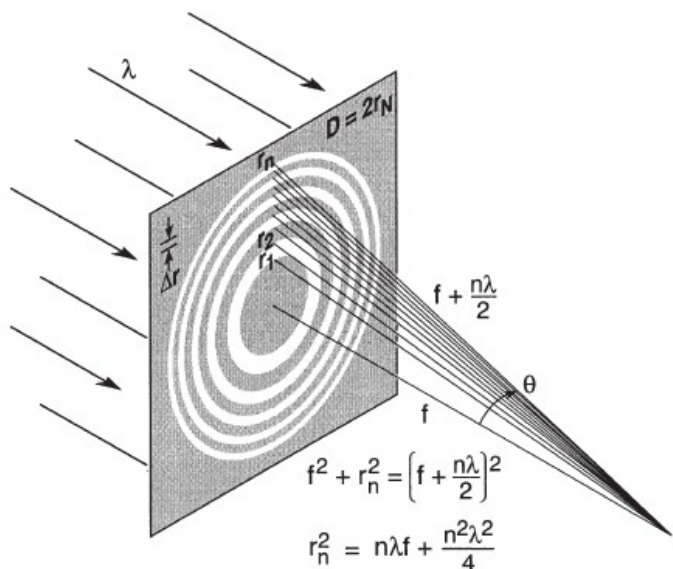
$$f_N = \frac{f_1}{N} \approx \frac{R}{2 \cdot N \cdot \delta} \sim \frac{0.2}{2N \cdot 5 \cdot 10^{-6}} \sim 10^4 / N \text{ [mm]}$$

Mnoho malých mikročoček za sebou relativně dlouhá ohnisková vzdálenost.  
 Problém absorpce – lehké materiály Be, Al  
 S absorpční délkou ~ 0.1 – 1 mm ( Be až 10mm)

# Optické prvky

## Fokusační optika

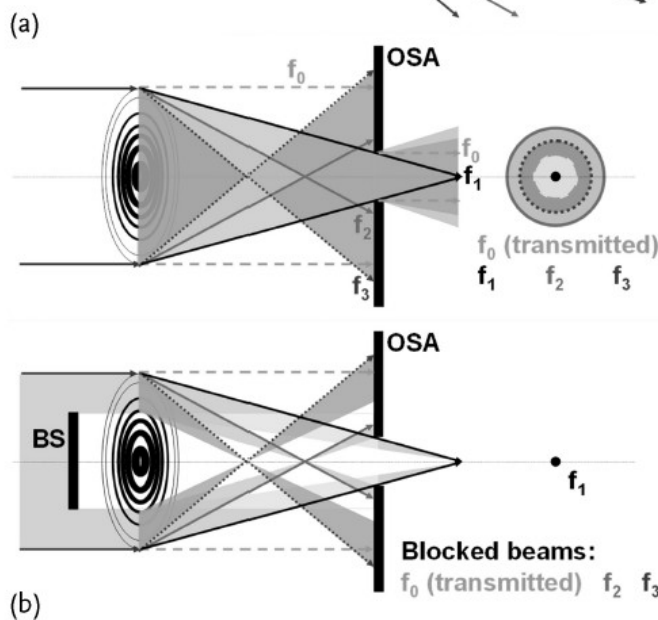
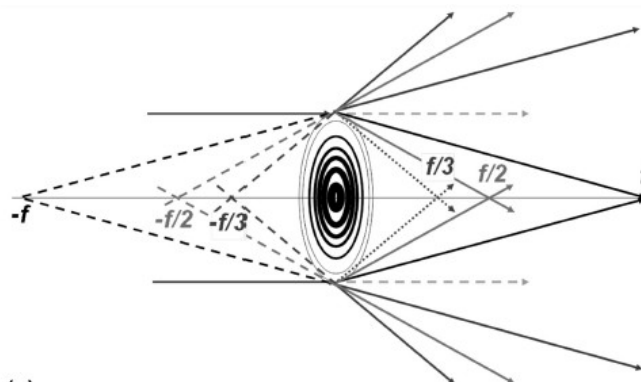
Fresnelovy čočky  
difrakční optika



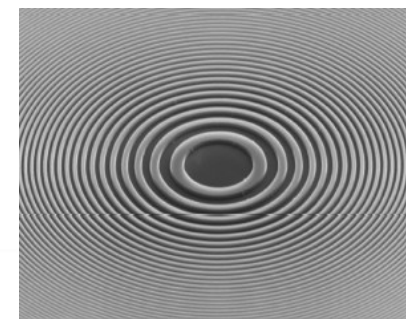
**Fig. 4-8.** A Fresnel zone plate lens with plane wave illumination, showing only the convergent (+1st) order of diffraction. Sequential zones of radius  $r_n$  are specified such that the incremental path length to the focal point is  $n\lambda/2$ . Alternate zones are opaque in the simple transmission zone plate. With a total number of zones,  $N$ , the zone plate lens is fully specified. Lens characteristics such as the focal length  $f$ , diameter  $D$ , and numerical aperture  $NA$  are described in terms of  $\lambda$ ,  $N$ , and  $\Delta r$ , the outer zone width. [Courtesy of Cambridge University Press, Ref. 3.]

Ize zanedbat

$$r_n^2 = n f \lambda + \frac{n^2 \lambda^2}{4}$$



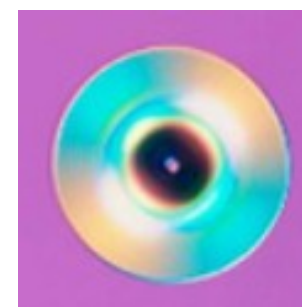
OSA - order sorting aperture



$$r_m^2 = m \cdot \lambda \cdot f$$

šířka m-té zóny

$$\Delta r_m \simeq \frac{\lambda f}{2r_m} = \frac{\sqrt{\lambda f}}{2\sqrt{m}}$$



# Optické prvky

## Základní veličiny charakterizující Fresnellovu čočku

- the *maximum number*  $N_{\max}$  of zones, if we know the diameter  $D$  of the zone plate:  
 $D = 2r_m$  can be calculated as:

$$N_{\max} \simeq \frac{D}{4\Delta r} = \frac{R_0}{2\Delta r} \Rightarrow D = 4N_{\max}\Delta r \quad (3.47)$$

with  $\Delta r$  being the width of the last zone,  $D$  the diameter of the ZP and  $R_0$  its radius ( $R_0 = r_{N_{\max}} = D/2$ ).

- the *focal distance* of the FZP can be calculated by considering the last zone ( $m = N_{\max}$ ). With the considerations above and using Eq. (3.46), one obtains:

$$f \simeq \frac{D\Delta r}{\lambda} \quad (3.48)$$

which is the focal distance for the first diffraction order.

- the *numerical aperture* (NA), still in the small angles approximation ( $f \gg D$ ):

$$\text{NA} \simeq \frac{D/2}{f} = \frac{\lambda}{2\Delta r} \quad (3.49)$$

- the *spatial resolution*, using Rayleigh criterion for a circular aperture:

$$\text{resolution(coherent)} = \frac{0.61\lambda}{\text{NA}} = 1.22 \cdot \Delta r = 1.22 \frac{\lambda f}{D} \quad (3.50)$$

- the *depth of focus*, DOF:

$$\text{DOF} = \pm \frac{1}{2} \frac{\lambda}{(\text{NA})^2} = \pm \frac{2(\Delta r)^2}{\lambda}$$

- the *spectral bandwidth*:

$$\frac{\Delta\lambda}{\lambda} < \frac{1}{2N_{\max}}$$

# Optické prvky

## Kapiláry, polykapiláry, vlnovody

Využívají totálního odrazu při malých úhlech podobně jako rtg zrcadla

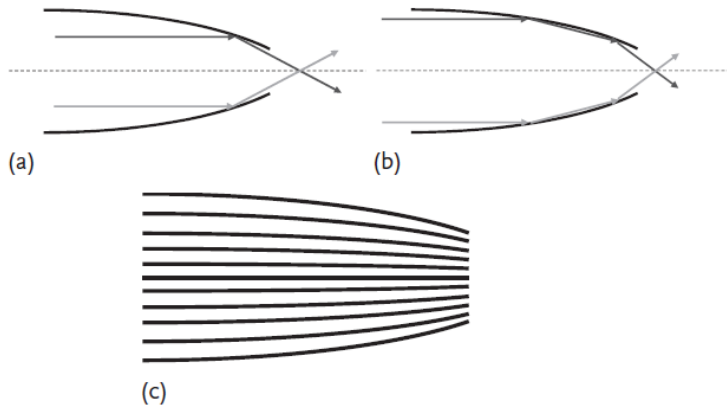
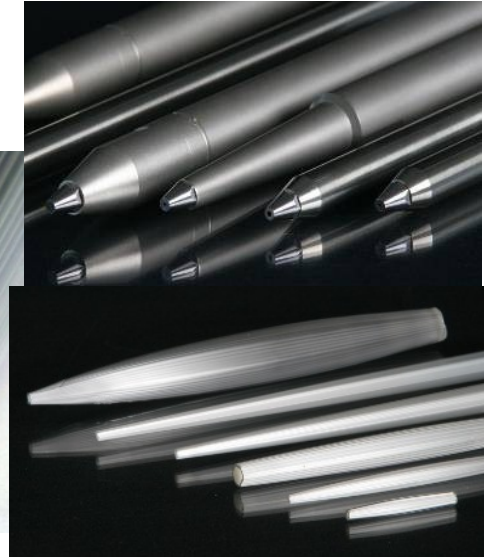
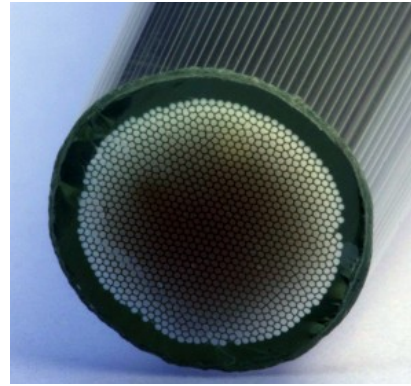


Figure 3.10 Schematic illustration of capillaries and focusing principle: (a) single bounce; (b) multiple bounce and (c) poly-capillaries (Kumakhov lens).

Rtg svazek „trpí“ mnohonásobnými odrazy  
-relativně malá intenzita  
-nízká divergence, ale velké místo fokusace

Často se používají také jen na tvorbu  
paralelního svazku



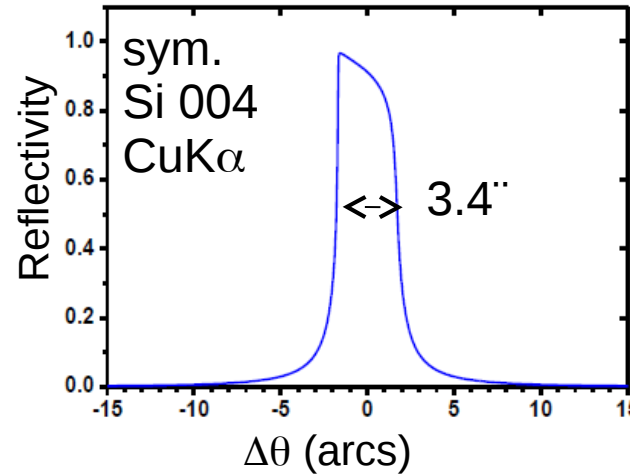
Výstupní divergence svazku je min. rovna nebo zpravidla větší než kritický úhel daného materiálu.

Problémem je také drsnost povrchu uvnitř kapilár.

# Monochromátory

Využívá se dynamické difrakce na monokrystalech  
Zpravidla Si nebo Ge

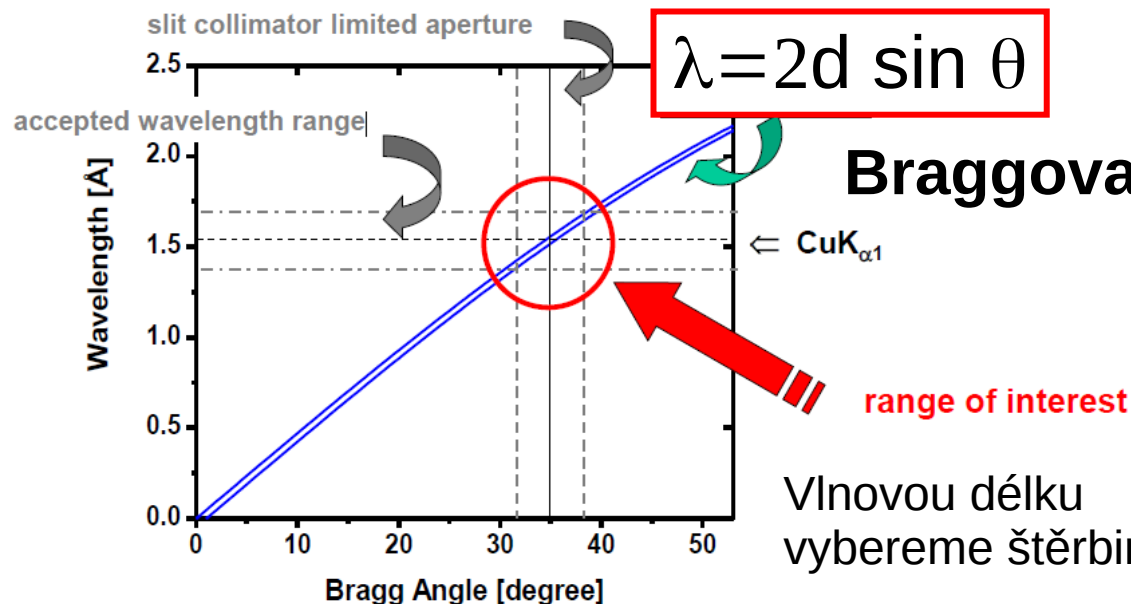
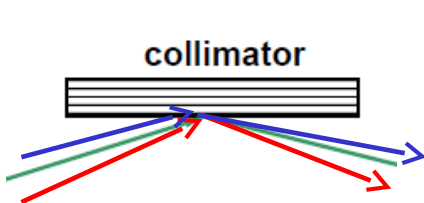
$$FWHM \cong \frac{2C|\chi_h|}{\sin 2\Theta_B} \sqrt{\frac{1}{|b|}}$$



faktor asymetrie  
 $b < 0$ ; Bragg  
 $b > 0$ ; Laue  
 $b = -1$  sym. Bragg

$$b = -\frac{\sin(\Theta_B + \phi)}{\sin(\Theta_B - \phi)}$$

$\phi$  Úhel mezi difraktujícími rovinami a povrchem



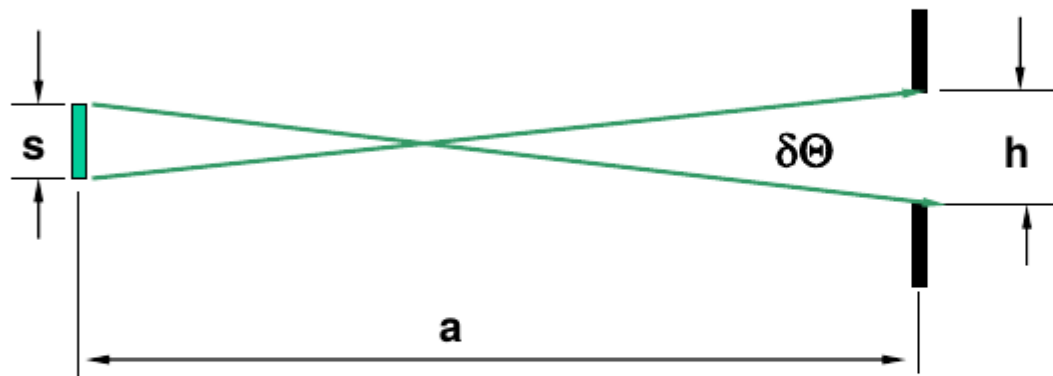


# Monochromátory



## Divergence

Limitations of single axis diffraction (slit system(s)):



Divergence:

$$\delta\Theta = (h+s) / a$$

Typical laboratory setup:  $\delta\Theta = (0.4\text{mm} + 0.5\text{mm}) / 500\text{mm} = 1.8 \cdot 10^{-3} \Rightarrow 370''$

**At least a double crystal diffractometer setup is required !**

Synchrotron :  $\delta\Theta = (0.2\text{mm} + 0.2\text{mm}) / 40\text{ m} = 1.0 \cdot 10^{-5} \Rightarrow 2''$

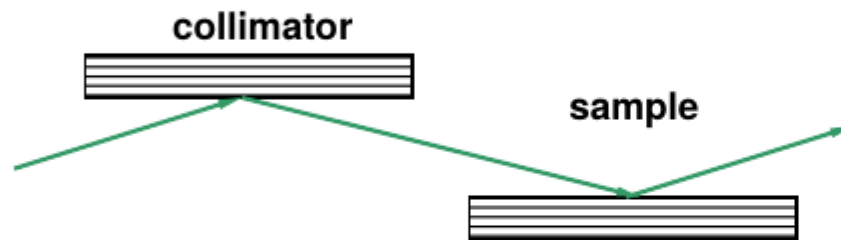
# Monochromátory



## Double Crystal Diffractometer (DCD) setups

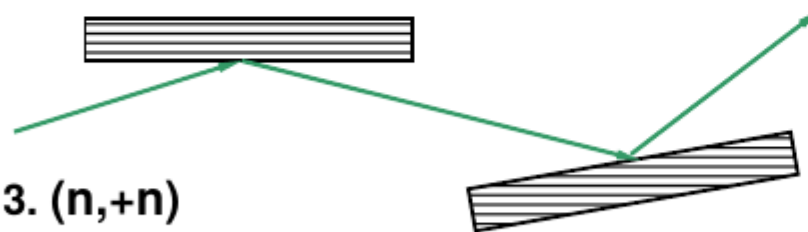
Three different setups of the 'classical' DCD

1. (n,-n)



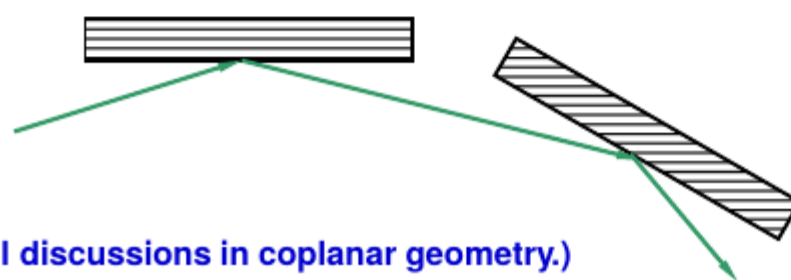
The same reflection (hkl) of collimator and sample in opposite direction.

2. (n,-m)



Different reflections of collimator  $(hkl)_c$  and sample  $(hkl)_s$  in opposite direction.

3. (n,+n)



The same reflection (hkl) of collimator and sample but in the same direction.

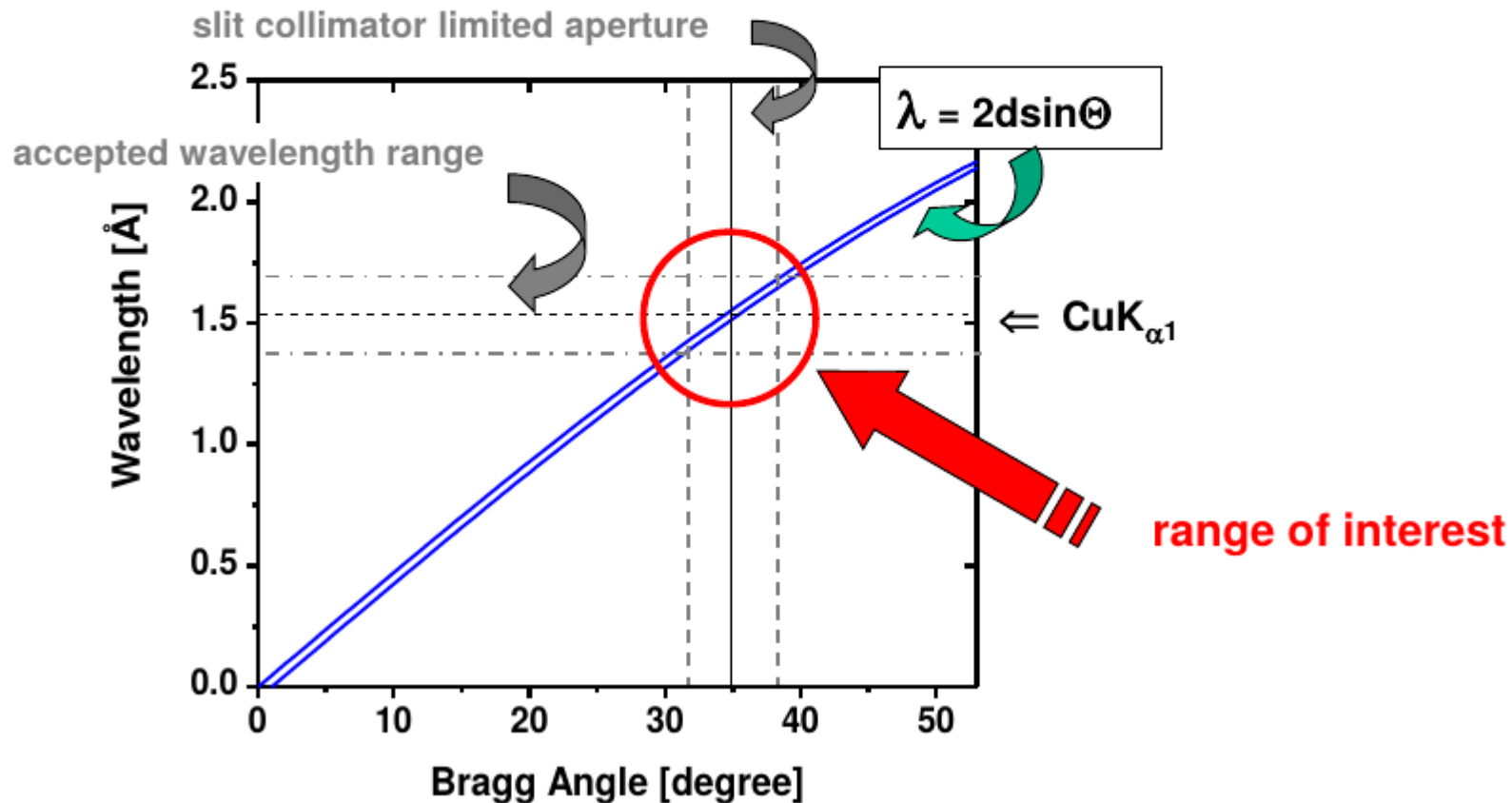
(All discussions in coplanar geometry.)

# Monochromátory



## DuMond Diagram

Graphical representation of Bragg's law showing the reflecting range

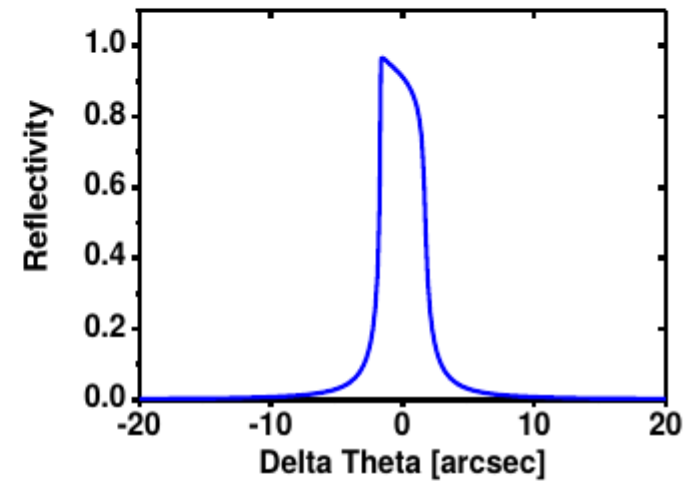
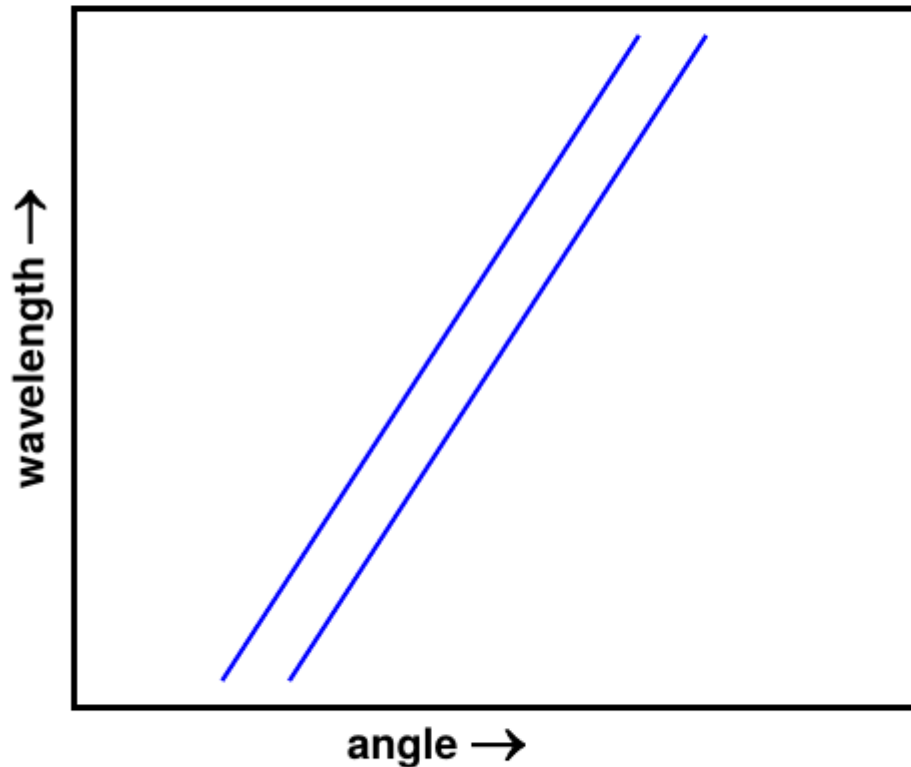


# Monochromátory



## DuMond Diagram / (n,-n) setup

Reflection curve of the collimator crystal



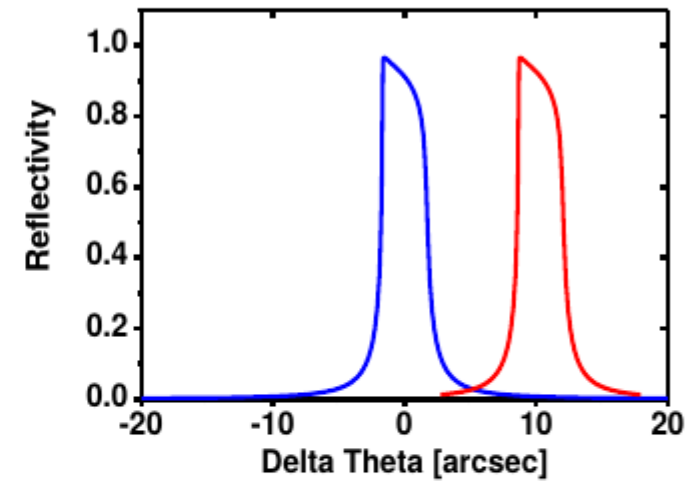
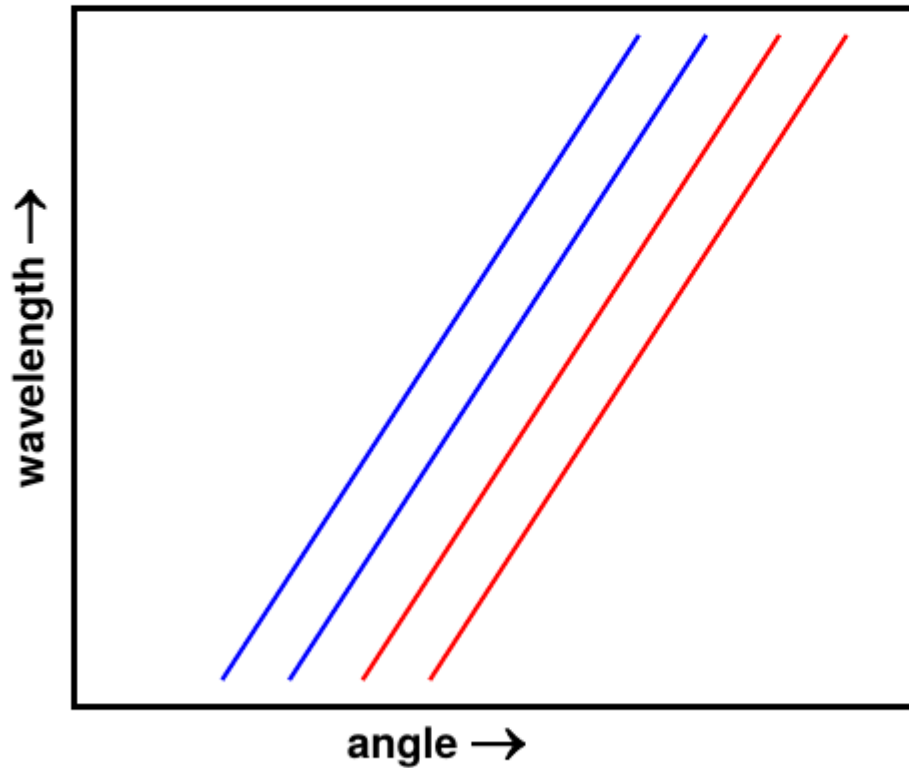
# Monochromátory



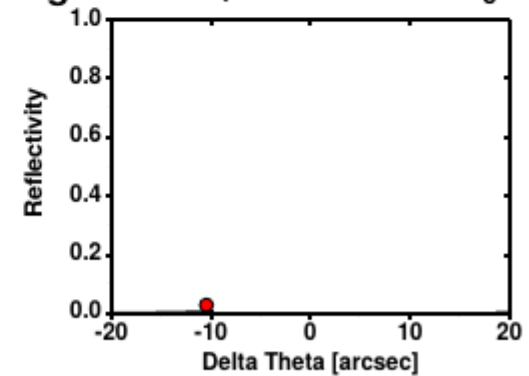
## DuMond Diagram / (n,-n) setup

Reflection curve of the collimator crystal

Reflection curve of the sample



Rocking curve (convolution  $R_c \times R_s$ )



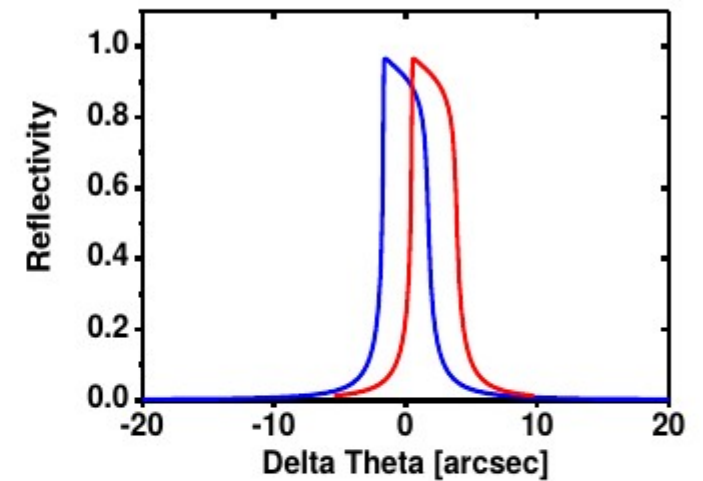
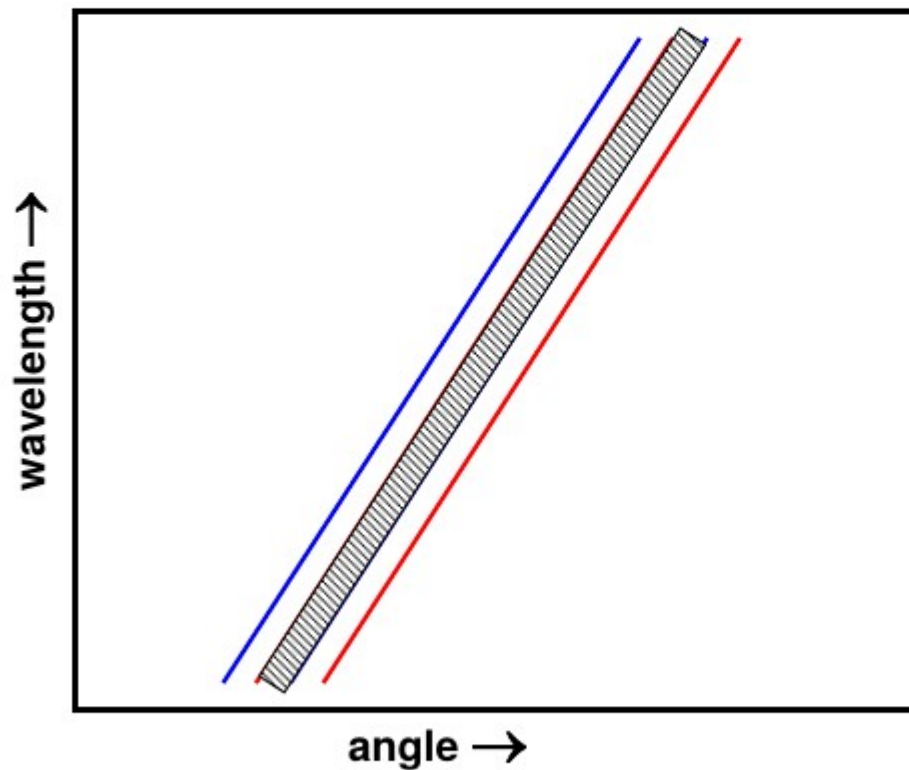
# Monochromátory



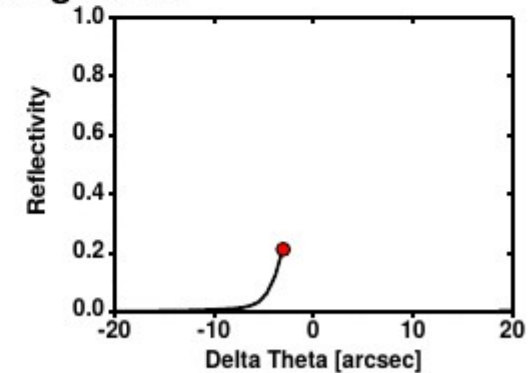
## DuMond Diagram / (n,-n) setup

Reflection curve of the collimator crystal

Reflection curve of the sample



Rocking curve



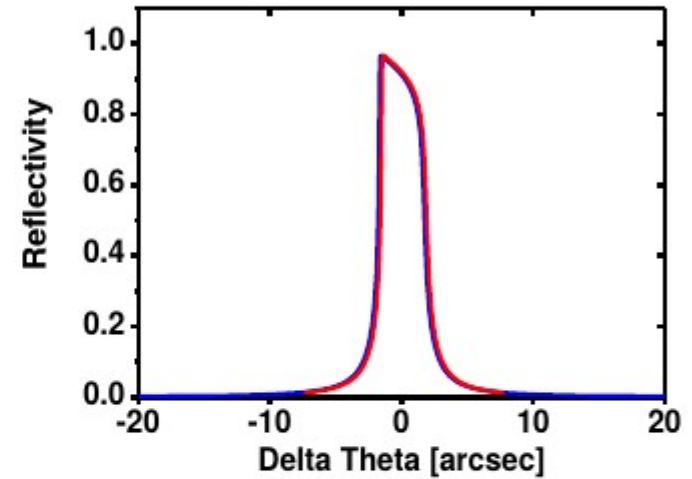
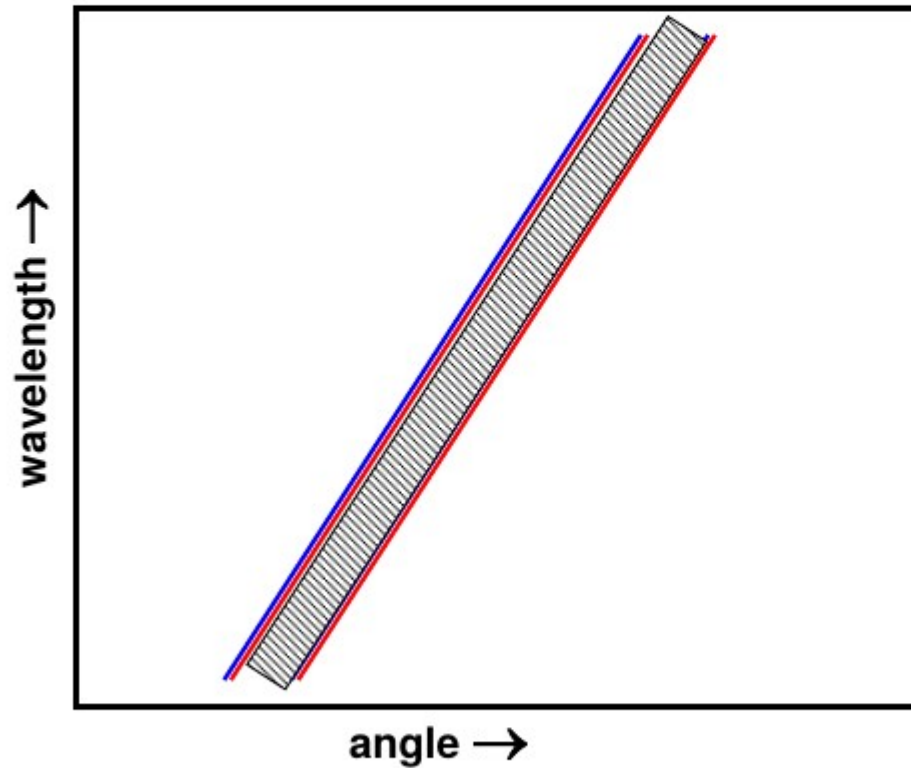
# Monochromátory



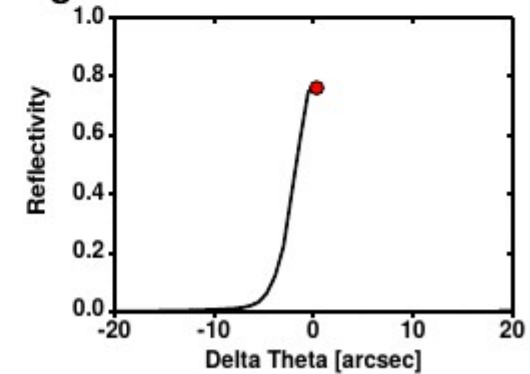
## DuMond Diagram / (n,-n) setup

Reflection curve of the collimator crystal

Reflection curve of the sample



Rocking curve



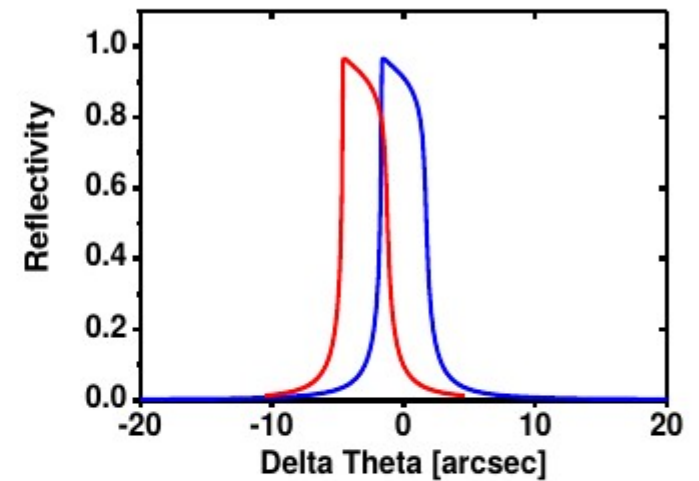
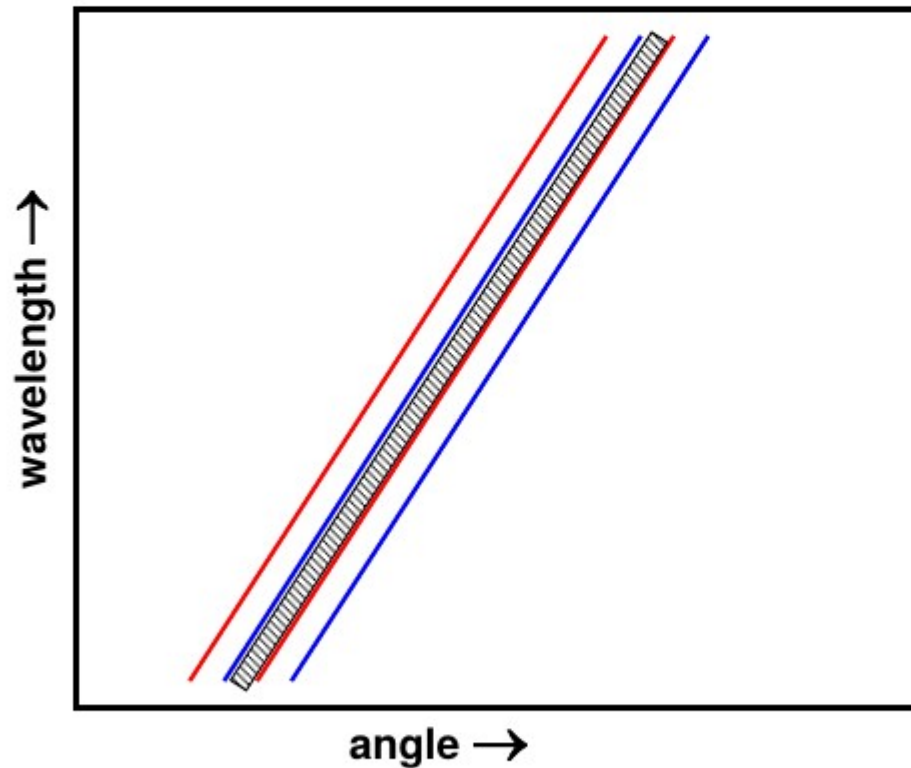
# Monochromátory



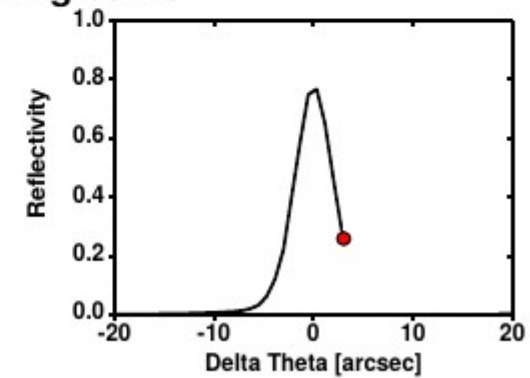
## DuMond Diagram / (n,-n) setup

Reflection curve of the collimator crystal

Reflection curve of the sample



Rocking curve





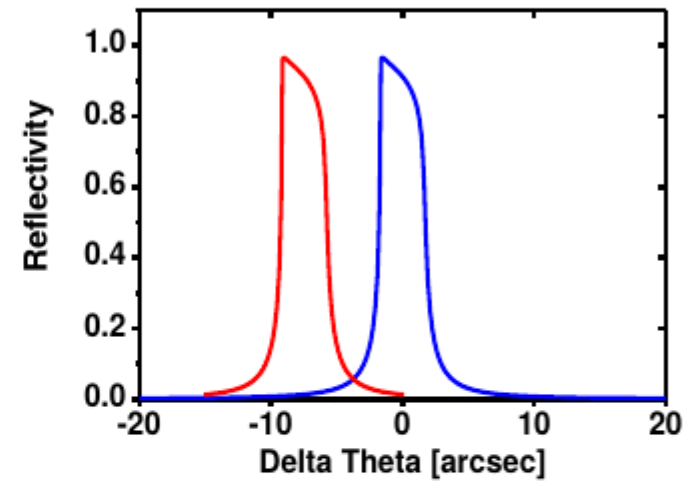
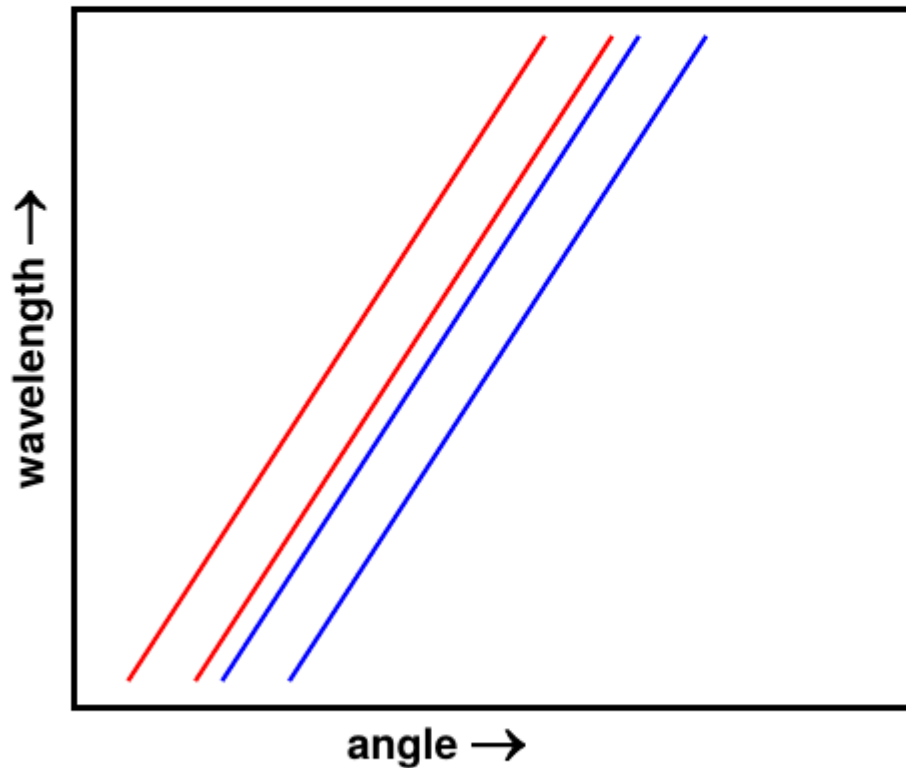
# Monochromátory



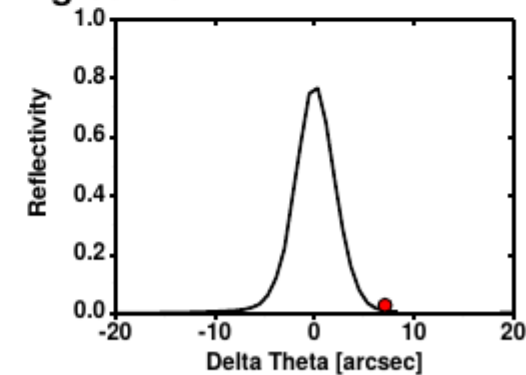
## DuMond Diagram / (n,-n) setup

Reflection curve of the collimator crystal

Reflection curve of the sample



Rocking curve



# Monochromátory



## Theoretical description (n,-n) setup

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Rocking curve:

$$R_c(\Delta\Theta) \propto K \int_{-\infty}^{\infty} C_1(x) C_2(x - \Delta\Theta) dx$$

$C_1, C_2$  - reflection curves of collimator and sample, respectively

$$R_c(0) = P \quad \text{percent reflection ( = 0.8 for absorption free case)}$$

**NO wavelength dependence of (n,-n) setup!**

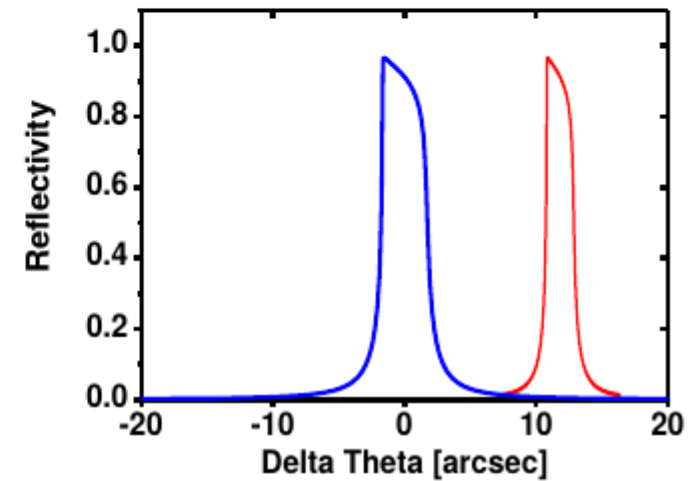
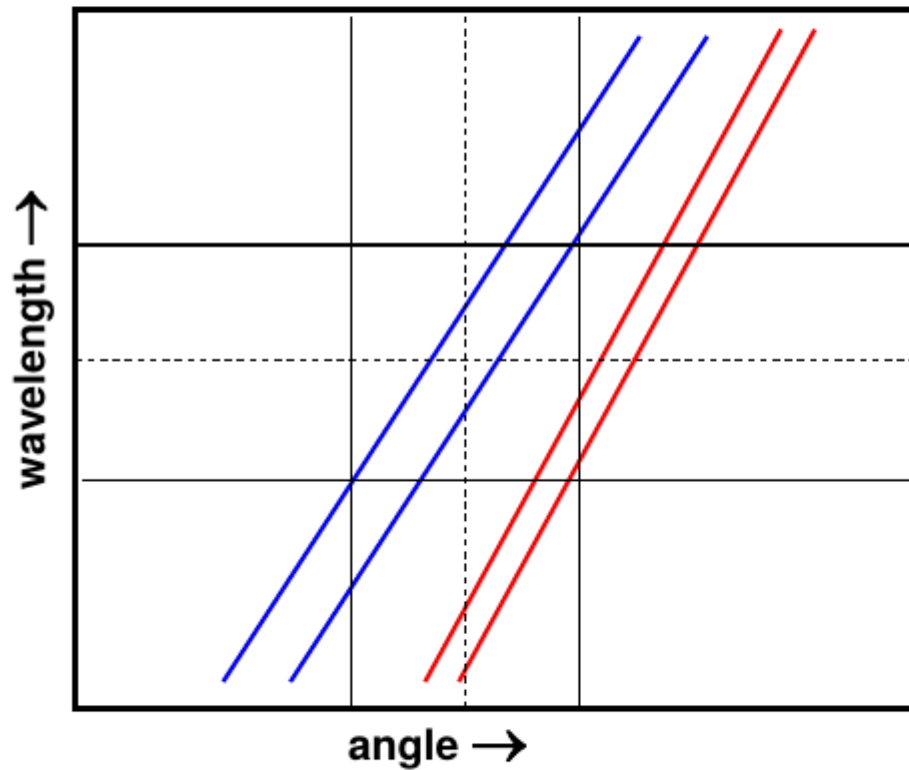
# Monochromátory



## DuMond Diagram / (n,-m) setup

Reflection curve of the collimator crystal  $(hkl)_c$

Reflection curve of the sample  $(hkl)_s$



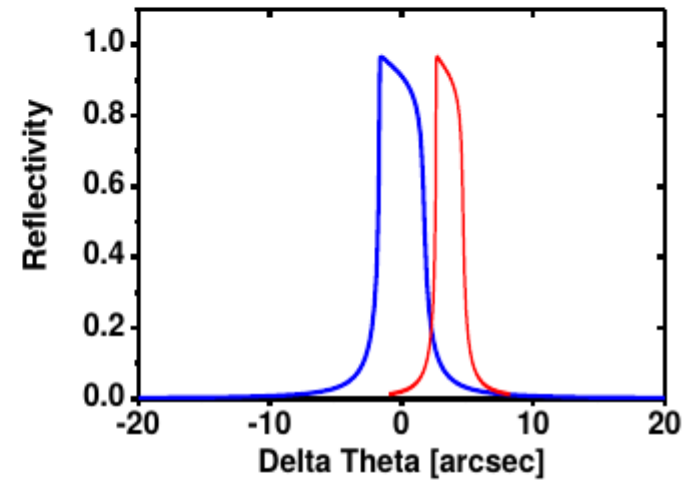
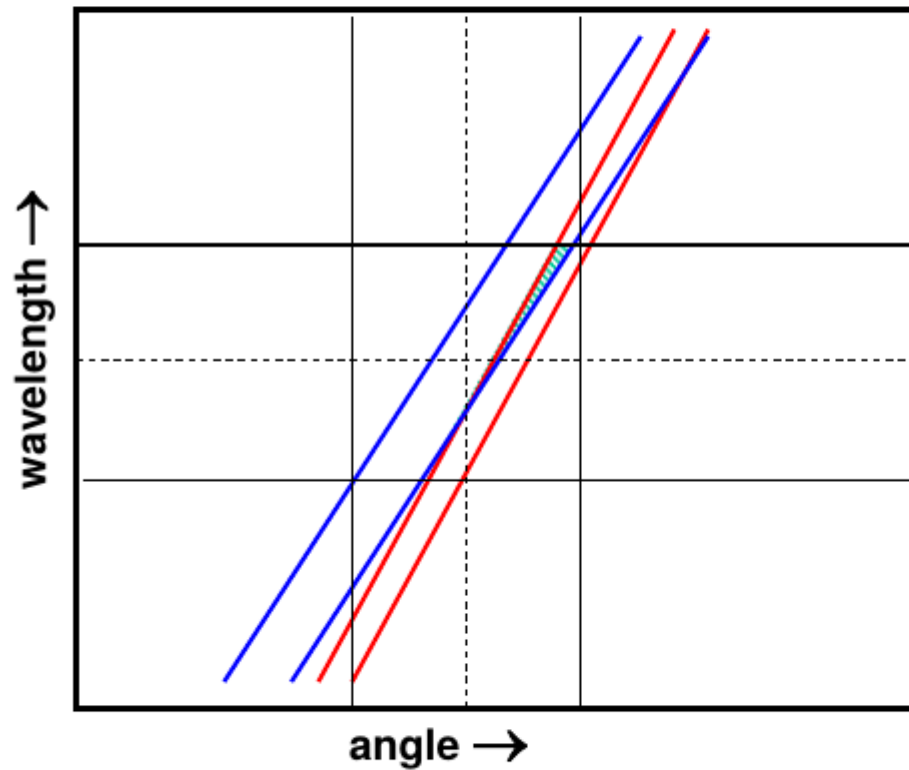
# Monochromátory



## DuMond Diagram / (n,-m) setup

Reflection curve of the collimator crystal  $(hkl)_c$

Reflection curve of the sample  $(hkl)_s$



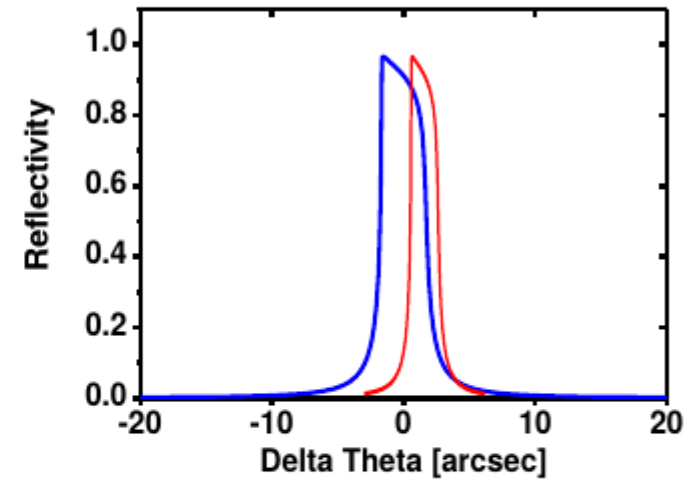
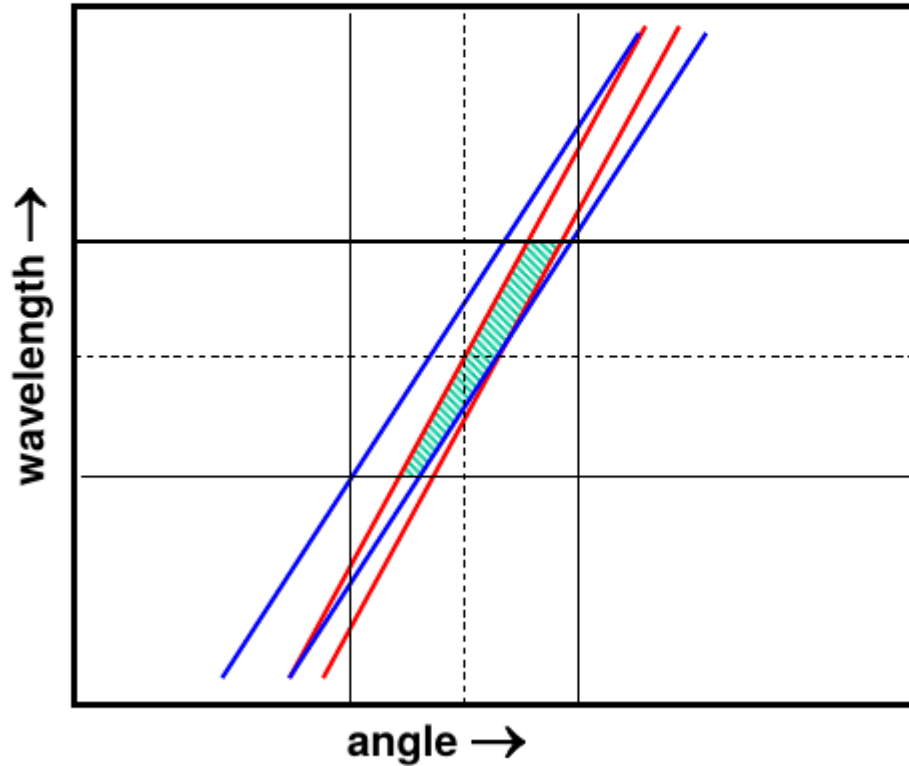
# Monochromátory



## DuMond Diagram / (n,-m) setup

Reflection curve of the collimator crystal  $(hkl)_c$

Reflection curve of the sample  $(hkl)_s$



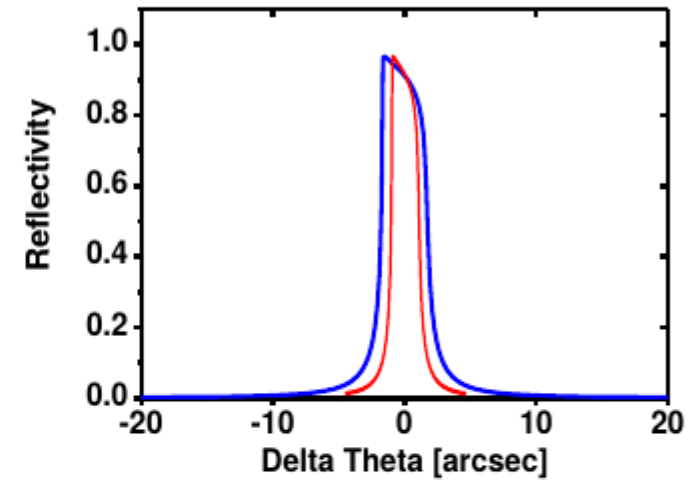
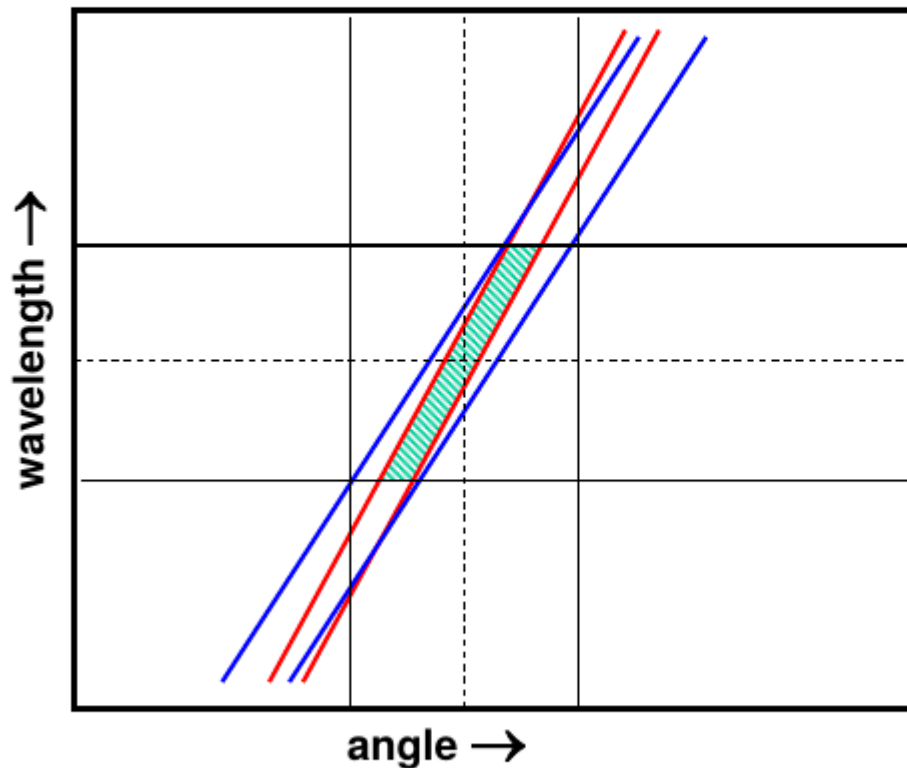
# Monochromátory



## DuMond Diagram / (n,-m) setup

Reflection curve of the collimator crystal  $(hkl)_c$

Reflection curve of the sample  $(hkl)_s$



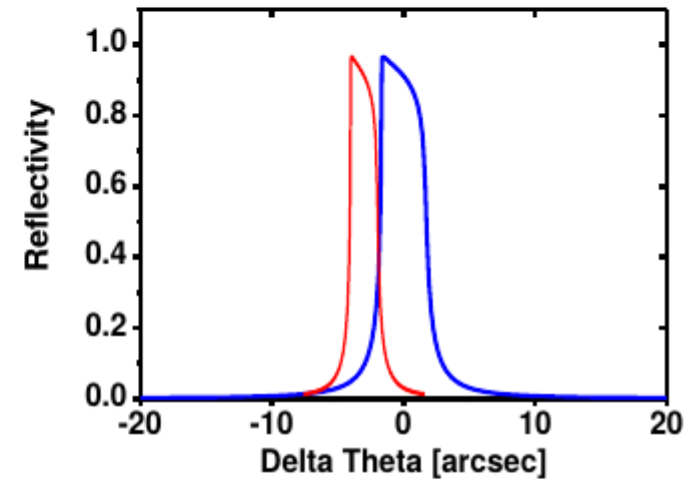
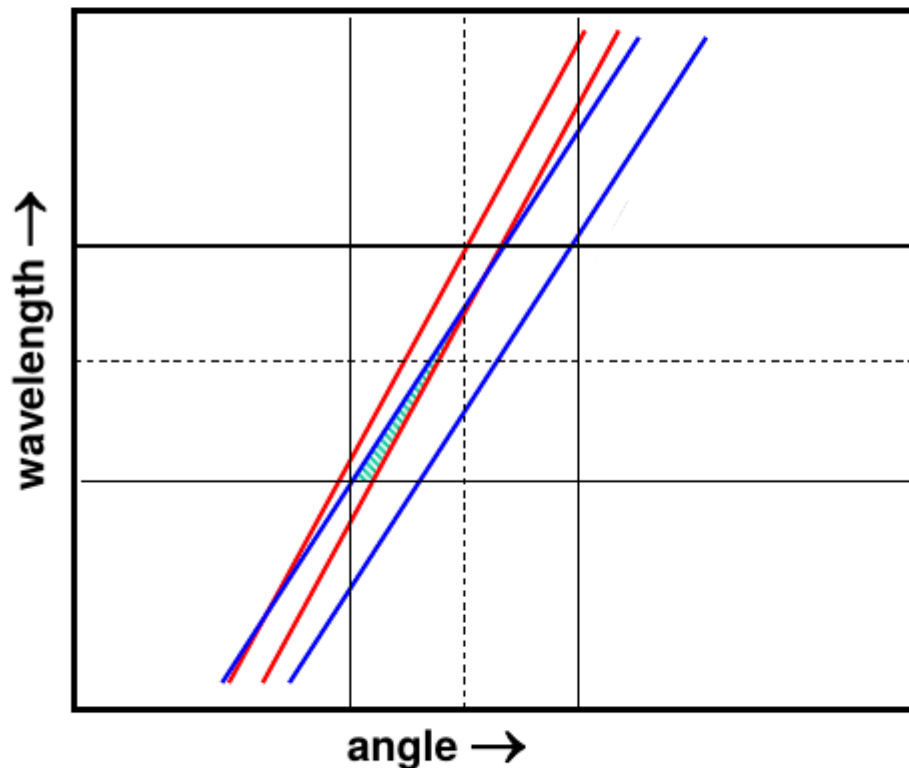
# Monochromátory



## DuMond Diagram / (n,-m) setup

Reflection curve of the collimator crystal  $(hkl)_c$

Reflection curve of the sample  $(hkl)_s$



The rocking curve of a (n,-m) setup is not only the convolution of two reflection curves.

Additional part by wavelength interval:

$$\delta\theta = \frac{\Delta\lambda}{\lambda} (\tan\theta_c - \tan\theta_s)$$

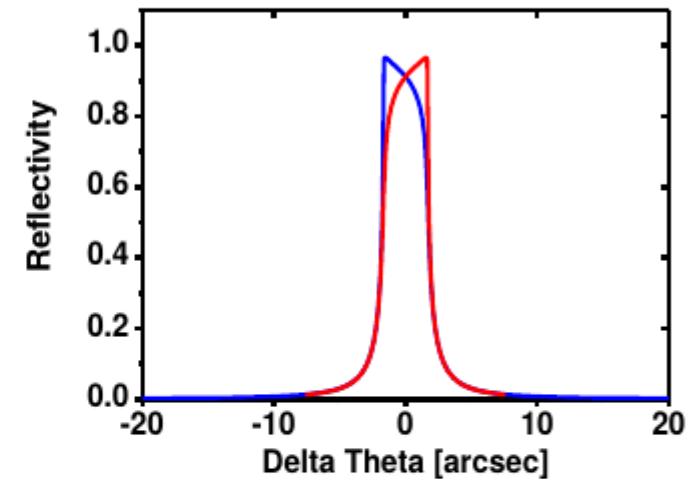
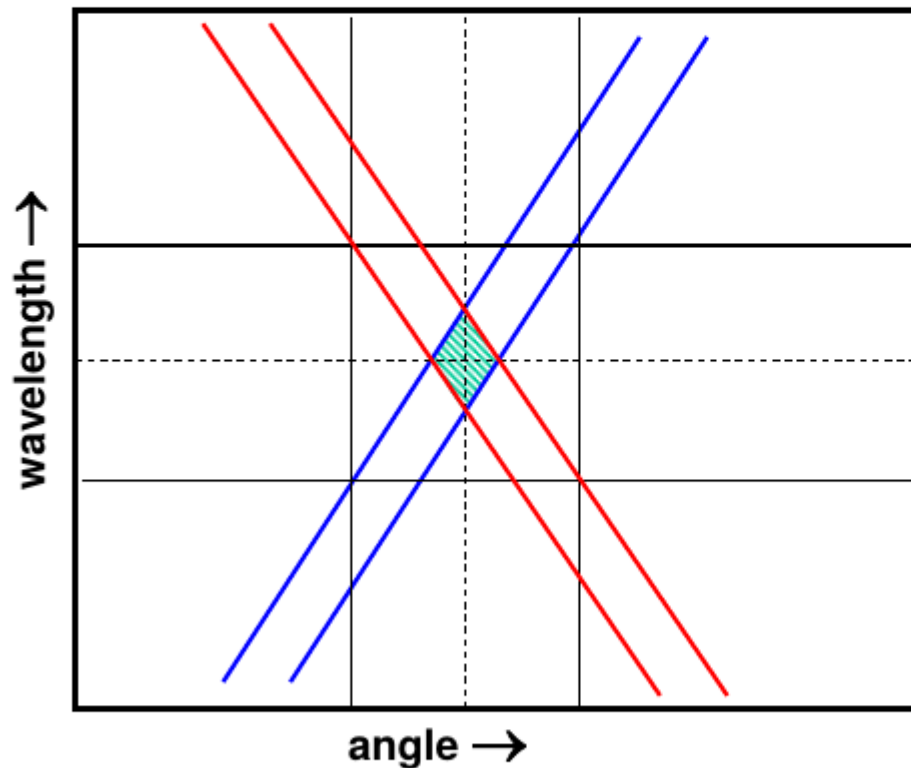
# Monochromator



## DuMond Diagram / (n,+n) setup

Reflection curve of the collimator crystal  $(hkl)_c$

Reflection curve of the sample  $(hkl)_s$



**Strongest influence of the wavelength interval:**

$$\delta\theta = \frac{\Delta\lambda}{\lambda} (\tan\theta_c + \tan\theta_s)$$



# Monochromátor



## Summary of DCD setups

**(n,-n)**  **parallel setup**

The diagram shows two parallel horizontal bars representing crystal surfaces. A green arrow enters from the left, hits the top bar, and reflects downwards. It then hits the bottom bar and reflects upwards, continuing in a parallel path to the right.

⇒ non-dispersive arrangement ⇒ **ideal for reflection curve analysis**  
⇒ **high intensity**

**(n,-m)** 

The diagram shows two crystal surfaces. The top one is horizontal, and the bottom one is tilted downwards. A green arrow enters from the left, hits the top surface, and reflects downwards. It then hits the tilted bottom surface and reflects upwards, continuing to the right.

⇒ slightly dispersive arrangement ⇒ dispersive increase in rocking curve  
width depends on the difference of both Bragg angles

**(n,+n)**  **anti-parallel setup**

The diagram shows two crystal surfaces. The top one is horizontal, and the bottom one is tilted downwards. A green arrow enters from the left, hits the top surface, and reflects downwards. It then hits the tilted bottom surface and reflects downwards, continuing to the right.

⇒ strong dispersive arrangement ⇒ **usable for monochromatization**  
⇒ **lower intensity**

# Monochromátory



## Crystal collimator optics

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These different double crystal setups can be used not only as diffractometer arrangements (collimator + sample), but also in different combinations as collimator / monochromator only !

⇒ **crystal collimator optics**

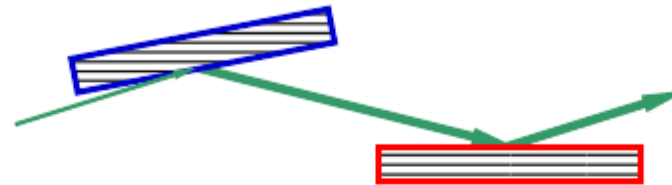
- **asymmetric reflection**
- **channel-cut**
- **Bartels monochromator**

# Monochromátory

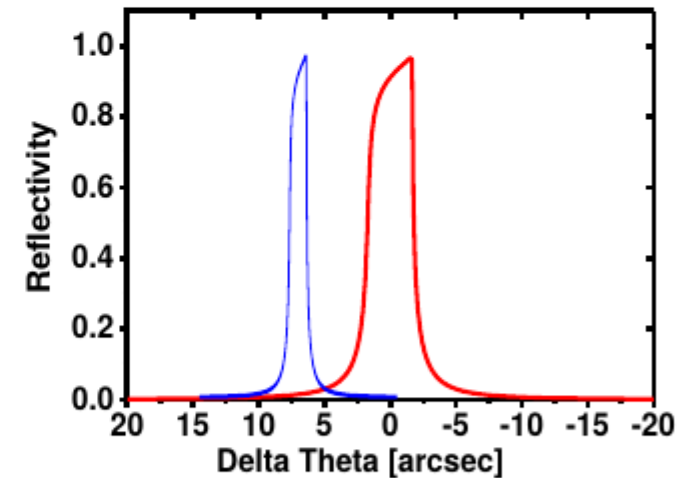
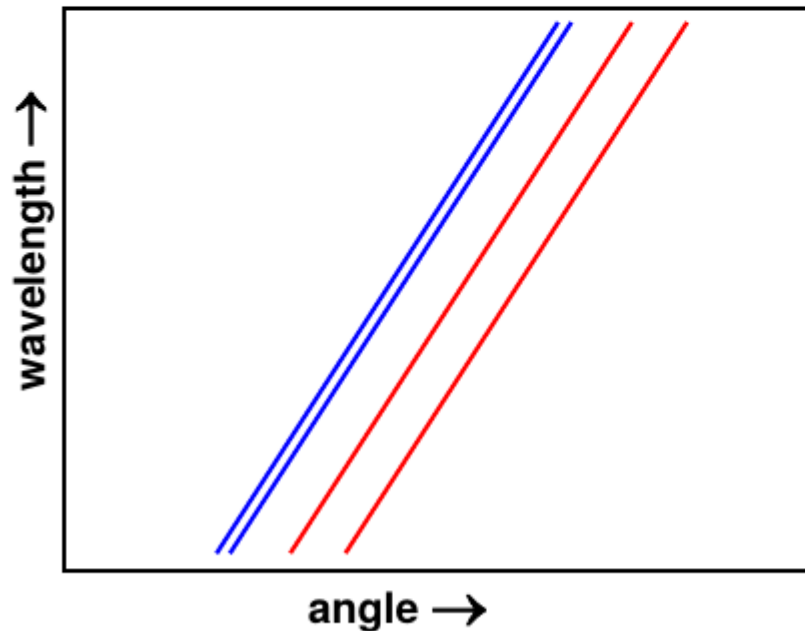


## Asymmetric reflection

asymmetric (n,-n)



beam divergency in/decreases with  $\sqrt{|b|}$  - beam width with  $\sqrt{\frac{1}{|b|}}$



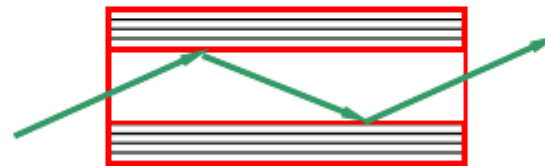
⇒ high angular resolution

# Monochromátory

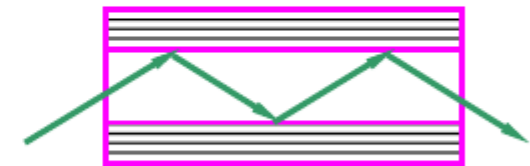


## Channel-cut

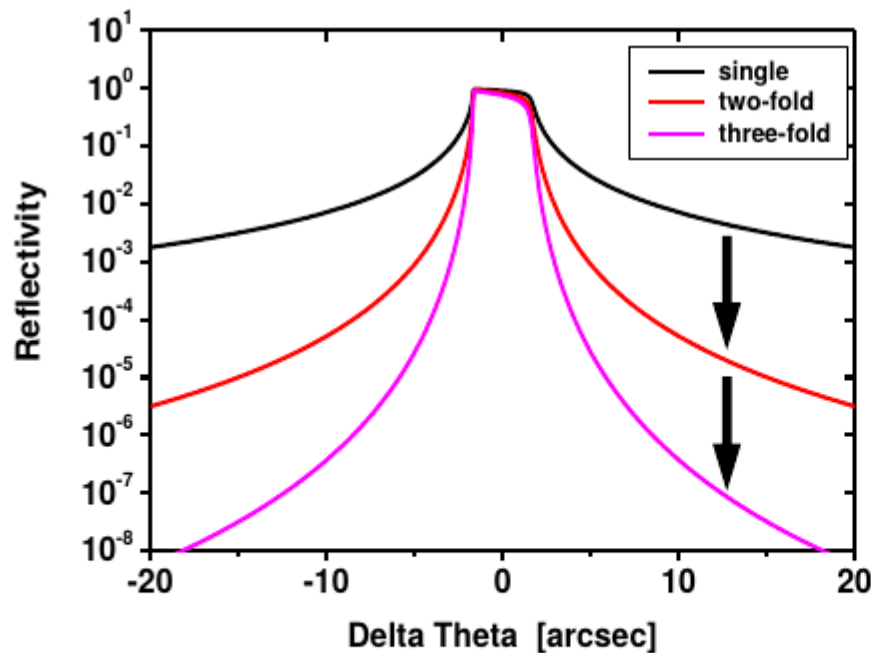
symmetric (n,-n) setup  
exactly parallel



two-fold



three-fold



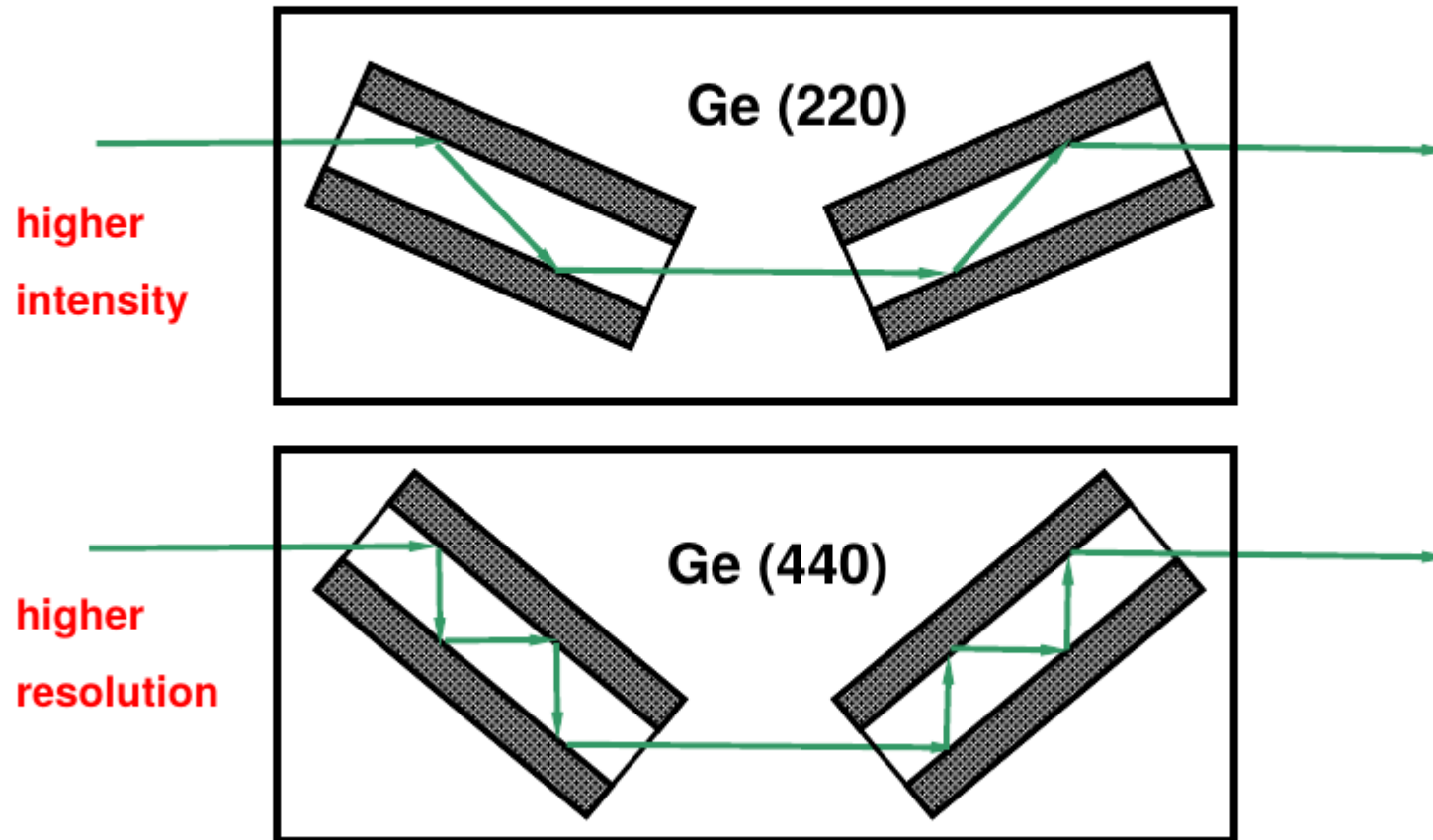
⇒ strong reduction of the  
reflection curve tails

# Monochromátory



## Bartels monochromator

(“4-bounce” beam conditioner, Beaumont-Hart Channel design)

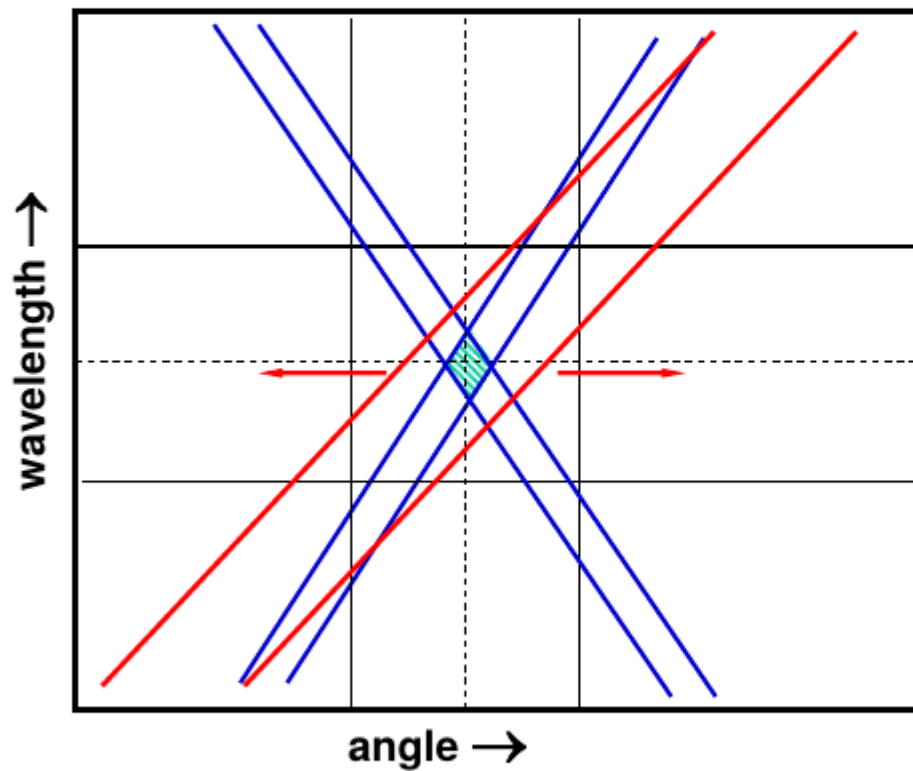


# Monochromátory



## DuMond Diagram / Bartels monochromator

The Bartels setup is monochromator and collimator in one !

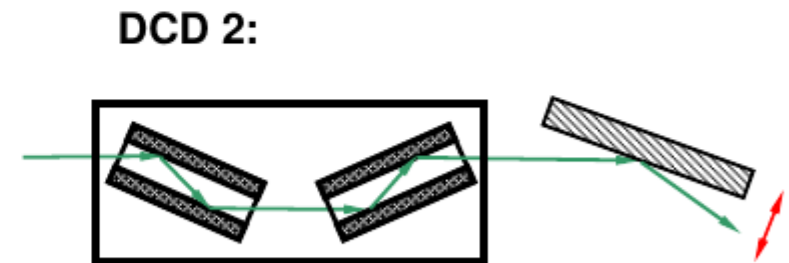
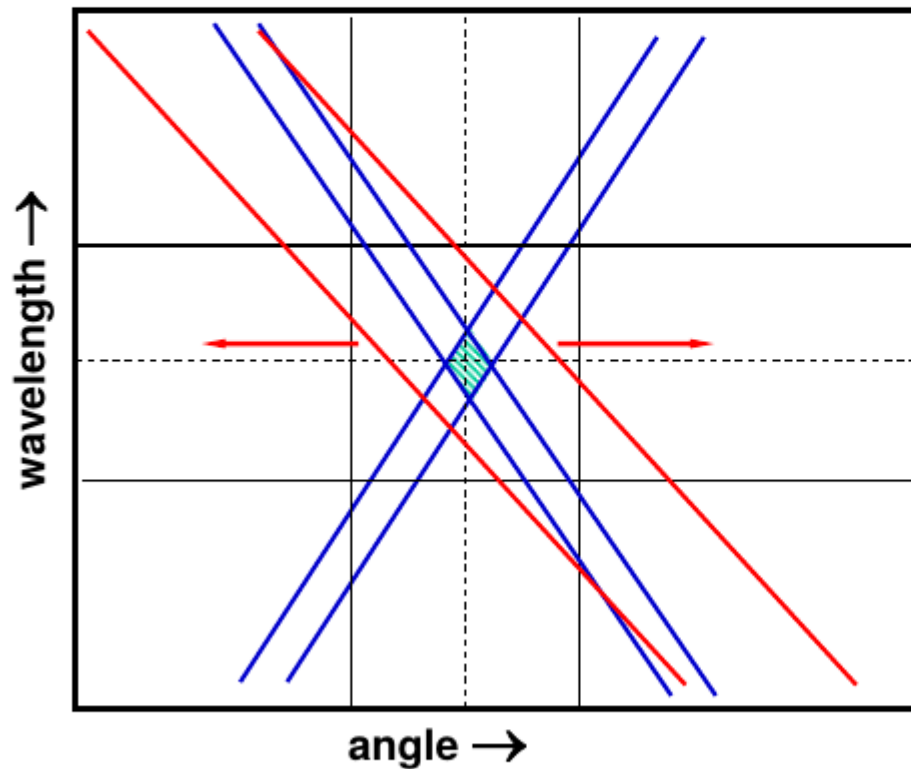


# Monochromátory



## DuMond Diagram / Bartels monochromator

The Bartels setup is monochromator and collimator in one !

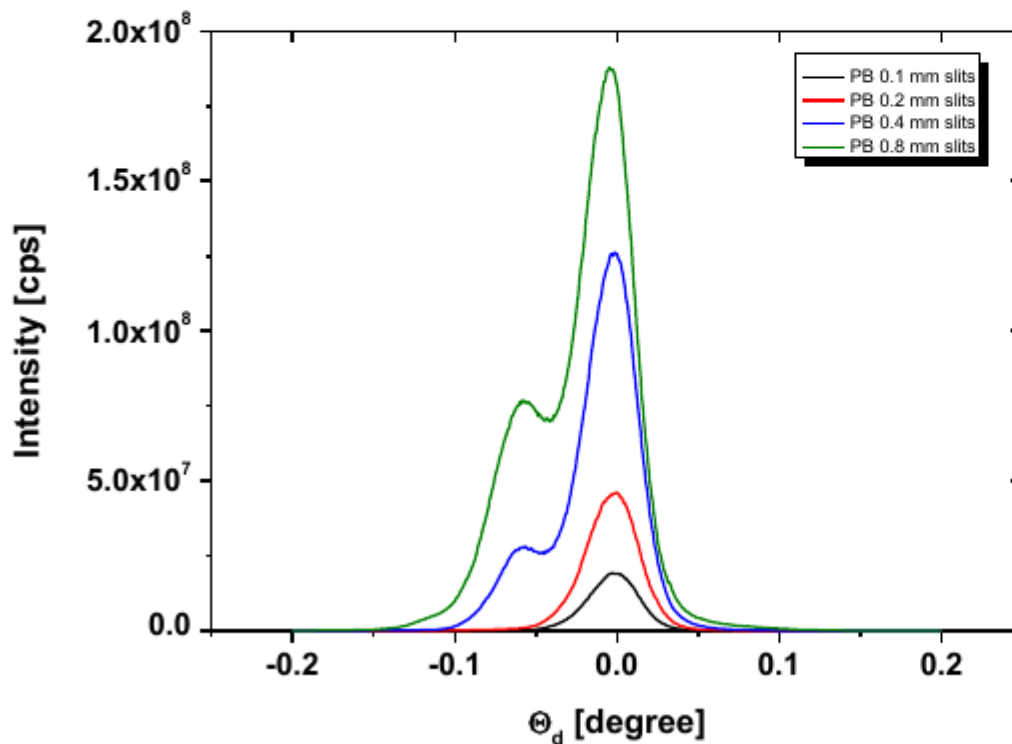
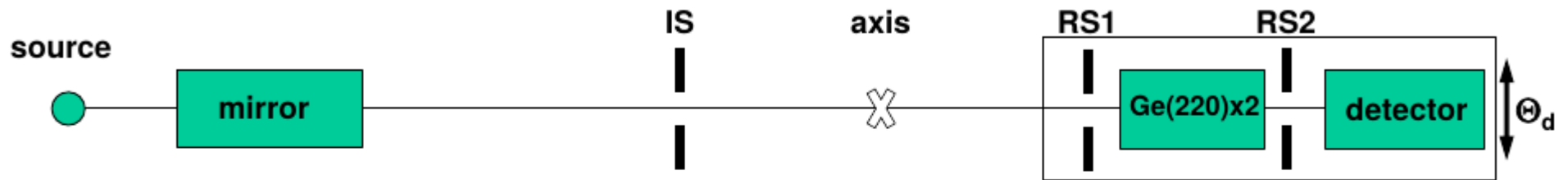


**Usable for all reflections !**

# Skenování



## Collimator test / 1

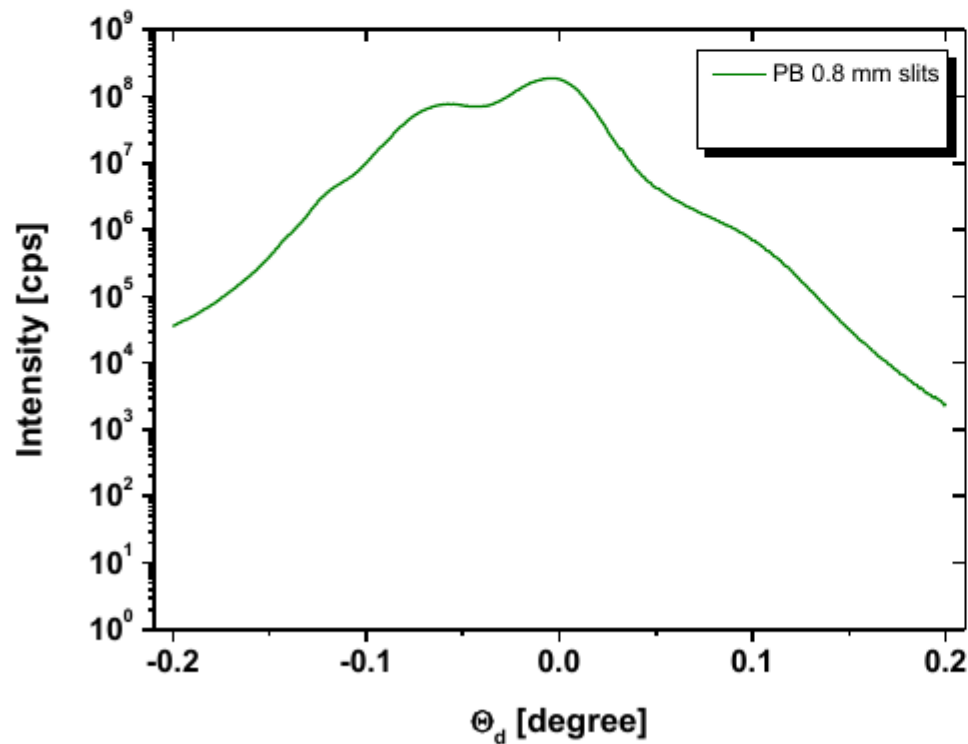




# Skenování



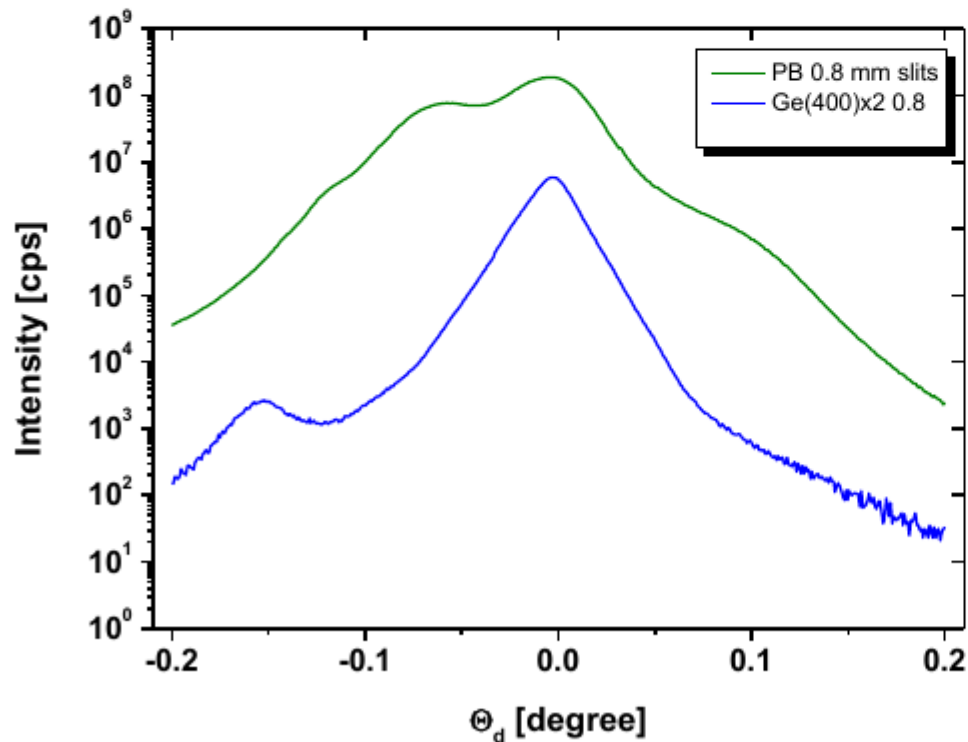
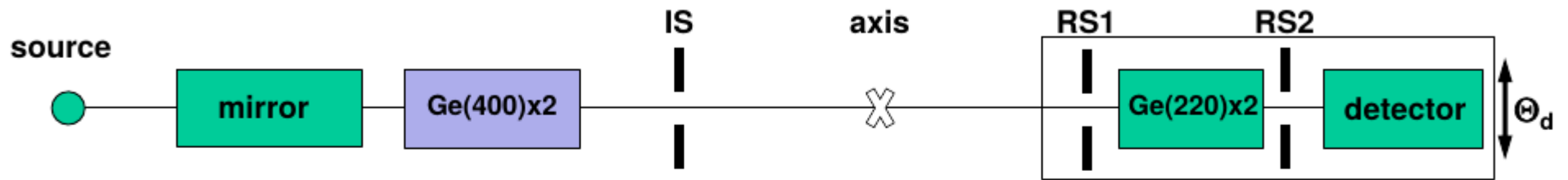
## Collimator test / 2



# Skenování



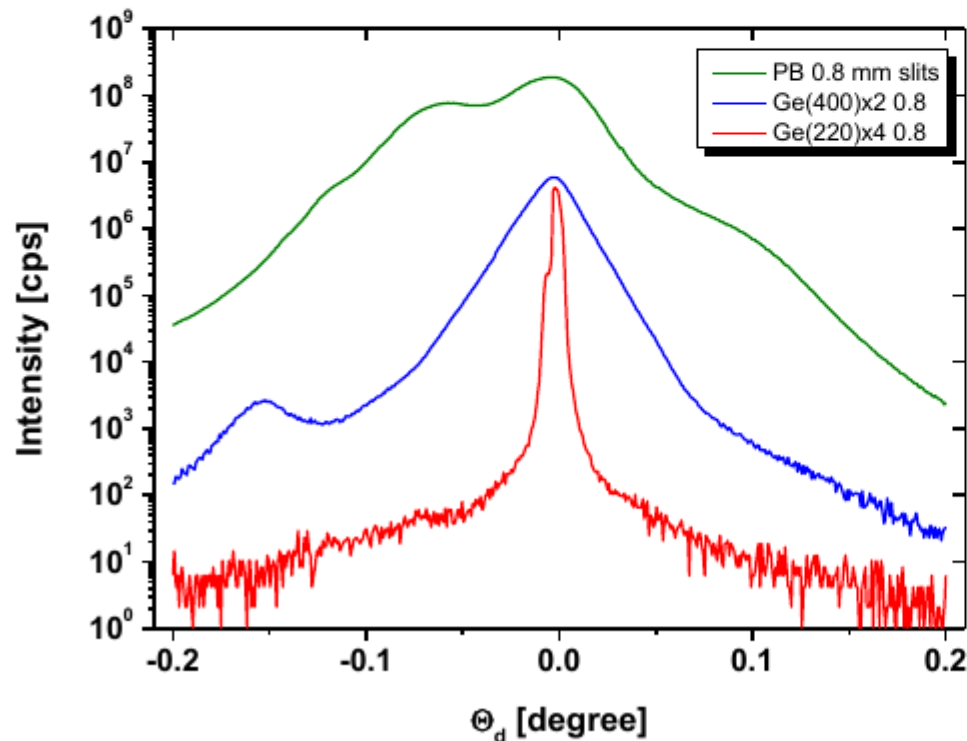
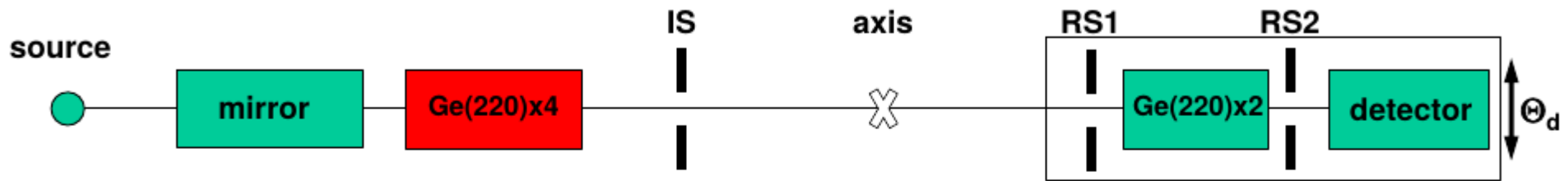
## Collimator test / 2



# Skenování



## Collimator test / 2

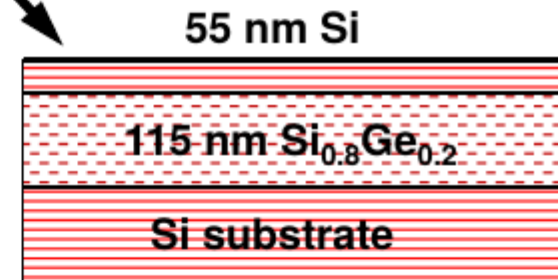
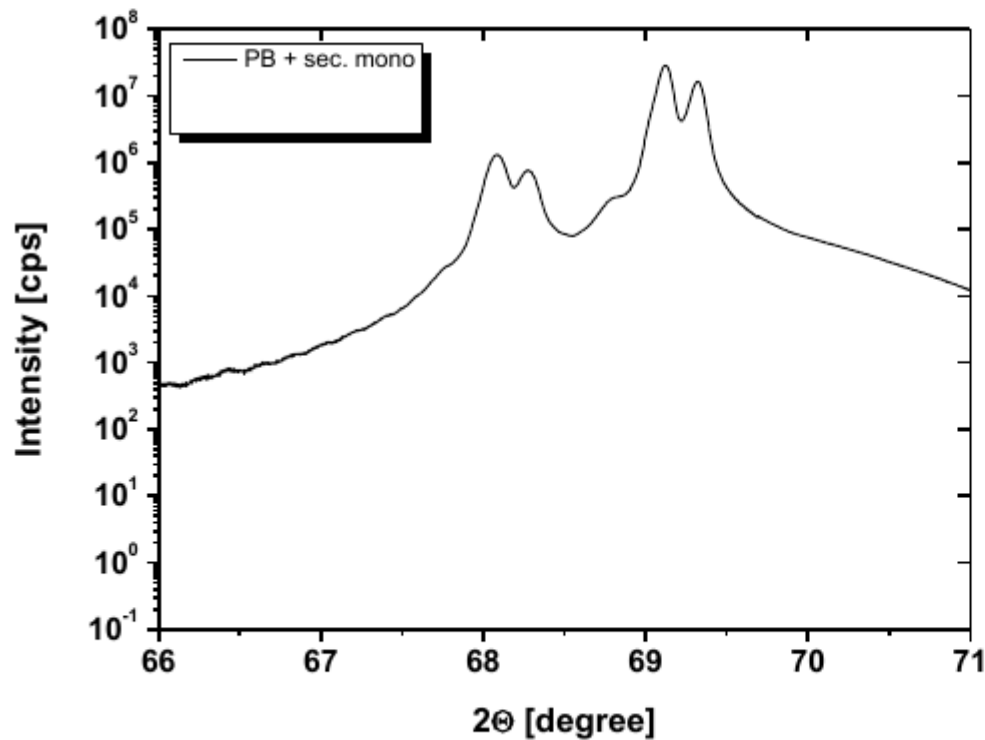
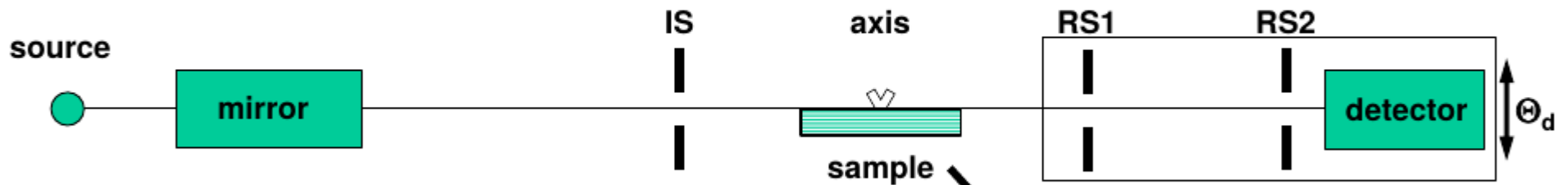


**Barthels monochromator generates the best defined beam**

# Skenování



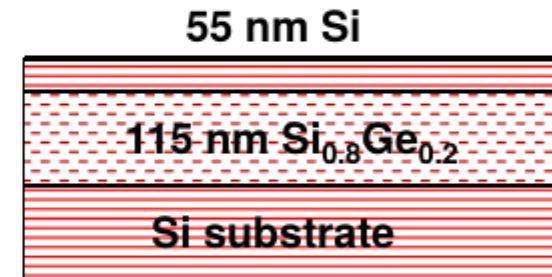
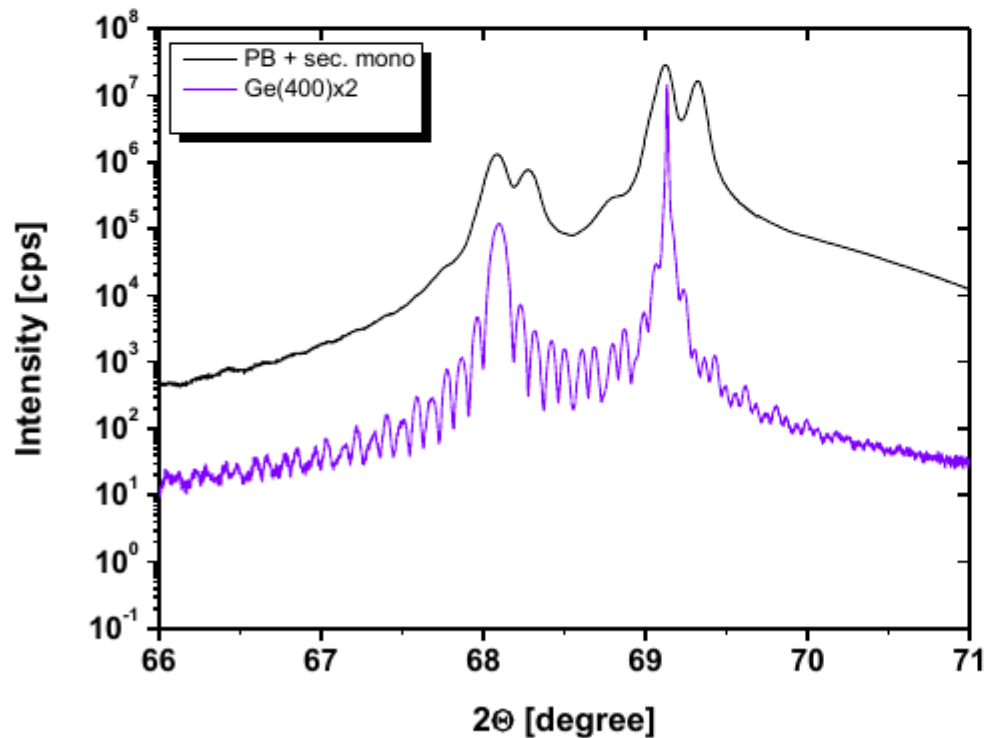
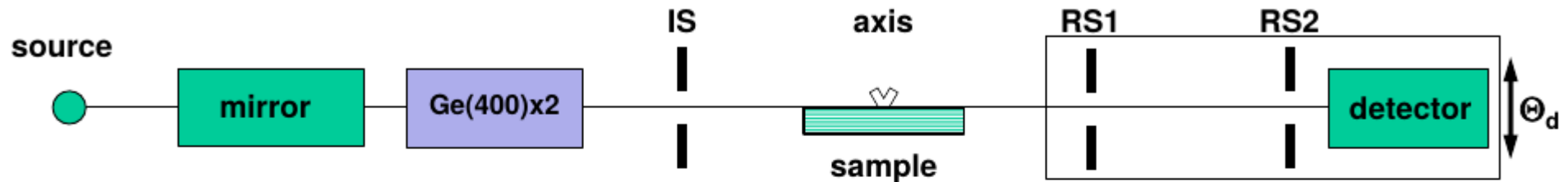
## Collimator test / SiGe sample



# Skenování



## Collimator test / SiGe sample

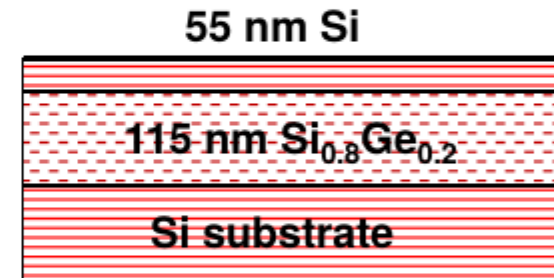
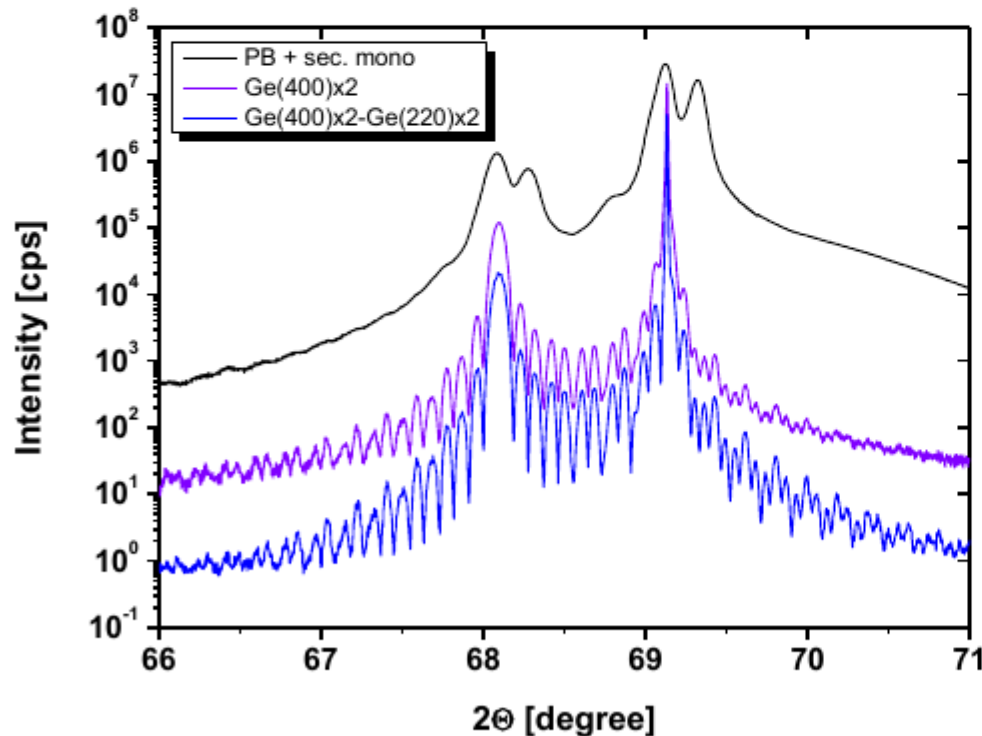
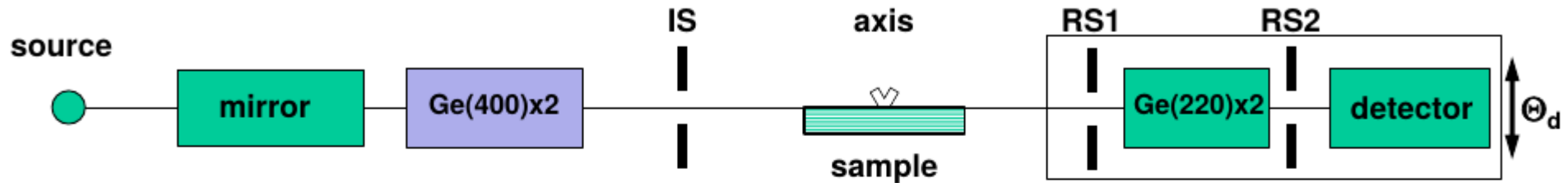


**PB configuration (without crystal collimator) makes no sense.**

# Skenování



## Collimator test / SiGe sample

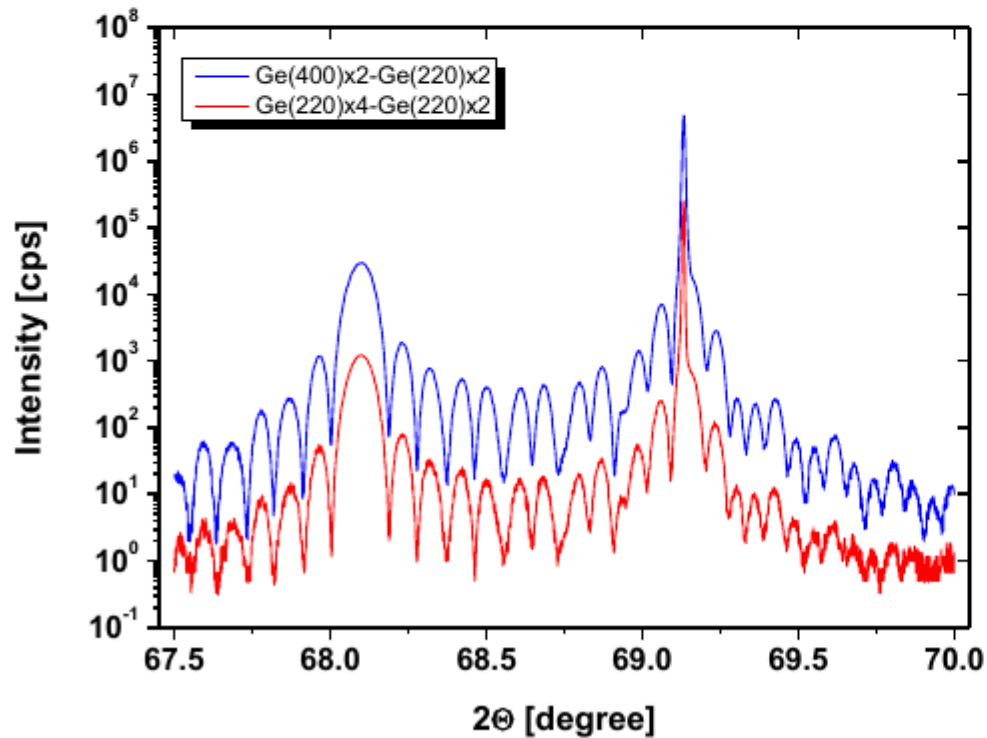
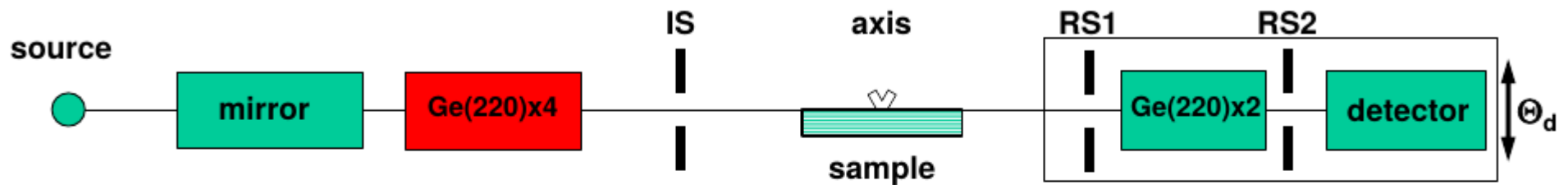


**Collimator + analyzer configuration gives best signal to noise ratio.**

# Skenování



## Collimator comparison / SiGe sample

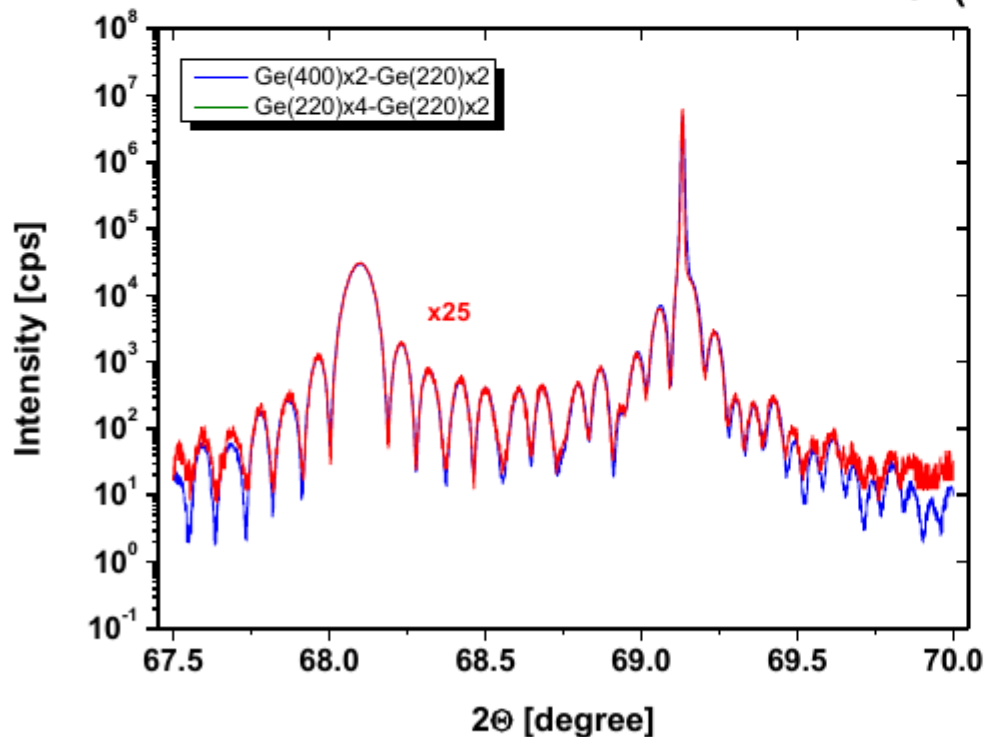
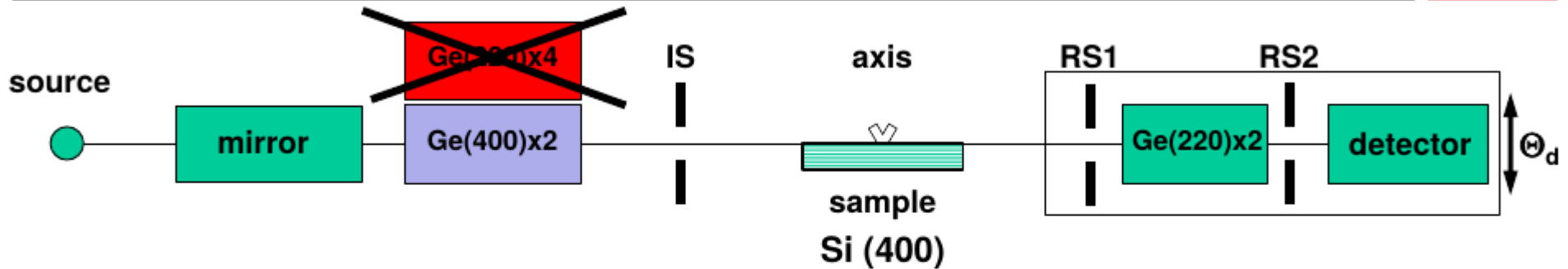


**Barthels collimator causes significantly lower intensity.  
But, is there something really better?**

# Skenování



## Collimator comparison / SiGe sample



answer: **NO !**

25 x less intensity,  
problems with background  
same resolution

$$\delta\Theta = \frac{\Delta\lambda}{\lambda} (\tan\Theta_c - \tan\Theta_s)$$

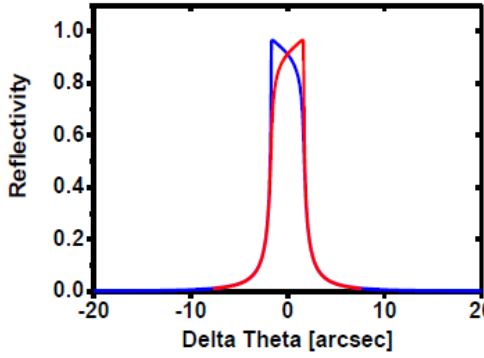
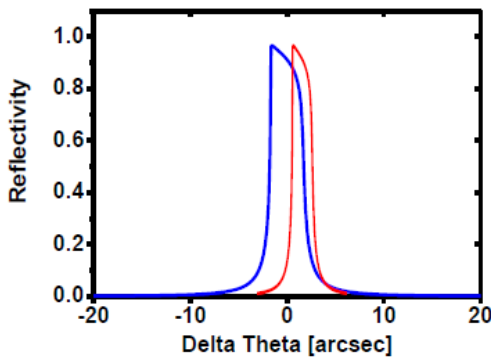
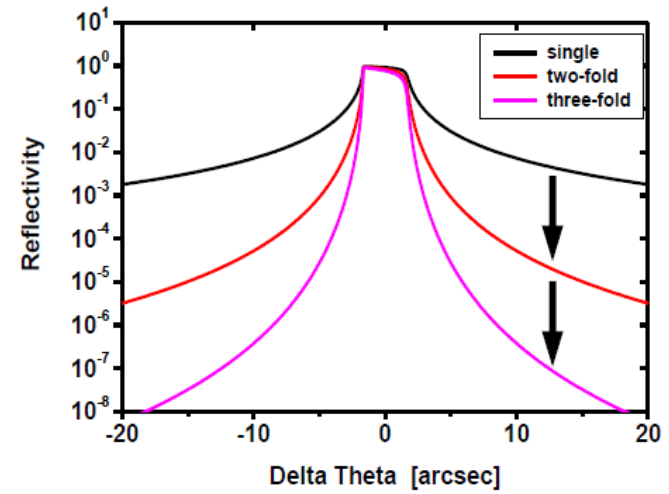
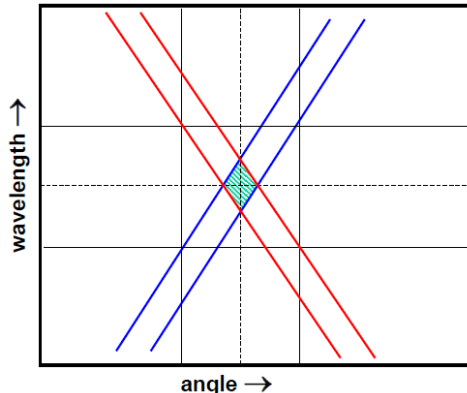
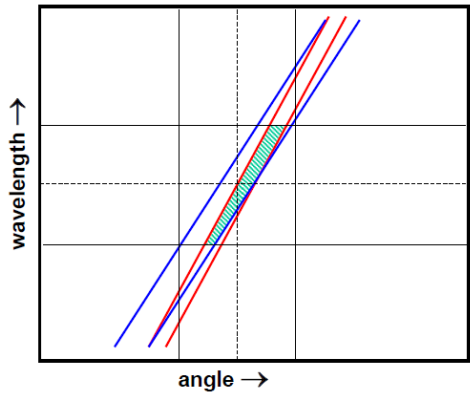
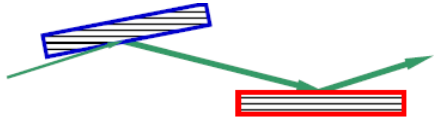
$$= 2.8 \cdot 10^{-4} (\tan 34.566^\circ - \tan 33.0^\circ)$$

$$\sim 2'' \text{ or } 0.0006^\circ$$

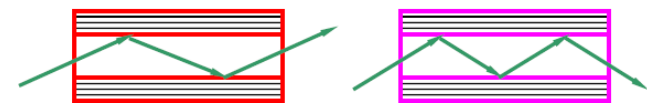


# Monochromátory

Nebo také dalším krystalem

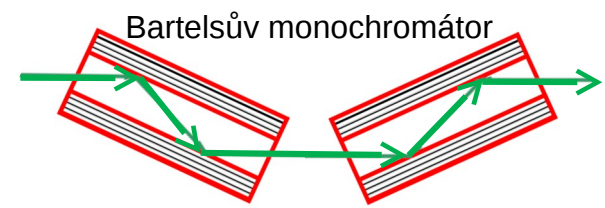


paralelní, nedisperzní usp.  
(n,-n)



paralelní,  
mírně disperzní usp.  
(n,-m)

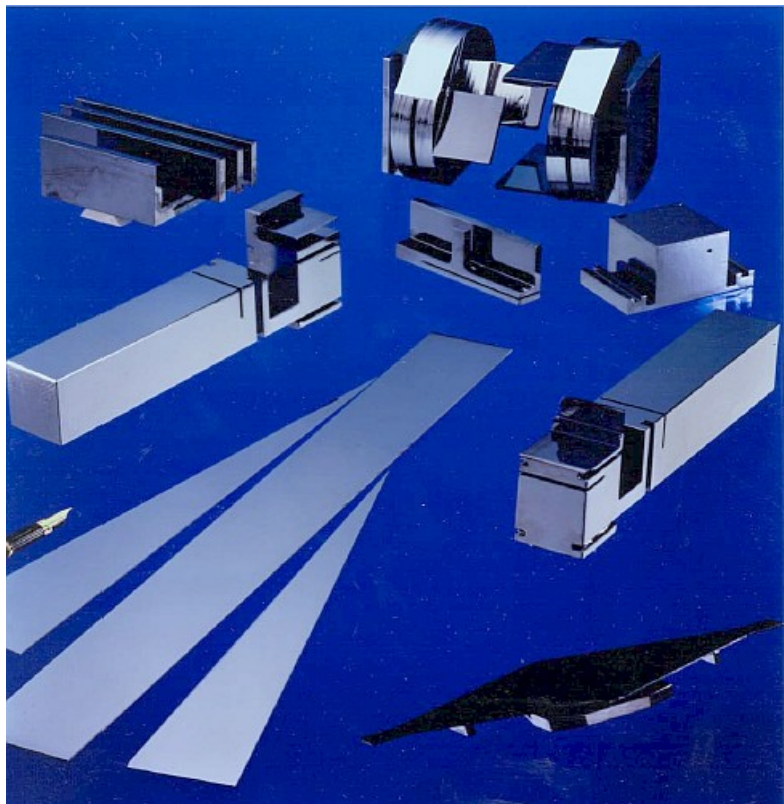
anti paralel.  
disperzní usp.  
pro monochmatizaci  
(n,+n)



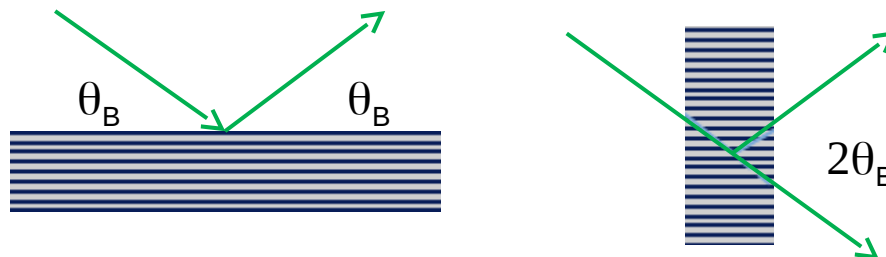
Monochromátor a kolimátor v jednom

# Monochromátory

Na synchrotronech se někdy používají sofistikované systémy krystalových monochromátorů



V uspořádání i na odraz i na průchod



Jedná se o dokonalé krystaly (Si, Ge, diamant, ...)

Upravené pro monochromátory – řezáním, leptáním, leštěním se správnou orientací

Bez deformace, správně upevněné  
Vyžadují náročný složitý chladicí systém

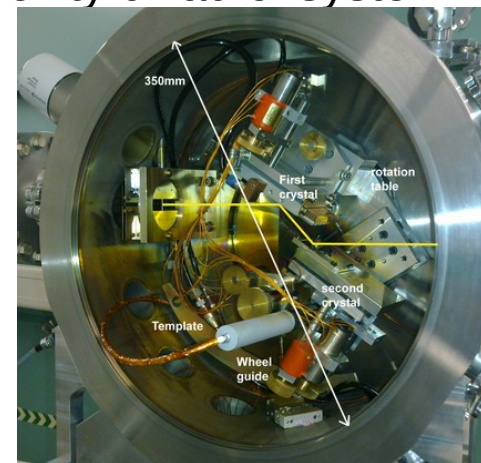
Monochromátory poskytující vysoké rozlišení

$$10^{-8} < \Delta E/E < 10^{-3}$$

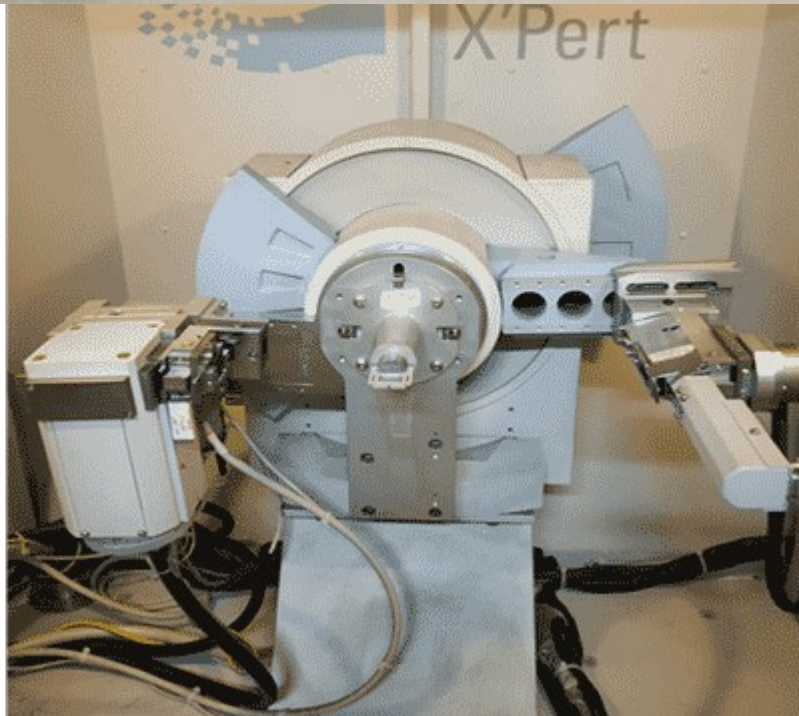
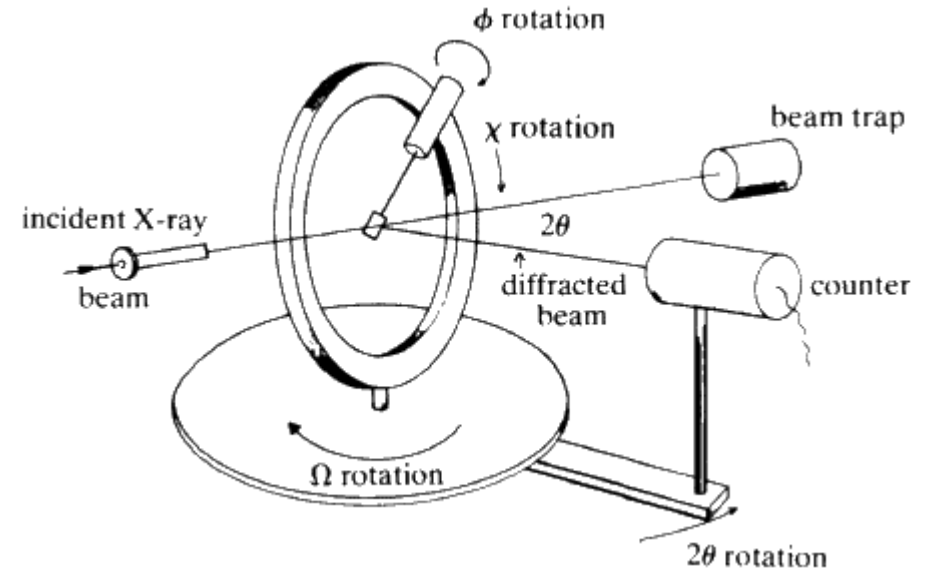
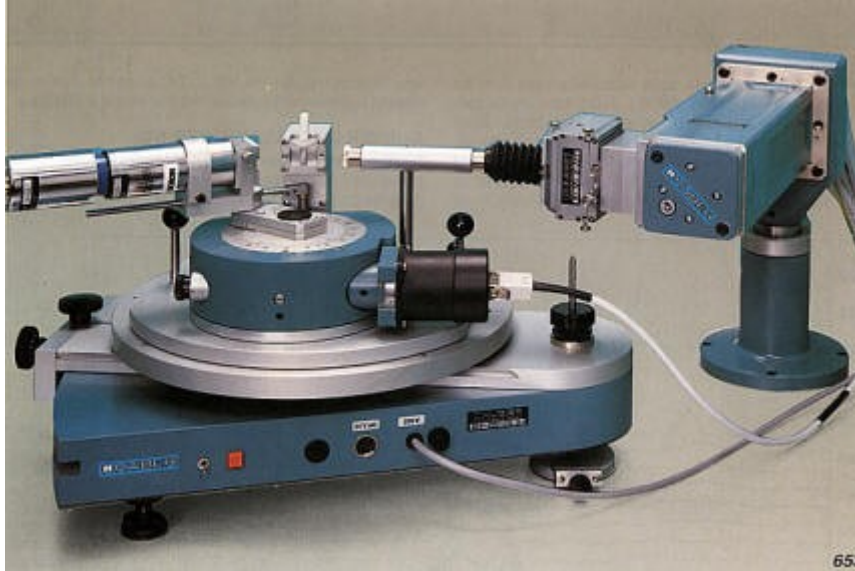
Monochromátory s fokusací – ohnuté krystaly

Kolimátory/ rozšiřovače svazků – asymetricky řezané

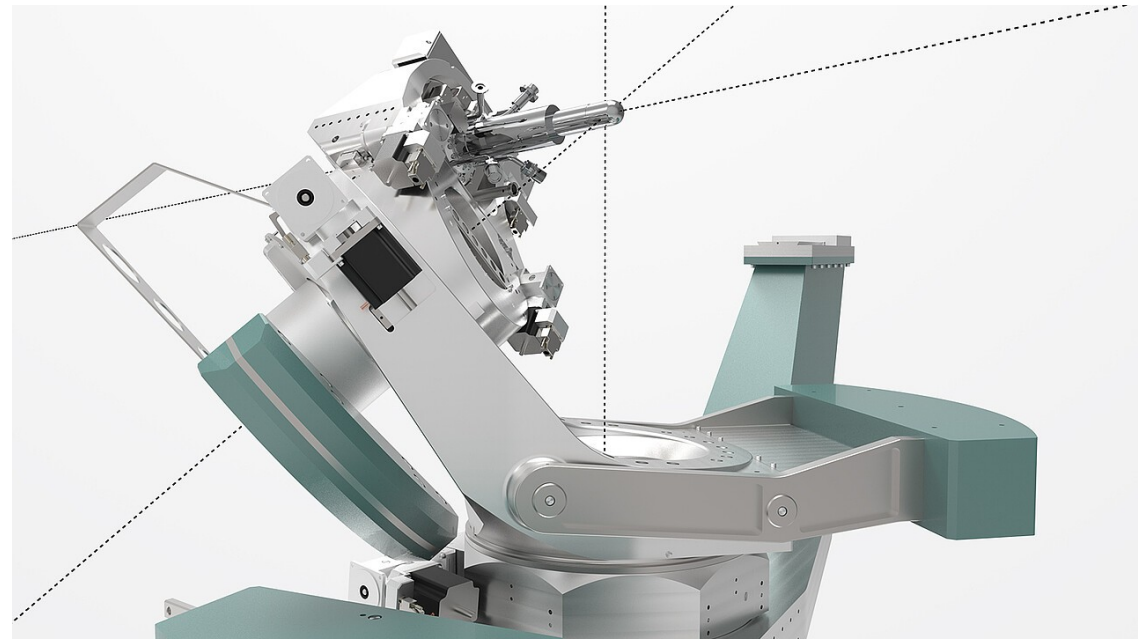
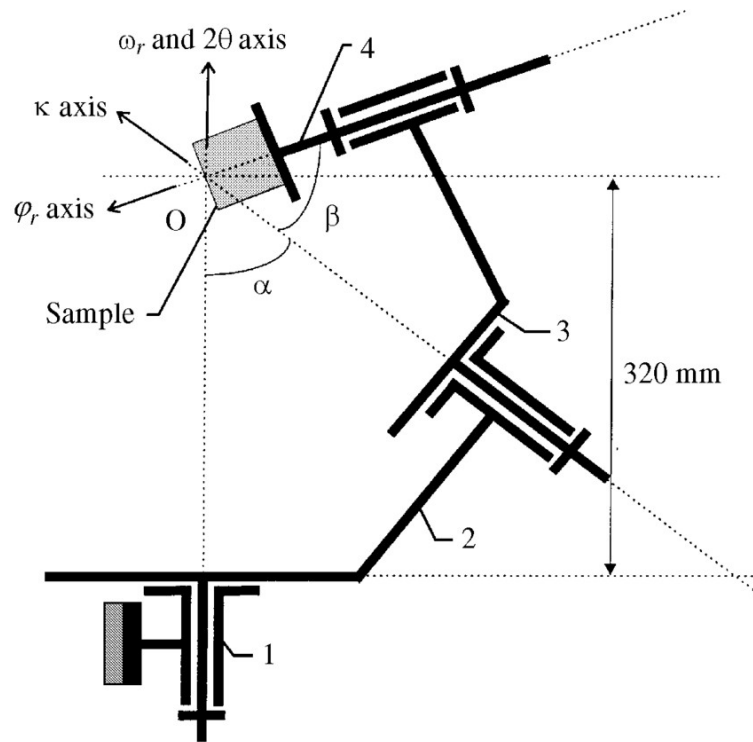
Fázové destičky



# Goniometry



# Goniometry



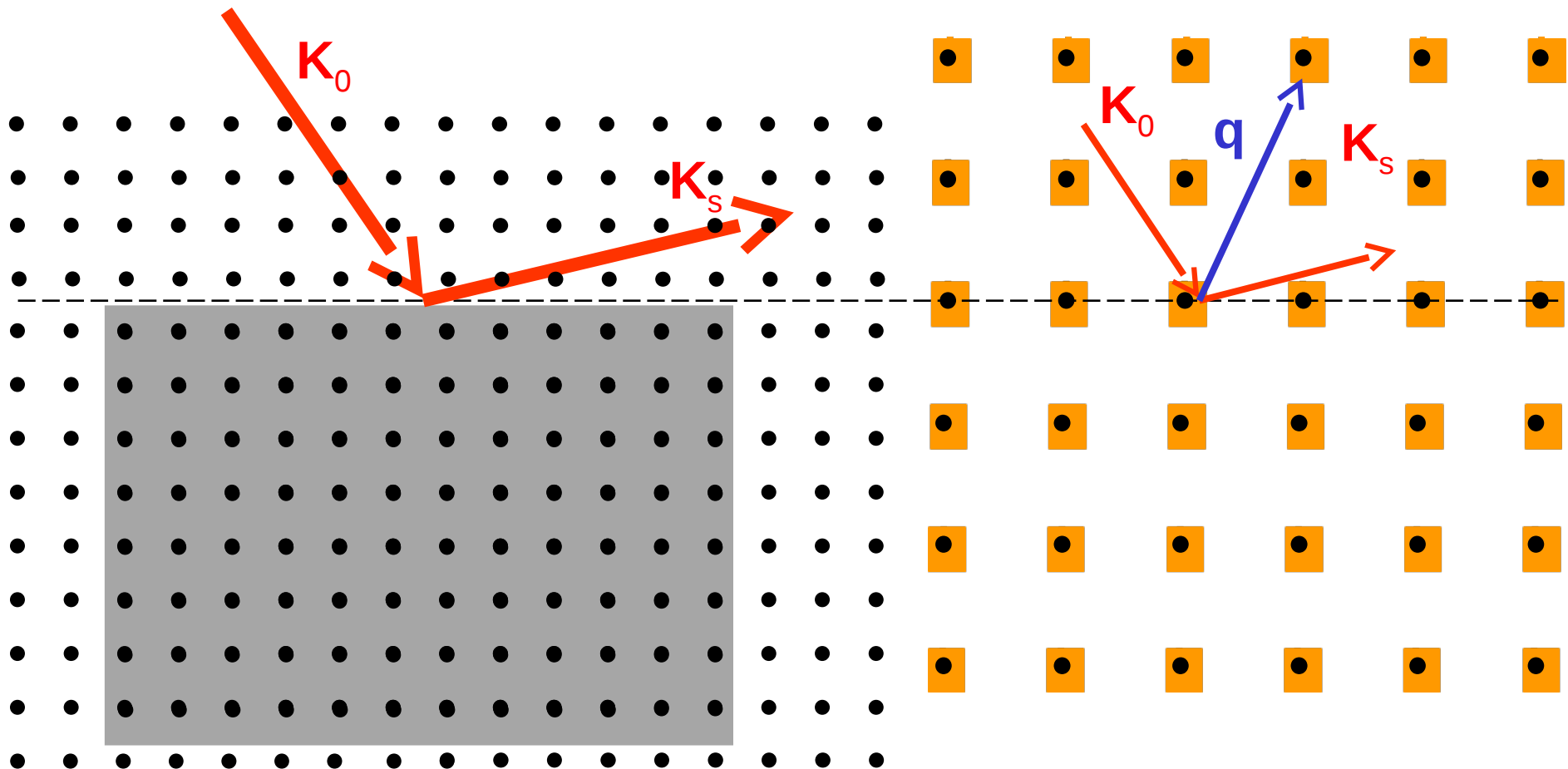
# Rozlišení v recipročním prostoru

Rozptýlená intenzita:  $I \sim \int d\Omega \ (d\sigma/d\Omega)$        $\mathbf{q} = \mathbf{K}_s - \mathbf{K}_0$

$$d\sigma/d\Omega \sim |\rho^{\text{FT}}(\mathbf{q})|^2 = \left| \sum_g \rho_g^{\text{FT}}(\mathbf{q}) S_g^{\text{FT}}(\mathbf{q}) \right|^2$$

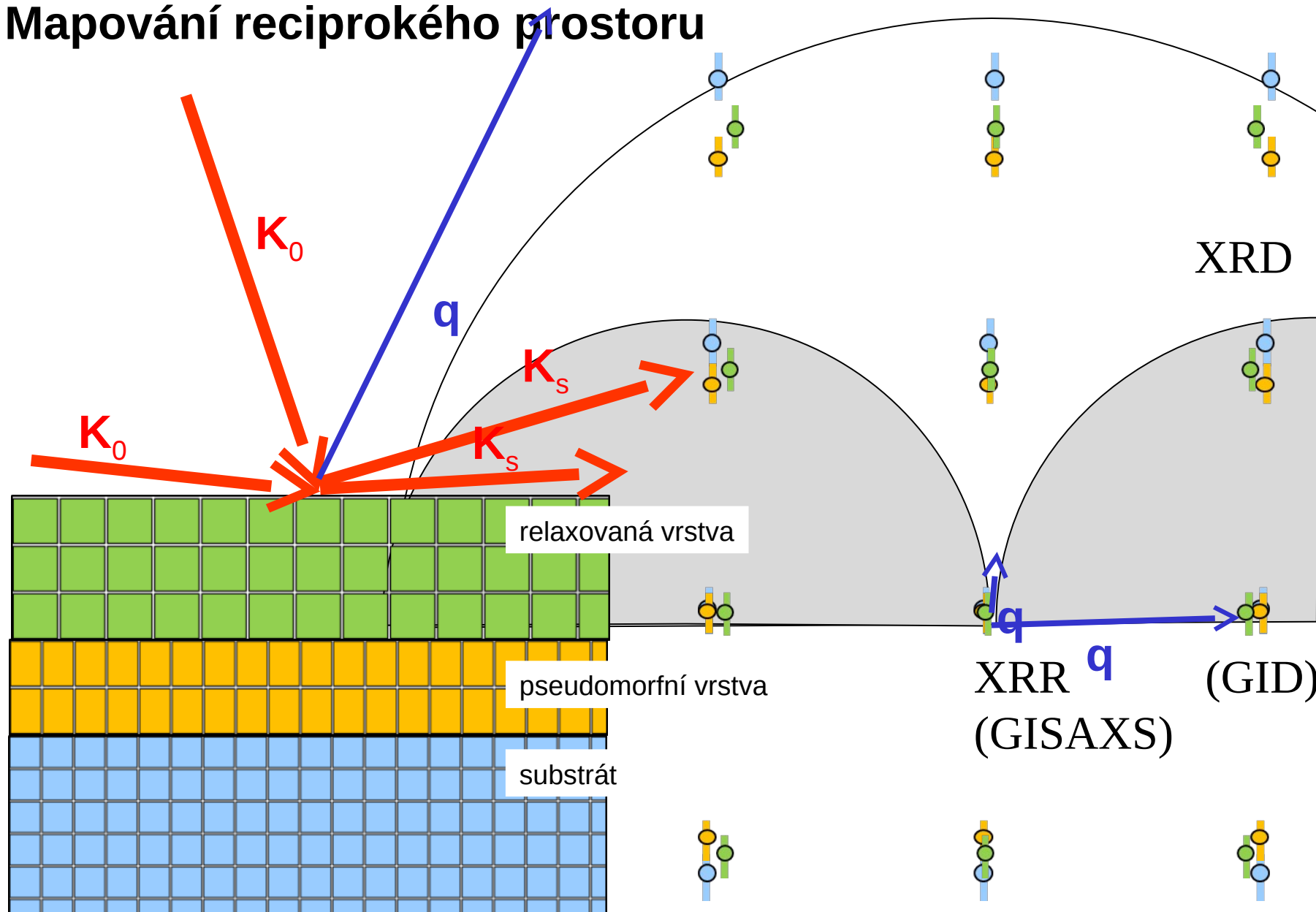
Přímý prostor

Reciproký prostor



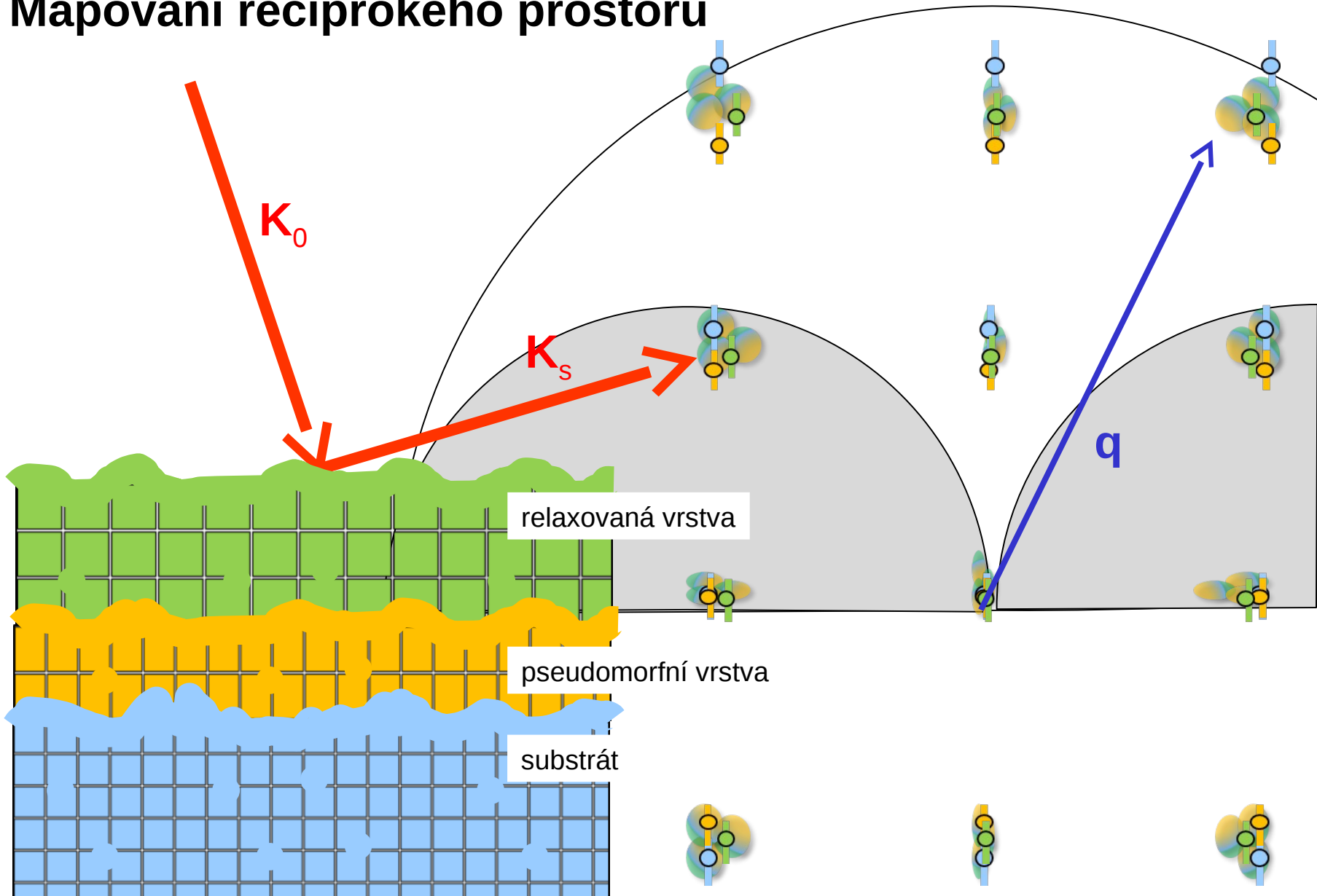
# Rozlišení v recipročním prostoru

## Mapování recipročního prostoru



# Rozlišení v recipročním prostoru

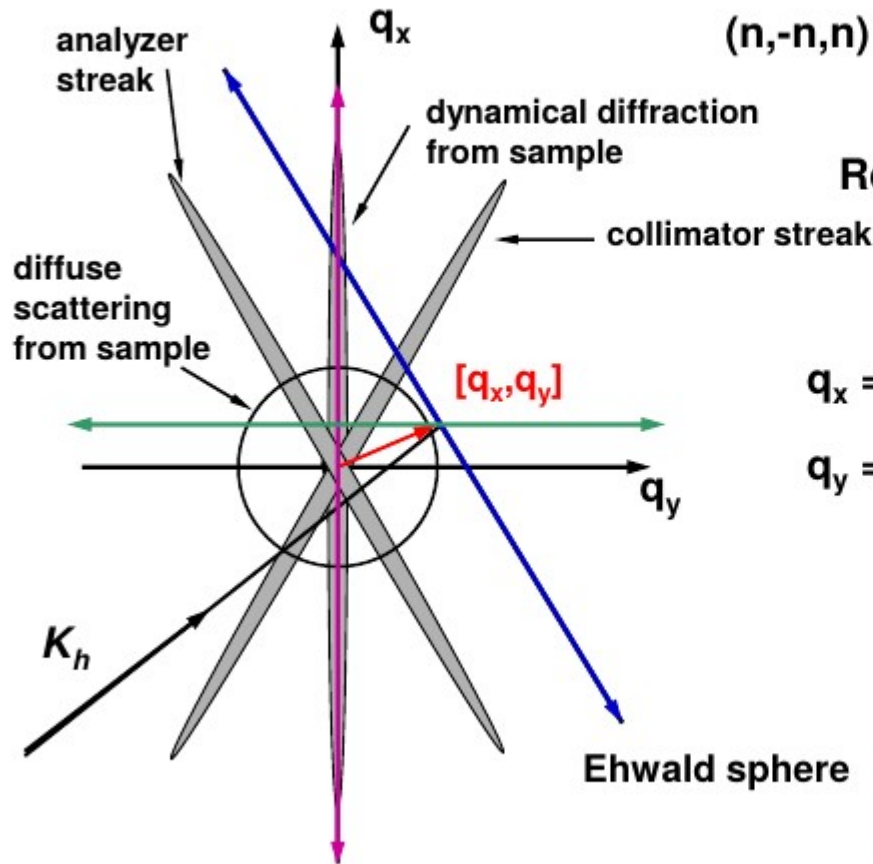
## Mapování recipročního prostoru



# Rozlišení v reciprokém prostoru



## TCD / detailed features in reciprocal space maps



(n,-n,n) TCD setup, symmetrical Bragg case

Reciprocal lattice point  $H$

$$q_x = \Delta\Theta \cos\Theta_B / \lambda = (\sin\omega + \sin(2\Theta - \omega)) / \lambda$$

$$q_y = (2\alpha - \Delta\Theta) \sin\Theta_B / \lambda = (-\cos\omega + \cos(2\Theta - \omega)) / \lambda$$

Possible scans:

1.  $\alpha/\omega = \text{fixed}$ ,  $\Delta\Theta/2\Theta = \text{variable}$
2.  $\alpha/\omega = \text{variable}$ ,  $\Delta\Theta/2\Theta = \text{fixed}$
3.  $\alpha/\omega = \text{variable}$ ,  $\Delta\Theta/2\Theta = 2\alpha/2\omega$

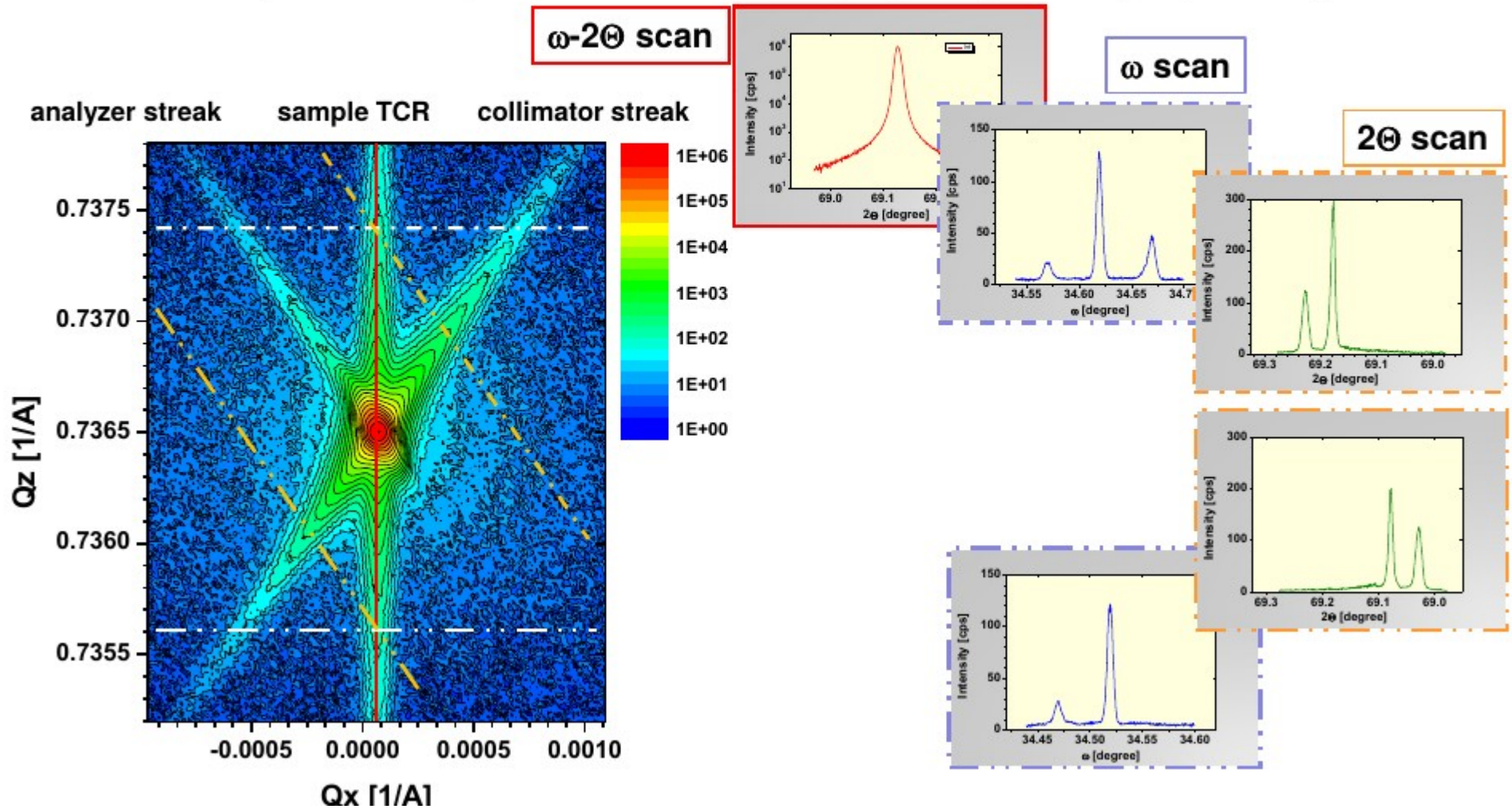


# Rozlišení v recipročném prostoru



RSM / Si(400)

SmartLab configuration: Ge(400)x2 collimator – Si (400) sample – Ge(220)x2 analyzer



# Rozlišení v recipročném prostoru

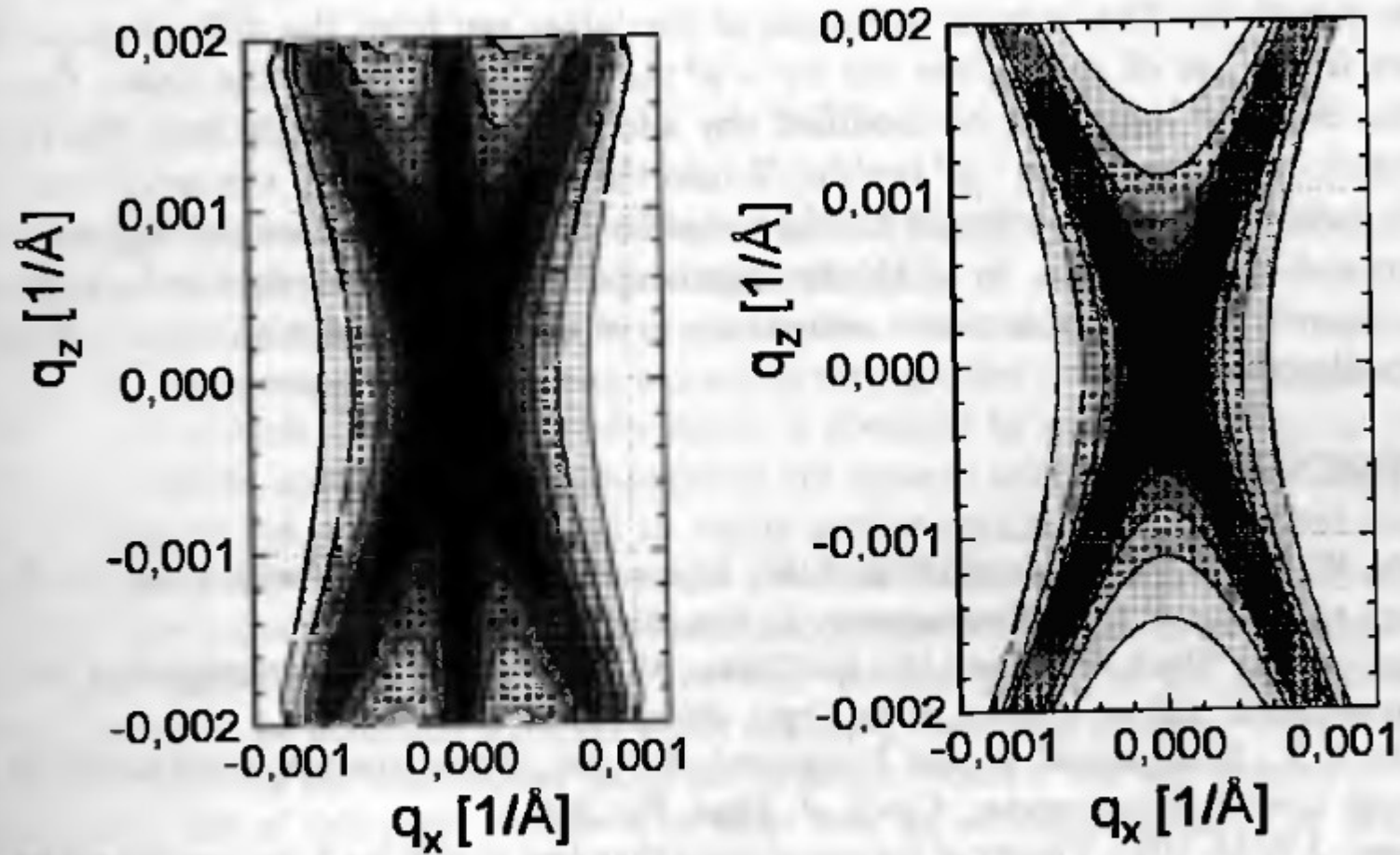
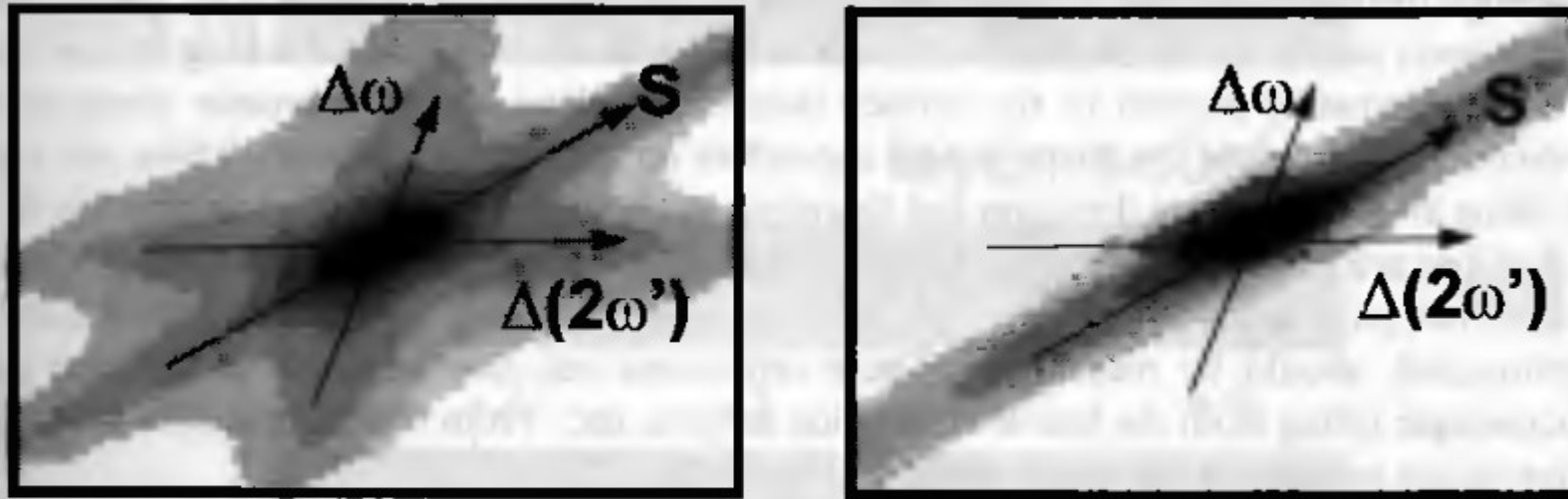


Figure 7. The device function of a triple axis diffractometer (left) and the detector signal (right). The diffractometer contains three Ge crystals, symmetrical diffraction 022  $\text{CuK}\alpha_1$ . The equi-intensity contours are logarithmic, their step is the half of the decade.

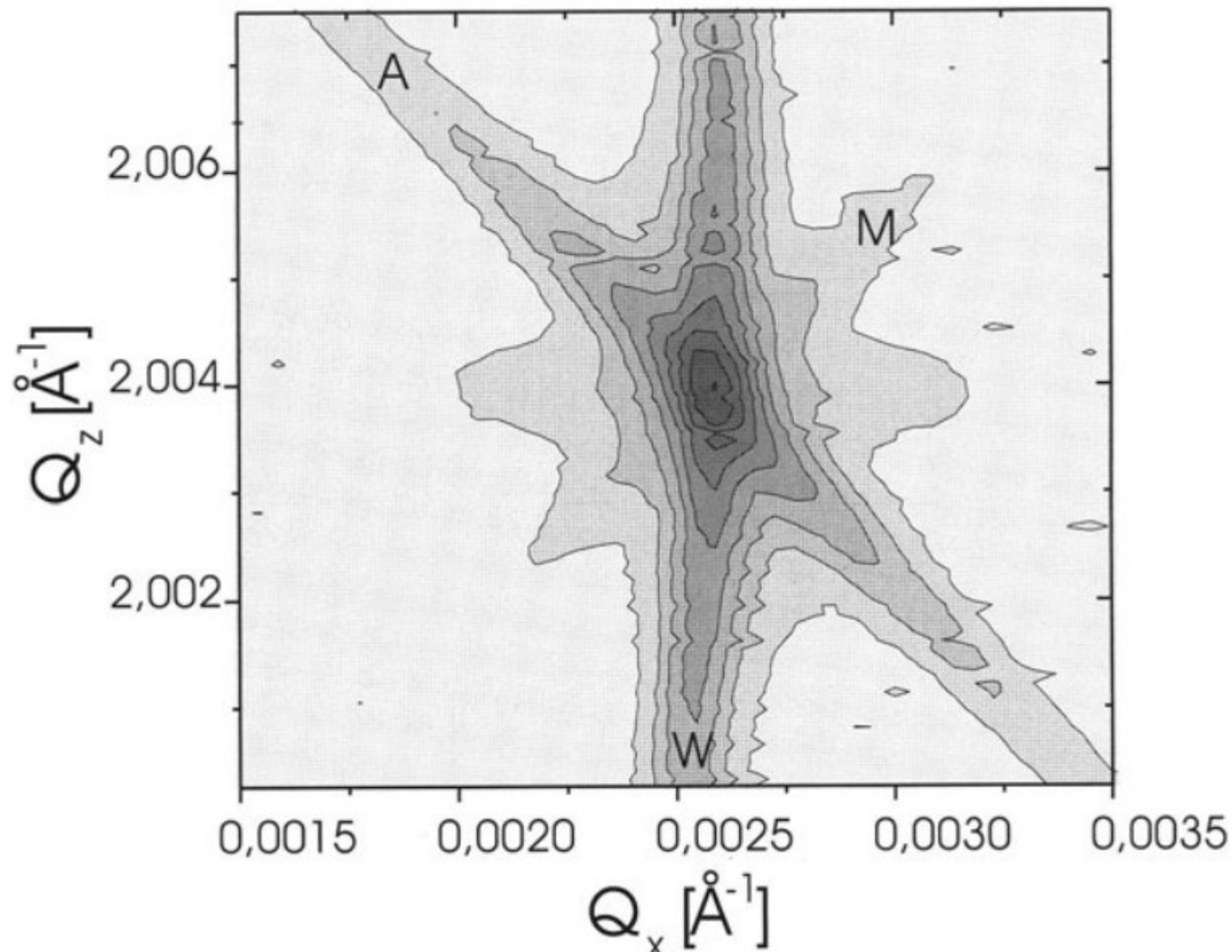
# Rozlišení v recipročním prostoru



**Figure 12.** The influence of the instrument function on a perfect crystal sample; left - the broadening and streaking caused by a three crystal three reflection diffractometer, and right - the negligible broadening caused by the instrument function of the HRMCMRD.

five-crystal eight-reflection diffractometer (HRMCMRD)

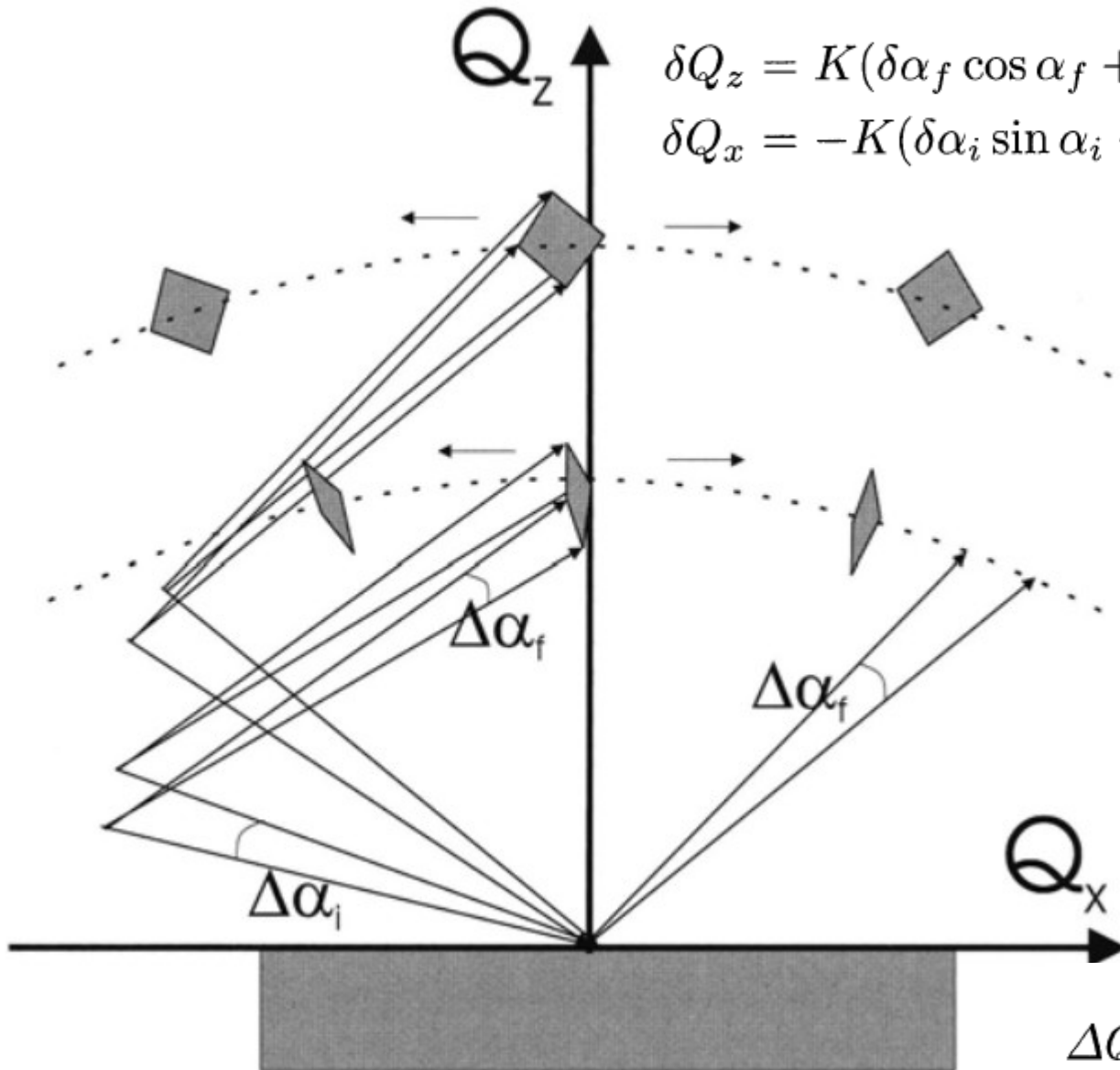
# Rozlišení v reciprokém prostoru



# Rozlišení v reciprokém prostoru

$$A_E = \Delta Q_x \Delta Q_z$$

$$\delta Q_z = K(\delta\alpha_f \cos \alpha_f + \delta\alpha_i \cos \alpha_i) + \delta K(\sin \alpha_i + \sin \alpha_f)$$
$$\delta Q_x = -K(\delta\alpha_i \sin \alpha_i - \delta\alpha_f \sin \alpha_f) + \delta K(\cos \alpha_f - \cos \alpha_i)$$



$$\Delta Q_x = K \sqrt{\sin^2 \alpha_i \Delta\alpha_i^2 + \sin^2 \alpha_f \Delta\alpha_f^2}$$

$$\Delta Q_z = K \sqrt{\Delta\alpha_i^2 \cos^2 \alpha_i + \Delta\alpha_f^2 \cos^2 \alpha_f}$$

# Rozlišení v recipročním prostoru

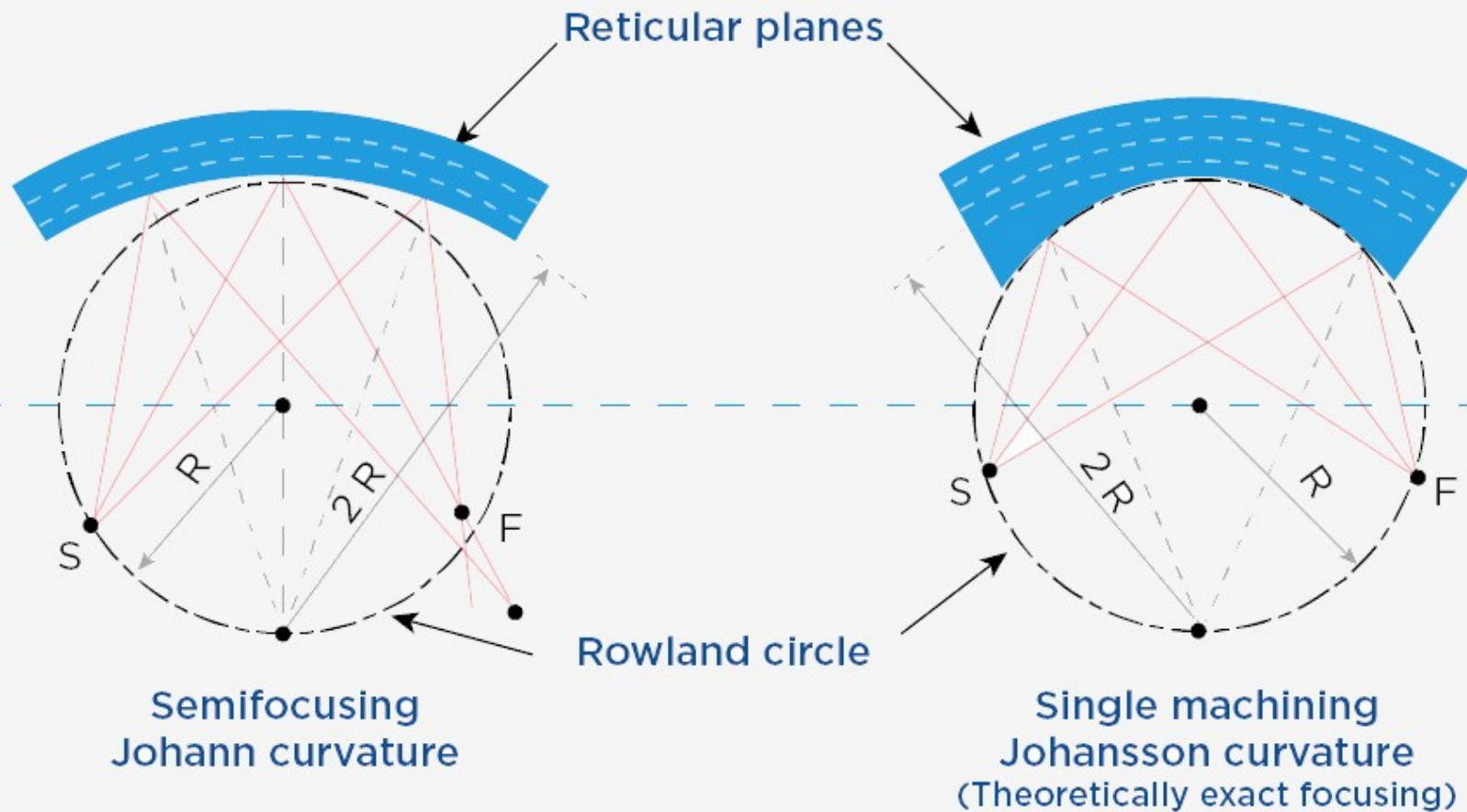
$$L_{s0} = \lambda \frac{R}{2r_s} \approx \frac{\lambda}{2\phi_s} \approx \frac{\lambda}{2\Delta\alpha_i},$$

$$L_{p0} = \frac{\lambda}{2} \frac{\lambda}{\Delta\lambda}.$$

$$L_p = \frac{L_{p0}}{\cos \alpha_i} \qquad L_s = \frac{L_{s0}}{\sin \alpha_i}.$$

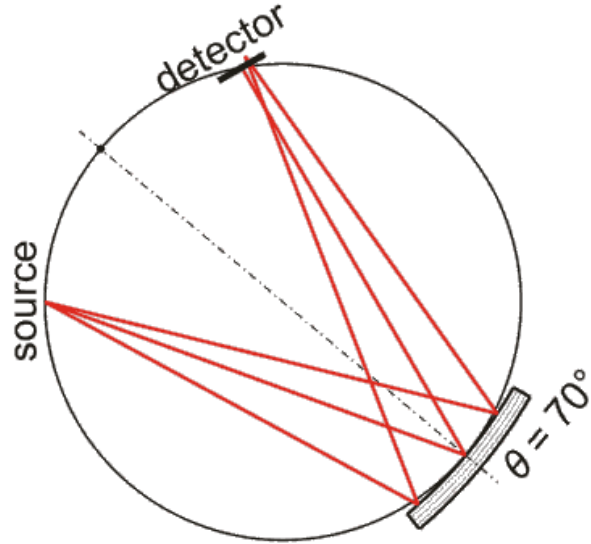
$$L_{\text{total}} = \frac{\lambda}{2} \left( \frac{1}{\Delta\alpha_i \sin \alpha_i} + \frac{1}{\Delta\alpha_f \sin \alpha_f} \right) + \frac{\lambda^2}{2\Delta\lambda} \left( \frac{1}{\cos \alpha_i} + \frac{1}{\cos \alpha_f} \right).$$

# Fokusuující monochromátory

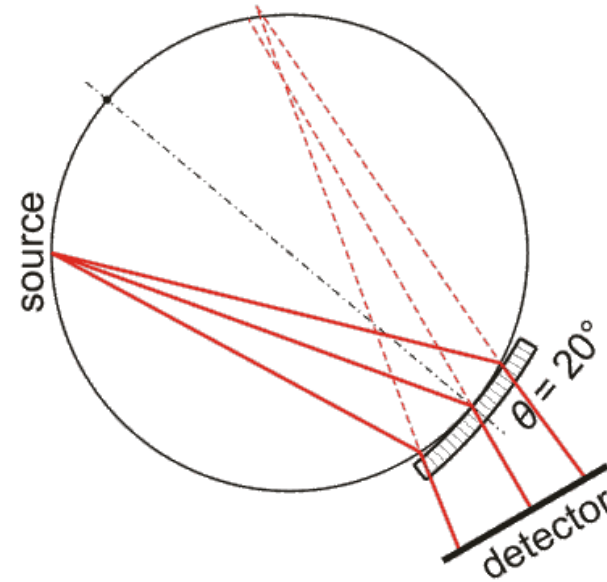


# Fokusující monochromátory

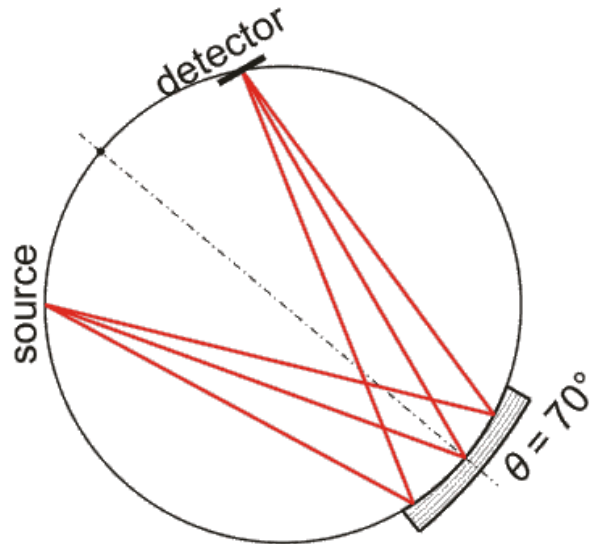
*Bragg bent (Johann)*



*Laue bent (duMond)*



*Bragg ground-bent (Johansson)*



*Laue ground-bent*

