Focusing neutron optics with elastically bent perfect crystals

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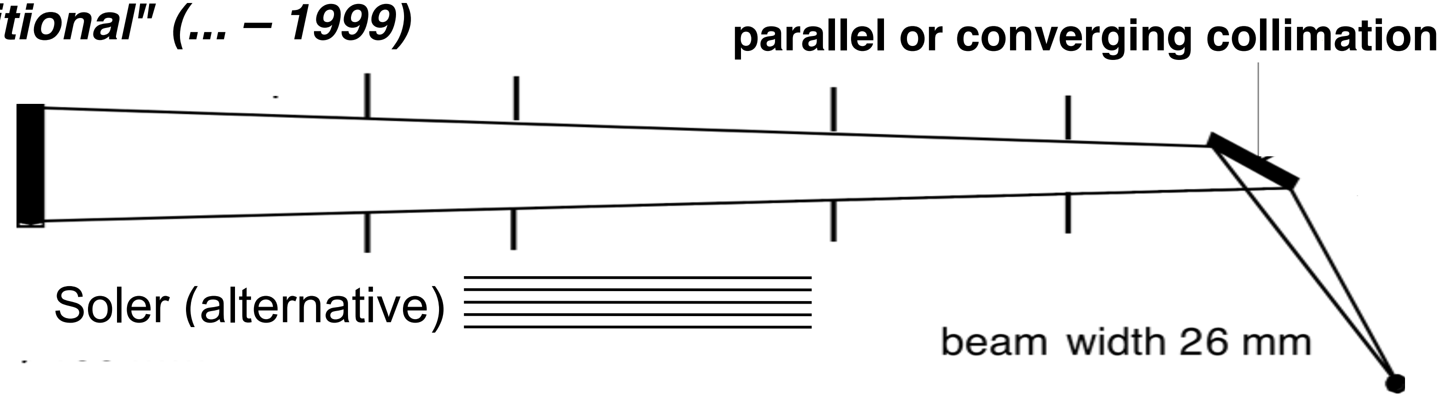
NEUTRONS FOR SOCIETY

Layout of the talk

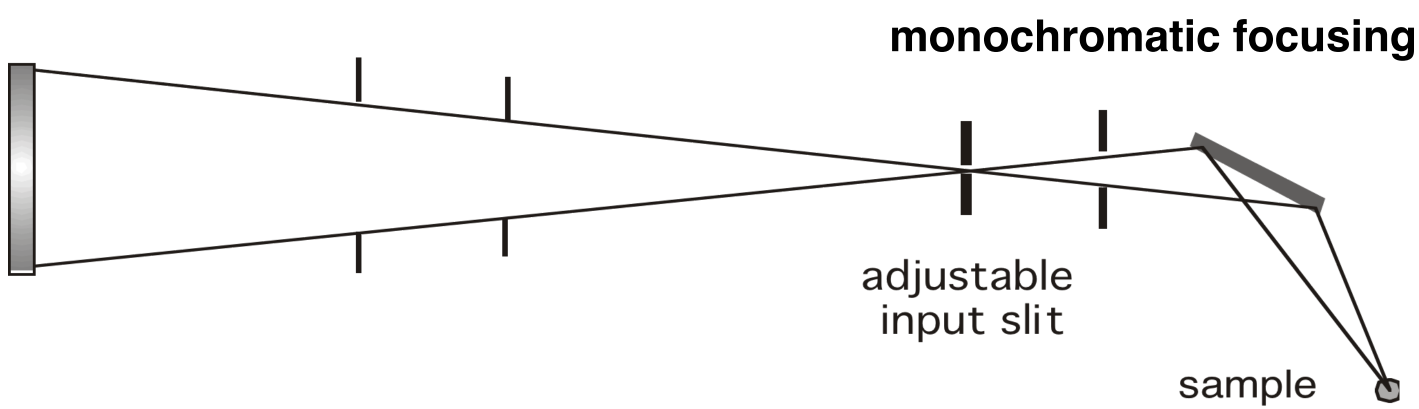
1. Optics
2. Technology
3. Applications
    1. General TAS
    2. Fine focusing reciprocal space
    3. Fine focusing real space
4. Conclusions

TAS layout

"traditional" (... – 1999)



"modern" (2000 - ...)

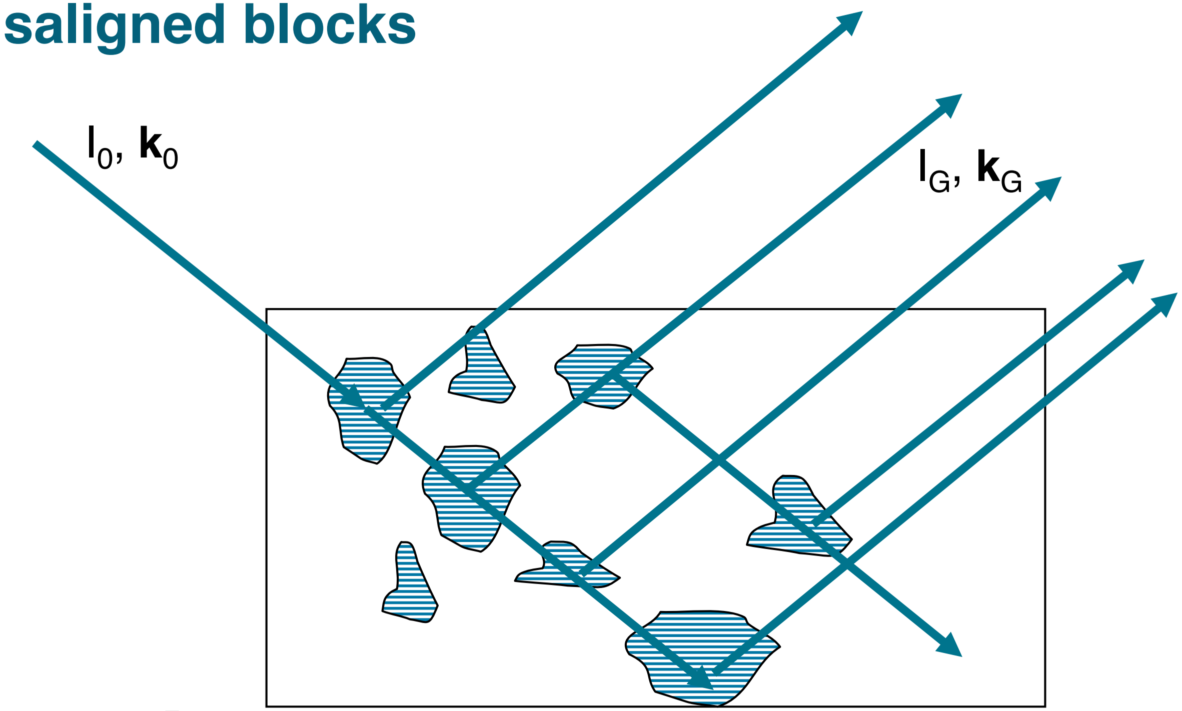


intensity gain ≈ 30x

sample size > 1 cm3 ➔ 100 mm3

Mosaic crystal

assembly of (slightly) misaligned blocks



Zachariasen's equations:

$$\partial I_0 / \partial s_0 = -\sigma(\varepsilon)(I_0 - I_G)$$

$$\partial I_G / \partial s_G = -\sigma(\varepsilon)(I_G - I_0)$$

$$\sigma(\varepsilon) = Q_{kin} w(\varepsilon) = \frac{F_G^2 \lambda^3}{v_0^2 \sin 2\theta} \frac{\exp\left[-(\varepsilon/\eta)^2\right]}{\eta\sqrt{\pi}}$$

$$\varepsilon = \Theta - \Theta_0$$

kinematic reflectivity

mosaic distribution (Gaussian)

angular deviation

Mosaic crystal reflectivity

Solutions to Zachariasen's eqs:

Bragg case:

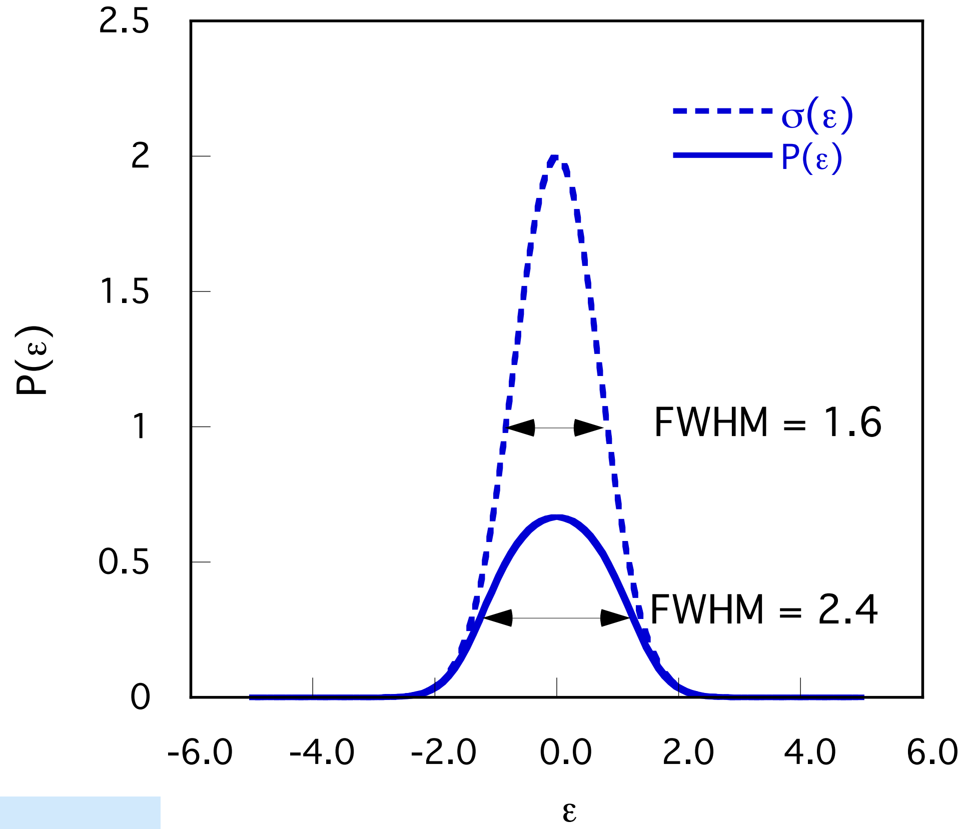
$$P(\varepsilon)=\frac{\sigma(\varepsilon)}{\mu+\sigma(\varepsilon)+u(\varepsilon)\coth ut}$$

$$P(\varepsilon)=\frac{\sigma(\varepsilon)}{\sigma(\varepsilon)+1}, \quad \mu=0$$

$$u=\sqrt{\mu(\mu+2\sigma)}$$

Laue case:

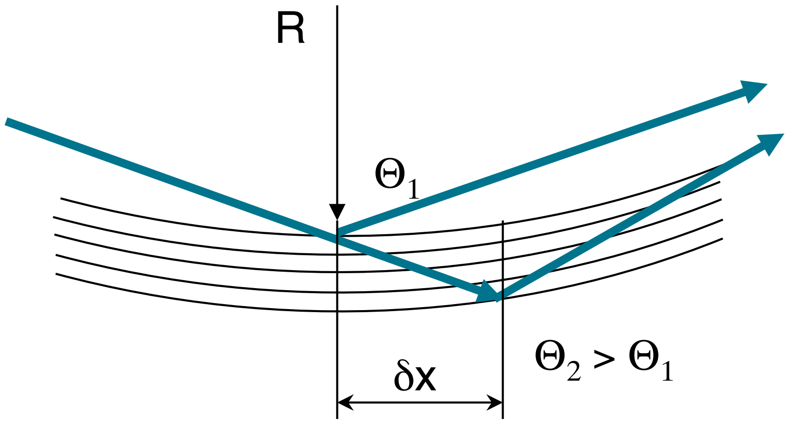
$$P(\varepsilon)=\exp\left[-(\mu+\sigma(\varepsilon))t\right]\sinh\left[\sigma(\varepsilon)t\right]$$



$$\sigma(\varepsilon)=Q_{kin}w(\varepsilon)=\frac{F_G^2\lambda^3}{v_0^2\sin 2\theta}\frac{\exp\left[-(\varepsilon/\eta)^2\right]}{\eta\sqrt{\pi}}$$

Gradient crystals

Simple bending

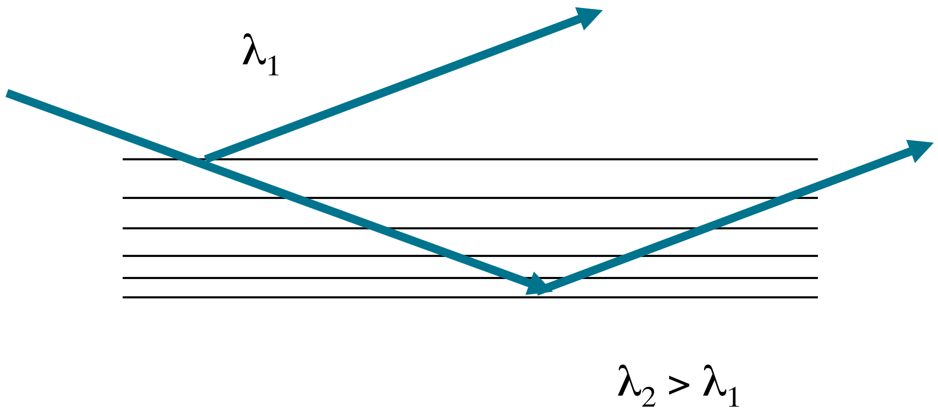


apparent mosaic width:

$$\delta\Theta = \frac{\delta x}{R}$$

wavelength band:

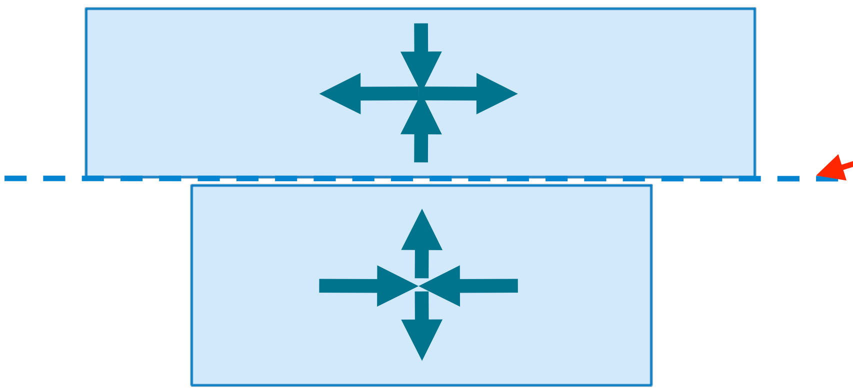
$$\Delta\lambda = 2\Delta d_{hkl} \sin\Theta$$



Simple d_{hkl} gradient)

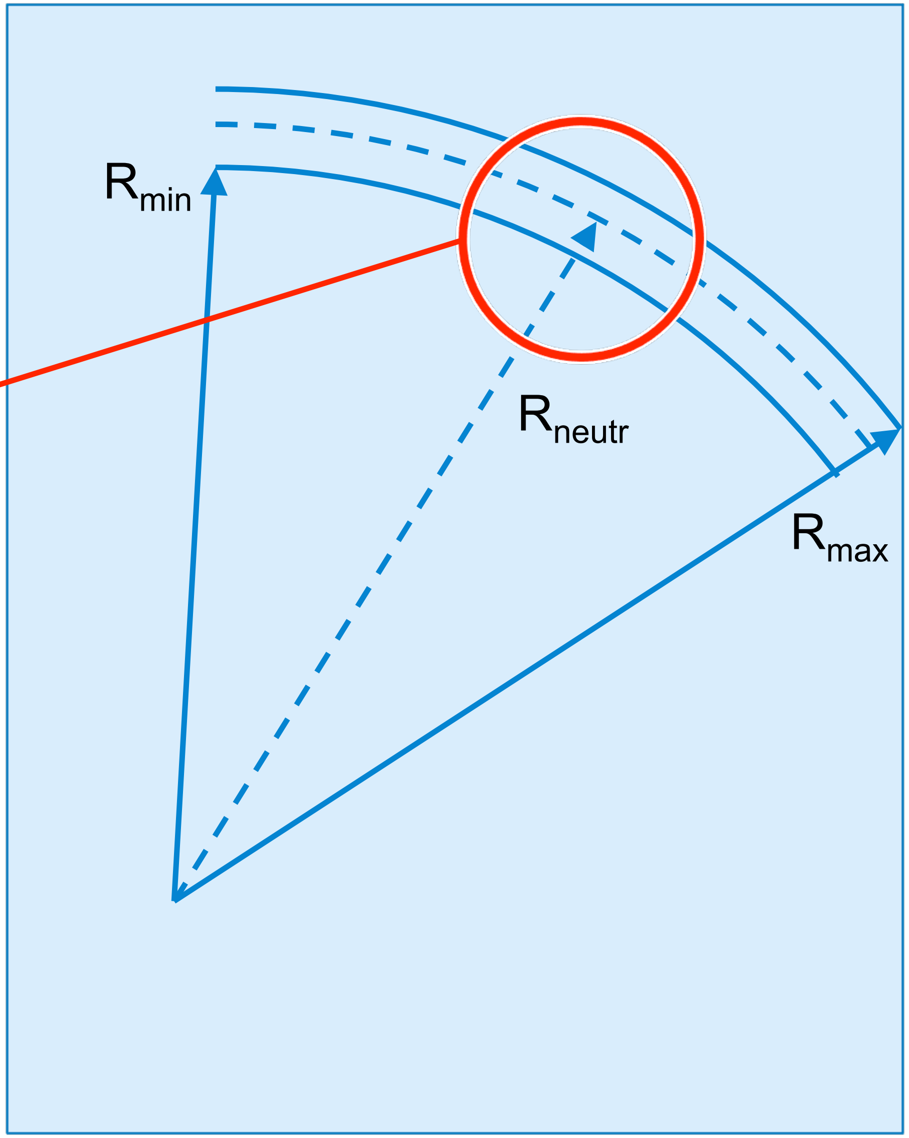
Gradient crystals

Elastically bent crystal



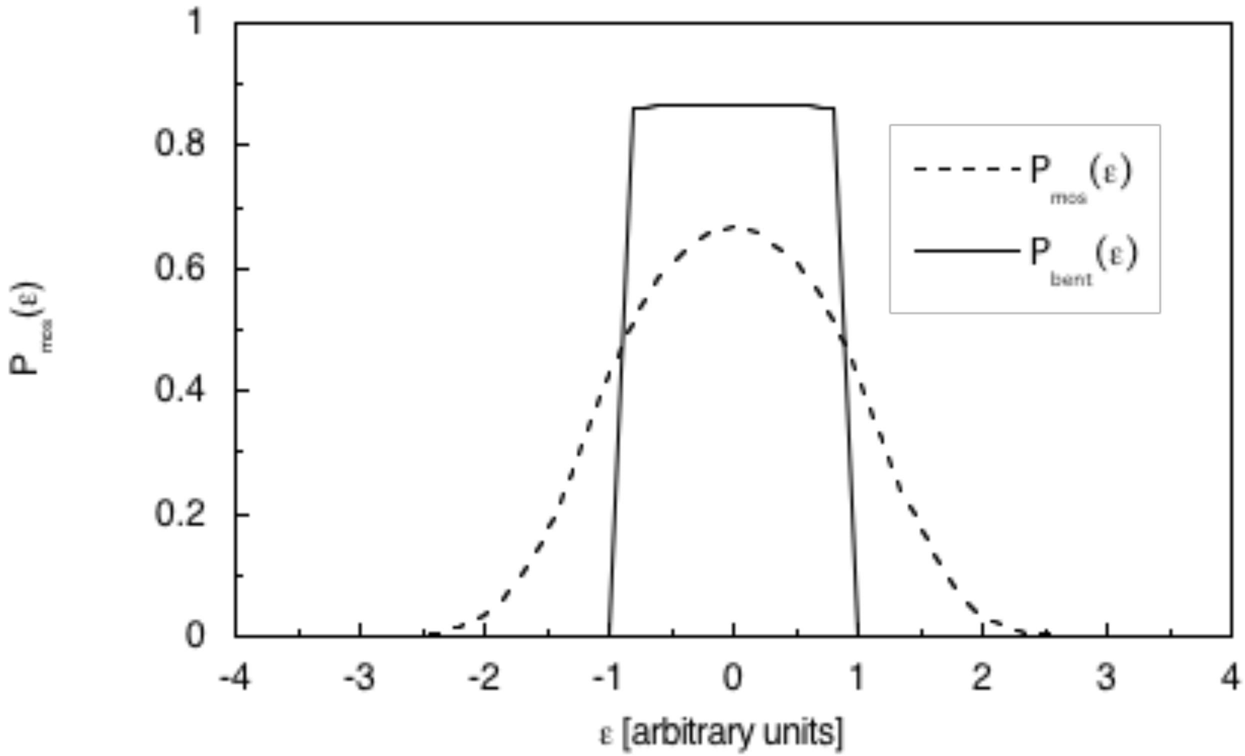
Effective bending radius variation
due to strain/stress equilibrium

analytically solvable
(cf. eg. Landau & Lifshitz)



Gradient *vers*. mosaic

Reflection profile



Integrated reflectivity

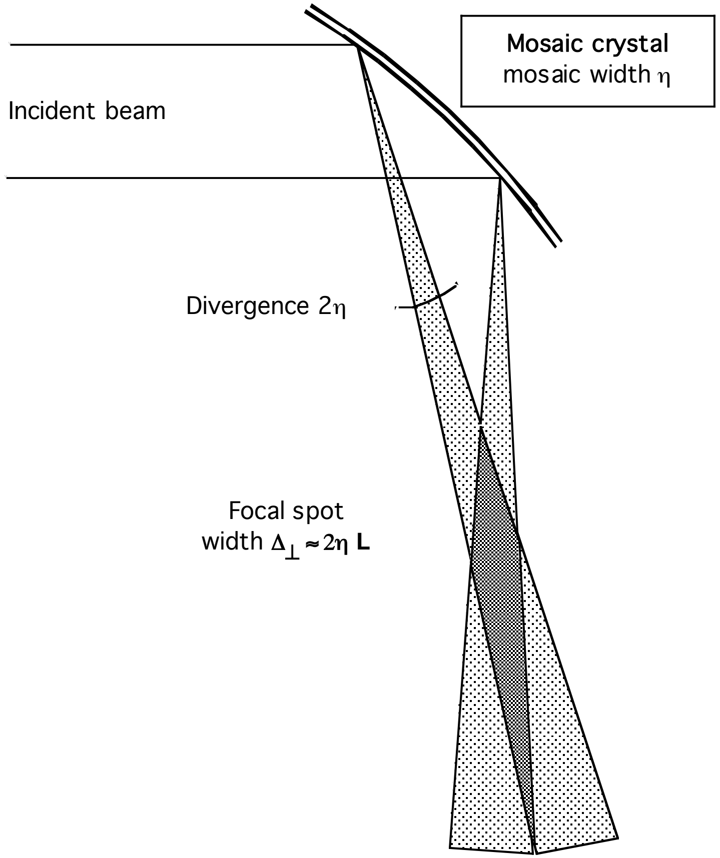
$$\rho(\Theta) = \frac{\Delta x}{R}\left[1 - \exp\left(\frac{Q_{kin} R}{\cos\Theta}\right)\right]$$

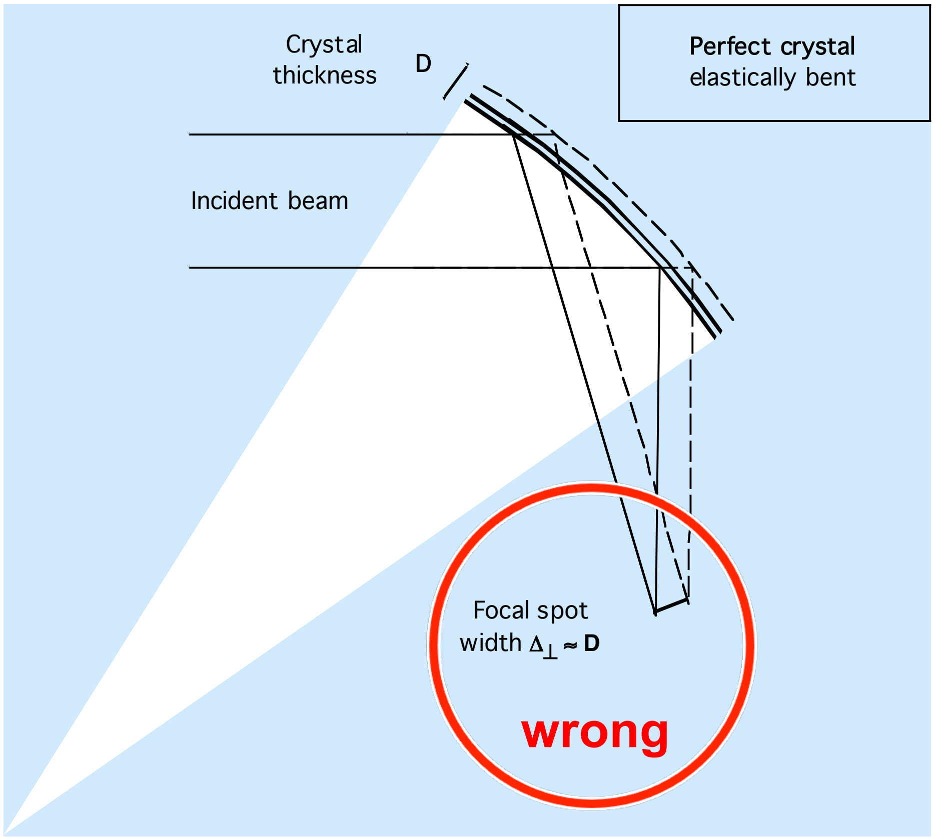
J. Kulda, Acta Cryst. A40 (1984) 120

- almost rectangular rocking curve with minimum tails
- smaller crystal thickness required to achieve given reflectivity

Focusing properties

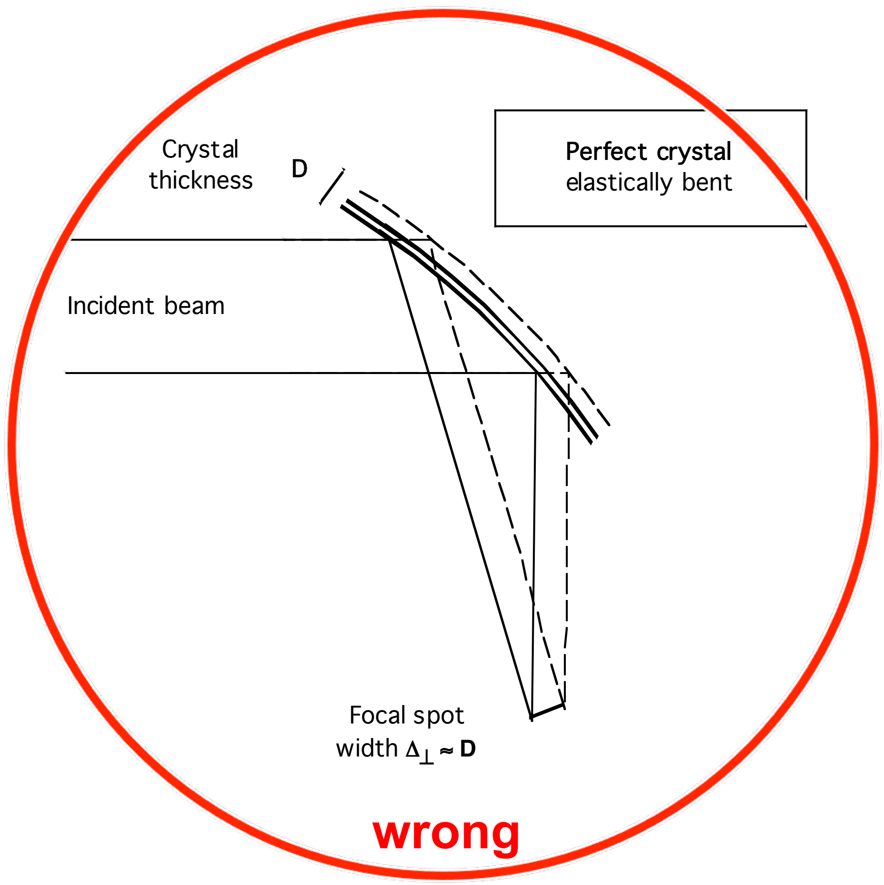
real space



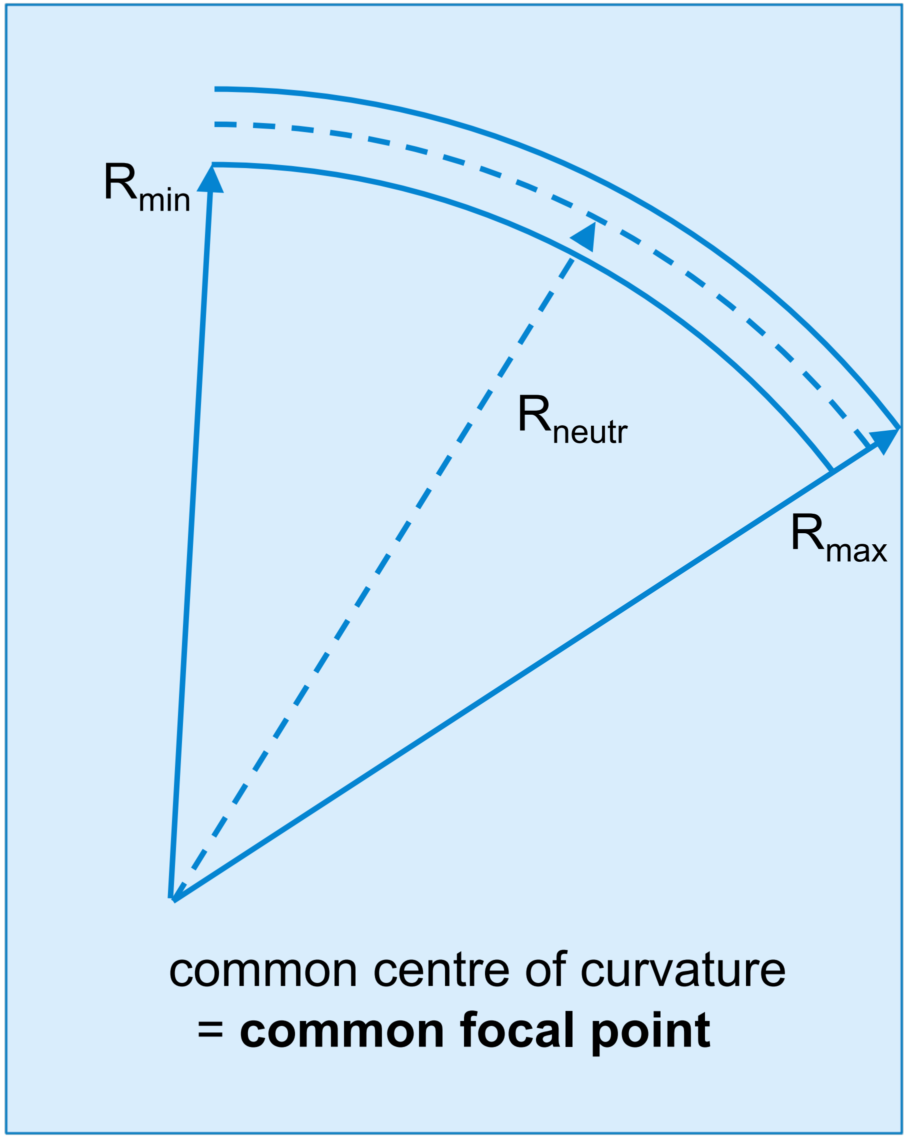


Kulda & Saroun, Nucl. Inst. Meth. A379 (1996) 155

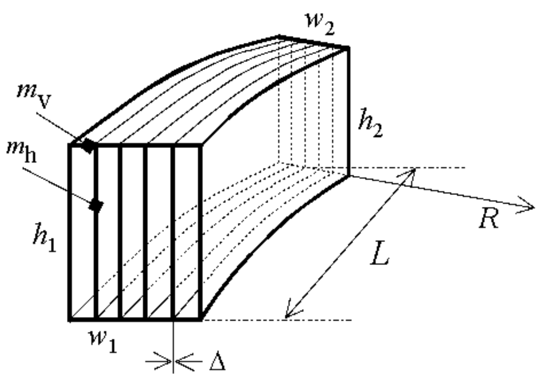
Gradient crystals



Kulda & Saroun, Nucl. Inst. Meth. A379 (1996) 155

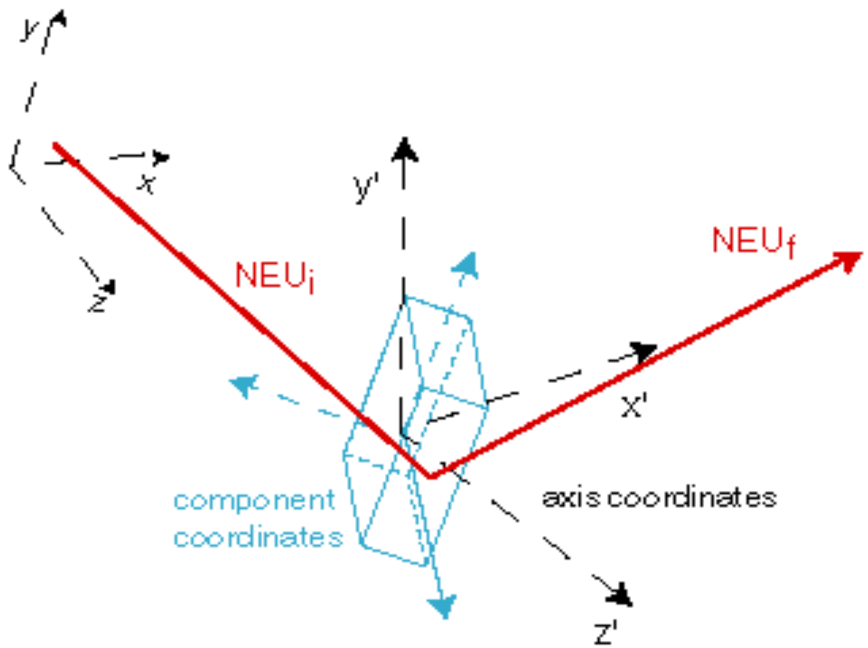


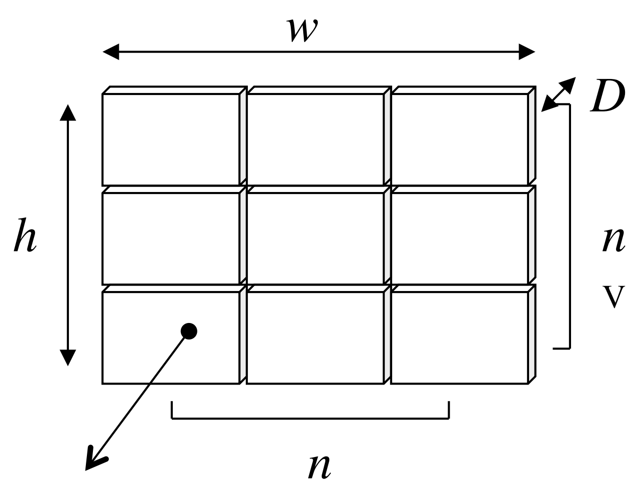
RESTRAX



- neutron ray-tracing or multi-Gaussian convolution
- diffraction/reflection optics of neutron instruments
- realistic crystal description (mosaic, elastically bent)
- highly optimized F77/F95 code

http://omega.ujf.cas.cz/restrax





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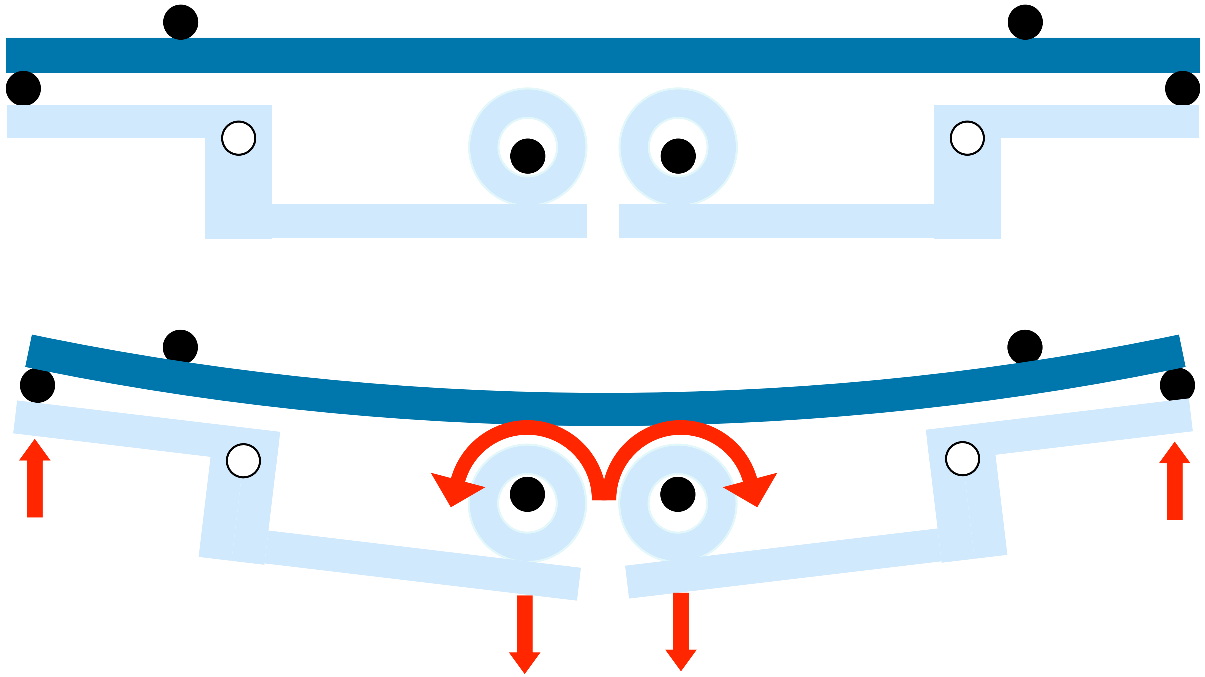
Si bender - function scheme

- **horizontal focusing**: four-point bending device

R_h = inf.

R_h = 1 - 20 m



- **vertical focusing**: inclining segments & bell-shaped cams

R_v = 0.2 m - inf.

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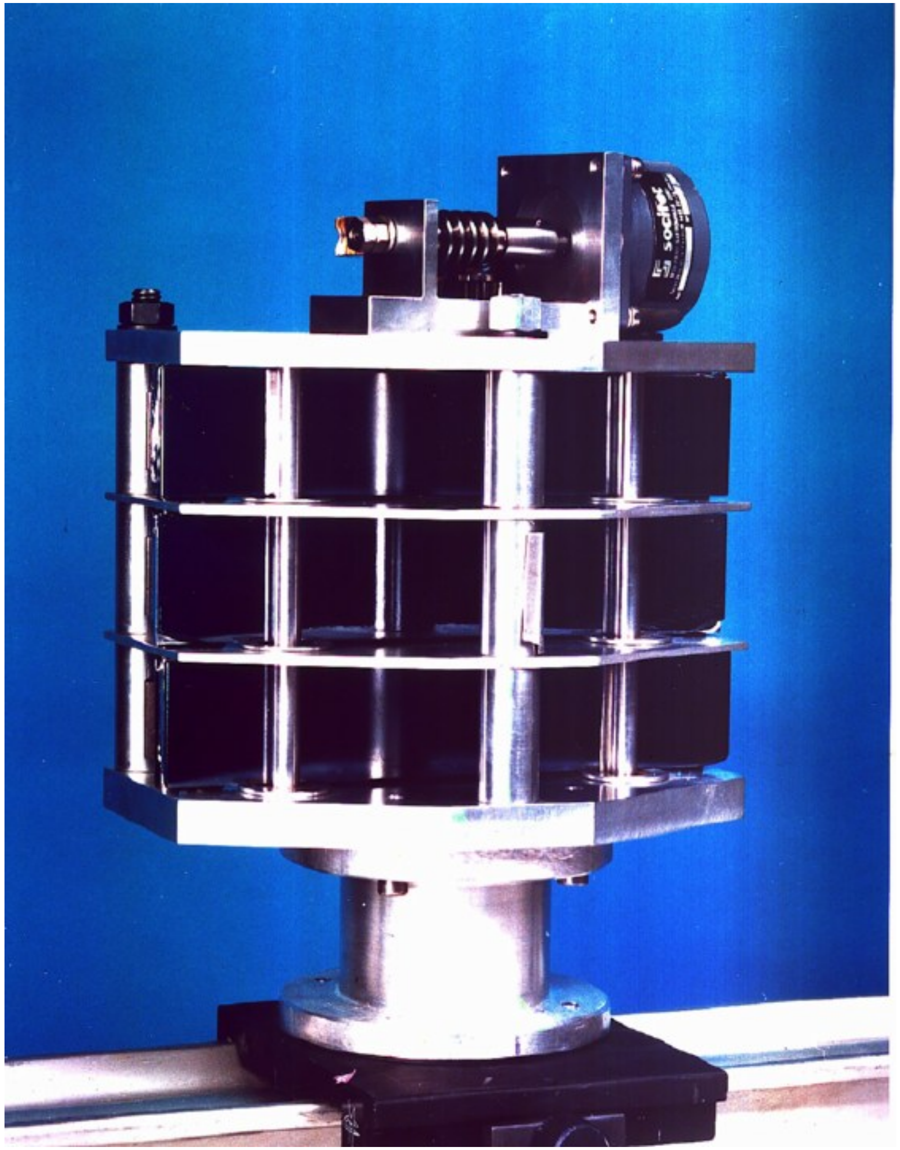
Si bender - 1^{st} generation



1st generation:

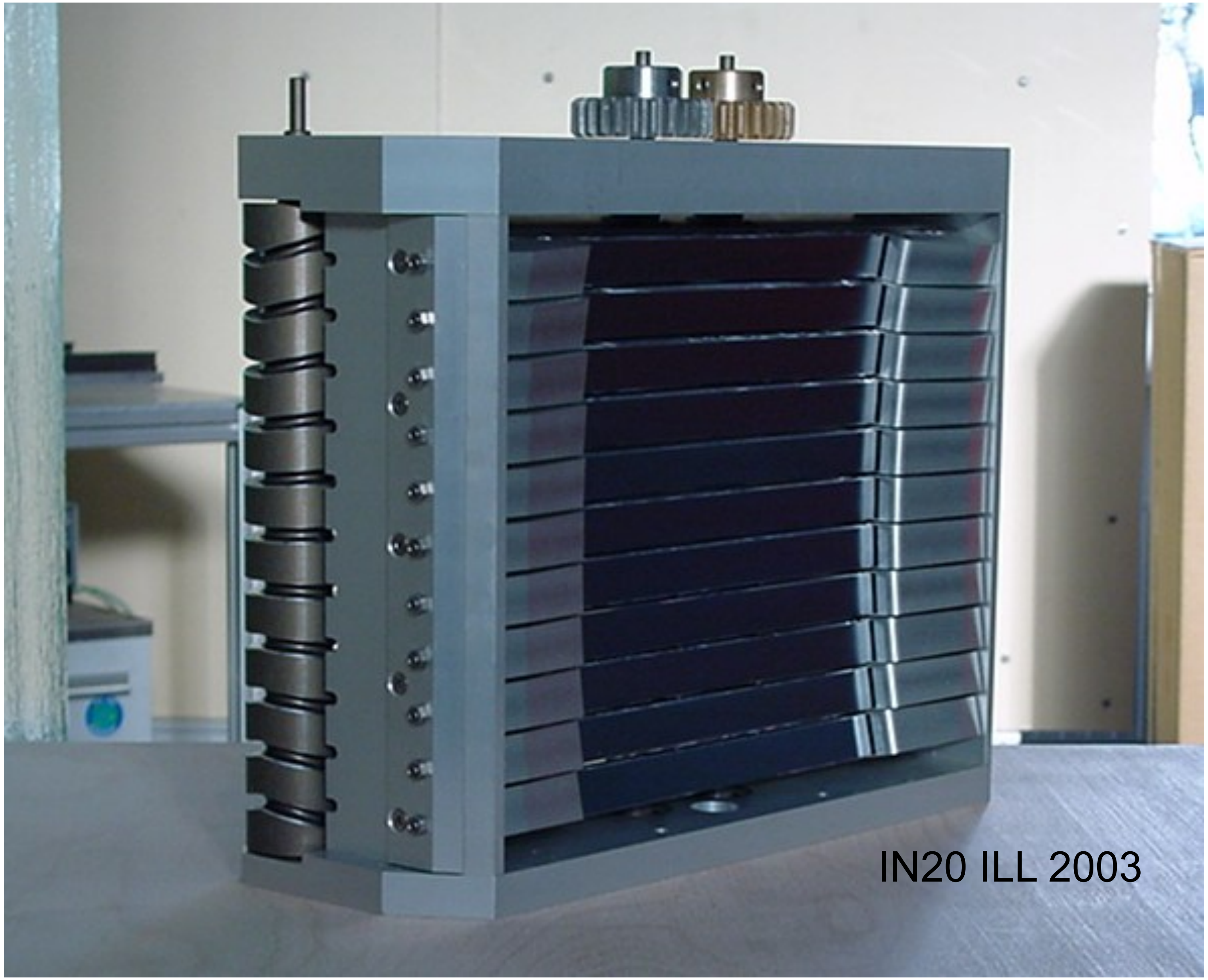
- variable horizontal curvature
- fixed vertical curvature
- 3 vertical segments (40 mm)
- blade thickness 3-5 mm
- active length 120 mm

↓

2nd generation:

- *variable horizontal* AND *vertical curvature*
- *segment height < 20 mm*
- blade thickness < 1 mm
  (> 10 per pack)

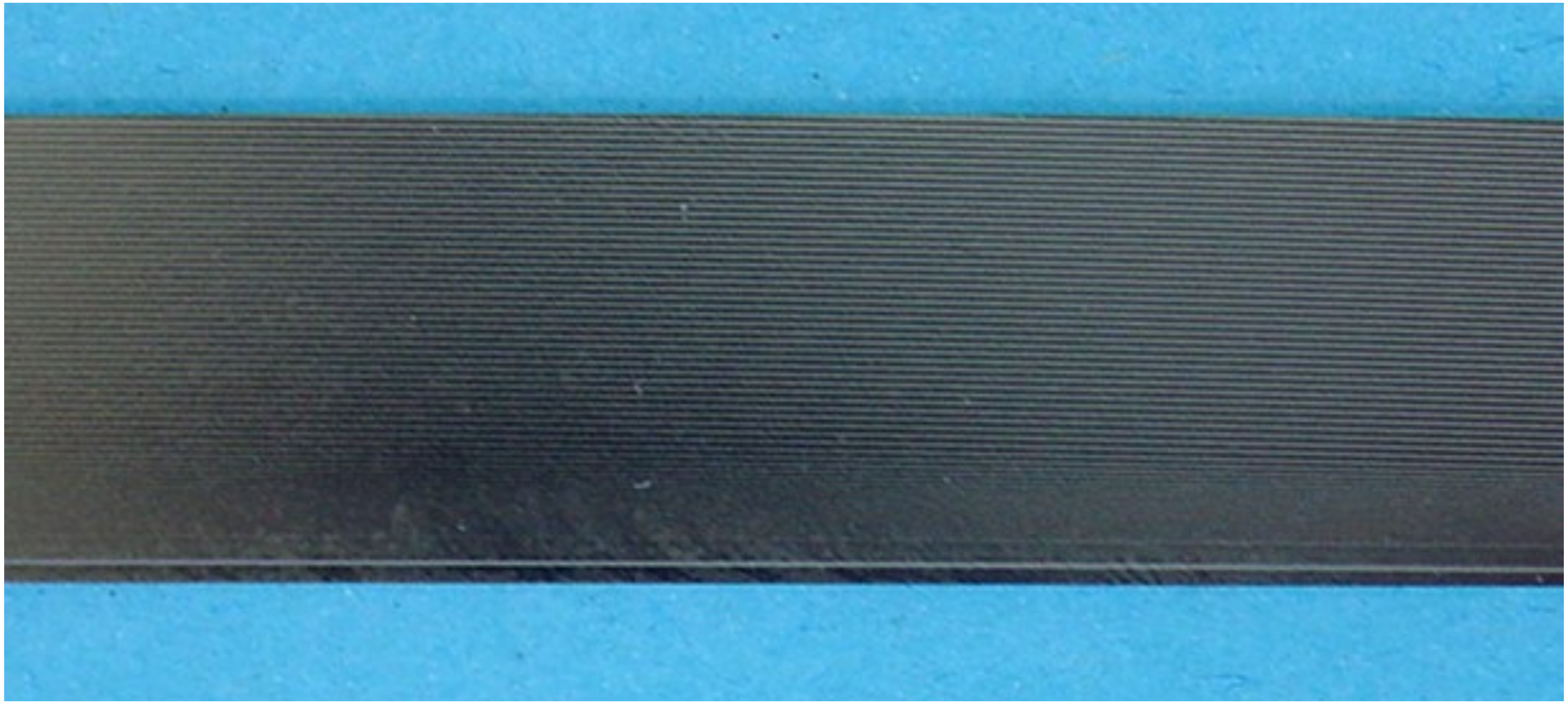
Si bender - front



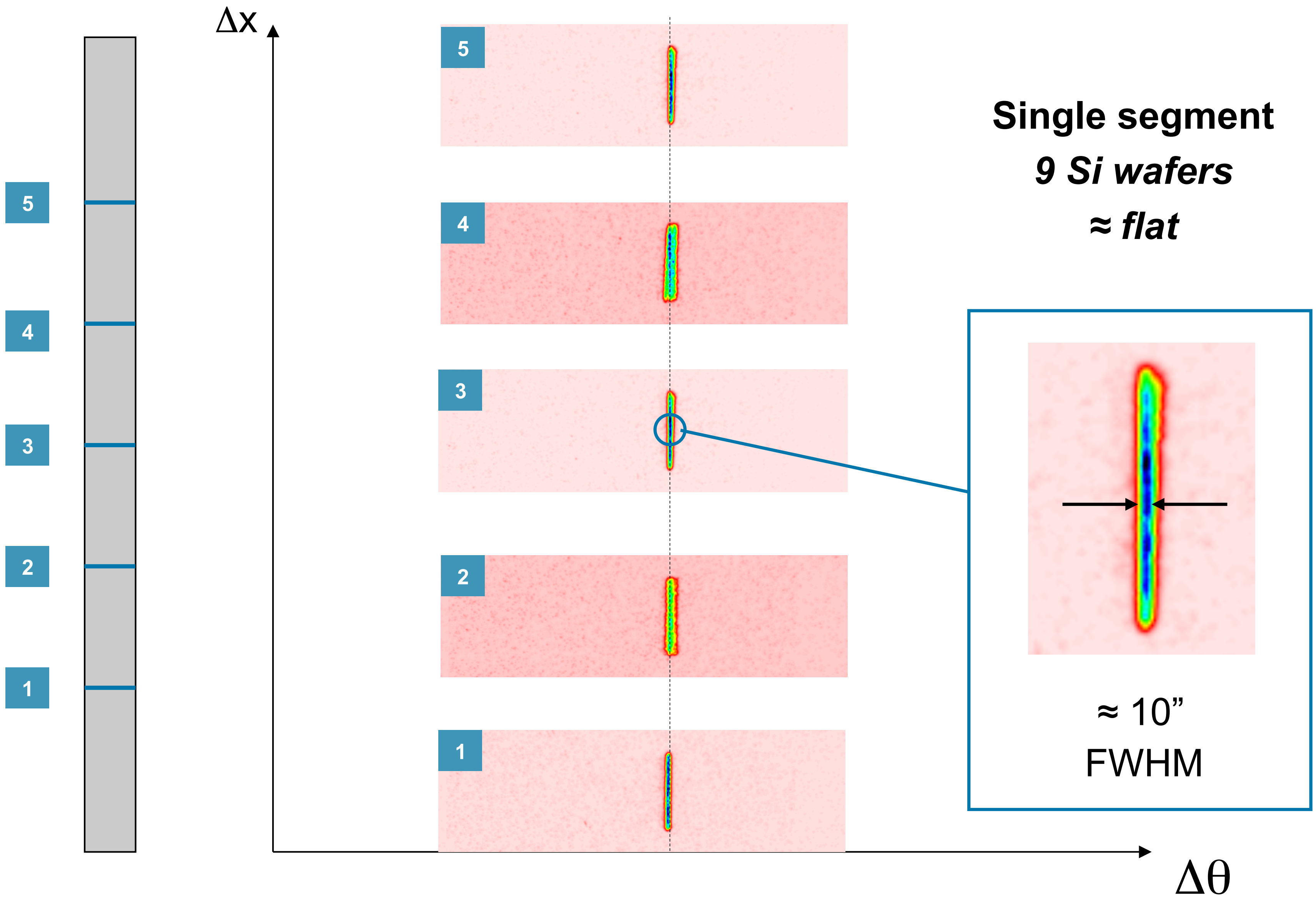
Si bender - back

Si wafers

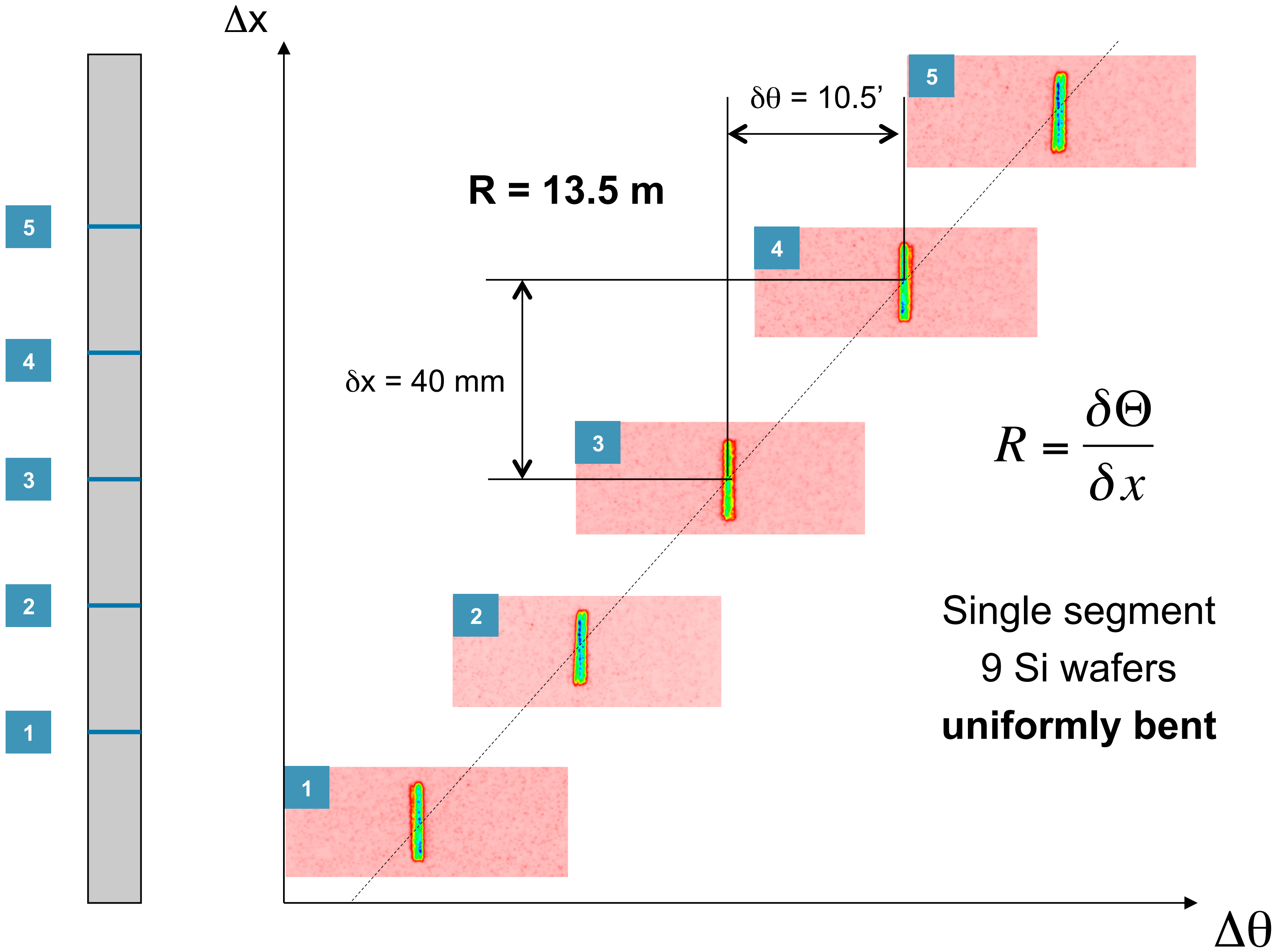
- 99 wafers (11 segments, 9 wafers each)
- size 265 x 17 x 1 mm^3
- largest face (111)
- surface as-cut (mutiwire saw!) & etched



X-ray tests (I)



X-ray tests (II)



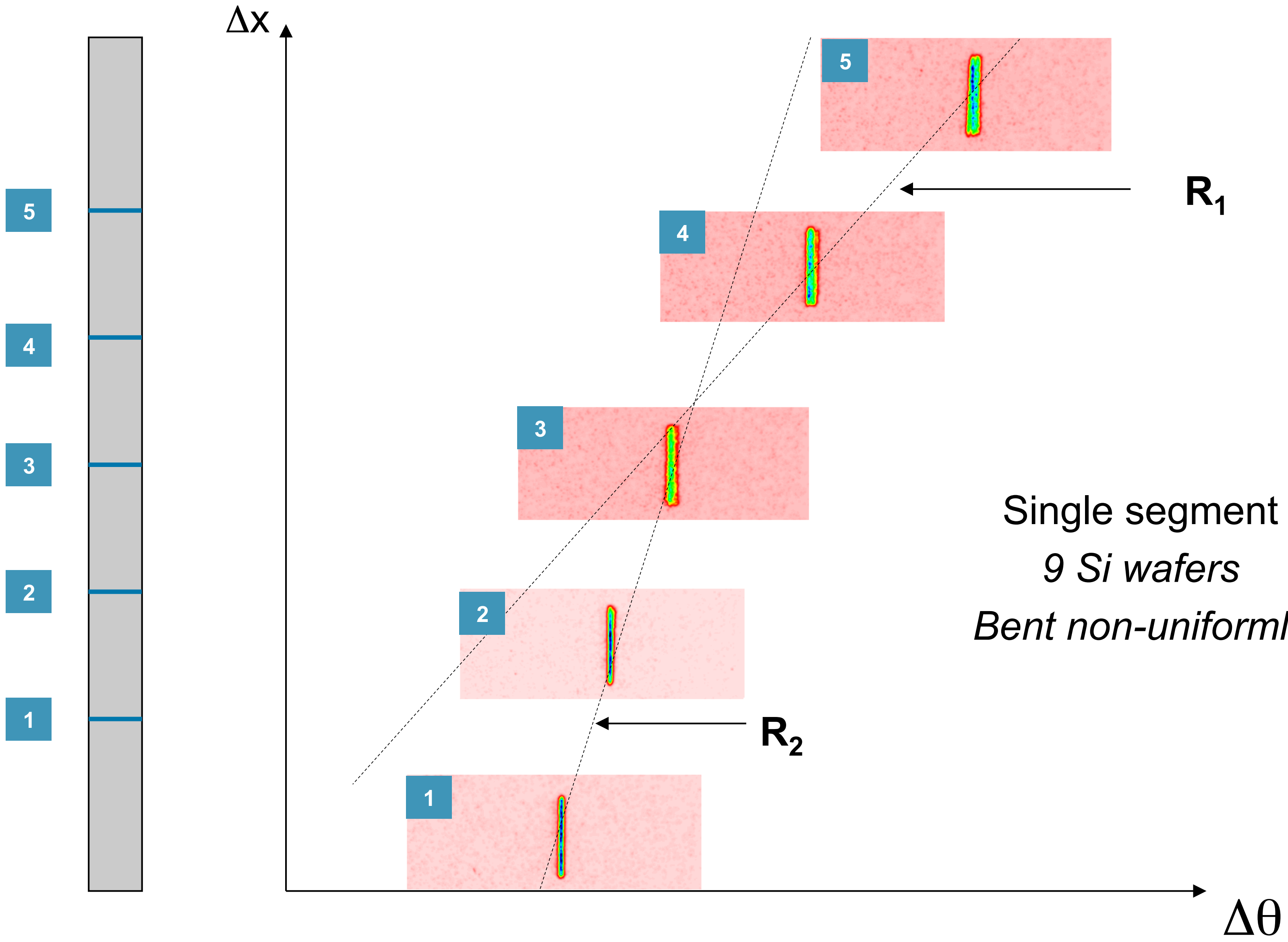
$$R = \frac{\delta\Theta}{\delta x}$$

Single segment

9 Si wafers

uniformly bent

X-ray tests (III)



Single segment

9 Si wafers

Bent non-uniformly

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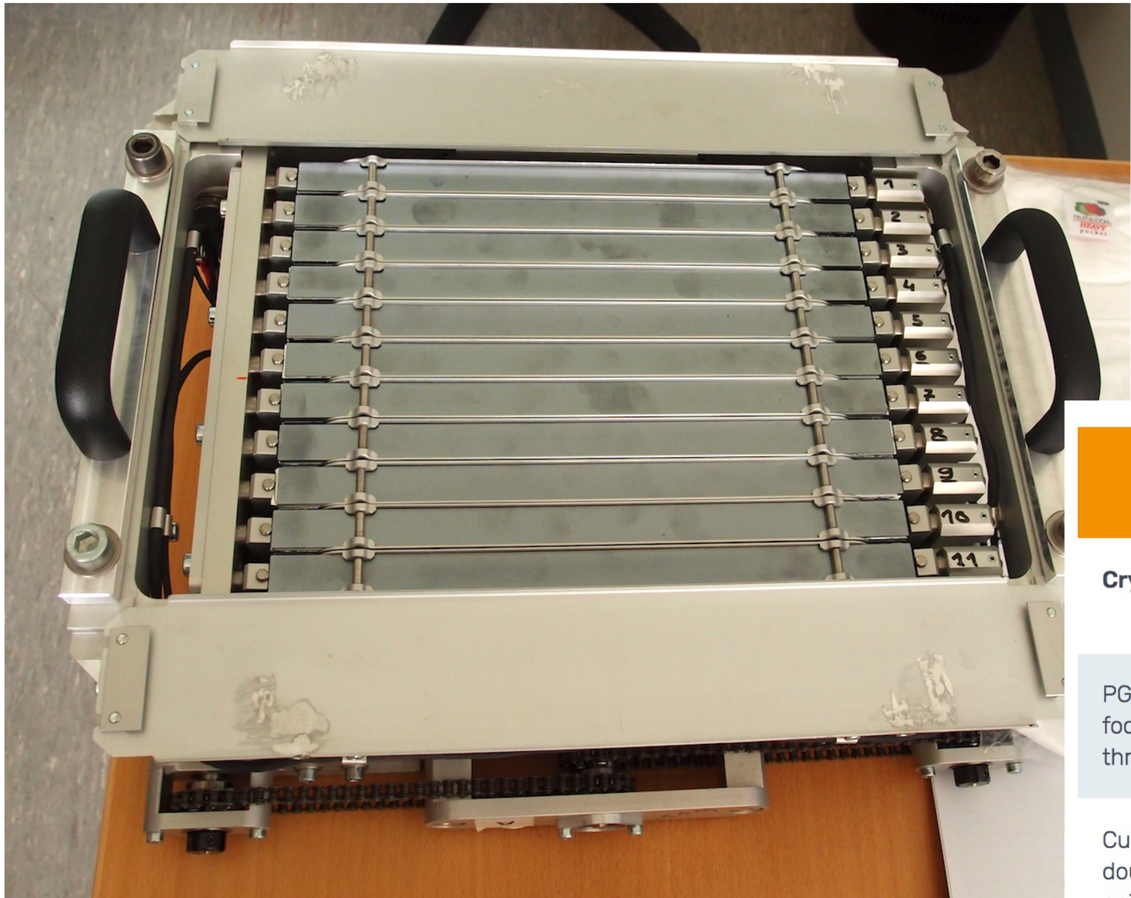
Si (111) vers. PG(002)



IN1, IN8, IN20, ThALES

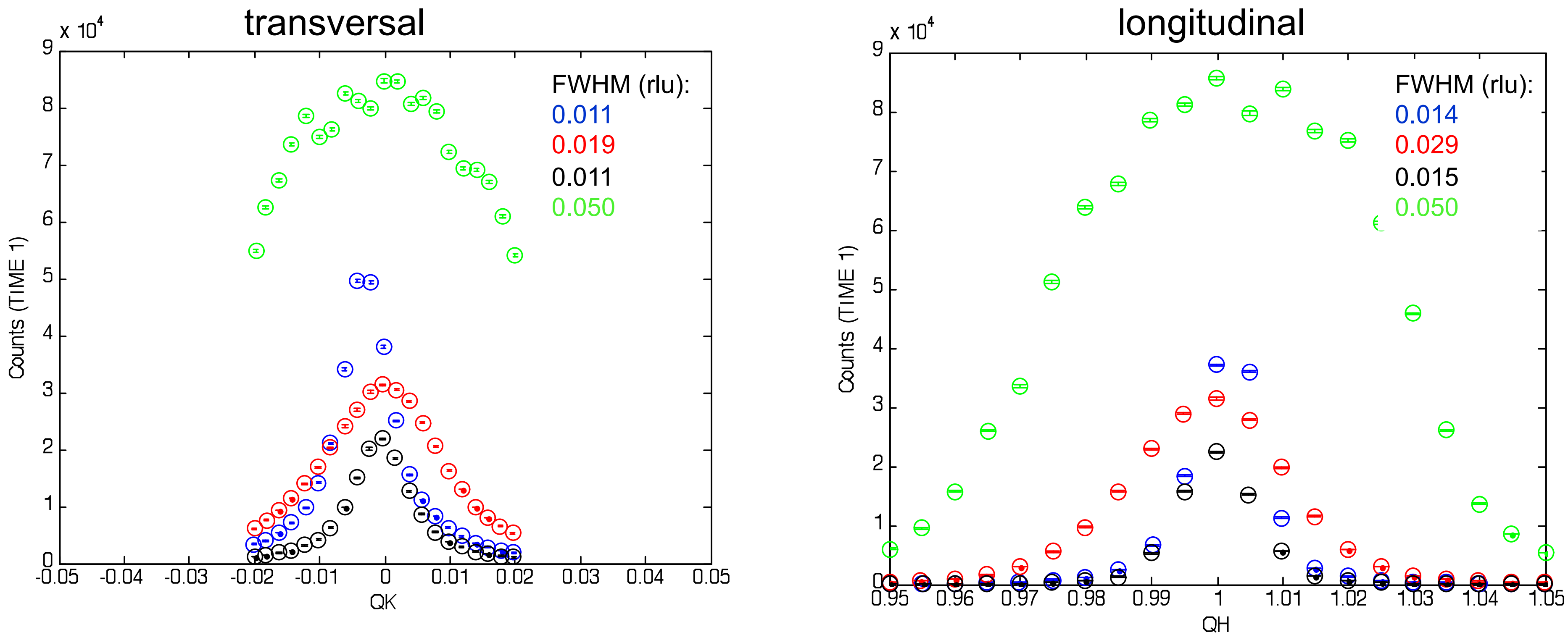
Monochromator			
Crystal	**W x H (mm^2)**	**ki/Å^{-1}**	**flux/10^8 n $cm^{-2}s^{-1}$**
PG (002) double focusing, three faces	233x197	2.662 4.1	2.0 6.5
Cu (200) variable double-focusing, anisotropic mosaic (h:25', v:10')	233x197	4.1 7.0	4.6 3.0
Si (111) bent perfect crystals, fixed horiz. curvature optimized for k=3.5Å^{-1}	180x197	2.662 4.1	0.8 3.4

monochromatic flux ≈ 1/3 PG

Si (111) vers. PG(002)

NEUTRONS FOR SOCIETY

Bragg width (PMN 100)



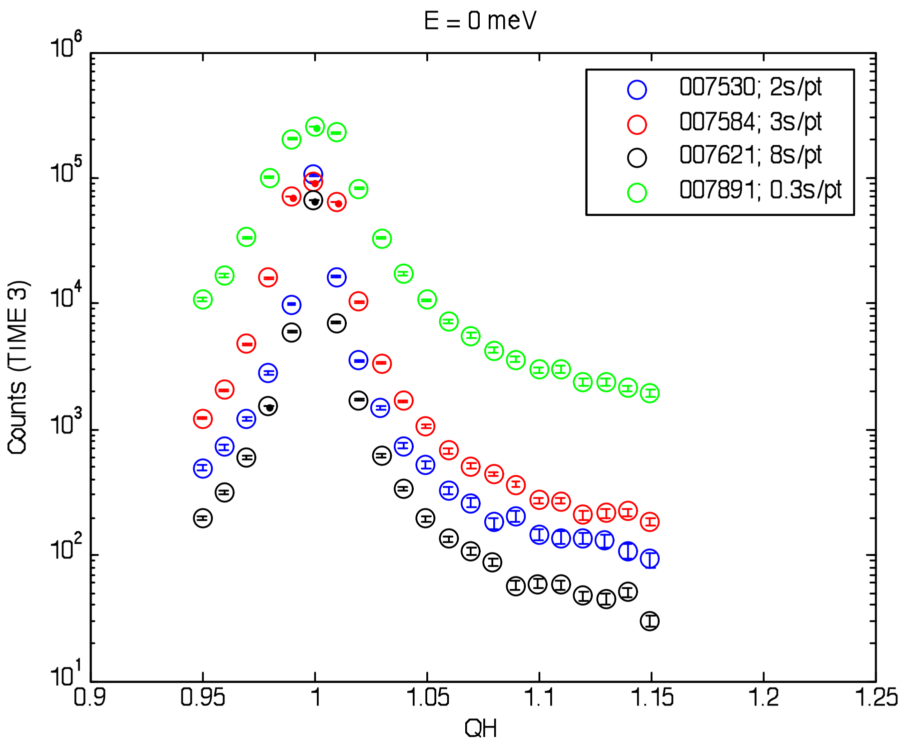
PG-PG	open	DTR 40
PG-PG	40' – 40'	DTR 40
Si-Si	open	DTR 10
Si-Si	40' – 40'	DTR 40

Si (111) vers. PG(002)

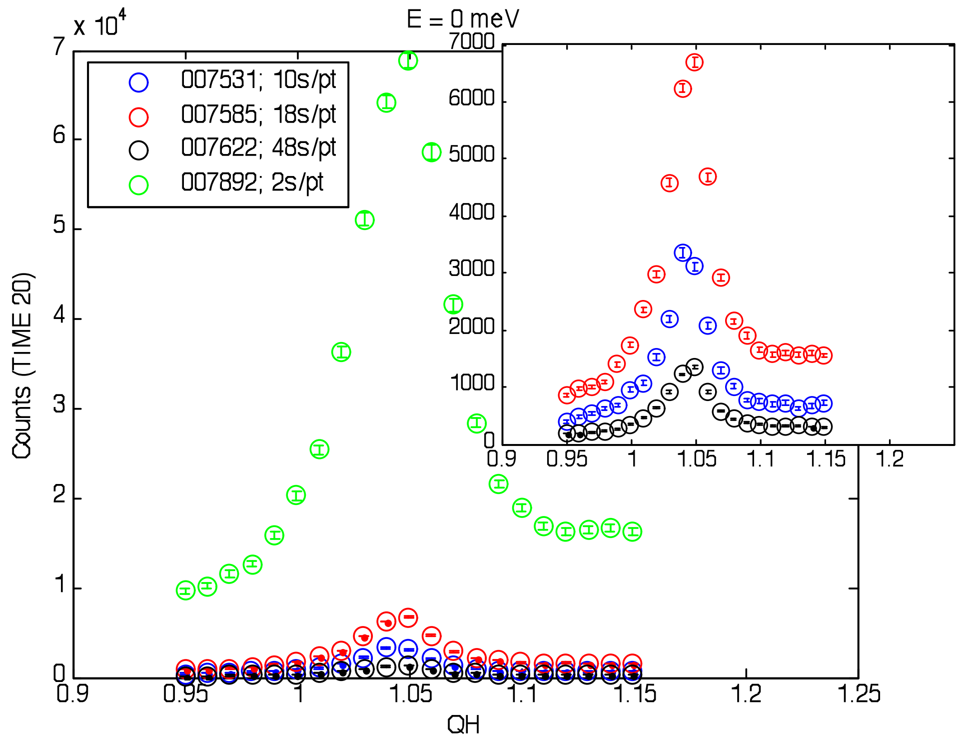
NEUTRONS FOR SOCIETY

Diffuse scattering (PMN 100)

Along diffuse streak
(1+q, -q, 0)



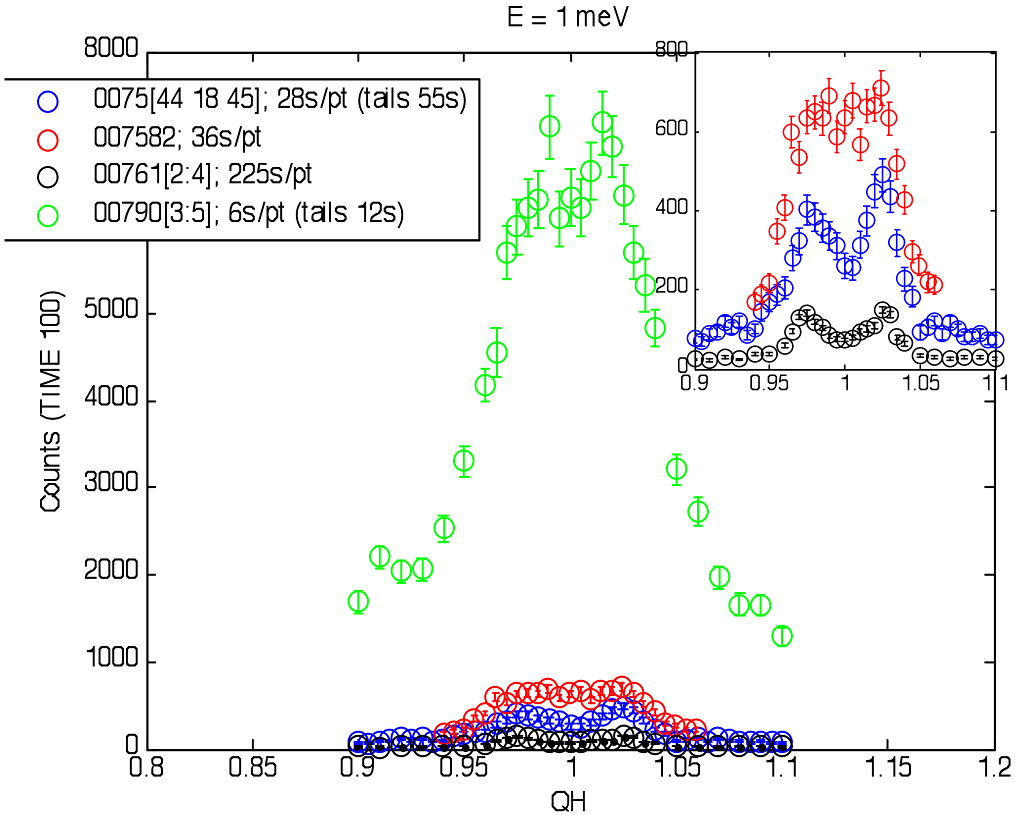
Across diffuse streak
at (1.05, -0.05, 0)

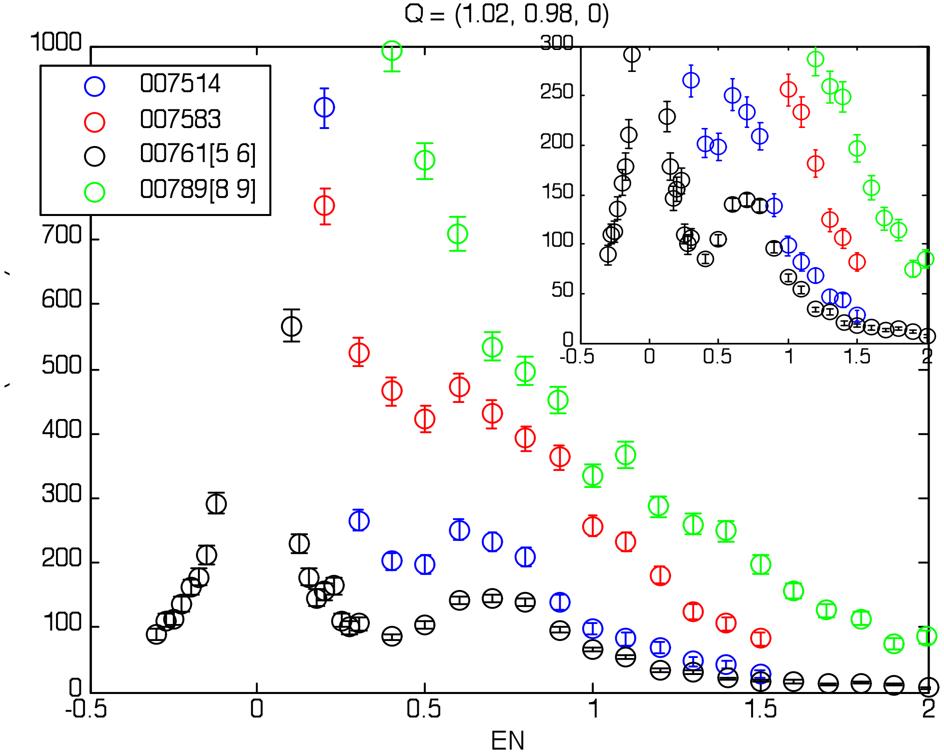


PG-PG	open	DTR 40
PG-PG	40' – 40'	DTR 40
Si-Si	open	DTR 10
Si-Si	40' – 40'	DTR 40

Si (111) vers. PG(002)

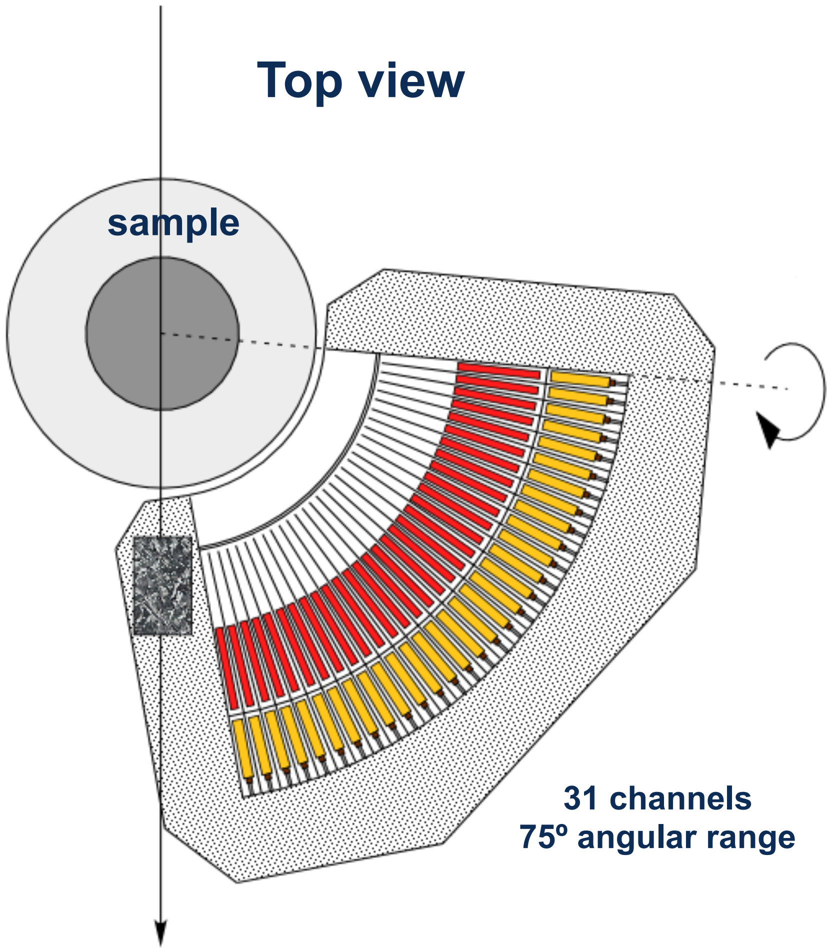
Phonons & QE signal (PMN 110)

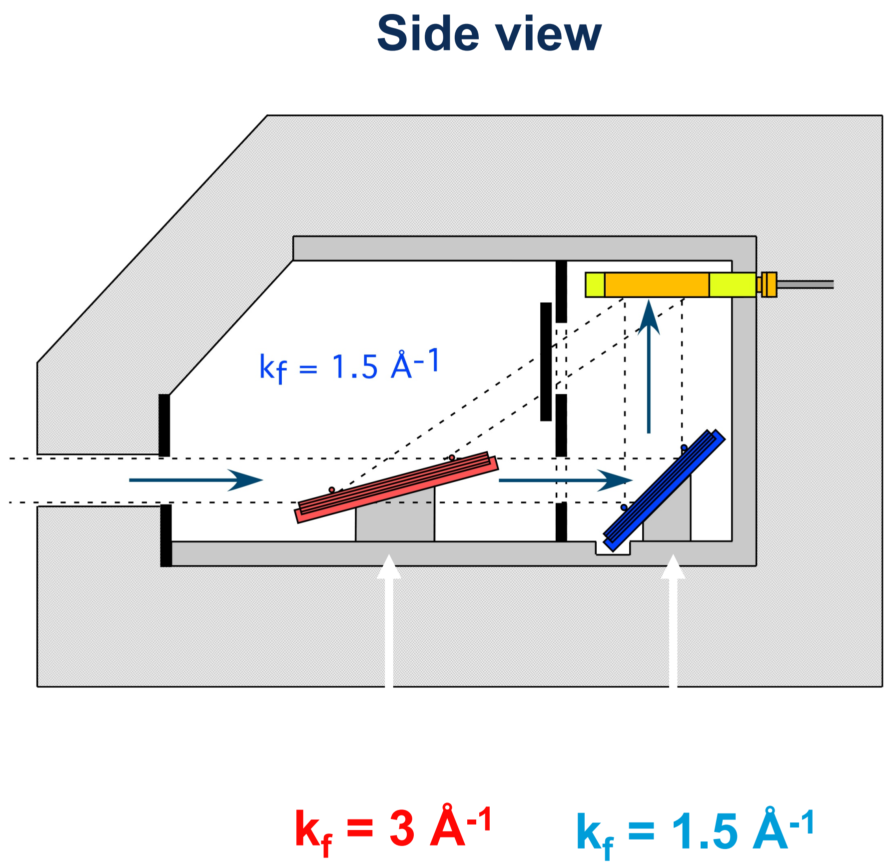




PG-PG	open	DTR 40
PG-PG	40' – 40'	DTR 40
Si-Si	open	DTR 10
Si-Si	40' – 40'	DTR 40

FlatCone multianalyzer

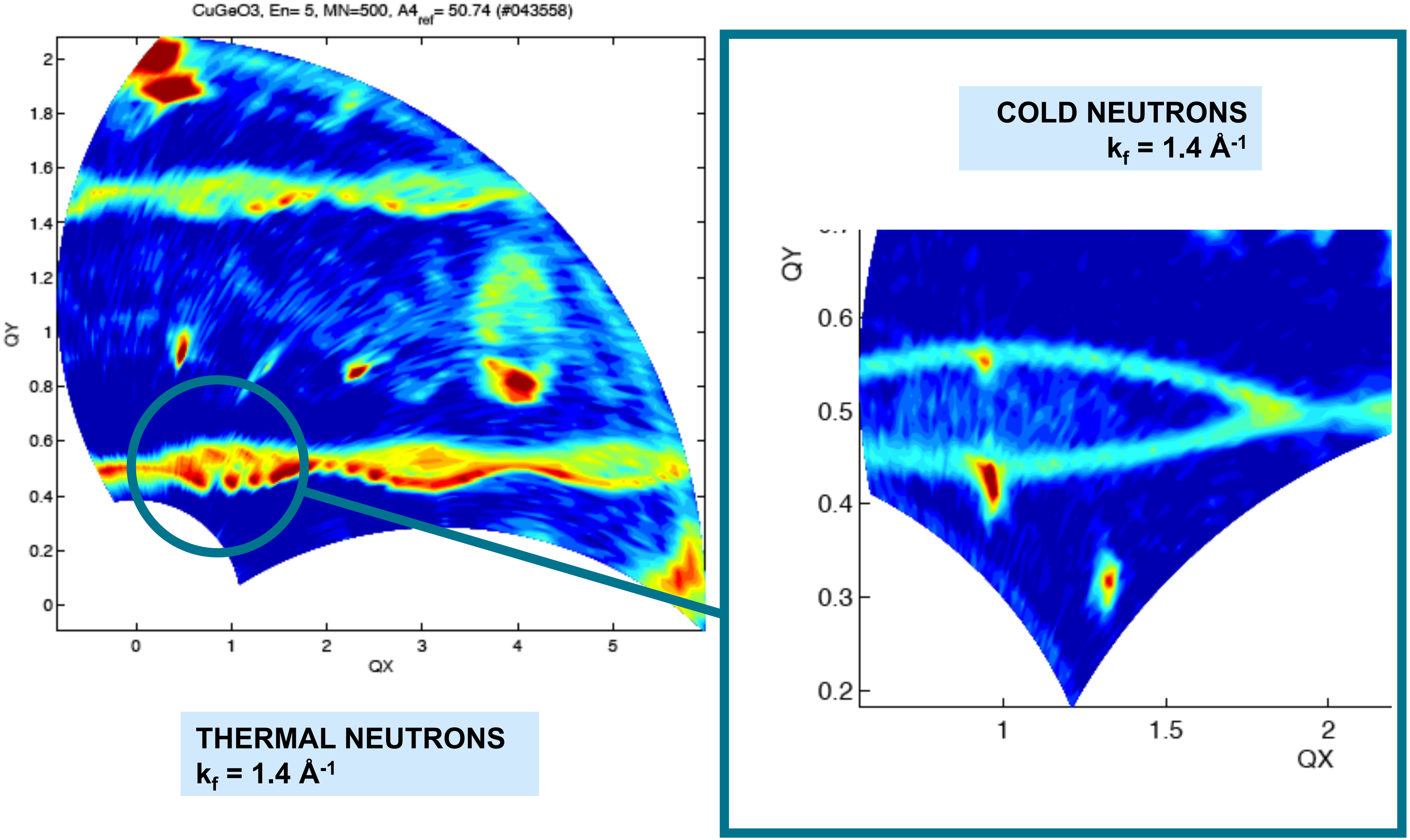




LANGEVIN


IN20, September 2006

$CuGeO_3$

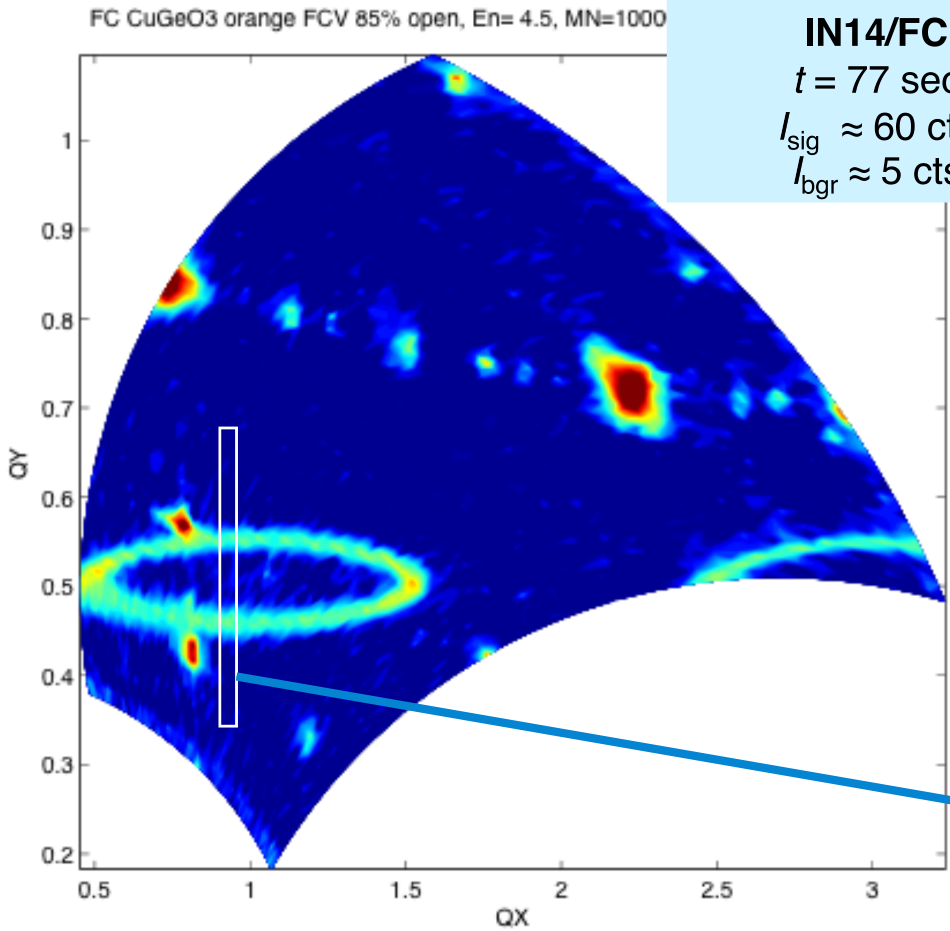


THERMAL NEUTRONS
k_f = 1.4 Å^{-1}

COLD NEUTRONS
k_f = 1.4 Å^{-1}

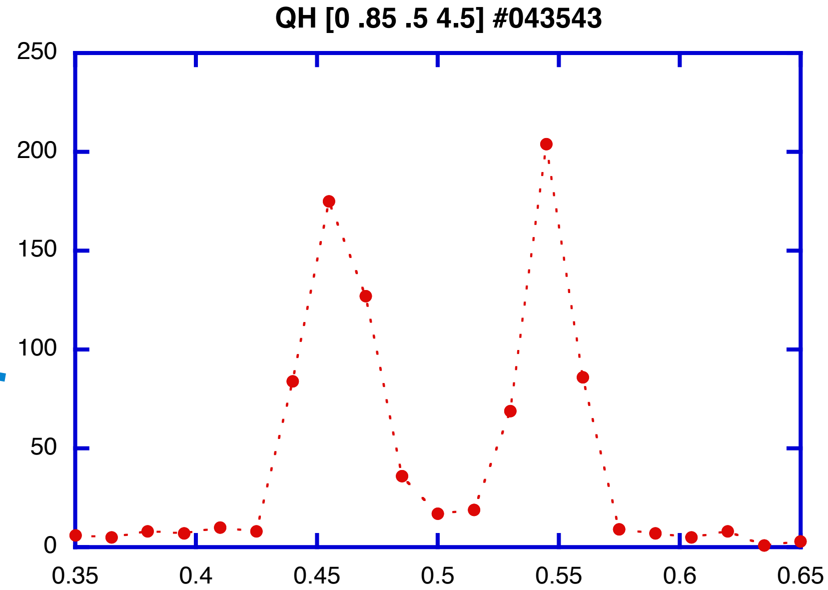
NEUTRONS FOR SOCIETY

$CuGeO_3$ with IN14/FC



IN14/FC
t = 77 sec
I_{sig} ≈ 60 cts
I_{bgr} ≈ 5 cts

IN14/TAS
t = 81 sec
I_{sig} ≈ 180 cts
I_{bgr} ≈ 5 cts



ΔE = 4.5 meV
k_f = 1.4 Å^{-1}

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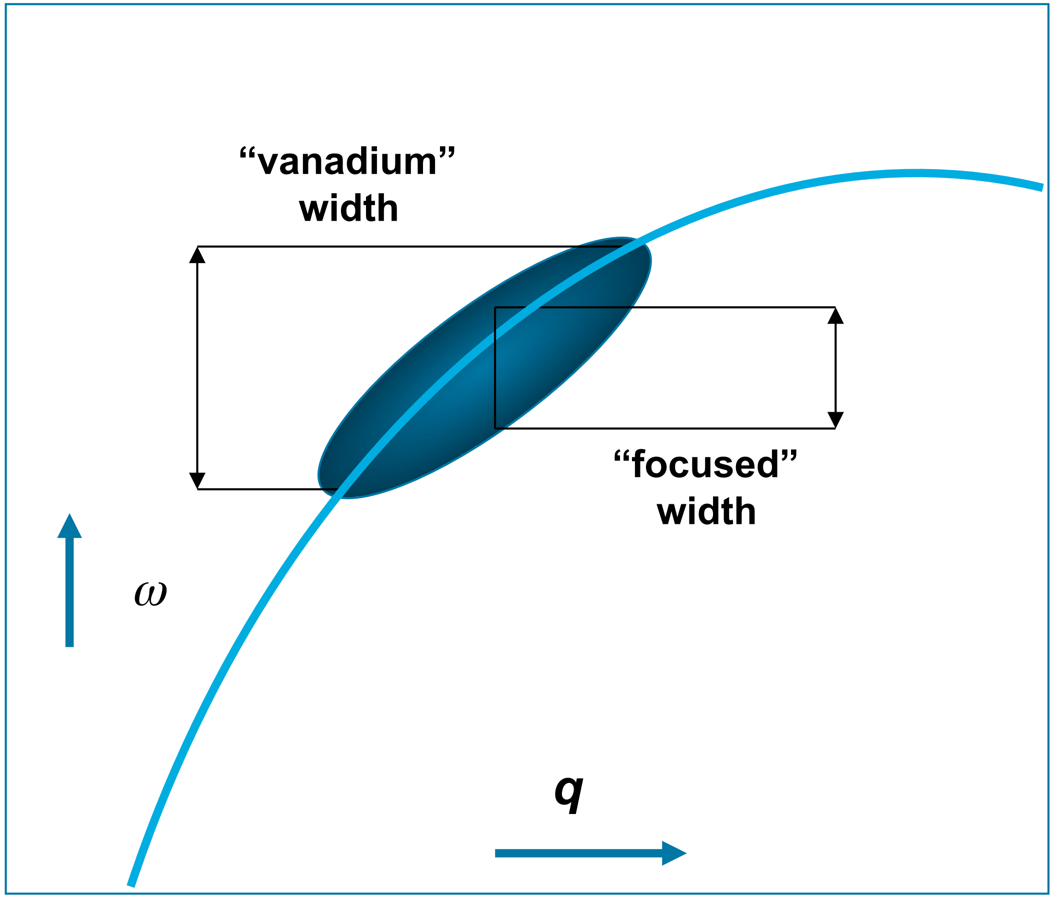
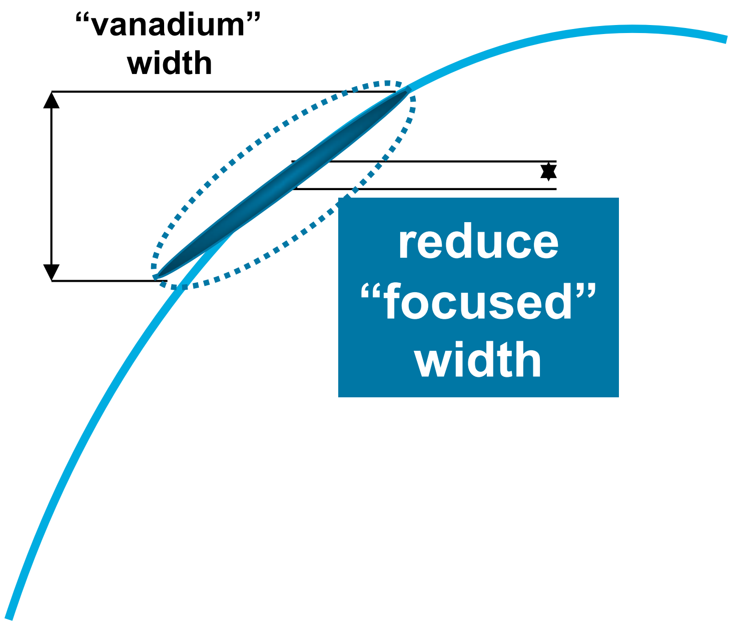
Neutron TAS

Neutron **T**hree-**A**xis **S**pectrometers:

- access to large Q,ω range
- energy resolution $\Delta E/E \approx$ 5-10%
- efficient for $\omega(q)$
- lacking resolution for $\Gamma(q)$

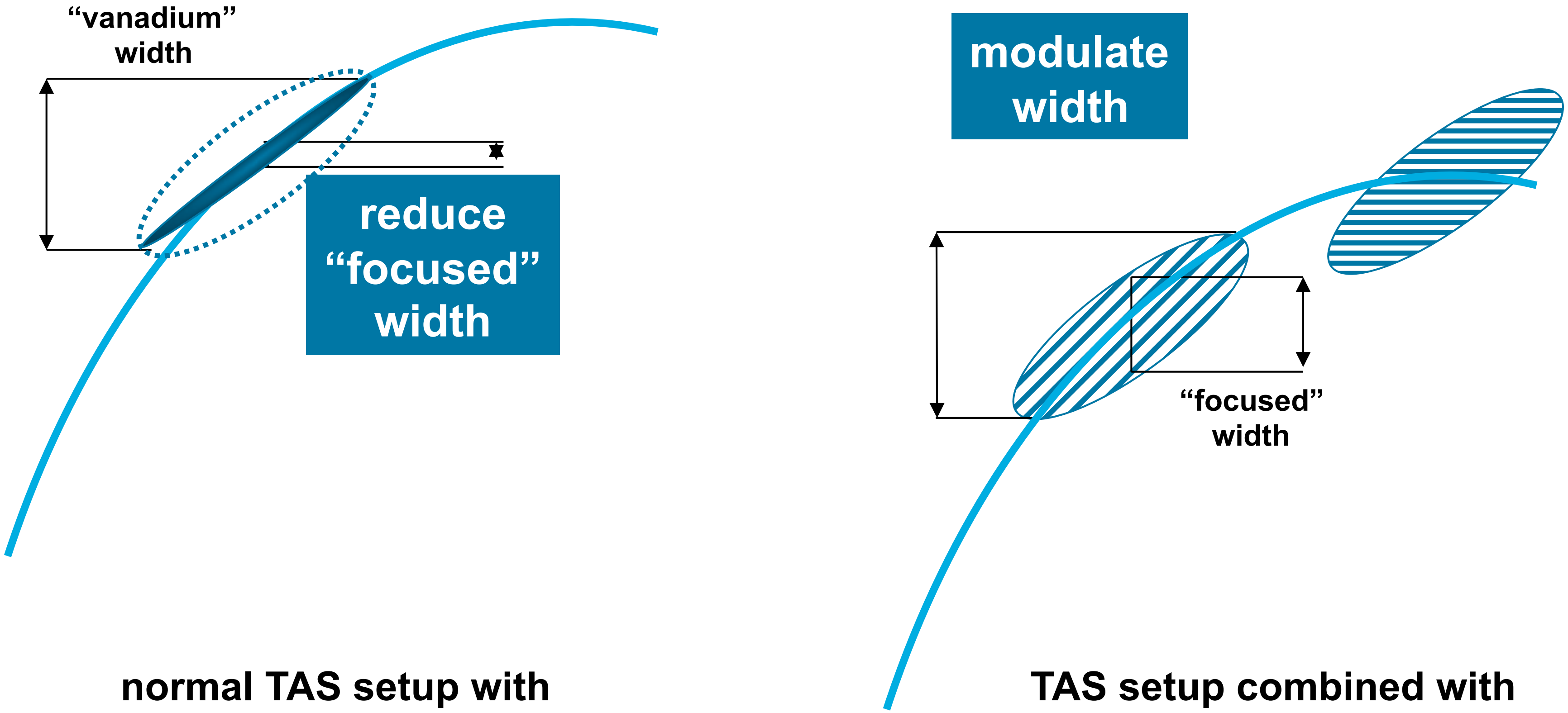


TAS resolution



normal TAS setup with perfect monochromator & analyzer crystals (Si, Ge)

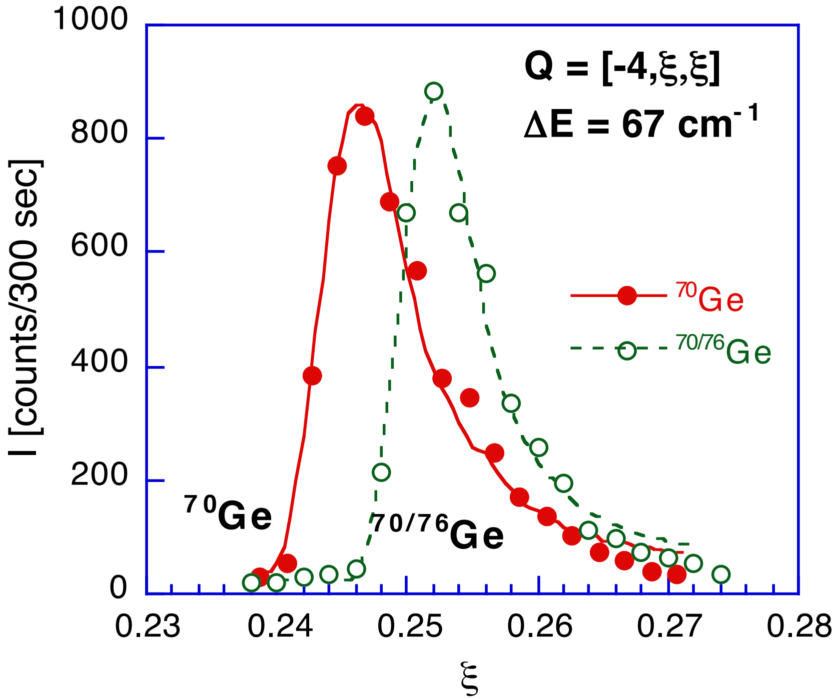
TAS resolution



normal TAS setup with perfect monochromator & analyzer crystals (Si, Ge)

TAS setup combined with spin-echo (TOF Fourier technique)

TASSE vers. high resolution TAS

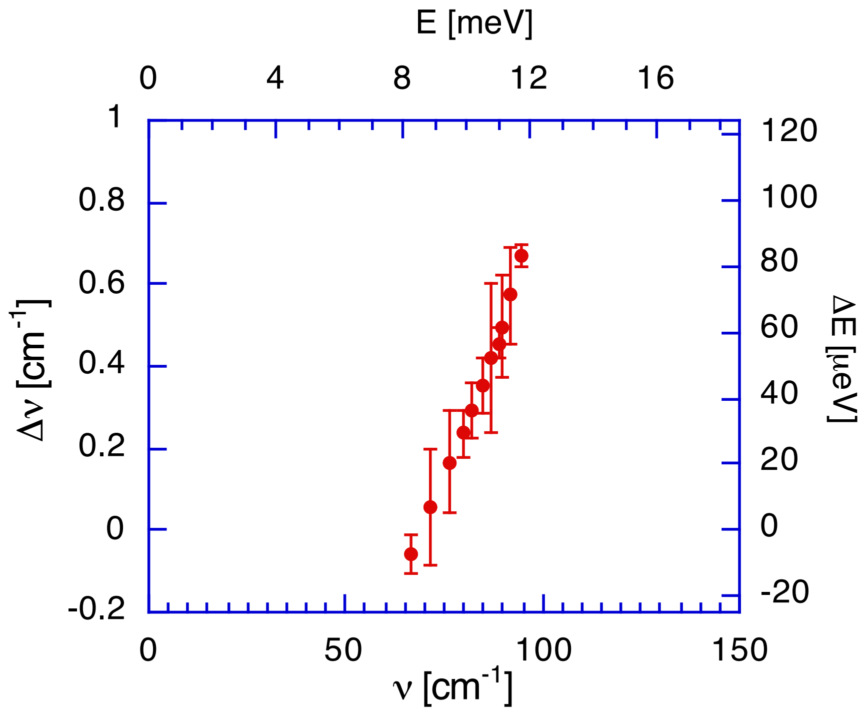


IN20

Si111/Si111

$R_M = R_A = 50$ m

sample volume < 0.5 cm^3



- *same position accuracy*
- *HR TAS faster and easier*
- *TASSE better for FWHM*

A. Goebel et al., Phys. Rev. B58 (1998) 10510

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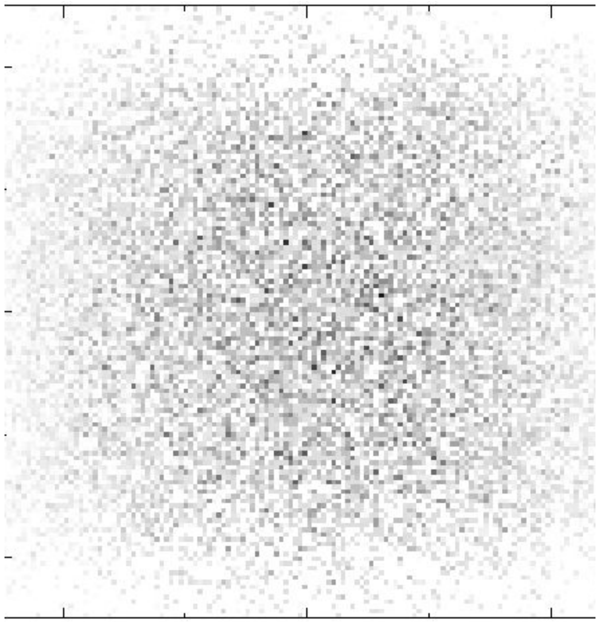
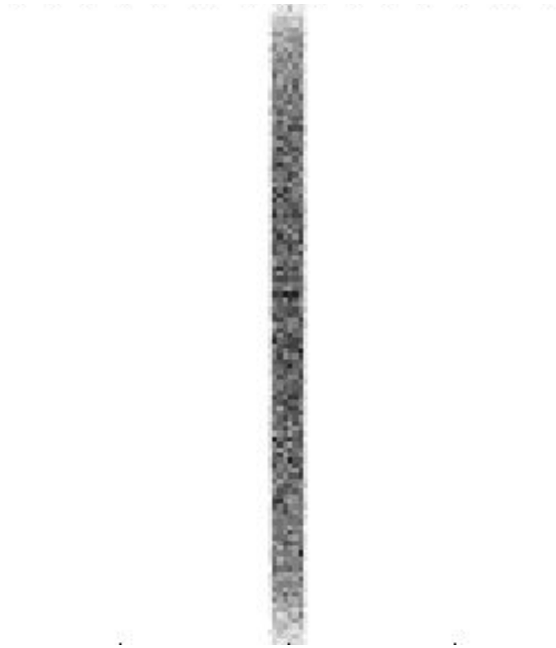
Microfocusing crystal optics



PG002 horizontal focus
(RESTRAX ray-tracing)

Paris-Edinburgh
High pressure cell

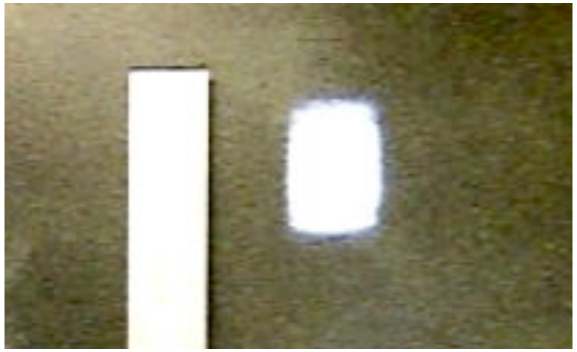


Si111 horizontal focus
(RESTRAX ray-tracing)

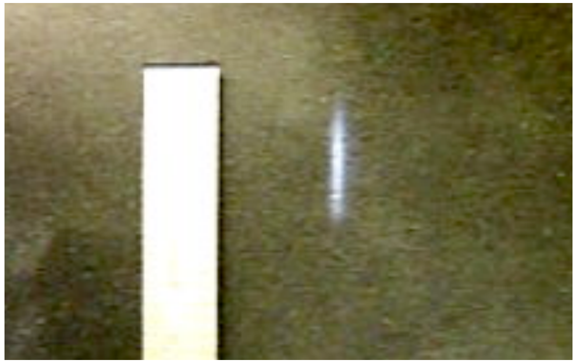
Si (111) microfocusing tests

IN20 (2009)

horizontal (focused)

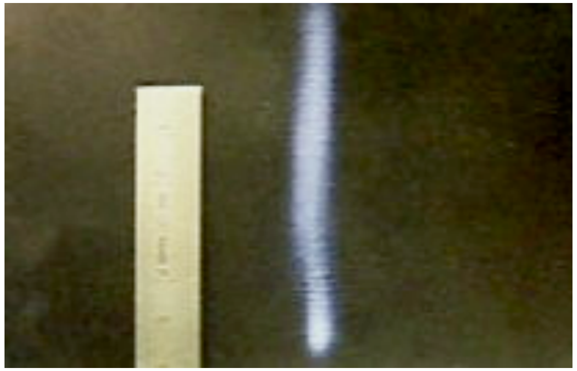


D ≈ 10 mm

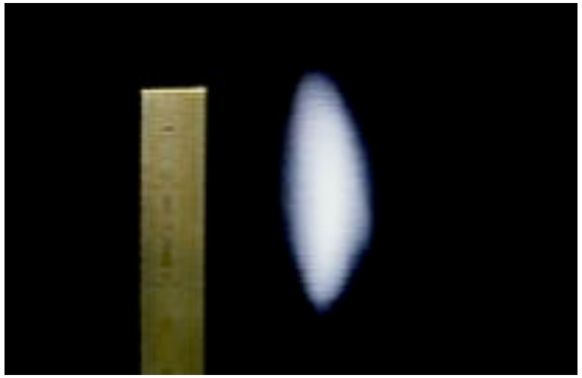


D ≈ 1 mm

vertical (D ≈ 2 mm)

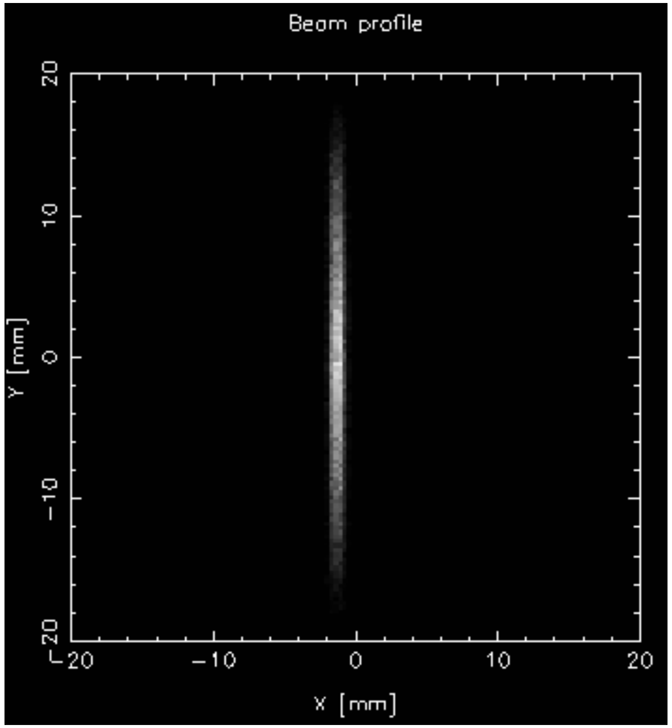


defocused



focused

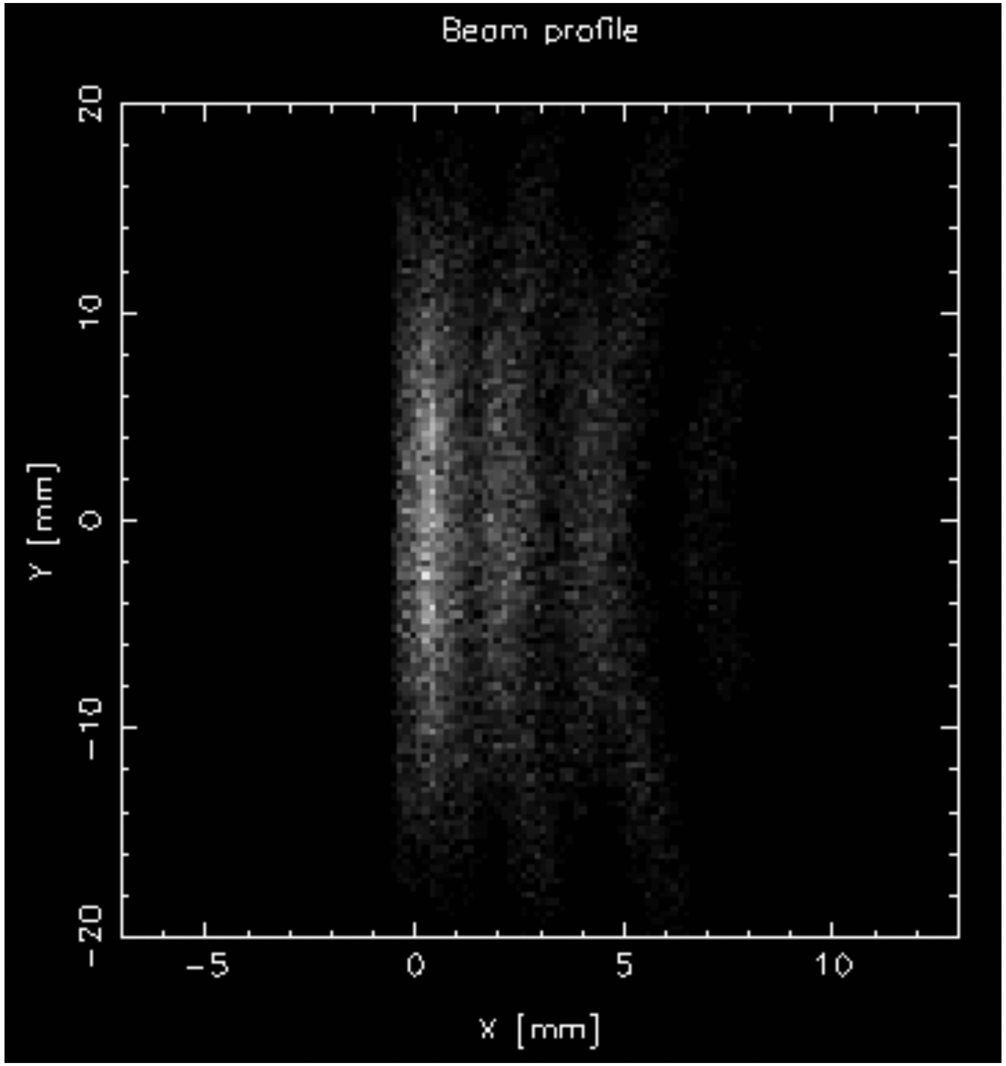
Vertical focusing Si111



1 segment

Restrax simmulation
real space (X-Y)

9 segments

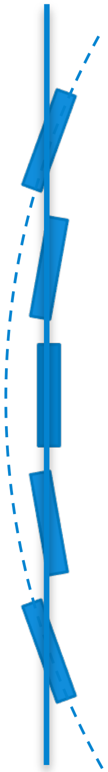


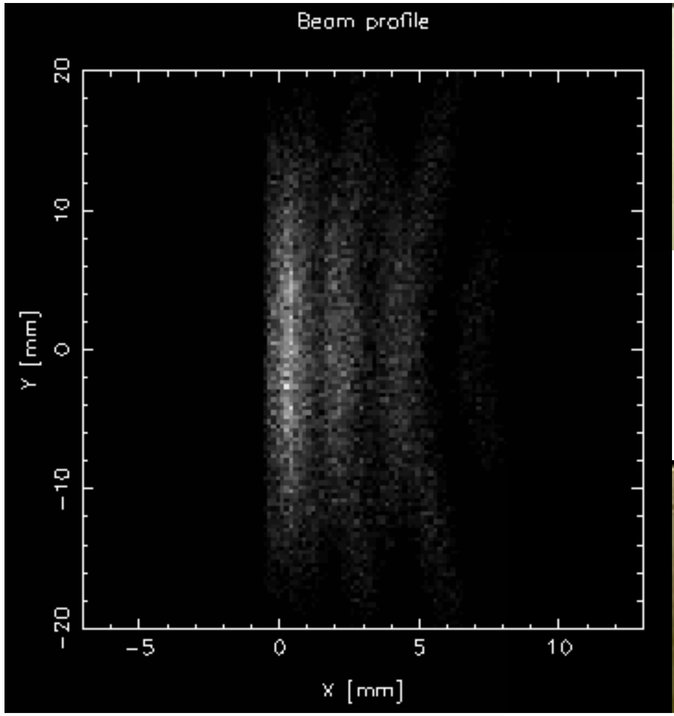
Vertical focusing aberrations

- standard TAS devices approximate cylindrical surface by a flat array of tilted slabs
- in high resolution mode aberrations due to varaitions in θ_B become apparent

➡ **develop a true sagitally focusing system**

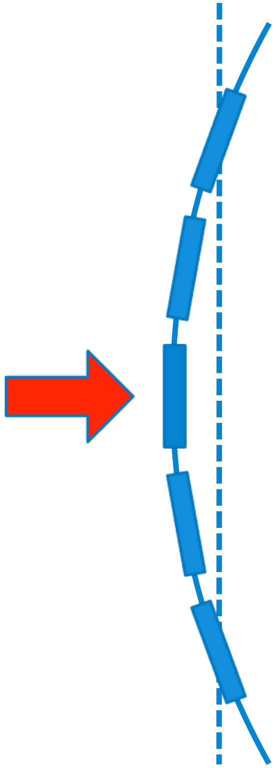
➡ **replace by a multichannel supermirror device**





defocused

focused



sagital focusing

Concluding remarks

Strong points

- deterministic behavior, sharp imaging
- almost rectangular reflection profiles
- absence of 2nd order contamination (Si, Ge, diamond)
- high transparence if Si (multicrystal alignments)

Caveats

- needs precise manufacturing/alignment
- reveals irregularities of samples (sample assemblies)
- aberrations visible in high-resolution setups
- silicon cutting issues