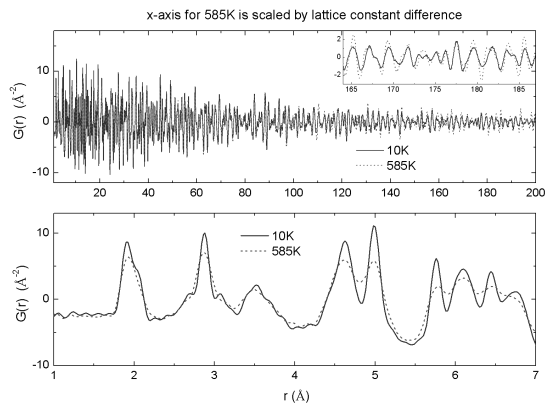


W0408

Nanometer Range Local Atomic Structure Probed by the PDF Method. T. Egami, Univ. of Tennessee, Knoxville, TN 37996-1508, Oak Ridge National Laboratory, Oak Ridge, TN 37831.

The method of atomic pair-density function (PDF) analysis has traditionally been applied mainly to study the short range structure within 0.5 nm or so. This is because the PDF analysis has been primarily used for liquid and glasses, which do not have much structure beyond nm. However, the PDF can be determined over larger distances, particularly when the measurement is made with higher Q-resolution. Using the NPDF of Los Alamos NL that has the Q resolution $\Delta Q/Q = 1.5 \times 10^{-3}$, the PDF can now be determined up to 30 nm. With this capability it is now possible to determine the hierarchical structure in different lengthscales. We discuss examples of such study, in 1) relaxor ferroelectrics in which the local atomic polarizations are non-collinear, and are different from the average polarization in nano-domains, 2) nickelate compounds in which the local environment of Ni ion is Jahn-Teller distorted, but shows no macroscopic distortion due to formation of sublattices and nano-domains. The figure shows the PDF of LiNiO_2 determined at 10 and 585 K.



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