# Comparable MC simulations of a powder diffractometer for the IFE research institute in Norway

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# Outline

- Comparison of simulations using VITESS and McStas
- Design improvement
  - Impile section
  - Monochromator
  - Detector
  - Parameters for high resolution and high intensity measurements
- Summary and Outlook

# Location and Purpose


IFE (Institute for energy technique) in Kjeller close to Oslo

- Main research subject: hydrogen storage

# Overall design

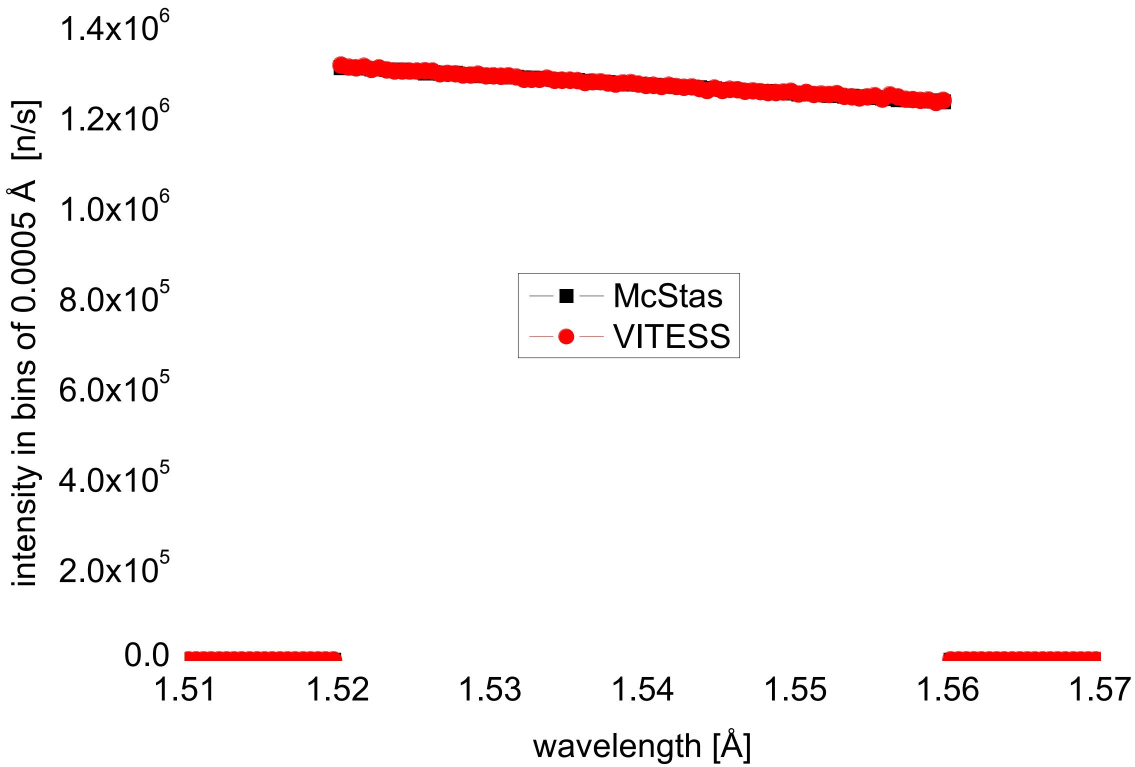
# McStas – VITESS Comparison: Intensities

- Instrument after first phase of design study
- Parameters:
  - 90 deg take-off angle, 1.540 Å
  - Sample: NAC, 0.5 cm diameter, 3 cm height
- Simulated with the McStas and the VITESS package

| | | | McStas | | VITESS | | | |
|---|---|---|---|---|---|---|---|---|
| component | monitor position | intensity [n/s] | error [n/s] | flux [n/(cm²s)] | intensity [n/s] | error [n/s] | difference in component | total difference |
| impile | out | 1.019E+08 | 6.E+03 | | 1.019E+08 | 2.E+04 | -0.01% | -0.01% |
| collimator | out | 1.172E+07 | 2.E+03 | | 1.171E+07 | 6.E+03 | -0.04% | -0.04% |
| monochromator | out | | | | 1.551E+06 | 3.E+03 | | |
| first slit in shielding | out | 1.564E+06 | 7.E+02 | | 1.551E+06 | 3.E+03 | -0.78% | -0.82% |
| focussing collimator | out | 1.463E+06 | 7.E+02 | | 1.448E+06 | 2.E+03 | -0.18% | -1.00% |
| sample | in | 1.563E+05 | 2.E+02 | 1.042E+05 | 1.536E+05 | 8.E+02 | -0.74% | -1.73% |
| detector | in | 246 | 1 | | 227 | 1 | -5.96% | -7.59% |
| detector | detected | | | | 133 | 1 | | |

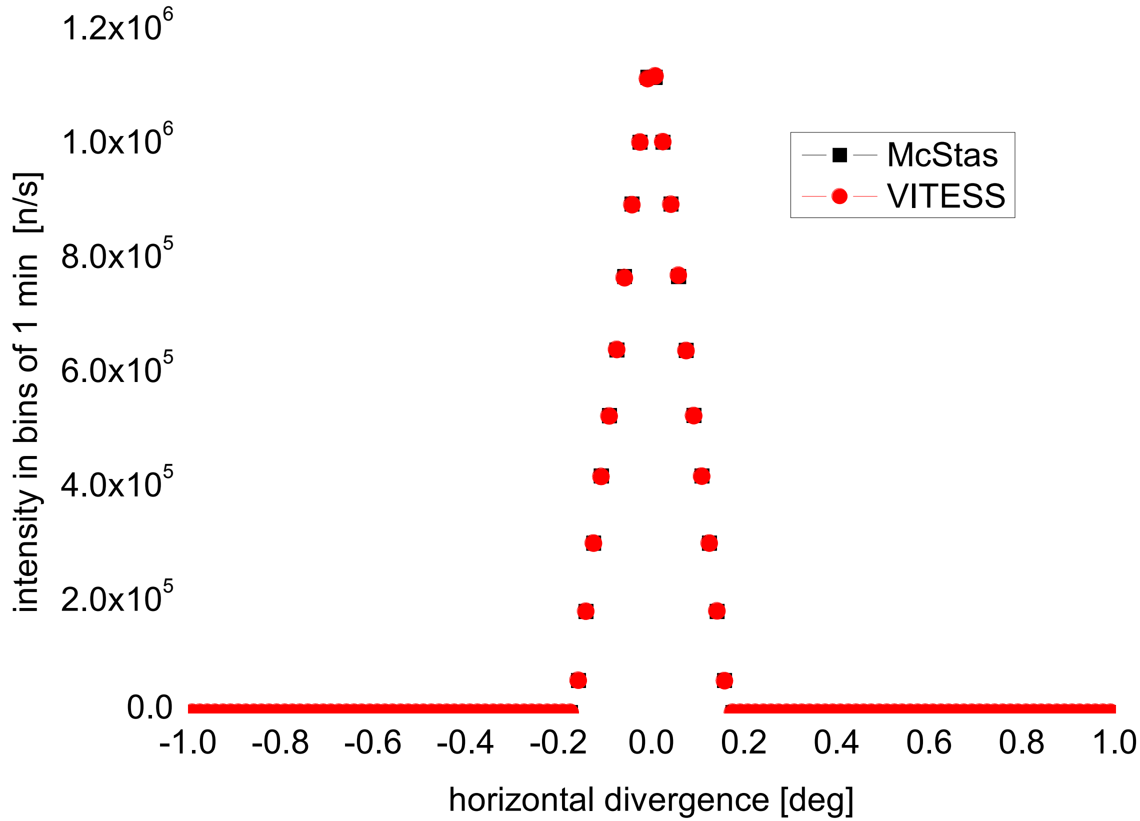
- Very good agreement except for sample
- Possible reason:
  - Different treatment of attenuation inside sample

# Comparison McStas – VITESS 1



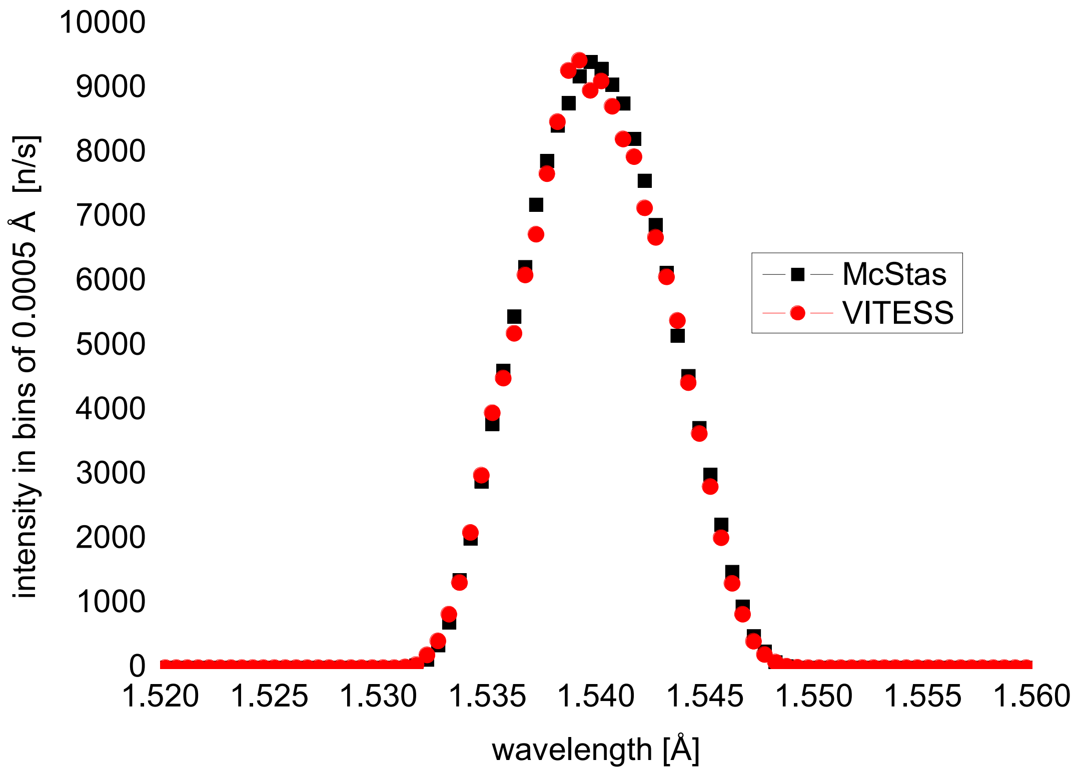

- Identical wavelength distribution at the end of the impile section

# Comparison McStas – VITESS 2



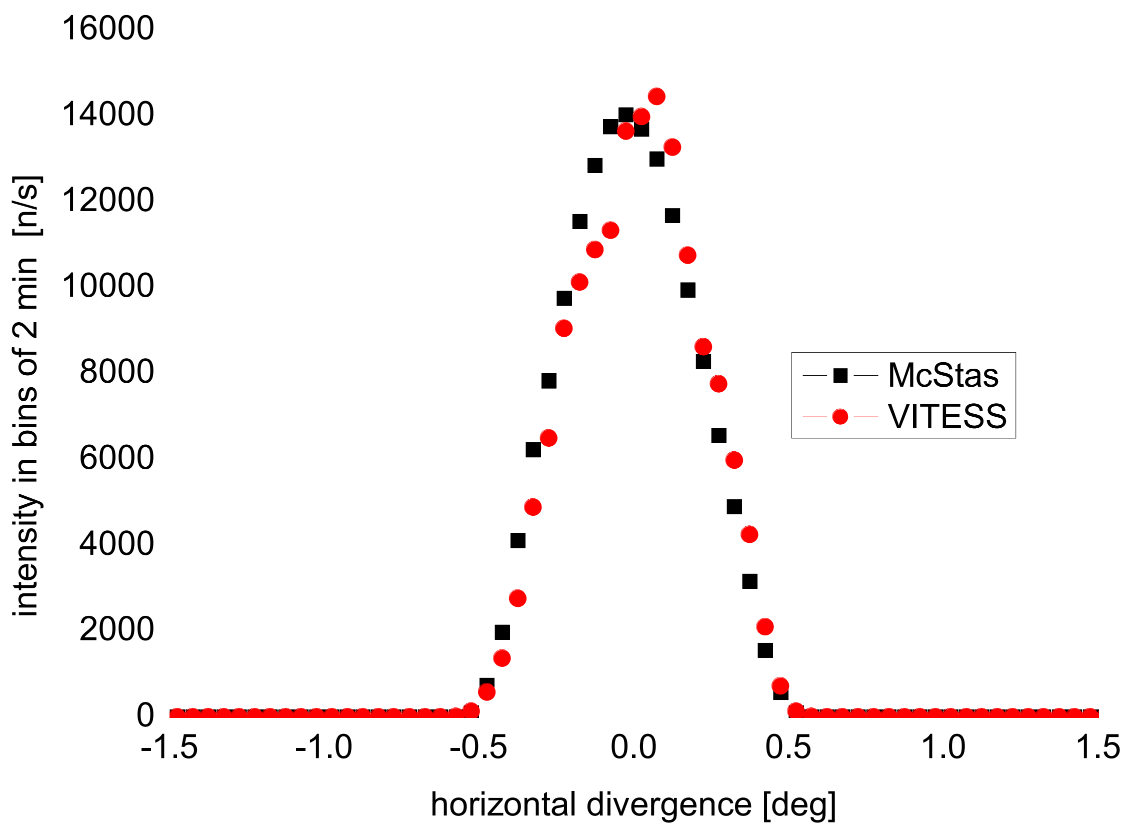

- Identical result after collimator

# Comparison McStas – VITESS 3



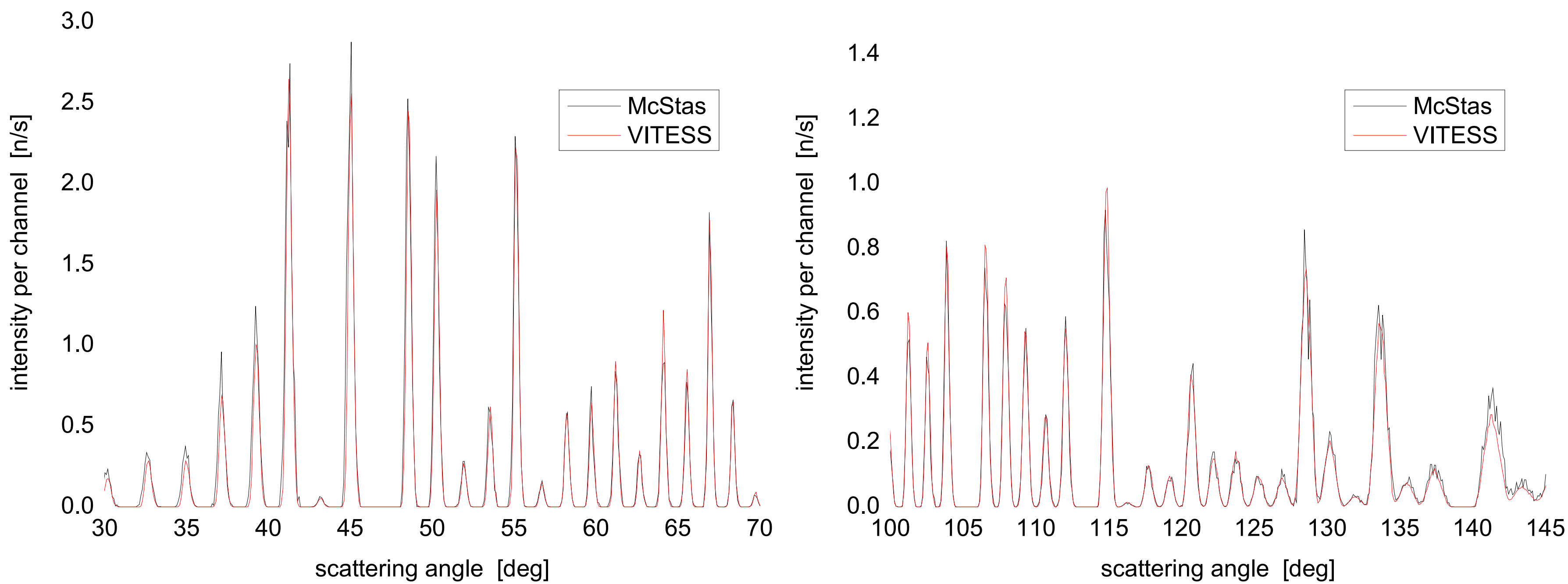

- Wavelength distribution at sample nearly identical

# Comparison McStas – VITESS 4




- Divergence distribution at sample very similar, but slightly shifted

# McStas – VITESS Comparison: Detector Signal

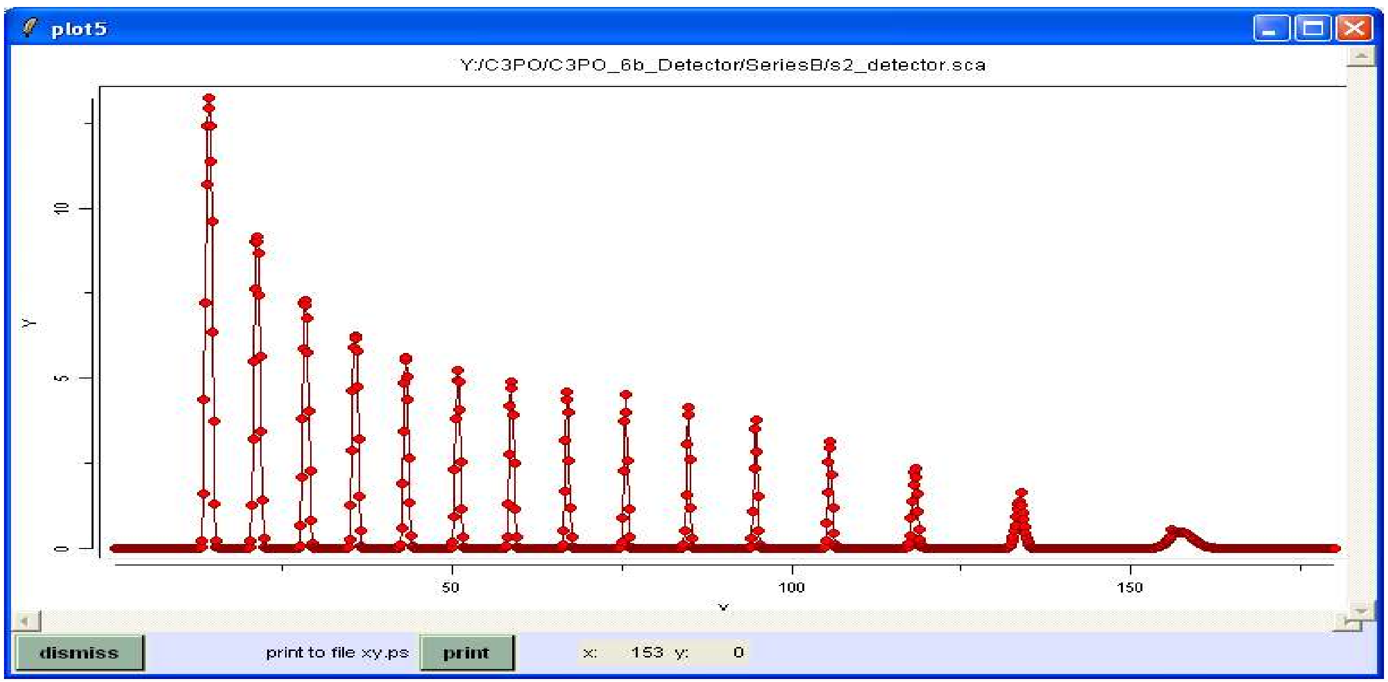



- Good agreement of line shape and relative intensities

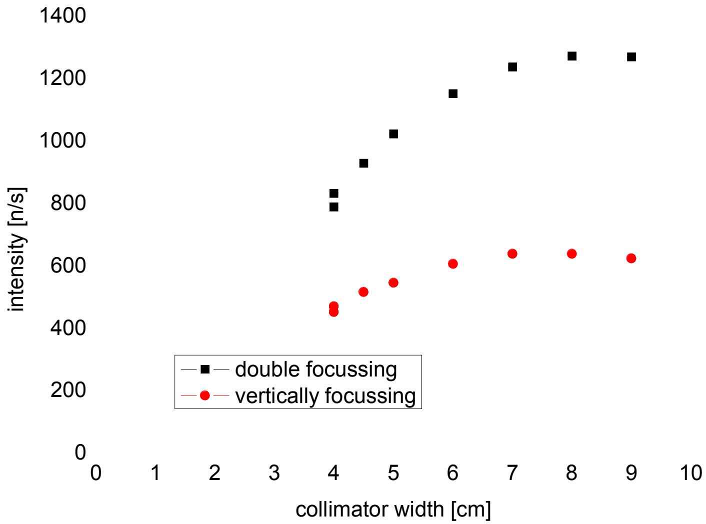
Comment: Vitess detector used in option 'Monitor only'

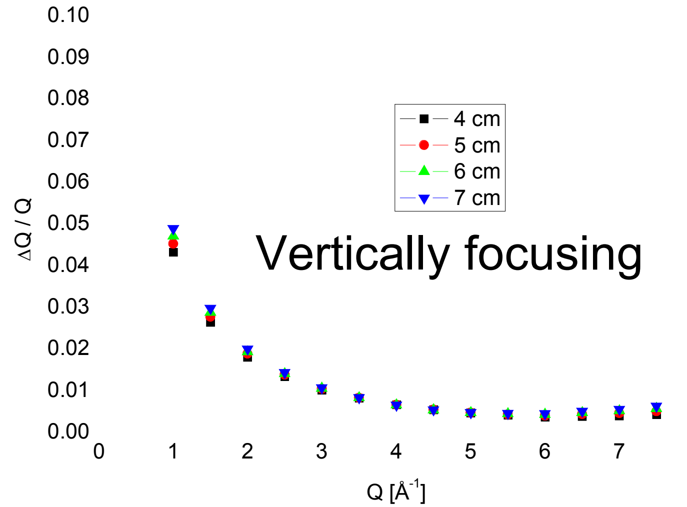
# Artificial sample

- The performance of an instrument is investigate by means of an artificial sample, which
  - Has reflections of identical intensity (and no internal line width)
  - Lines are well separated to allow simple line width determination
  - In this case, reflections occur for Q = 1, 1.5, 2, ……8 $Å^{-1}$
- The resulting diffraction pattern (for λ=1.54 Å) looks like that:

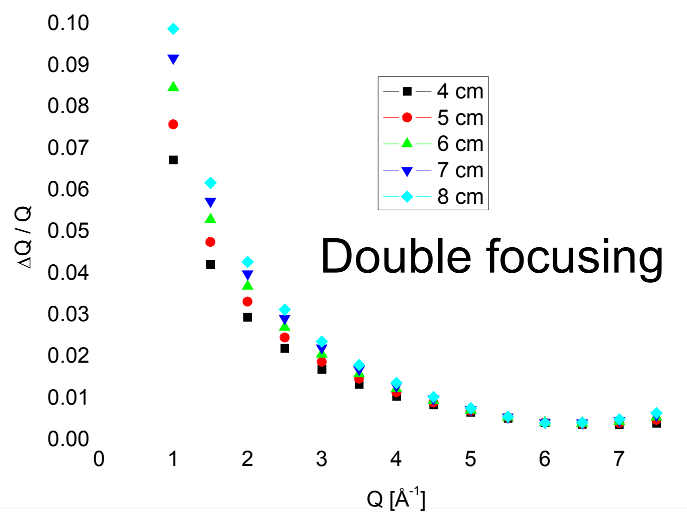


# Size of the Impile Section



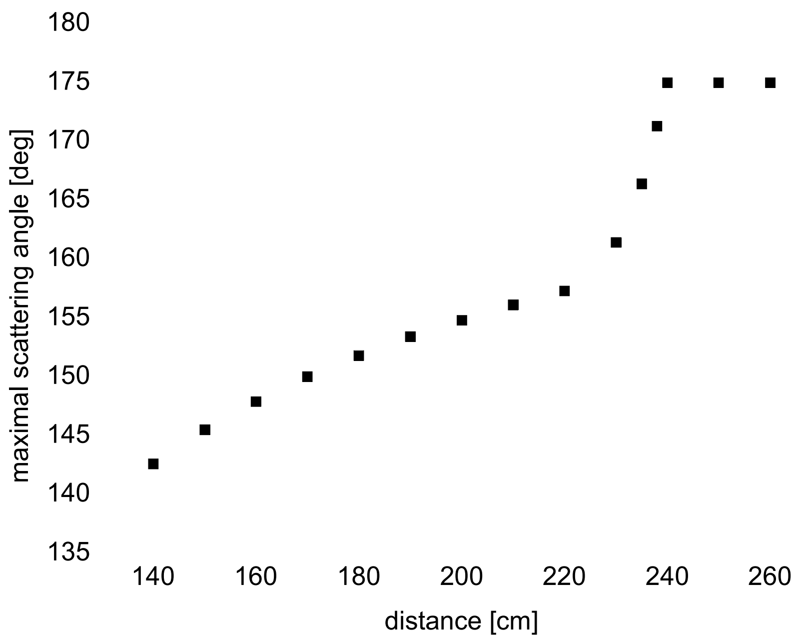




- Method:
  rectangular cross-sections chosen that fit into the tube of circular profile
- Result:
  increasing the width from 4 to 8 cm yields a gain of about a factor of 1.5 in intensity, but results in a loss of resolution
- Value for following simulations: 70 x 120 $mm^2$
- Idea:
  large cross-section here and variable aperture in front of the sample

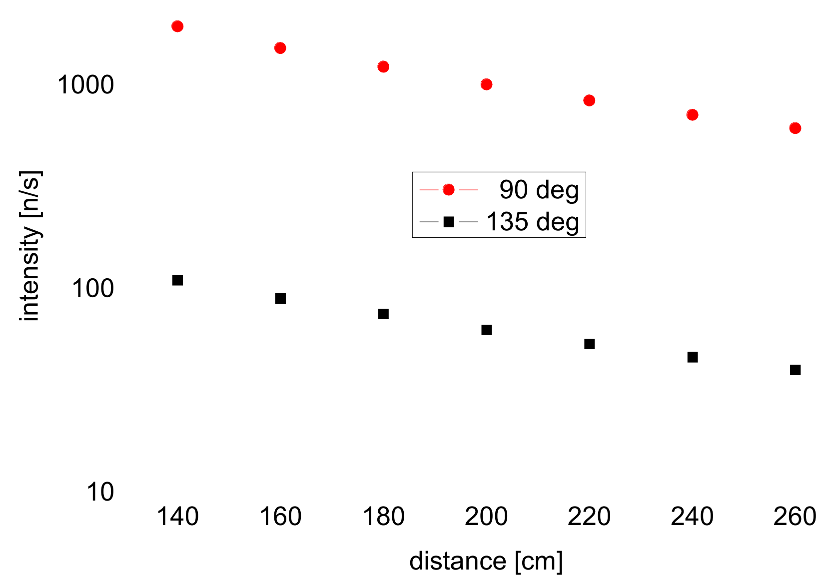


# Variation of Monochromator – Sample Distance 1

**Maximal angle of detection as a function of monochromator – sample distance**



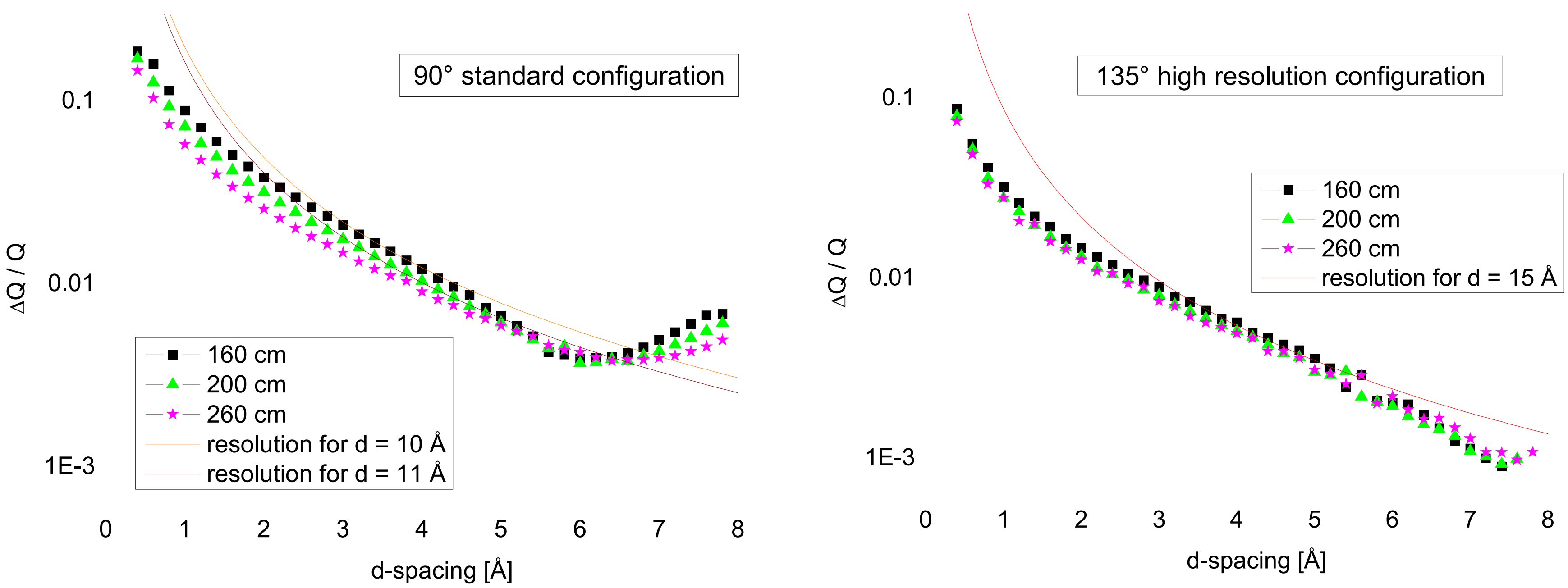

**Intensity as a function of distance monochromator - sample**




- Maximal detection angle drops down rapidly to about 155° below 2.4 m and then decreases further for shorter distances
- Intensity increases significantly with decreasing monochromator – sample distance

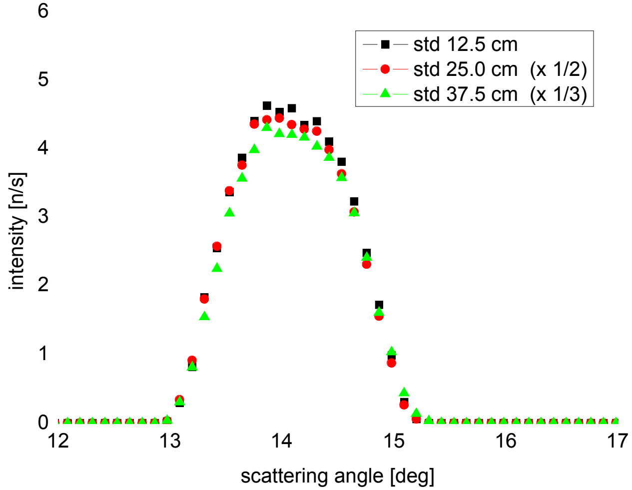
# Variation of monochromator – sample distance 2

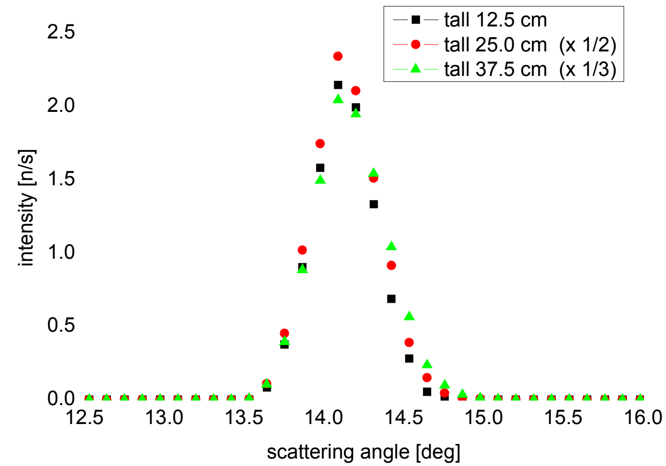
**Resolution as a function of distance monochromator - sample**




- Resolution worsens with decreasing monochromator – sample distance, only for the standard configuration not for the high resolution option

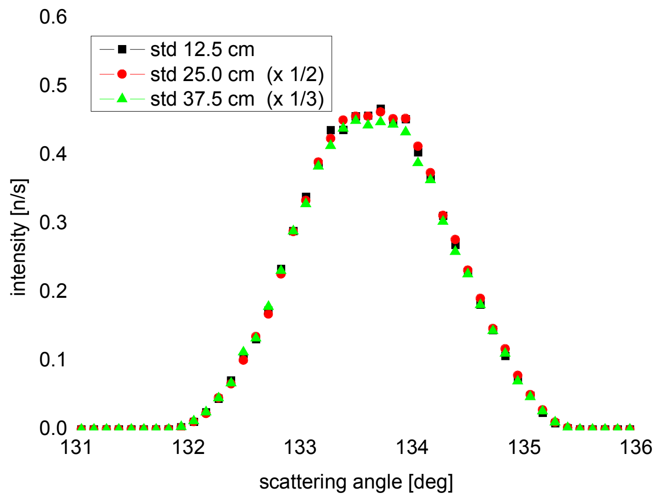
# Line Shapes for Different Detector Heights

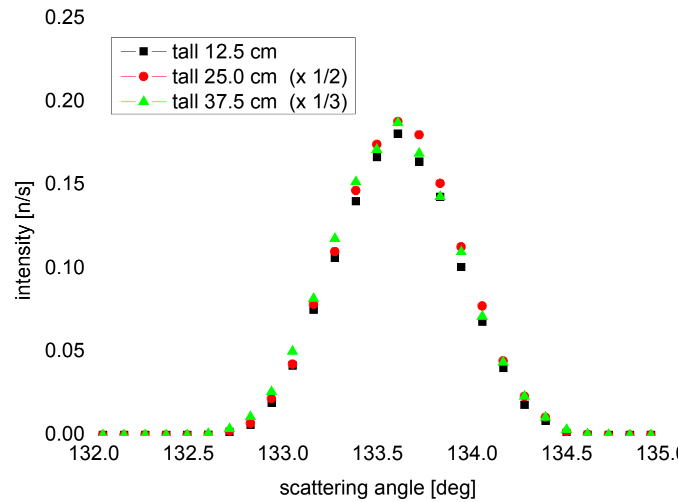



**monochromator slit 60 x 110 mm²**

**monochromator slit 20 x 170 mm²**




- Significant influence of detector height on the line shape exists only for narrow tall slit and low scattering angle

# Influence of Detector Cell Size on Instrument Resolution 1

Necessary resolution to resolve lines of a cubic lattice of cell constant $d_0$ is:

$$\Delta d/d = d^2 /( 2\, d_0^2)$$

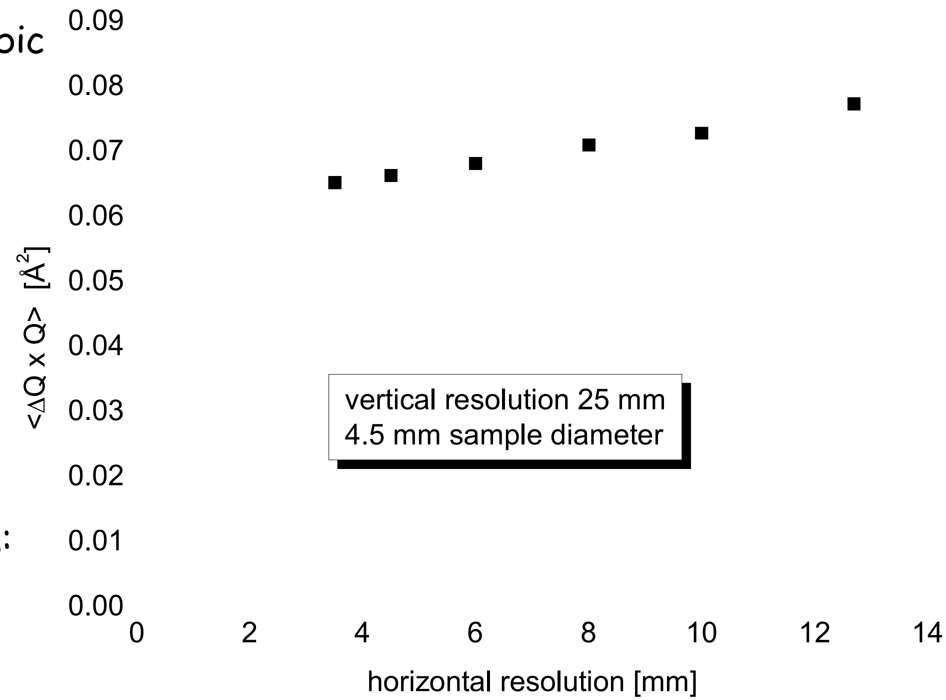
That is in Q:

$$\Delta Q/Q = Q_0^2 /(2\, Q^2)$$

$$\Rightarrow \quad \Delta Q \cdot Q = Q_0^2/2 = const$$

Number used to determine overall resolution:

$$\langle \Delta Q \cdot Q \rangle = 1/N \;\Sigma\; \Delta Q_i \cdot Q_i$$

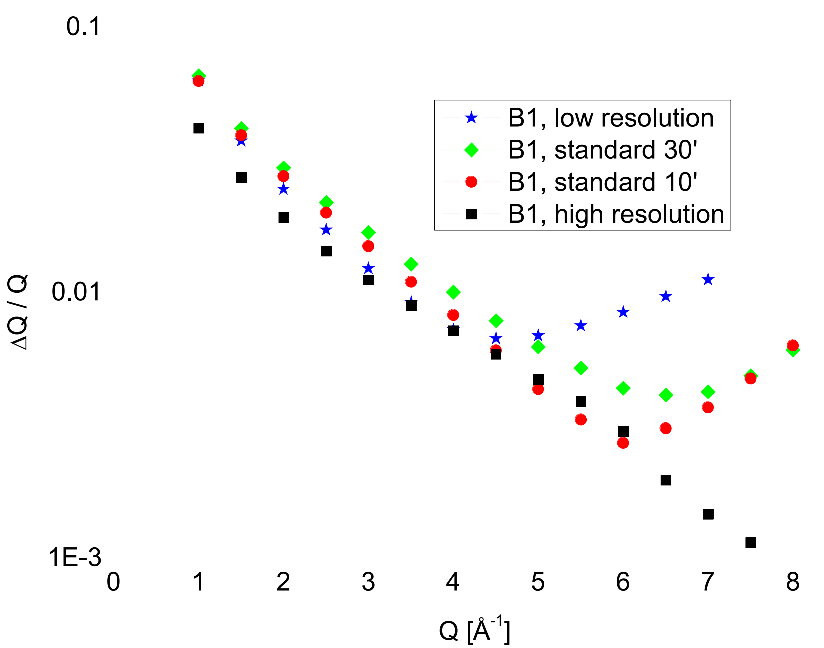


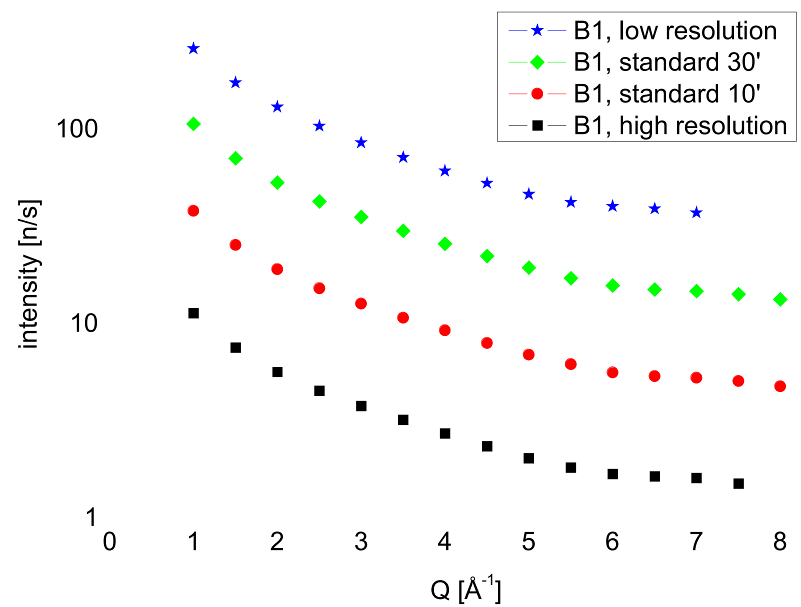

| vertical resolution | | | horizontal resolution | | | |
|---|---|---|---|---|---|---|
| | 3.5 mm | 4.5 mm | 6 mm | 8 mm | 10 mm | 12.7 mm |
| 10 mm | 0.0651 | 0.0665 | 0.0682 | 0.0707 | 0.0728 | 0.0775 |
| 15 mm | 0.0650 | 0.0666 | 0.0683 | 0.0710 | 0.0727 | 0.0777 |
| 20 mm | 0.0652 | 0.0665 | 0.0683 | 0.0709 | 0.0730 | 0.0777 |
| 25 mm | 0.0653 | 0.0664 | 0.0683 | 0.0711 | 0.0729 | 0.0775 |

# High and Low Resolution Set-ups

| take-off [deg] | h | k | l | lambda [Å] | coll 1 [min] | slit [cm] | A [cm] |
|---|---|---|---|---|---|---|---|
| 60.0 | 1 | 1 | 3 | 1.706 | 30.0 | 9.2 | 16.4 |
| 90.0 | 1 | 1 | 5 | 1.540 | 30.0 | 6.0 | 11.0 |
| 90.0 | 1 | 1 | 5 | 1.540 | 10.0 | 6.0 | 11.0 |
| 135.0 | 3 | 3 | 5 | 1.594 | 10.0 | 4.0 | 7.0 |

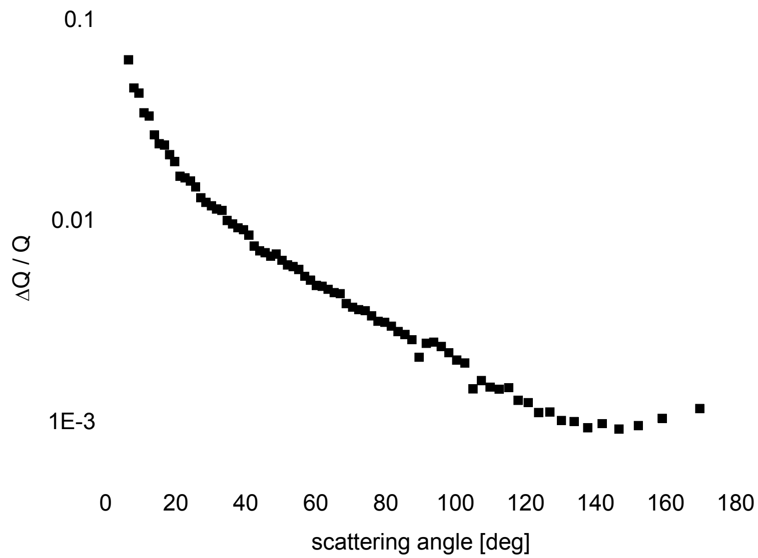
- Intensity and resolution vary a lot

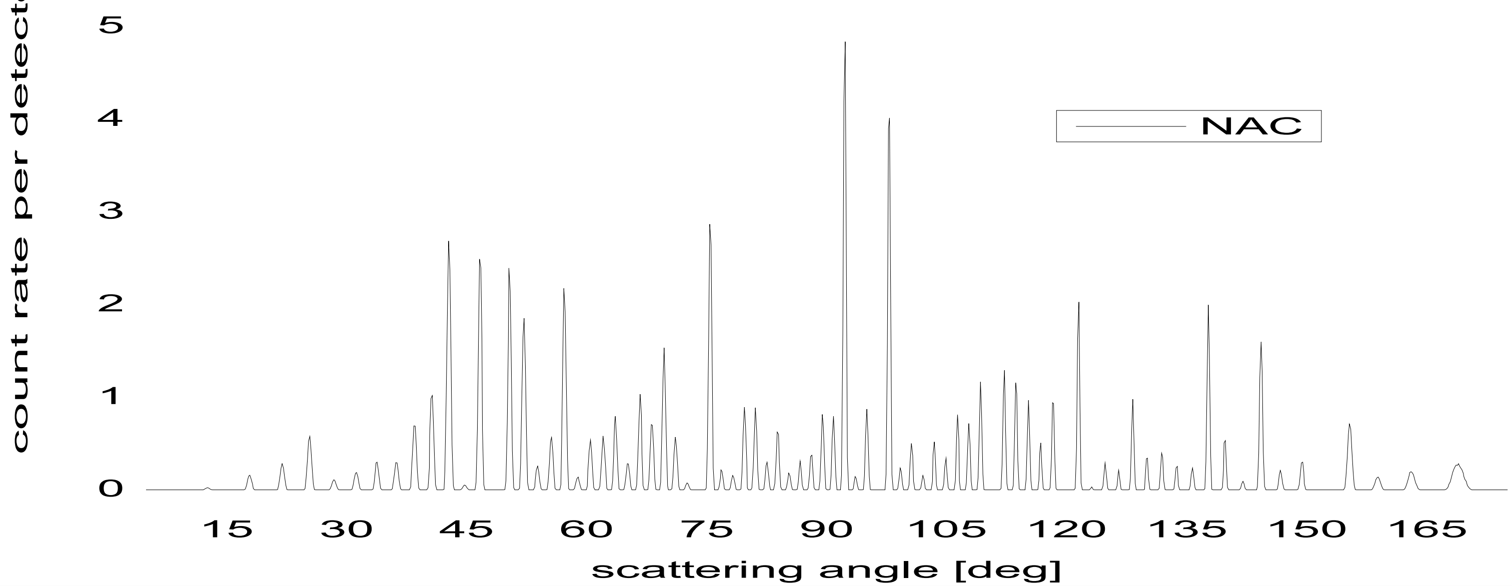


# NAC in the High-resolution Option

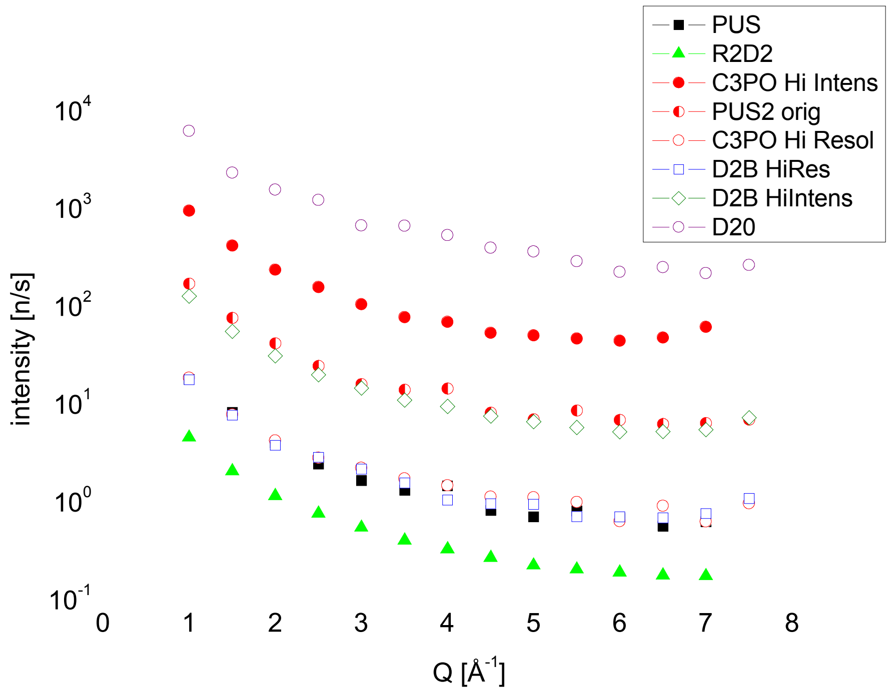
- Parameters
  - Take-off angle 135°
  - 10' collimation
  - Monochromator slit 20 x 70 mm²
  - (335) reflection, 1.594 Å
  - Mosaicity 16'
  - Distance monochromator – sample: 2.0 m
  - Sample size 6 x 30 mm²
  - Detection: 5° - 175°°, 3.5 x 25 mm² cells

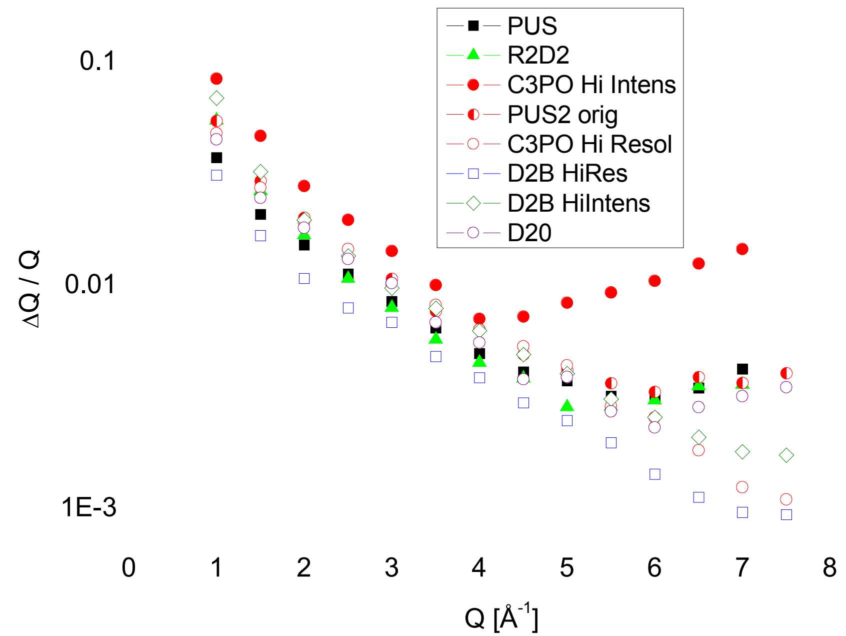


# Updated Performance Comparison

- Performance of the high intensity and the high resolution option in comparison to the instruments shown before

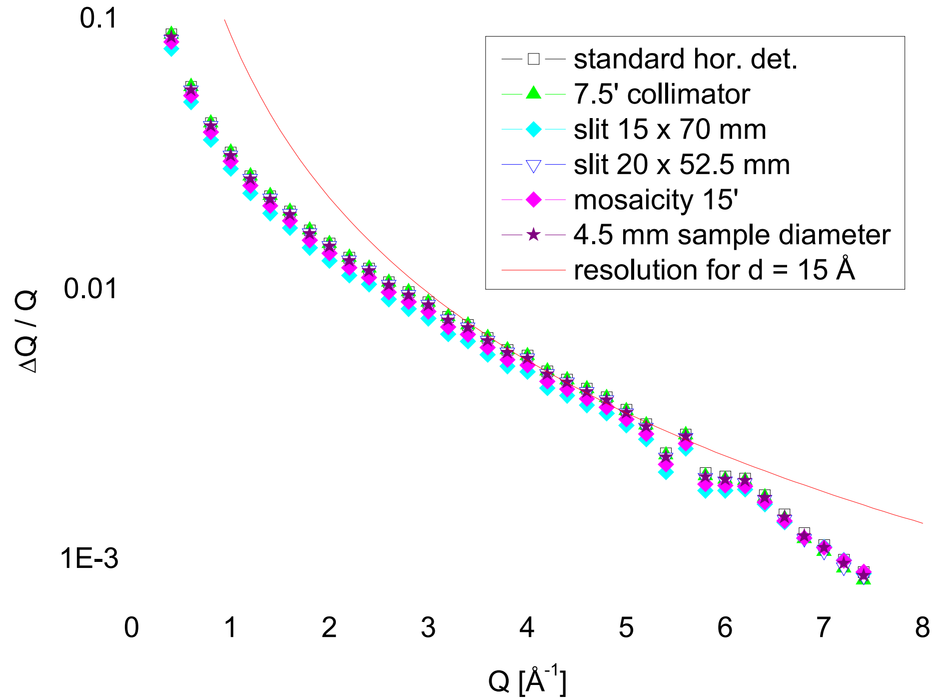



- High intensity option satisfactory
- High resolution option of C3PO could still be better

# Resolution Limiting Factors

- New standard parameter set
  - Take-off angle 135°
  - 10’ collimation
  - Monochromator slit 20 x 70 mm²
  - (335) reflection, 1.594 Å
  - Mosaicity 20’
  - Distance monochr. – sample: 1.6m
  - Sample size 6 x 30 mm²
  - Detector: 5° - 147.9°, 3.5 x 25 mm² cells




- Results
  - Reducing the slit width has the largest effect on resolution, but only up to 105°
  - Reducing the mosaicity improves the resolution in the same range, but to a lower degree
  - The other parameters have hardly any influence.
  - Lines around Q=4.5Å (2θ=70°) are hardest to resolve

# Summary and outlook

- Comparison VITESS – McStas
  - Good agreement for source, collimator and detector
  - Identical shape of spectrum
  - Differences in absolute flux values after monochromator and powder sample in the order of 10 – 25 %

- Features of the Diffractometer
  - The new powder diffractometer will be very flexible by
    - Variable take off angles (60° - 120°)
    - Variable slit size
    - 2 different collimations
  - High intensity is easier to achieve than high resolution
  - Optimal set-up for a given resolution shall be received by numerical optimization of the whole instrument
    - Possible because of the short simulation times using VITESS

Thank you for your attention