Monte-Carlo Modeling of Multiplexed Neutron Spectrometers

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Standard Triple Axis Spectrometers

A1(θ_M): Angle of the Monochromator

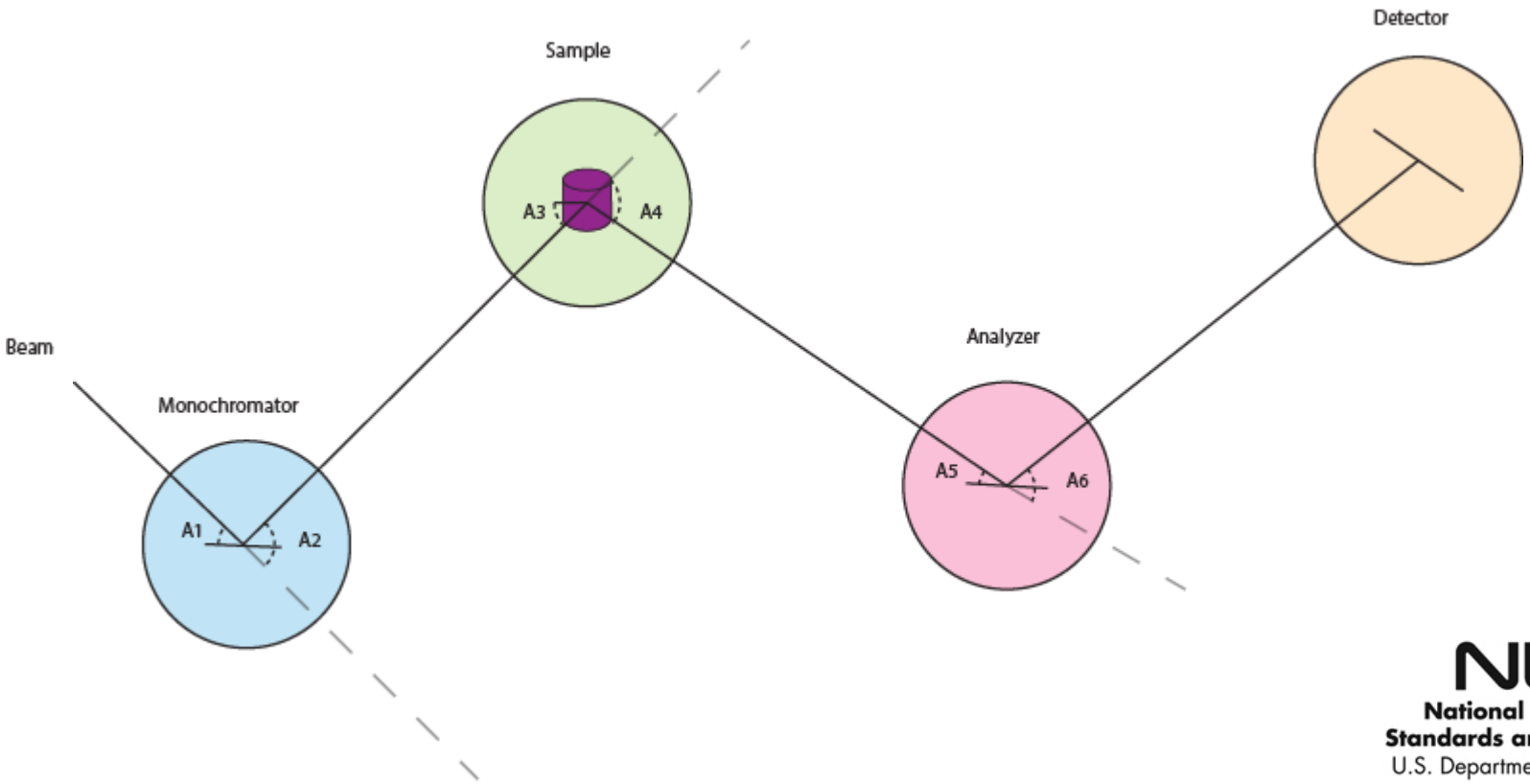
A2($2\theta_M$): Take-off angle from the Monochromator

A3(θ_S): Angle of the Sample

A4($2\theta_S$): Take-off angle from the Sample

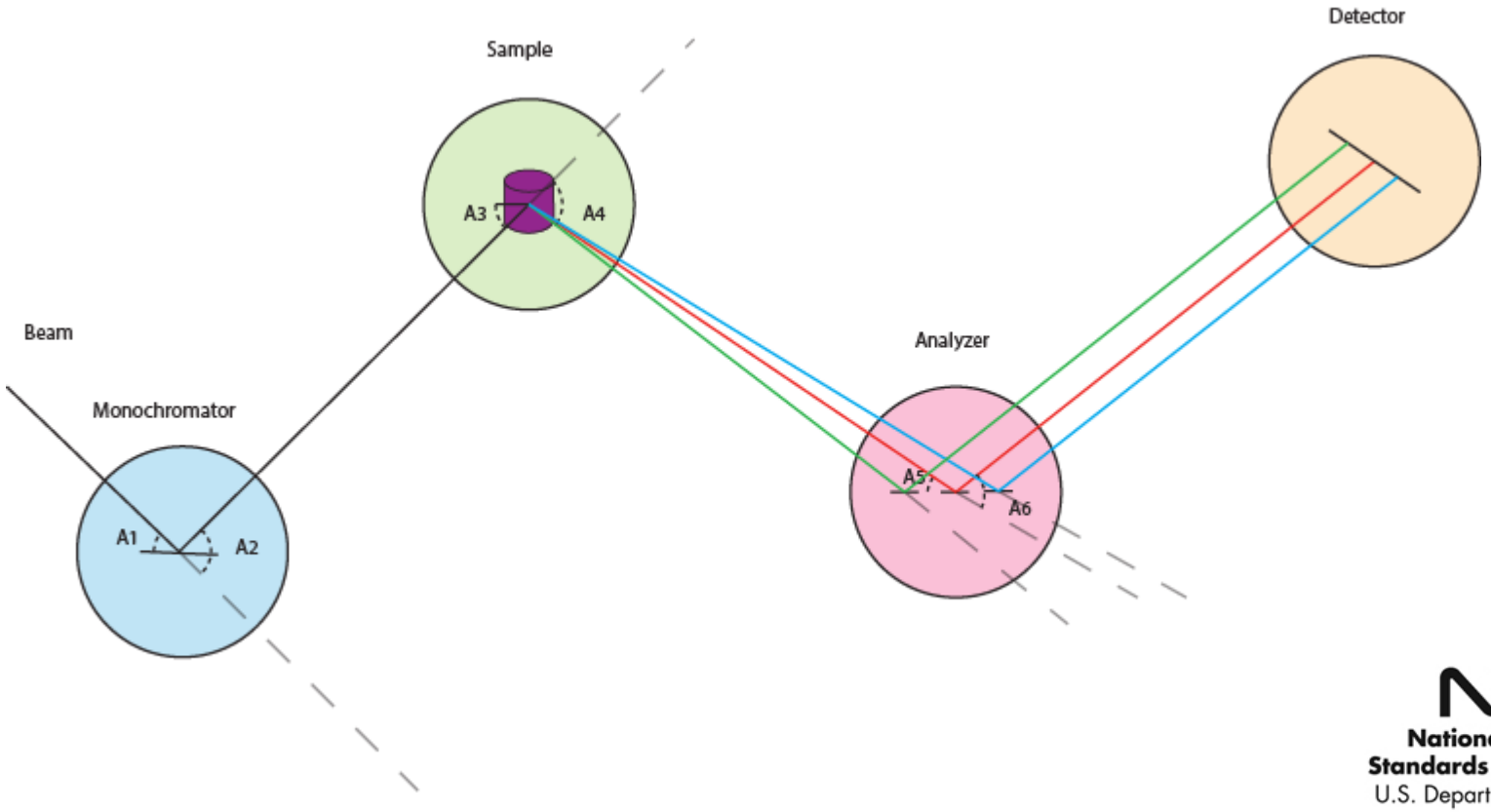
A5(θ_A): Angle of the Analyzer Crystal Group

A6($2\theta_A$): Take-off angle from the Analyzer Crystals



RITA-Style Multiplexed Triple Axis Spectrometers

- In order to cover a larger A4 range, multiple analyzer crystals are aligned along A5 in order to form an Analyzer Crystal Group
- Each crystal can then be individually rotated to scatter a different energy



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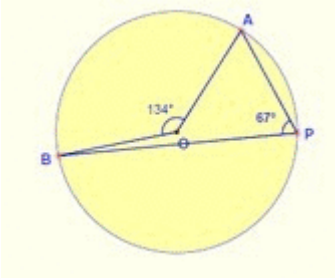
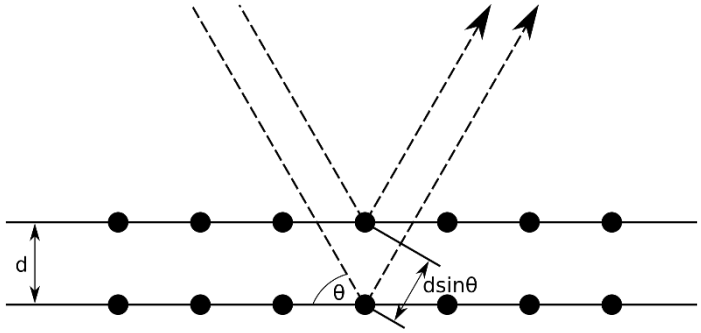
Rowland Geometry

- Uses the Central Angle Theorem



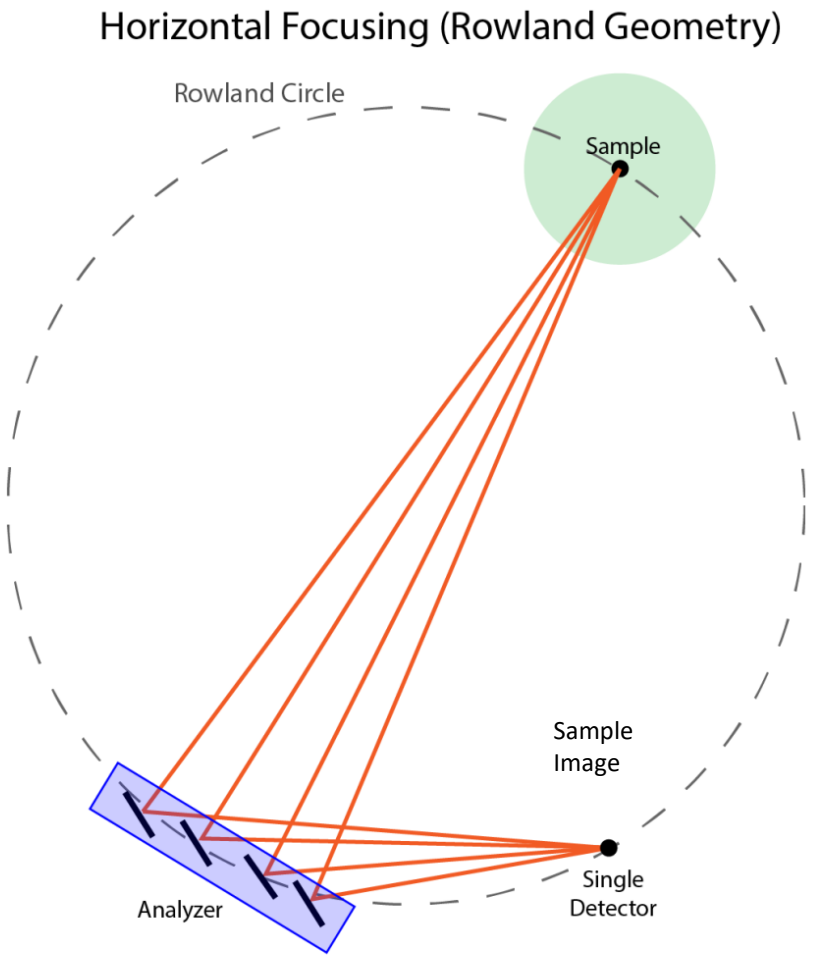
http://www.mathopenref.com/arccentralangletheorem.html

- Bragg's Law
  - Waves are scattered from lattice planes whose interplanar distance is d. The angle necessary for this scattering process to take place is the Bragg angle (θ_B). The waves then scatter off at an angle of $2\theta_B$.
  - $n\lambda=2d\sin\theta_B$



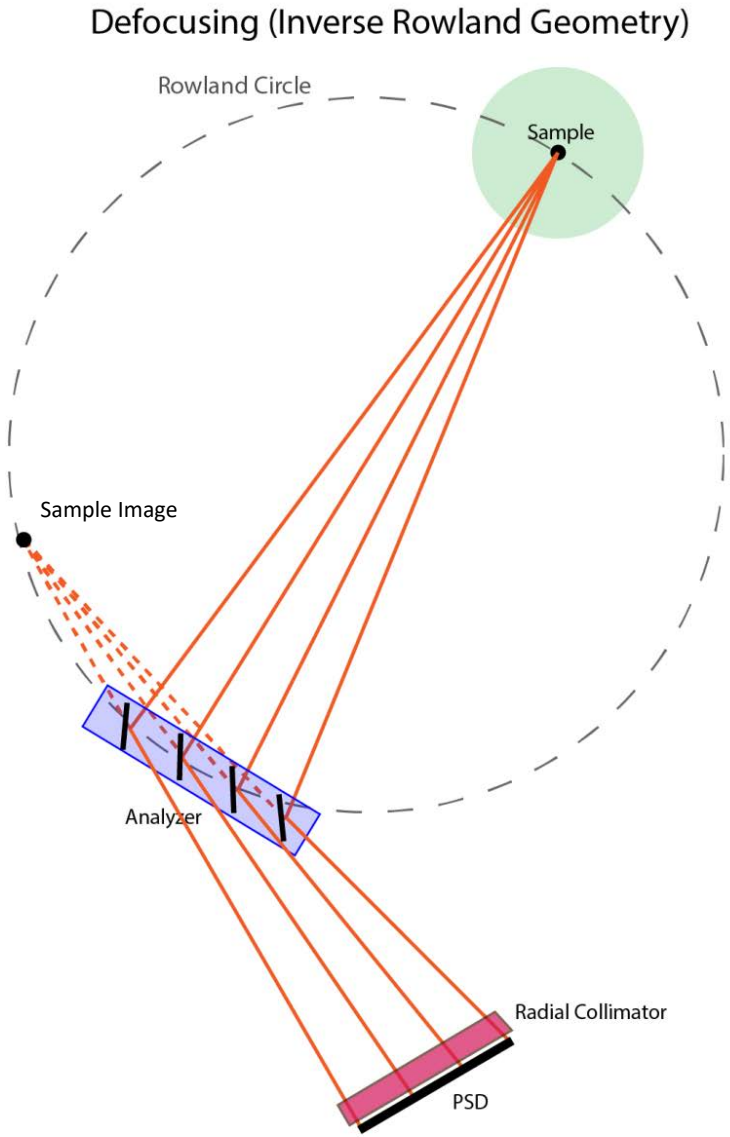
https://en.wikipedia.org/wiki/Bragg%27s_law#/media/File:BraggPlaneDiffraction.svg

Rowland Geometry



- Typically, this simple geometry is used throughout the world in triple axis spectrometers
- A wide A4 range created by the sample is compressed to produce a sample image at the position of a single detector
- The analyzer crystal group is placed tangent to the circle
- In fixed-E_f mode (our primary mode of interest), each analyzer crystal is individually rotated such that each reflect off the same energy
- This results in a relaxed Q-resolution due to the loss of the A4 information

Inverse Rowland Geometry



- This is a new geometry developed for RITA style multiplexed spectrometers by Leland Harriger and Igor Zaliznyak
- A sample image reproduced by the multiplexed analyzer is projected onto the Rowland circle and then viewed by a position sensitive detector (PSD) through a radial collimator.
- This ability to use a radial collimator just before the PSD greatly increases the signal-to-noise ratio.

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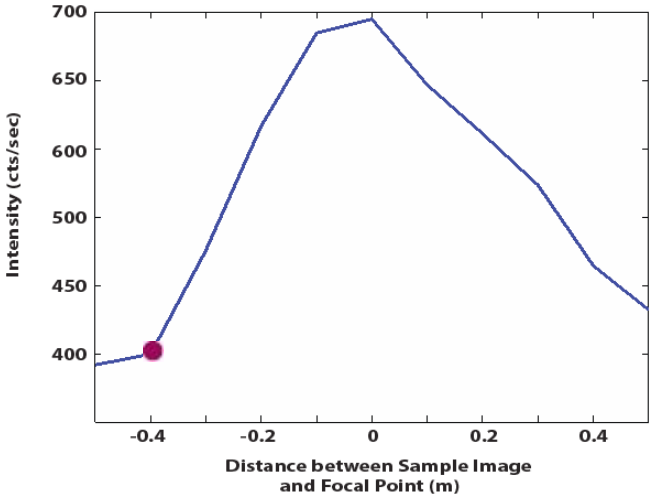
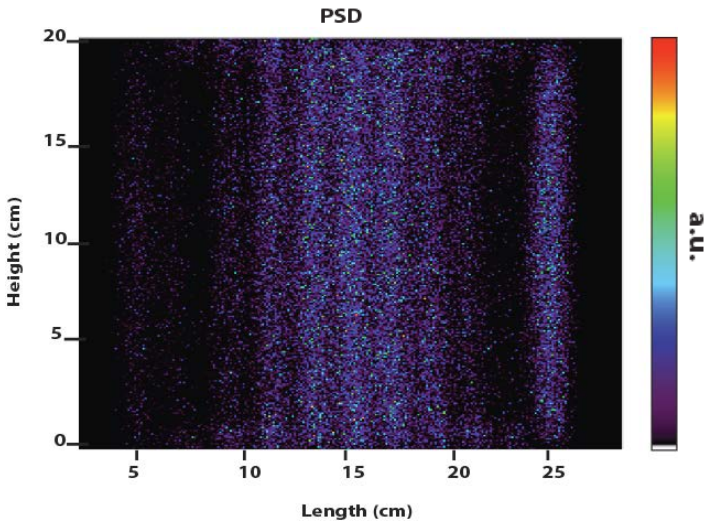
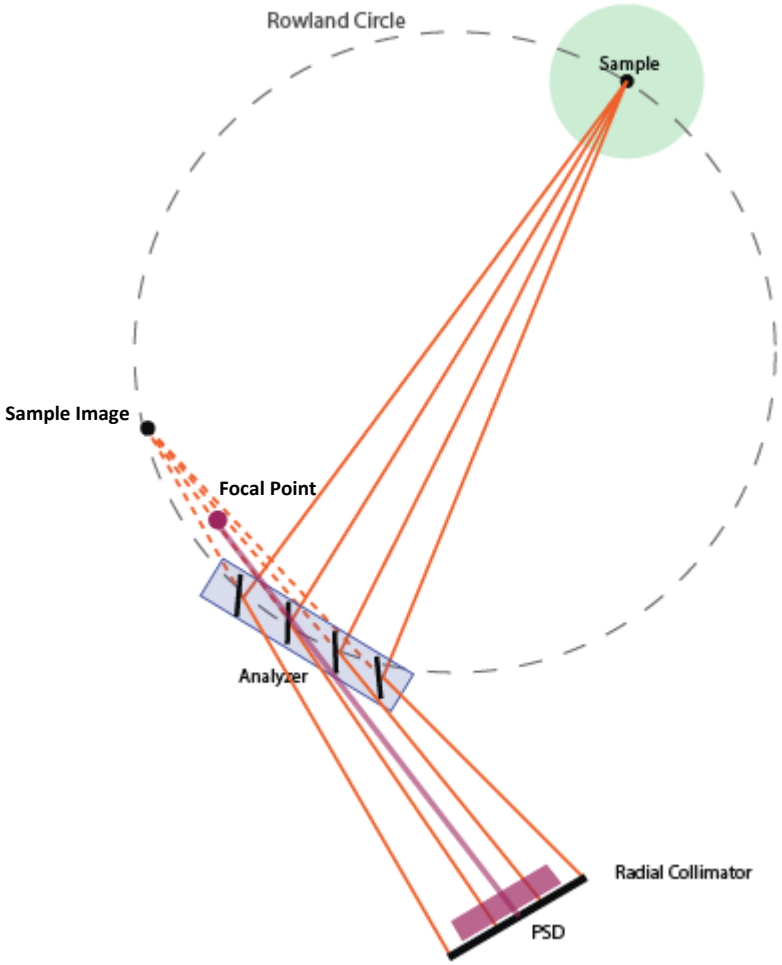
Monte-Carlo Simulations

- All simulations were run using McStas, a neutron ray-trace simulation package.
  - http://www.mcstas.org/
- I built a virtual triple axis spectrometer that mirrors SPINS in McStas where neutron ray paths were determined component by component using the Monte-Carlo method
- Monte-Carlo simulations use a repeated random sampling process rather than an analytical calculation to determine neutron ray paths

Focal Length at Sample Image







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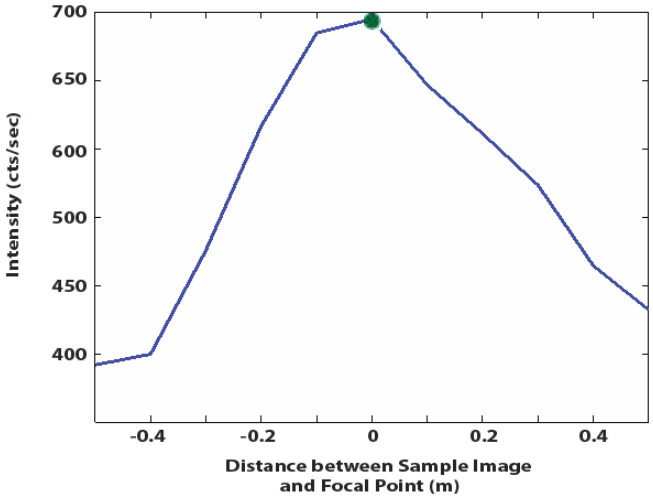
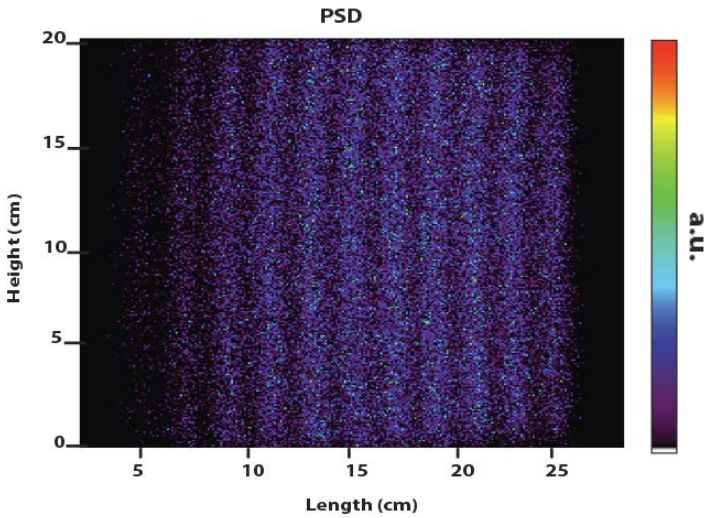
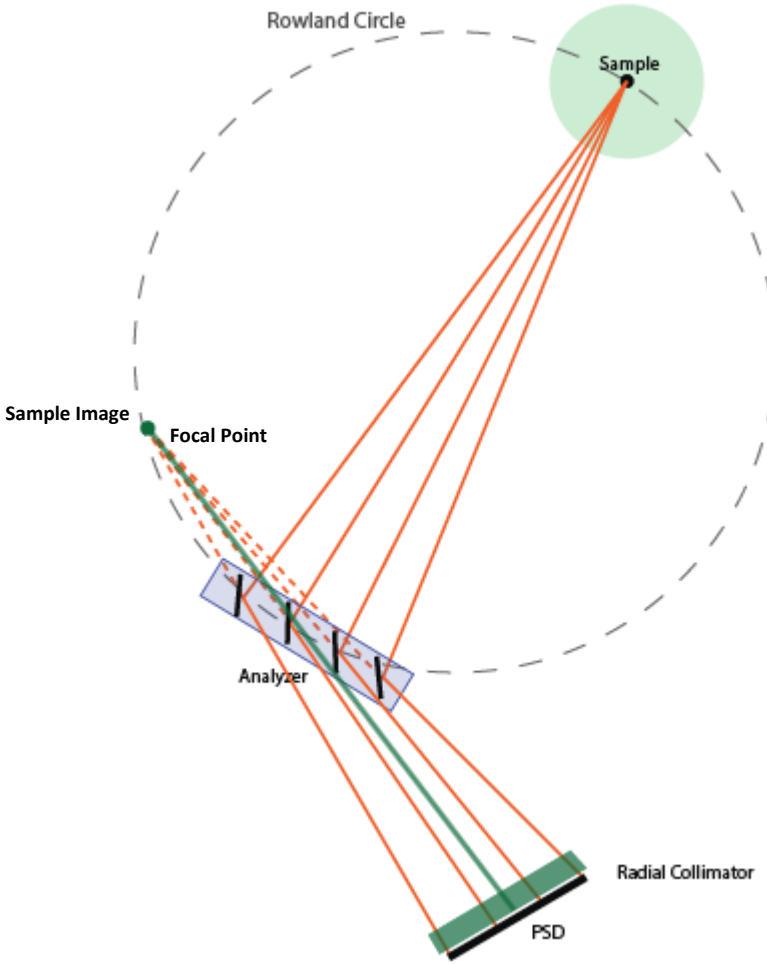
Focal Length at Sample Image







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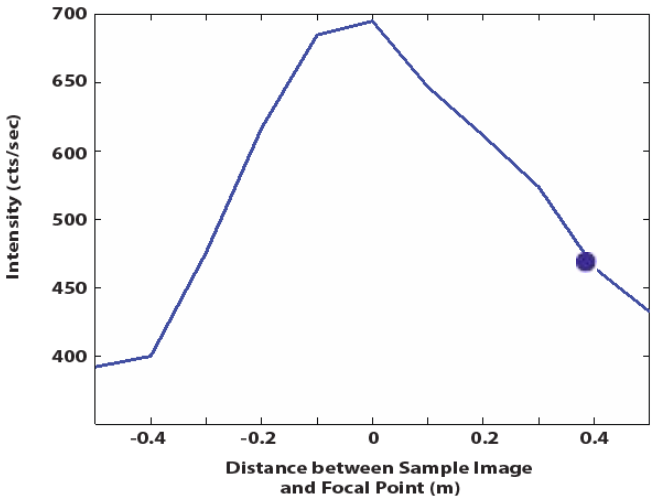

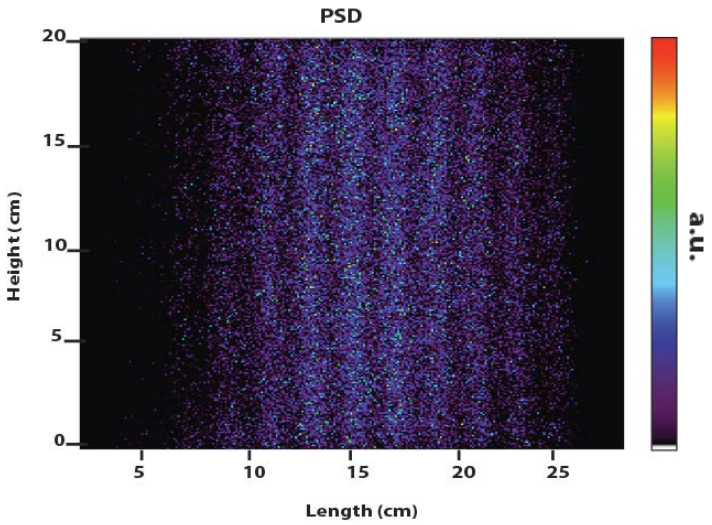

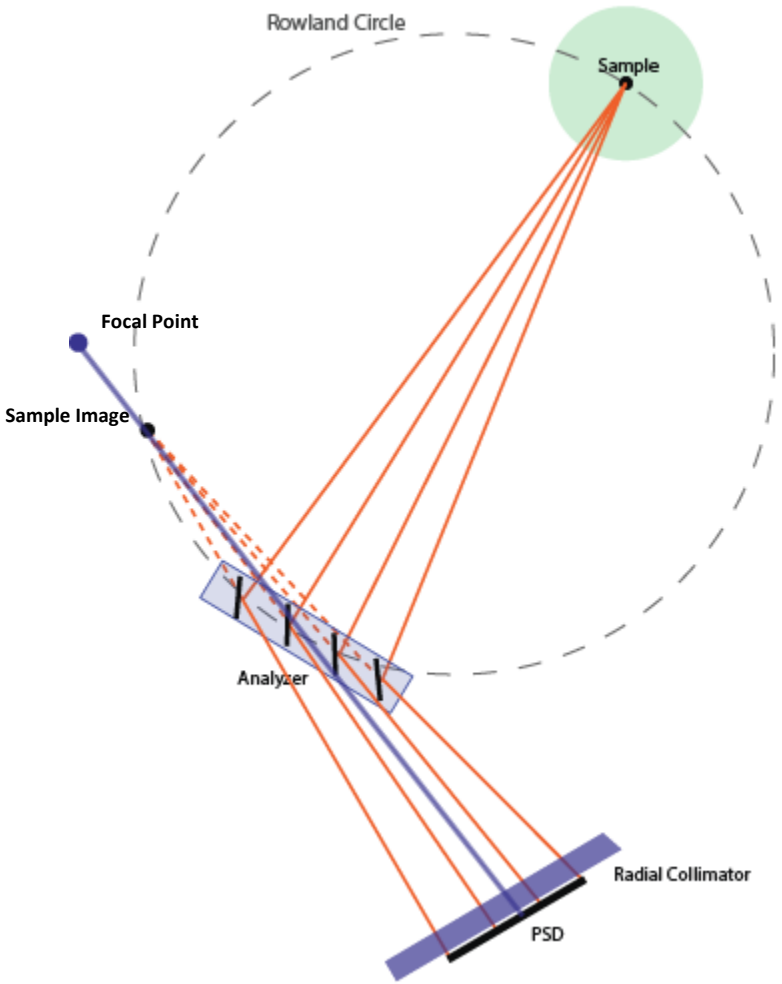

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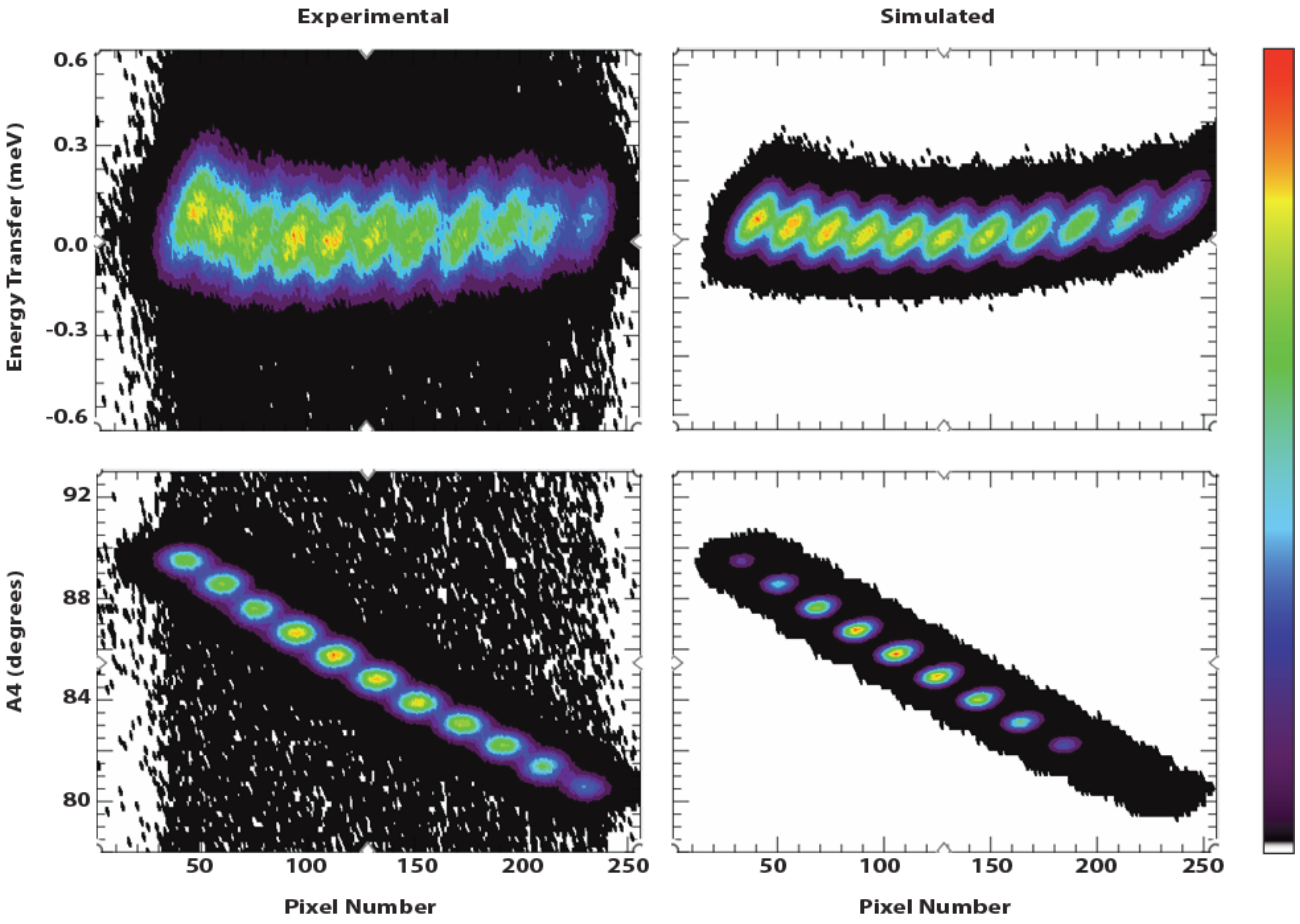
Calibration Results



- The elastic lines from a simulation of a spectrometer using Rowland defocusing is consistent with real data from SPINS
- The A4 scans are also very similar

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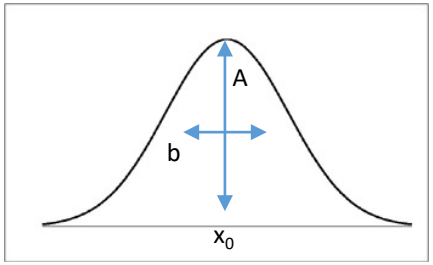
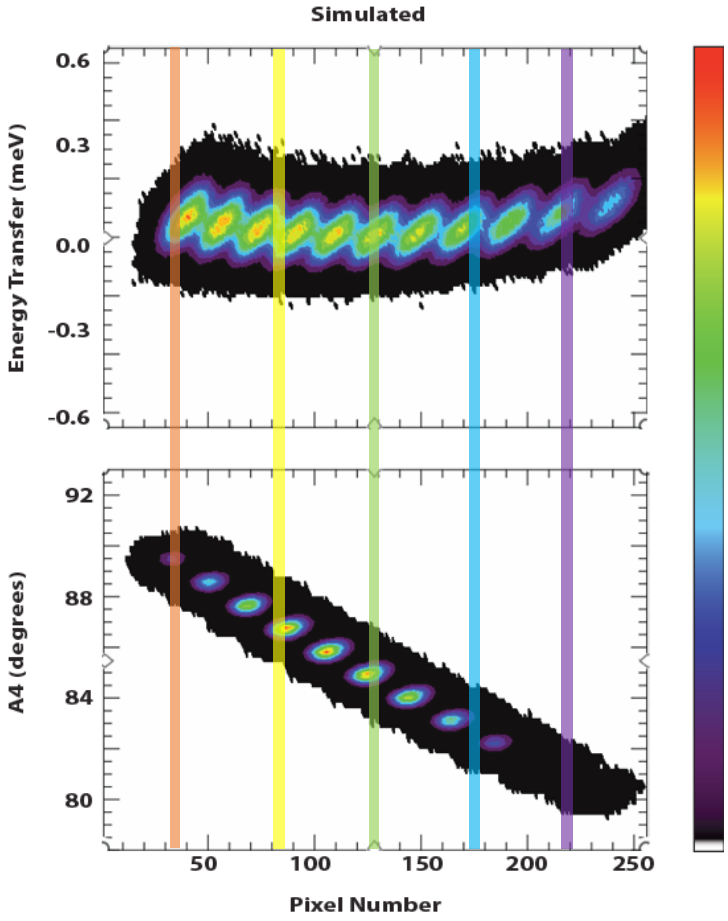
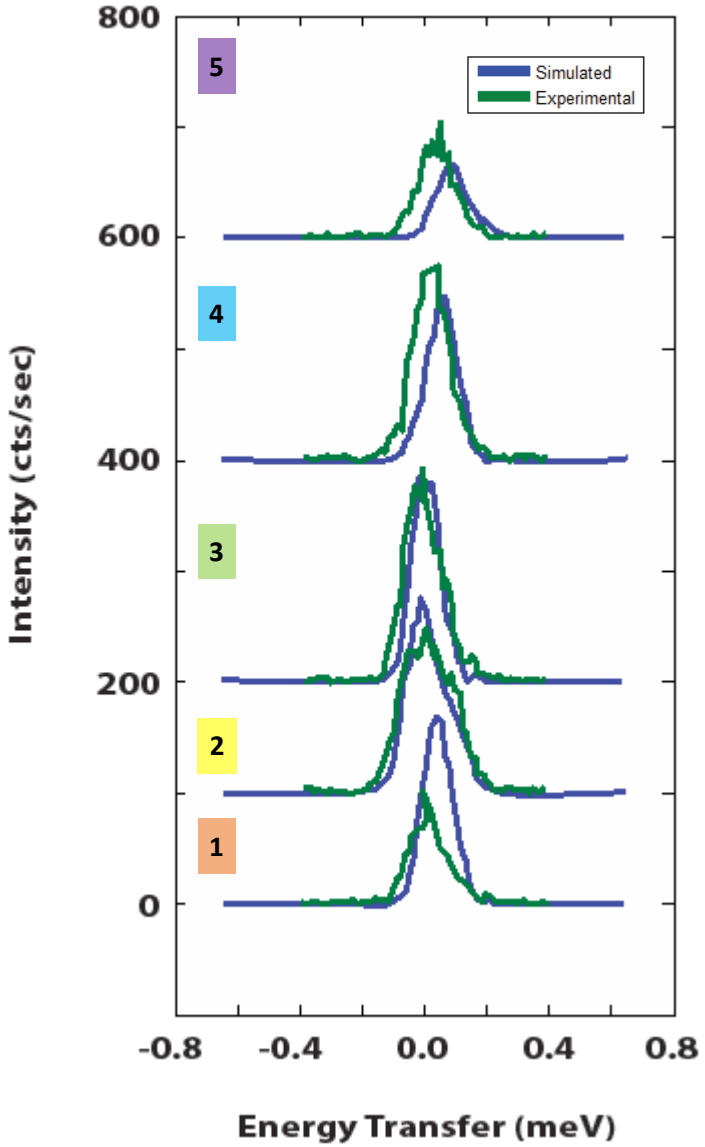
Calibration Results







- All Monte-Carlo results were restructured to mimic real data files and DAVE was then used to run calibrations.
- The peak and width (A, b) are use to determine the sensitivity of each pixel.
- The center (x_0) is used to determine the A4/Ef value sampled by each pixel.

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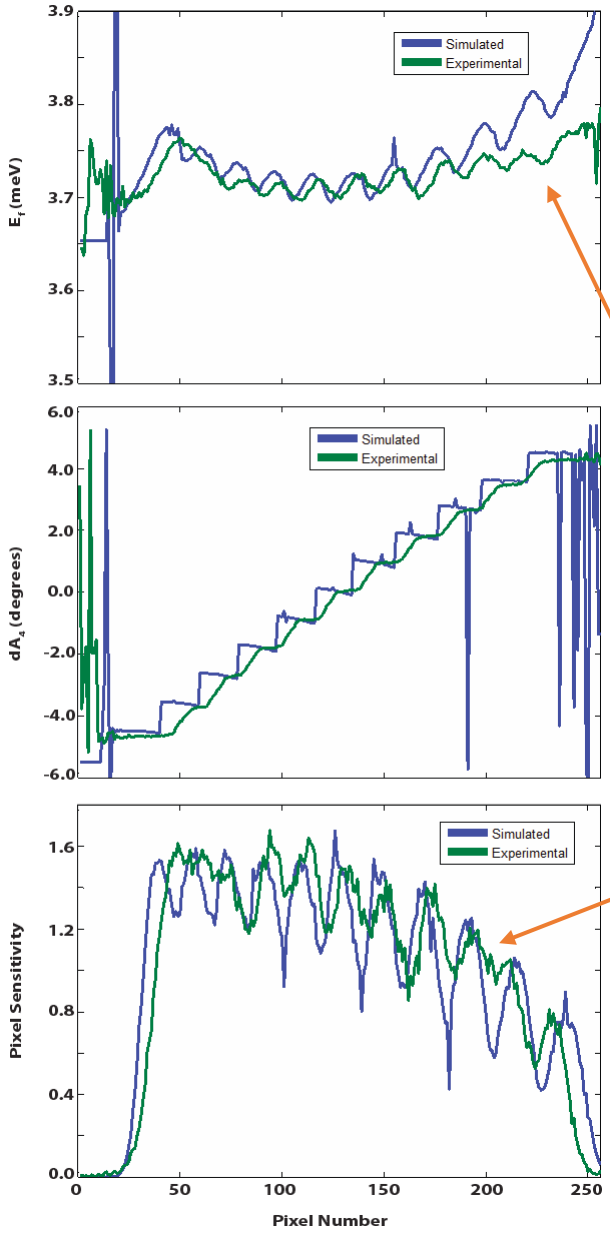
Calibration Results



- Fits were then run in DAVE using the previous calibrations to produce these plots
- Curved shape of the energy plot is a result of the crystals lying tangent to the Rowland circle
- Intensities are not uniform across the crystals for this same reason as seen in the sensitivity plot

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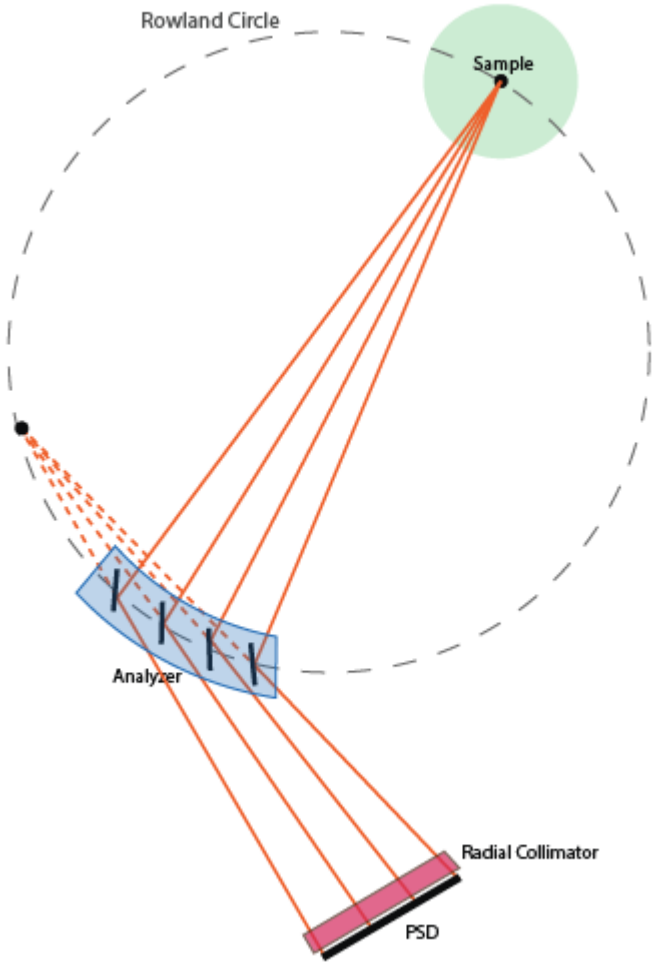
Simulating a ‘Perfect’ Rowland Triple-Axis Spectrometer



- The analyzer crystal group is placed along the circle as opposed to tangent to it
- Each crystal is then rotated to produce the A5 value relative to their individual position on the circle.

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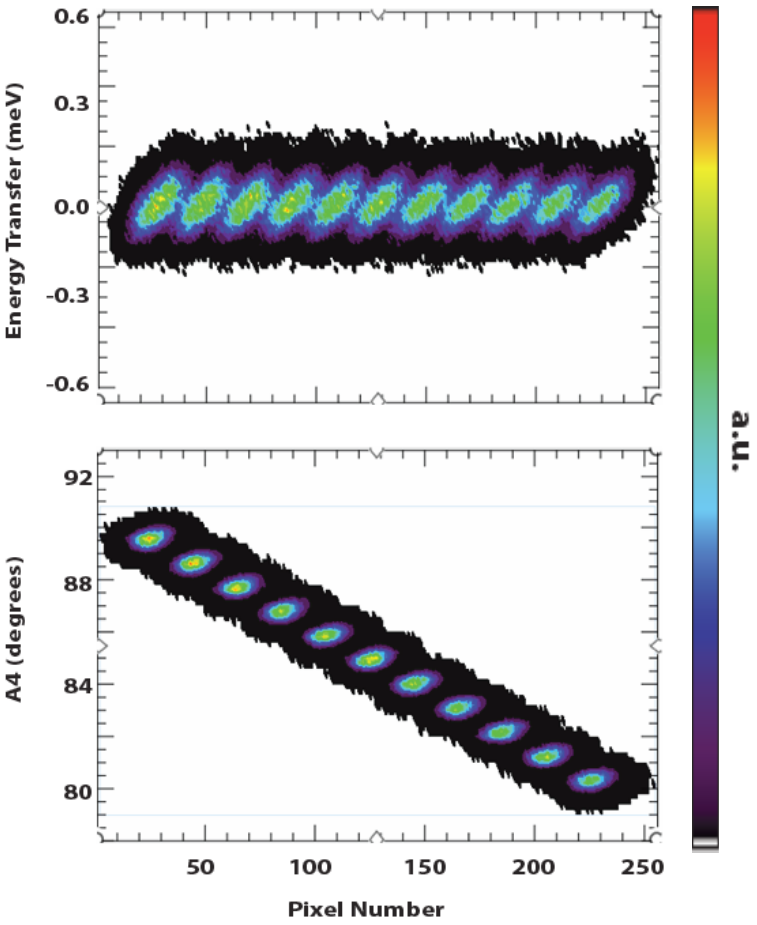
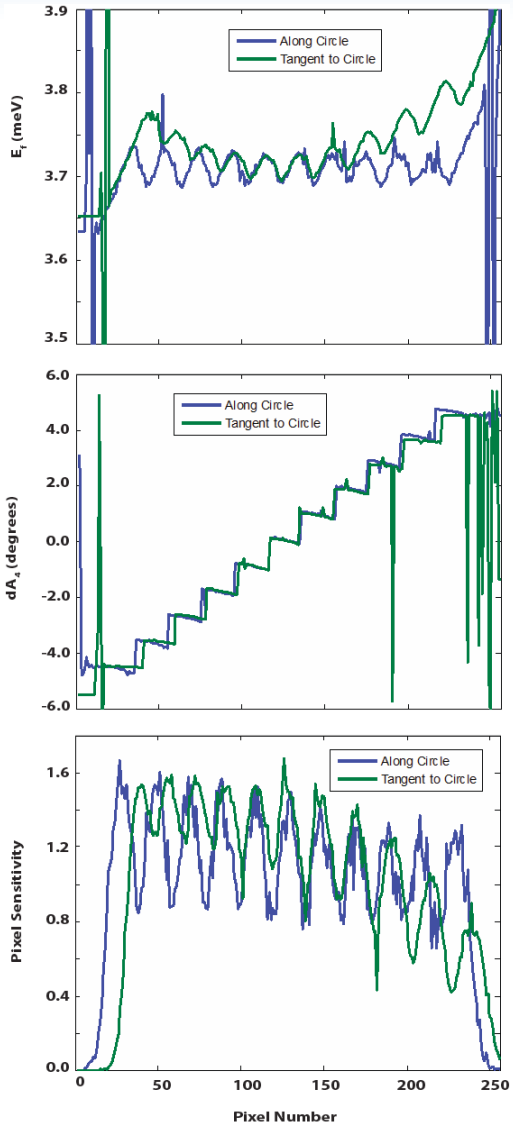
Results





- Uniform intensity across crystals is due to a reduction in beam depletion caused by being further and further away from the sample

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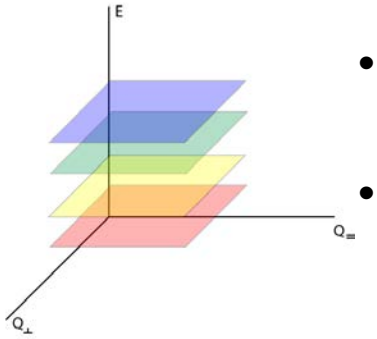
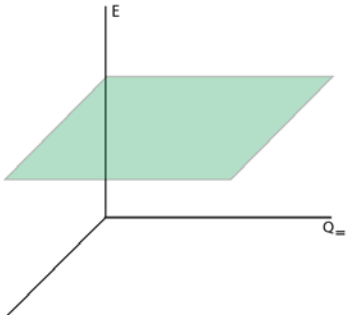
Wide Angle Designs

IRIS (**I**nverse **R**owland **I**nelastic **S**pectrometer)

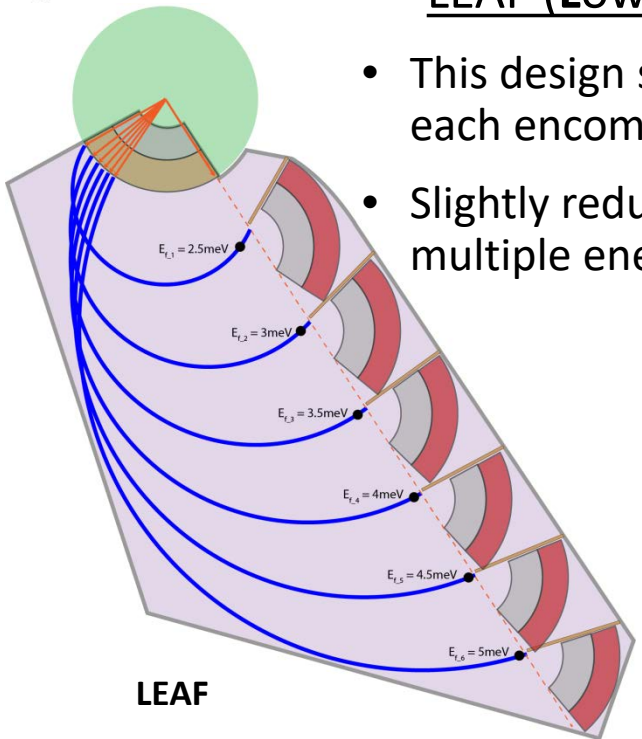


- We can expand the multiplexing of analyzer crystals to a 150° A4 coverage by closely packing the crystals
- The PSD is then converted into a large detector bank

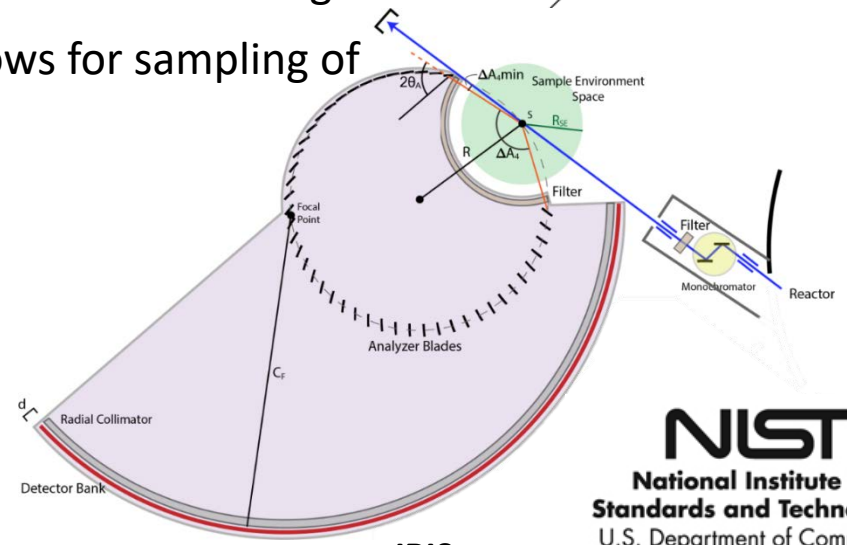


LEAF (**L**ow **E**nergy **A**nti-**F**ocusing Spectrometer)

- This design superimposes multiple Rowland circles with each encompassing its own reduced IRIS design
- Slightly reducing Q-space allows for sampling of multiple energies at once



LEAF



IRIS

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Conclusions

- Multiplexing a triple axis spectrometer increases throughput considerably.
- Rowland defocusing can be applied to triple axis spectrometers immediately
- Monte-Carlo results agree very well with experimental results for a Rowland defocused triple axis spectrometer
- Monte-Carlo results for wide angle designs can now be carried out with a high level of confidence

Acknowledgments

- Leland Harriger
- Jeff Lynn
- Julie Borchers and the other SURF Directors
- NSF and CHRNS

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