POWGEN: A Versatile 3rd Generation Neutron Powder Diffractometer

Bragg's Law

$$\lambda = {h}/{mv} = {ht}/{mL} = 2d \sin\theta$$

$$L = L_1 + L_2$$

L_1 = source to sample, L_2 = sample to detector

t = neutron time of flight

$$t = KLd \sin\theta \qquad d = {t}/{KL \sin\theta}$$

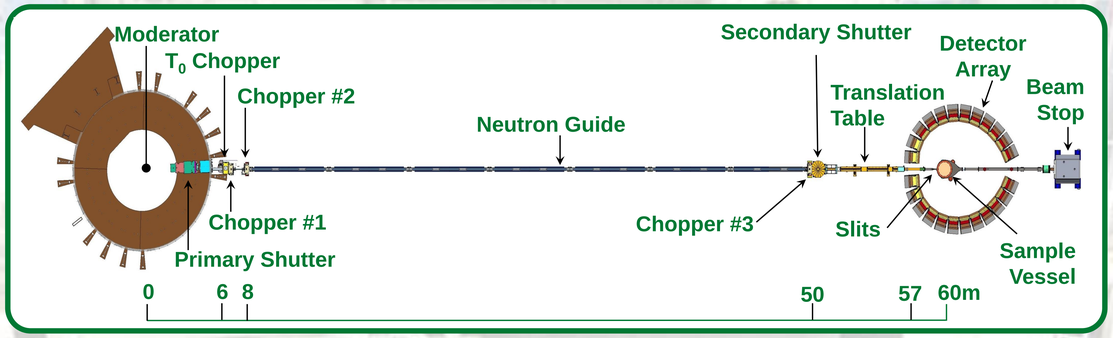
TOF → d Conversion

$$t = DIFC * d + DIFA * d^2 + \frac{DIFB}{d} + ZERO$$

$$t = DIFC * d + \Delta t$$

Resolution

$$R(d) = \Delta d/d = [(\Delta t/t)^2 + (\Delta L/L)^2 + (\Delta\theta)^2 \cot^2\theta]^{1/2}$$



Freq (Hz)	Wavelength (Å) center	min	max	d (Å) min	max	Q (Å^{-1}) min	max	Bank
60	0.533*	0.15	1.066	0.075	7.50	0.82	83.45	0*
60	0.800	0.27	1.333	0.134	8.00	0.76	46.88	1
60	1.500	0.97	2.033	0.485	13.00	0.48	12.95	2
60	2.665	2.13	3.198	1.070	21.00	0.30	5.87	3
60	4.797*	4.26	5.33	2.140	38.00	0.17	2.94	4*

* Setting not part of standard calibration

Profile Function

The Powgen peak profile is a convolution of pseudo-Voigt and back-to-back exponential functions.

$$H(x) = pV(x) \otimes E(x) = \int pV(x-t)E(t)dt$$

$$E(t) = \begin{cases} \frac{\alpha\beta}{\alpha+\beta} e^{\alpha t} & t \le 0 \qquad \alpha = {\alpha_0}/{d} \\ \frac{\alpha\beta}{\alpha+\beta} e^{-\beta t} & t > 0 \quad \beta = \beta_0 + {\beta_1}/{d^4} \end{cases}$$

The pseudo-Voigt function is a linear combination of Gaussian (σ) and Lorentzian (γ) functions.

$$\sigma^2 = \sigma_0^2 + \sigma_1^2 d^2 + \sigma_2^2 d^4 + \sigma_q^2/d^2$$

$$\gamma = \gamma_0 + \gamma_1 d + \gamma_2 d^2$$

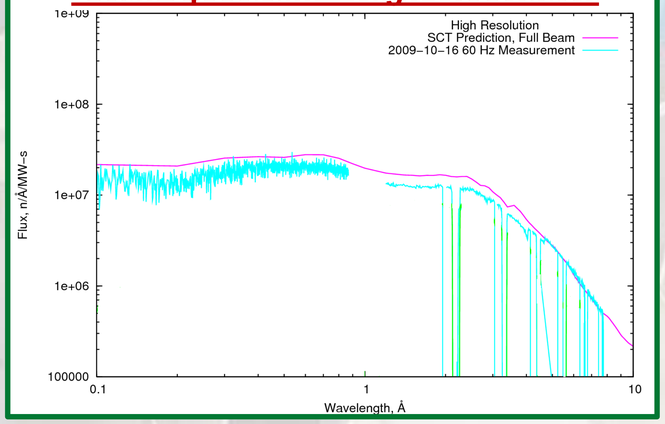
Normalization

Background is subtracted and data are normalized by uniform scatterer (vanadium).

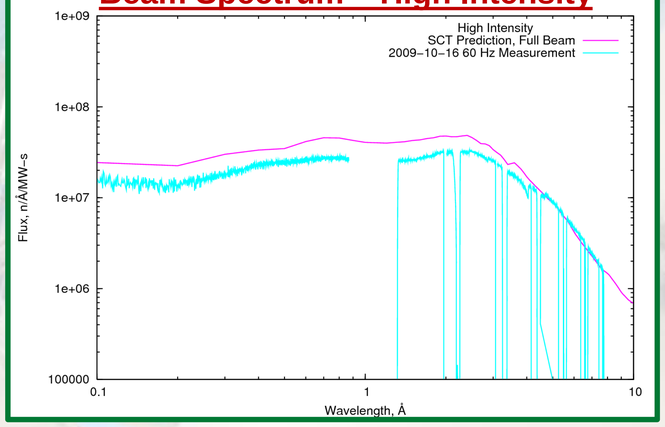
$$I_n = \frac{\text{Sample} - \text{Empty can}}{\text{Vanadium} - \text{Empty V}}$$

Beam Power (MW)	Pcharge (C) per hour
0.850	3.3
1.0	3.7
1.1	4.3
1.2	4.5
1.3	4.7
1.4	5.0
1.55	5.3

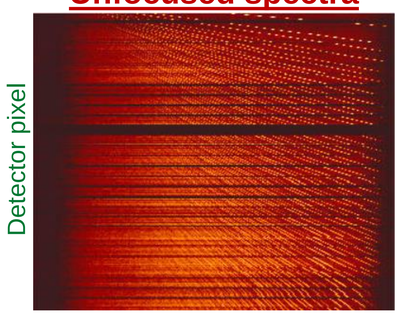
Beam Spectrum – High Resolution



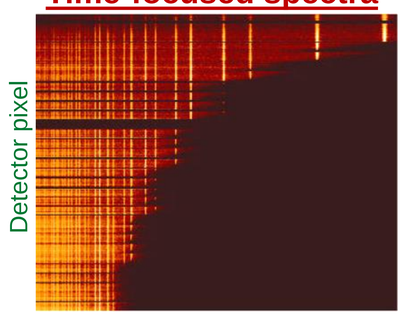
Beam Spectrum – High Intensity



Unfocused spectra



Time-focused spectra

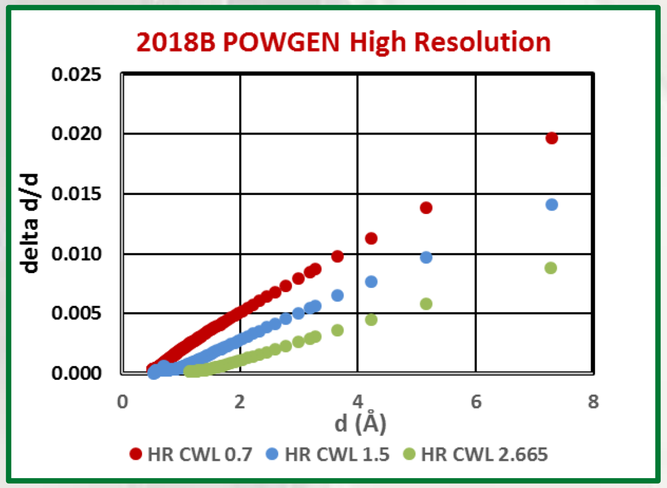


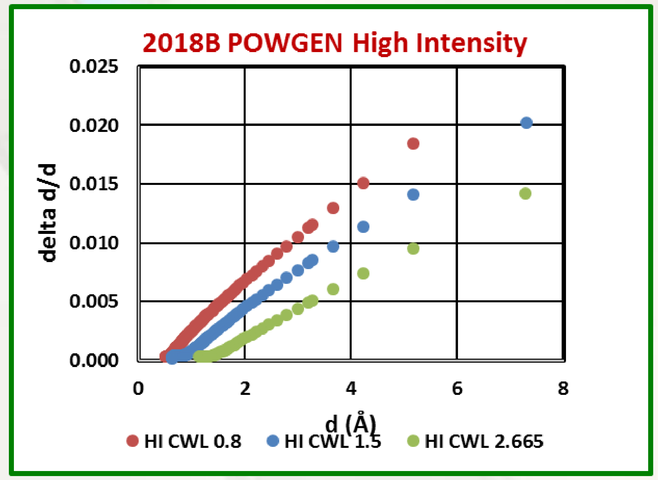
Time Focusing

In order to sum all detectors, data are time-shifted as if all detectors were at 90° 2θ.

$$t_i = KdL_i \sin\theta_i \quad \text{measured} \qquad t_f = KdL_f \sin\theta_f \quad \text{focused}$$

$$\frac{t_f}{t_i} = \frac{L_f \sin\theta_f}{L_i \sin\theta_i} \qquad \theta_f = 90° \qquad L_f = 63.18\text{m}$$





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