Static and Dynamic Pair Correlation Functions Determined by Neutron Scattering and Inelastic Correction to Total Scattering

Takeshi Egami, *University of Tennessee, Department of Materials Science and Engineering and Department of Physics and Astronomy, Knoxville, TN 37996, and Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*. E-mail: egami@utk.edu

The atomic pair-density function (PDF) is obtained as the Fourier-transform of the total scattering function. In case of x-ray scattering the PDF gives a snap-shot, a time averaged same-time correlation function, since the speed of light is so fast. However, the situation is more complex with neutrons, since the velocities of neutrons and atoms are comparable. On the other hand, it is easier to carry out inelastic scattering measurement with neutrons. The dynamic structure factor, S(Q, E), thus obtained, can be Fourier-transformed to give the dynamic PDF, or the frequency-resolved PDF. We show how the dynamic PDF helps to understand the nature of dielectric response of relaxor ferroelectric oxide, $Pb(Mg_{1/3}Nb_{2/3})O_3$, by direct observation of dynamic local ferroelectric polarization. The PDF obtained by powder diffraction without energy discrimination contains both static and dynamic information. For neutron scattering the dynamic part requires correction commonly known as the Placzek correction. We show how ineffective, or even damaging, this correction is, and show that the correct inelastic correction can be made within the Debye model of lattice vibration.

Keywords: total scattering, static and dynamic PDF, inelastic effects