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

$$t = KLd\sin\theta \quad d = {}^{t}/_{KL\sin\theta}$$

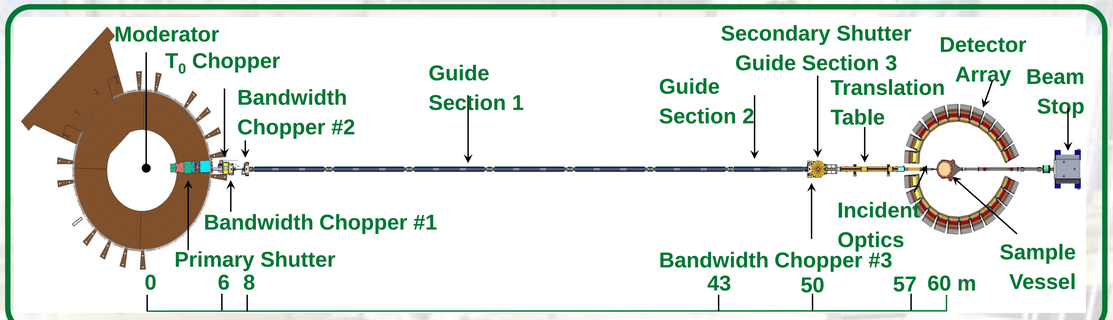
TOF→d Conversion

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

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

Resolution

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



Freq (Hz)	WL center	WL min	WL max	dmin	dmax	Qmin	Qmax	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

Profile Function

Peak profile is a convolution of psuedo-Voigt and back-to-back exponential functions.

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

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

Pseudo-Voigt is a linear combination of Gaussian (σ) and Lorentzian (γ)

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

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

Normalization

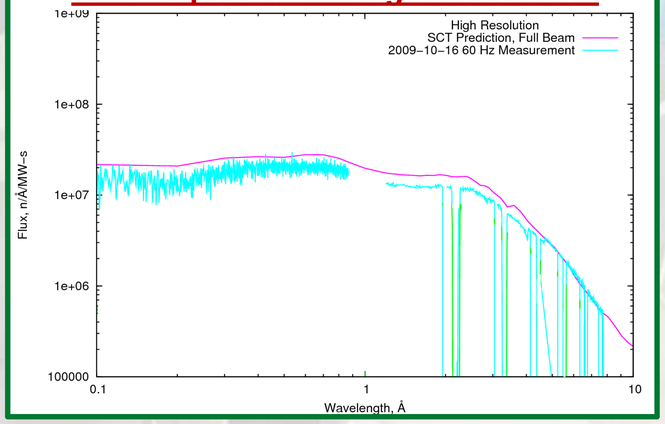
Background is subtracted and data are normalized by uniform scatterer (vanadium).

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

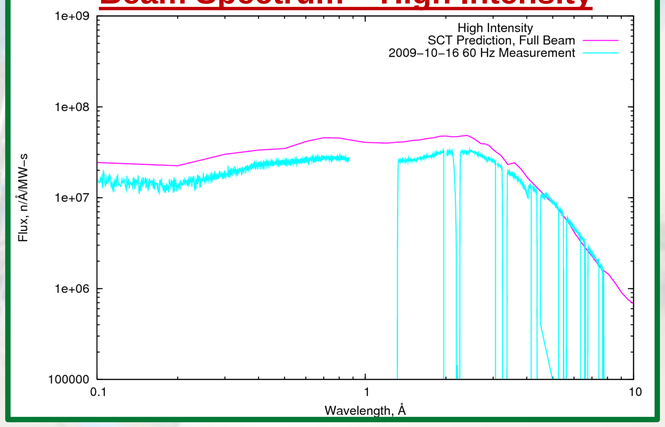
Proton Charge

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	5.4

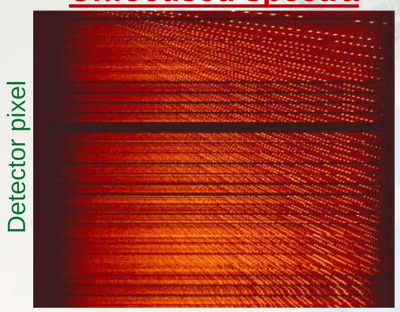
Beam Spectrum – High Resolution



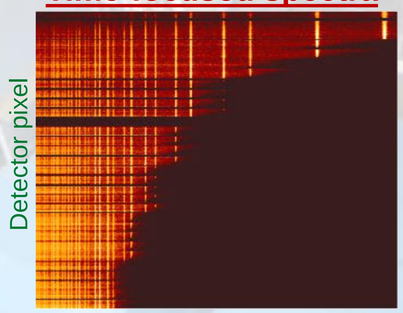
Beam Spectrum – High Intensity



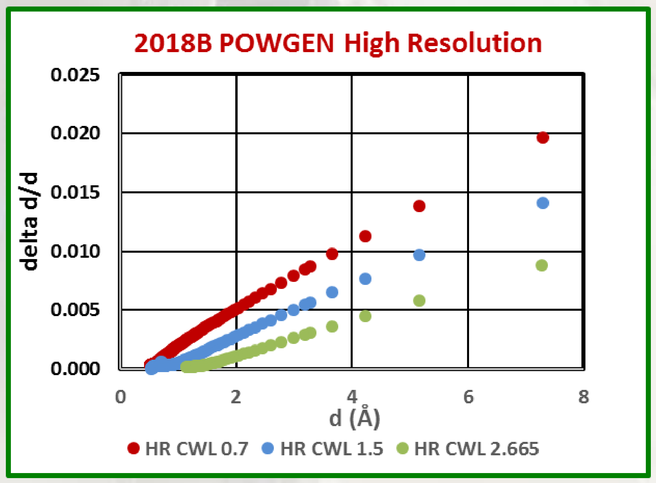
Unfocused spectra



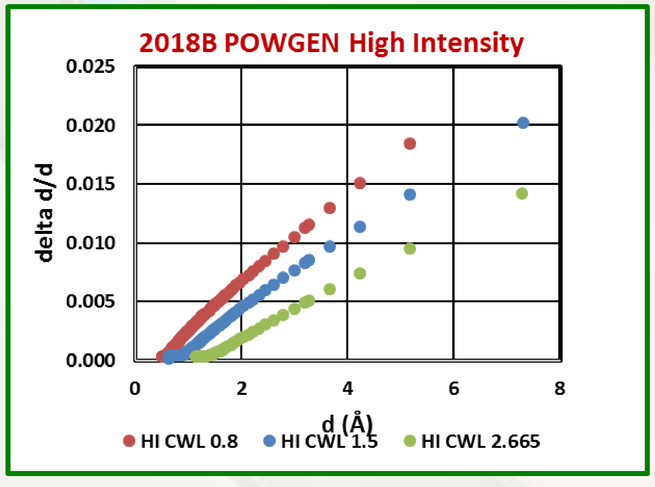
Time-focused spectra



2018B POWGEN High Resolution



2018B POWGEN High Intensity



Time Focusing

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

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

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

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

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