JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 54 (2021)

Supporting information for article:

Simulating and benchmarking neutron total scattering instrumentation from inception of events to reduced and fit data

Peter C. Metz, Thomas Huegle, Daniel Olds and Katharine Page

S1. What is a “3-hat” peak shape?

Topas (Cheary & Coelho, 1992) applies a series of convolutions to compute the profile of a particular peak. In a typical powder diffraction calculation, the crystallographic structure factor (F_{hkl}) is computed, and each reflection is convoluted with any instrumental and sample specific aberrations.

Often, these peak profiles are well described by canonical profile functions like the Gaussian, Lorentzian, or Voigt distributions. During our exploration of peak profiles suitable to describe the forward scattering banks of NOMAD, we found the usual Voigt profile fit some peaks inadequately, particularly those at low-Q. This was not the usual problem of an asymmetric profile shape typical of time-of-flight diffractometers and often found in back scattering, which is largely a consequence of the neutron moderator (see e.g. (Ikeda & Carpenter, 1985)). Rather, the profiles appeared symmetric but somewhat squared-off at the top.

Although we have not arrived at a fundamental explanation for this profile shape, introducing a peak profile given by the convolution of 3 hat functions of identical width produced the observed profile shape better than a Gaussian. In the text we describe this profile shape as similar to a gaussian but with sharper tails, which we have highlighted in the inset of Figure S1.

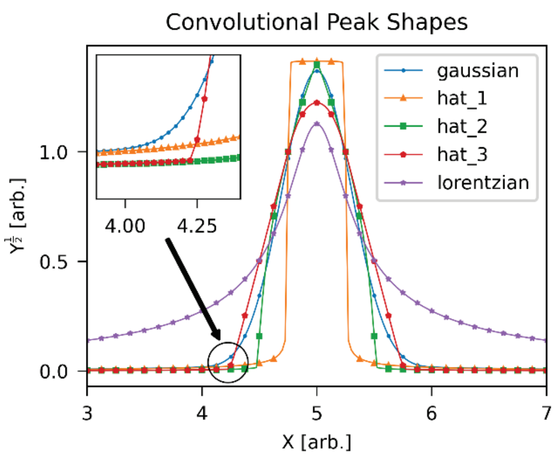


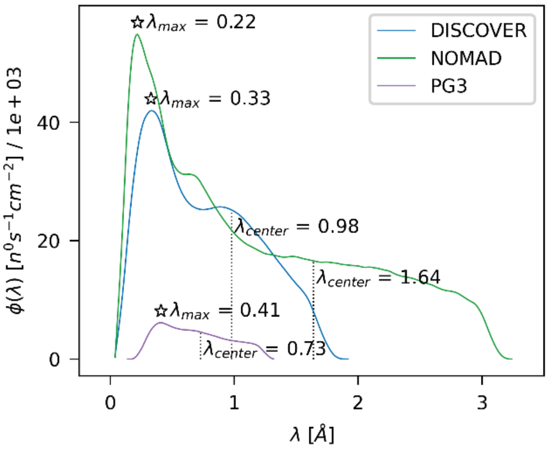
Figure S1. Comparison of the standard Gaussian and Lorentzian peak shapes with convolutional peak shapes produced by 1, 2, and 3 hat functions with FWHM = 0.5. Note square root vertical axis.

S2. DISCOVER incident spectrum

The DISCOVER beamline concept has a 32 m guided primary flight path. The guide design, which is the subject of additional optimization, has a graded reflectivity from m=3.6 at the upstream end to m=6 at the downstream end (m-value being defined as the ratio of the critical angle of total external reflection of a mirror relative to nickel).

Whereas NOMAD is optimized to deliver a maximum of short-wavelength neutrons in order to deliver rapid neutron pair distribution function data, DISCOVER aims to perform as a rapid medium resolution powder diffractometer and balances transport of short and long wavelength neutron.

The incident spectrum simulated in McStas utilized in this work is presented in Figure S2. Spectra shown are truncated with the relative tolerance 5E-05 $\phi(\lambda = \lambda_{max})$.



References

Cheary, R. W. & Coelho, A. (1992). *J. Appl. Crystallogr.* **25**, 109–121.

Ikeda, S. & Carpenter, J. M. (1985). *Nucl. Inst. Methods Phys. Res. A*. **239**, 536–544.