E0018

Pair Distribution Function Analysis: The Dependence of Entropic PDF's upon Non-Uniform Priors. R.J. Papoular, Laboratoire Léon Brillouin CEA/CNRS UMR12, Gif sur Yvette 91191, France.

Since their original introduction to study the local structure of crystals in the 1980's by Egami's group (e.g., [1] and references therein) , PDF analyses have undergone tremendous developments. Evolving alongside with the latter are the quest for the accuracy of PDF's [1], efficient programs such as PDFFIT [2] to compute them and the proper assessment of the standard uncertainties associated with them [3]. The present work focuses on yet another aspect linked to the reliability of PDF's: how many of them can be computed from a single dataset S(Q)? Whilst conventional PDF analyses involve a straightforward Sine Fourier transform, we use Maximum Entropy (MEM) to obtain g(r) from S(Q), as initially pioneered by Daniell's group in the 1980's to study liquids and amorphous materials [4]. We show that the retrieved PDF's are much dependent upon a MEM related device: the non-uniform PDF prior (NUP), which may range from totally disordered (liquid) to fully ordered (perfect crystal). The related PDF deviations are compared with the standard uncertainties.

[1] Toby *et al*., *Acta Cryst*. A**48**, 336(1992).
[2] Proffen *et al*., *J. Appl. Cryst*. **32**, 572(1999).
[3] Toby *et al*., *Acta Cryst*. A**60**, 315(2004).
[4] Daniell *et al*., *Maximum Entropy & Bayesian Methods, Skilling* (ed.), Kluwer(1989).