

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

A Novel Approach to Extracting the Pair Distribution Function of Bulk Liquids and Liquid Surfaces¹ DAVID VAKNIN, WEI BU, ALEX TRAVESSET, Ames Laboratory and Department of Physics and Astronomy, Iowa — The liquid structure factor $S(Q; \alpha)$ of water was measured by synchrotron X-rays in a reflection mode using a liquid surface diffractometer up to $Q \approx 6 \text{ \AA}^{-1}$ at various angles of incident beam α . The measurements were conducted at incident beam angles above and below the critical angle for total reflection. We calculated the geometrical and penetration depth corrections to $S(Q; \alpha)$ s above the critical angle that collapse them into a single bulk $S(Q)$ within experimental error. A new approach to determining the pair distribution function (PDF) from X-ray measured $S(Q)$ was used to analyze the data. The approach involves the calculation of $S(Q)$ from a model PDF, constructed by a linear combination of Error functions, and refined by non-linear least square fit procedure to the measured $S(Q)$. The advantages of this procedure is that no absolute scaling of the intensity is necessary and the PDF is determined with uncertainties. The methodology is currently implemented to determine the PDF at water and other liquid surfaces.

¹The work was supported by the DOE, Office of BES under contract number W-7405-Eng-82.

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Date submitted: 16 Nov 2006

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