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Treatment of hydrogen background in bulk and nanocrystalline neutron total scattering experiments

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Nuclear incoherent neutron scattering contributions present a challenge in the structural characterization of many classes of materials. This article introduces methods for the correction of nanoparticle, bulk crystalline and amorphous powder neutron scattering data with significant incoherent contributions from hydrogen, and describes the effects the corrections have on the resulting atomic pair distribution function data sets. The approach is presented in the context of the *PDFgetN* data-reduction program [Peterson, Gutmann, Proffen & Billinge (2000). *J. Appl. Cryst.* **33**, 1192].

1. Introduction

Neutron diffraction is a powerful method for probing and characterizing the atomic structure of a material. The analysis of both diffuse and Bragg scattering, the 'total scattering', can yield direct information about the interatomic distances in materials in the form of the pair distribution function (PDF) (Egami & Billinge, 2003). The PDF, $G(r)$, is defined in real space as a function of the pair density, $\rho(r)$,

$$G(r) = 4\pi r[\rho(r) - \rho_0\gamma_0], \tag{1}$$

and in reciprocal space as a sine Fourier transform of the normalized total scattering structure function, $S(Q)$,

$$G(r) = \frac{2}{\pi}\int_0^\infty Q[S(Q) - 1]\sin(Qr)\,\mathrm{d}Q. \tag{2}$$

In these relationships, r is the real-space distance between two atoms, Q is the magnitude of the scattering vector [$Q = (4\pi/\lambda)\sin(\theta/2)$, where θ is the scattering angle and λ is the wavelength of the incident radiation], ρ_0 is the average number density in the sample and γ_0 is a characteristic function for finite-sized objects, often called the nanoparticle form factor (Farrow & Billinge, 2009). $\rho(r)$ gives the probability of finding two atoms i and j separated by a distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ in real space, weighted by the scattering lengths b_i and b_j and averaged over all pairs of atoms in the sample (Faber & Ziman, 1965):

$$\rho(r) = \frac{1}{4\pi r^2}\sum_{ij}\frac{b_i b_j}{\langle b\rangle^2}\delta(r - r_{ij}). \tag{3}$$

There are numerous correlation functions commonly used for describing the total scattering function (Keen, 2001). The form shown here is that described by Egami & Billinge (2003), implemented in the data-reduction program *PDFgetN* (Peterson *et al.*, 2000) and the data-analysis software packages *DISCUS* (Proffen & Neder, 1997) and *PDFgui* (Farrow *et al.*, 2007). The construct is convenient for studying crystalline and nanocrystalline materials because the $G(r)$ function scales with r and oscillates around 0 at high r, clearly distinguishing structure up to nanometre length scales.

The quantity measured in a neutron scattering experiment is the double differential cross section per unit solid angle and energy interval (Squires, 1978; Keen, 2001). A number of approximations and corrections are necessary in order to isolate the scattering function $S(Q)$ (containing both diffuse and Bragg scattering) utilized above. This routinely includes a static approximation and corrections for sample-independent background, absorption, multiple scattering and elastic incoherent scattering. The relationships of different correlation functions to elastic, inelastic, coherent and incoherent scattering, and the scattering contributions that warrant empirical subtraction of the corrections described in this paper, are summarized in Fig. 1. The intensity of elastic coherent neutron scattering $I(Q)_{\mathrm{E,coherent}}$ is proportional to the Fourier transform in space of the static pair correlation function $G(r, \omega = 0)$, the probability of finding a particle at position r if there is a particle at $r = 0$ at the same time in the static structure. However, the static scattering function, $S(Q, \omega = 0)$, is not the function commonly accessed experimentally and used in total

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