

Abstract Submitted  
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**A New Approach for Extracting the Pair Distribution Function of Liquids from X-Ray Scattering Experiments**<sup>1</sup> DAVID VAKNIN, YAROSLAV CHUSHAK, ALEX TRAVESSET, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — A new approach for determining the pair distribution function (PDF,  $g(r)$ ) from X-ray liquid structure factor in a reflection mode is described and applied to those of pure water and dilute water-salt solutions. The approach involves the construction of a model PDF function using parameterized generating functions that is refined by least square fitting procedure to the measured liquid  $S(Q)$ . First, a histogram of the PDF is constructed using step-like functions that are convolved with width-varying gaussians for each interfacial step of the PDF to produce a smooth  $g(r)$ . The structure factor  $S(Q)$  is then calculated from  $g(r)$  which is given by a linear combination of Error Functions. The fitted parameters are the positions and widths of the peaks of the  $g(r)$ . The advantages of this procedure is that no absolute scaling of the intensity is necessary and it provides the uncertainties in calculated  $g(r)$ . Measuring the  $S(Q)$  in reflection mode at grazing-angles of incidence (in particular below the critical angle for total reflectivity - GIXD mode) enables to obtain the liquid-gas interfacial  $S(Q)$  for which the new approach can be readily extended.

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