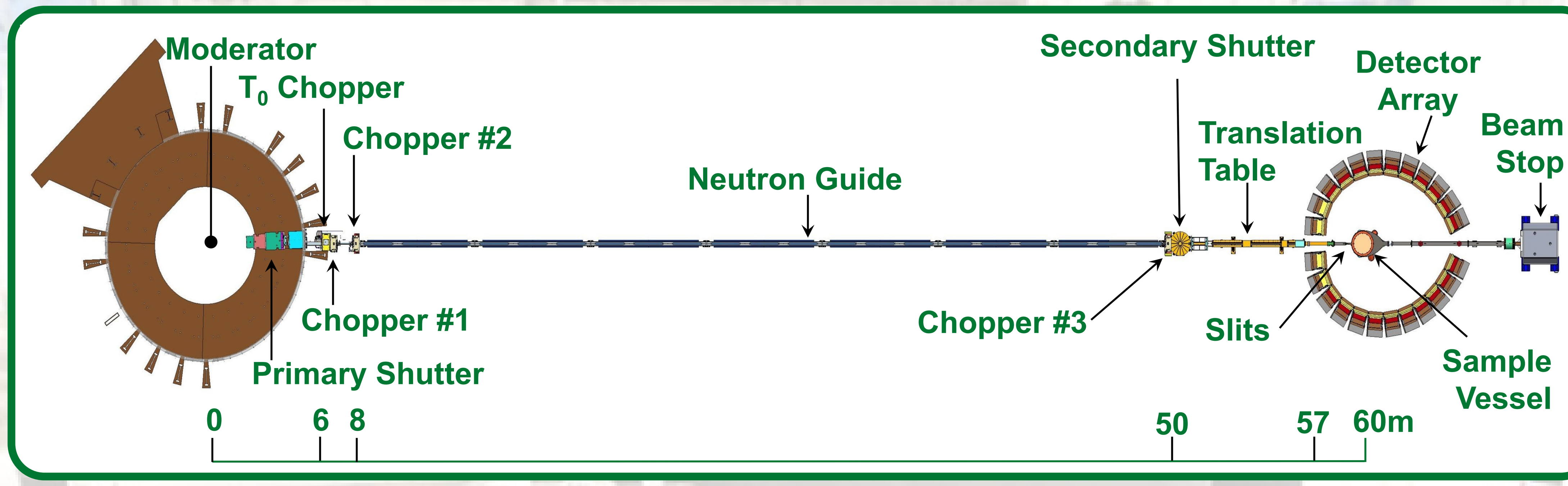
POWGEN: A Versatile 3rd Generation Neutron Powder Diffractometer



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, m = neutron mass
h = Planck constant

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

TOF → d Conversion

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

Chopper Settings and Neutron Bandwidth

Freq	Wavelength (Å)			d (Å)		Q (Å⁻¹)		Bank
(Hz)	center	min	max	min	max	min	max	
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

Profile Function

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

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

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

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

$$\sigma^2 = \sigma_0^2 + \sigma_1^2 d^2 + \sigma_2^2 d^4 + \sigma_q^2/d^2$$
$$\gamma = \gamma_0 + \gamma_1 d + \gamma_2 d^2$$

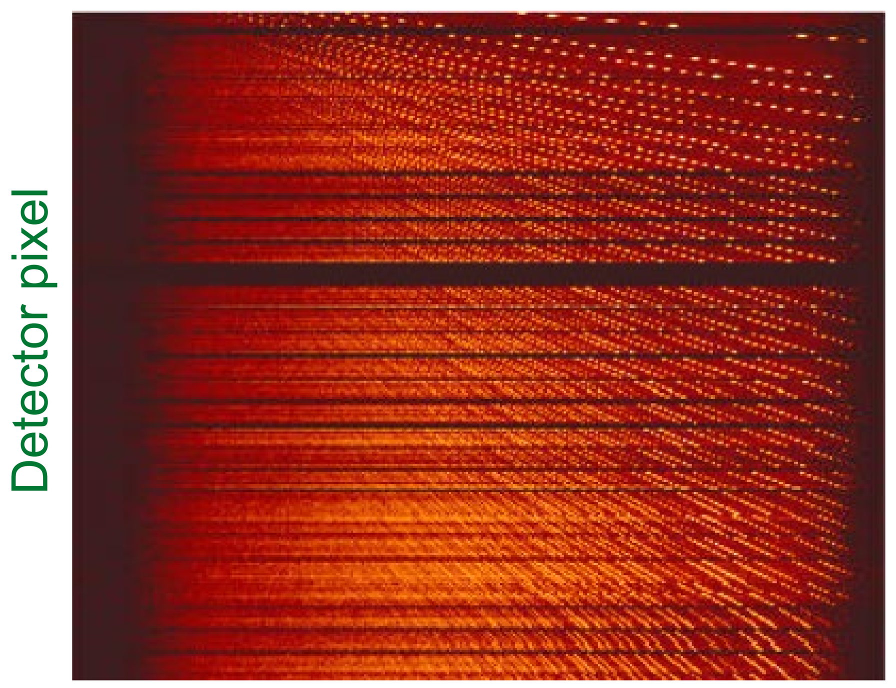
Time Focusing

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

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

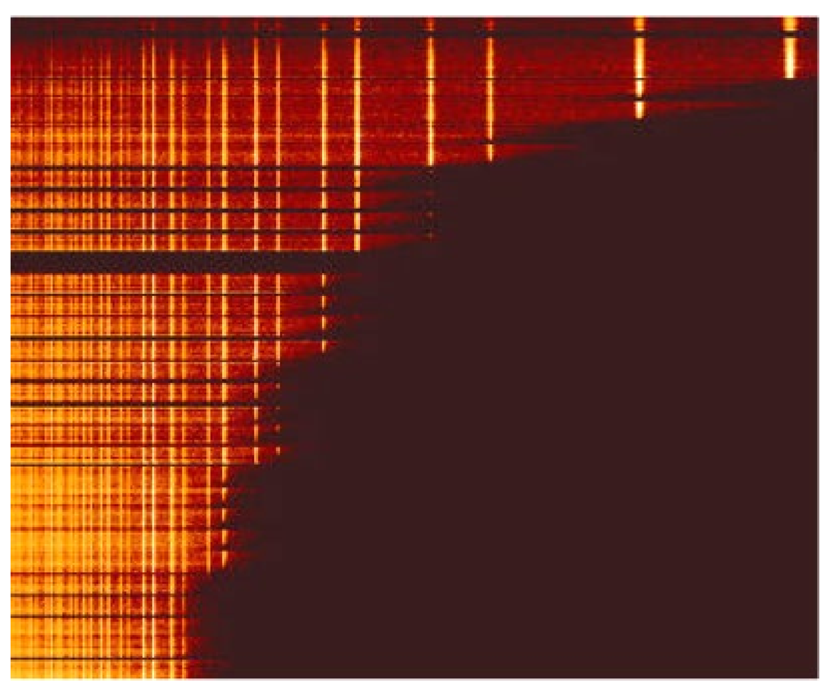
$$\frac{t_f}{t_i} = \frac{L_f\sin\theta_f}{L_i\sin\theta_i} \qquad 2\theta_f = 90° \qquad L_f = 63.18\text{m}$$

Unfocused spectra

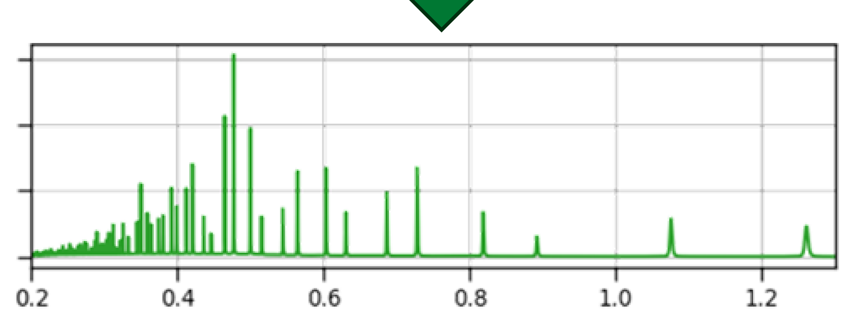


Time-of-flight, measured

Time-focused spectra

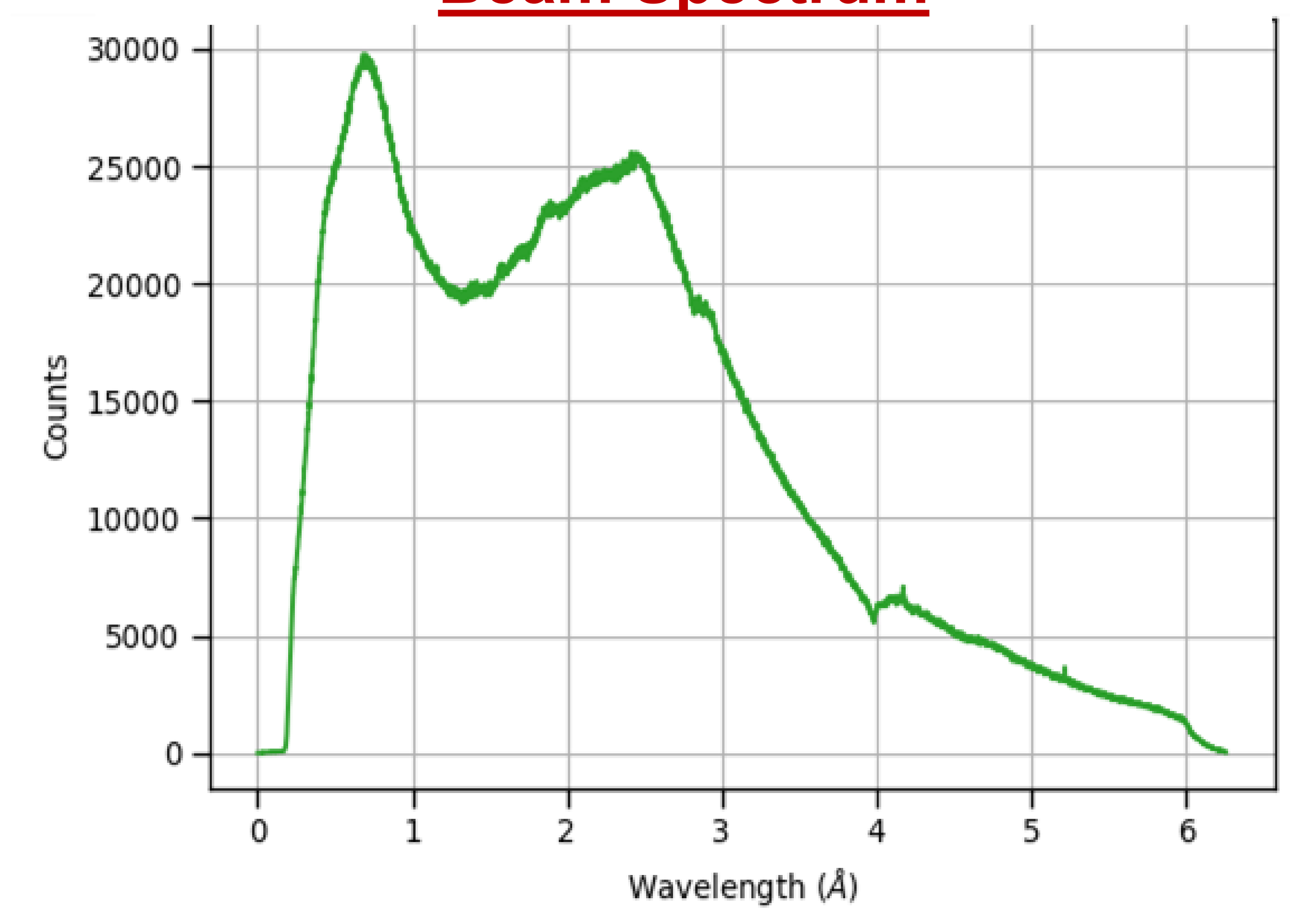


Time-of-flight, focused



d-spacing (Å)

Beam Spectrum



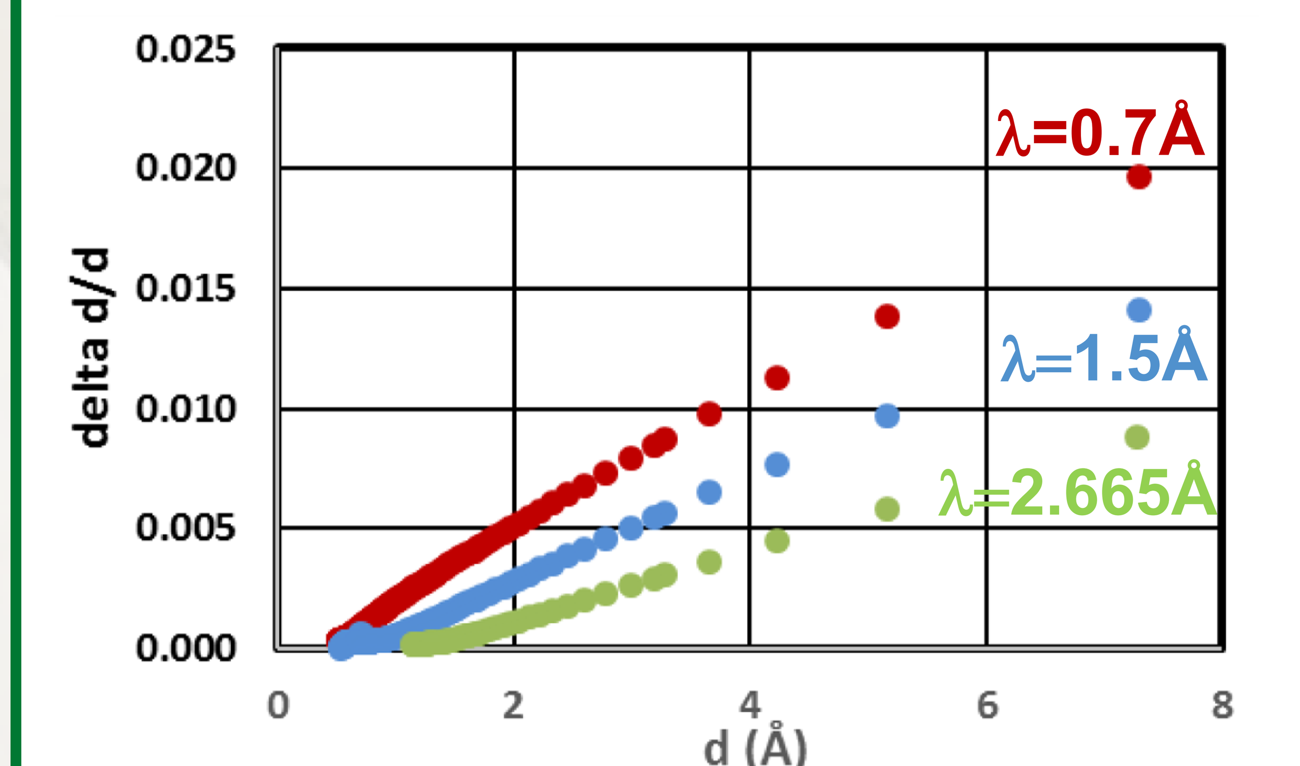
Beam Power (MW)	Pcharge (C) per hour
0.850	2.4
1.0	2.8
1.5	4.2
1.6	4.4
1.7	4.6
1.8	5.0
1.9	5.3
2.0	5.5

Normalization

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

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

Resolution



$$R(d) = \Delta d/d = [(\Delta t/t)^2 + (\Delta L/L)^2 + (\Delta\theta)^2\cot^2\theta]^{½}$$

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