

RECENT ADVANCES IN THE PDF TECHNIQUE

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The method of atomic pair-density, or pair-distribution, function (PDF) has long been used primarily for the study of liquids and glasses with x-ray or neutron diffraction, because crystallography is powerless for these materials which lack lattice periodicity. However, many of the useful real materials are not strictly periodic either in the atomic structure, and often deviations from the lattice periodicity determine their properties. The PDF method is well suited to capture such local deviations from the perfect periodicity, for instance those due to defects, alloying, and intrinsic local distortions pinned by chemical disorder. The advent of the synchrotron based radiation sources, such as synchrotron x-radiation sources and pulsed spallation neutron sources, made this application possible because of high energy x-rays and neutrons they produce. The wavelengths of rays from regular laboratory x-ray sources or neutrons from reactors are too long to determine the PDF with sufficient accuracy. The concepts, fundamentals and early applications of the PDF method on crystals with disorder are treated in the book co-authored with Simon Billinge [1].

Since then Simon developed the wonderful 2D rapid PDF technique which made the x-ray PDF really popular among many researchers. It is an exceptionally powerful technique when applied to nano-materials, and this session is focusing on this important development. W. Dmowski and I applied this technique to various nano-particles, and indeed obtained critical information as he will discuss later. At the same time we pushed the PDF technique further to apply on anisotropic materials and to describe the atomic dynamics in real space. The anisotropic PDF was developed earlier [2], but we recently applied this to examine the elasticity of a metallic glass under stress, and discovered that a significant portion of the apparently elastic response of a metallic glasses actually is anelastic. This discovery is leading to a deeper understanding of the mechanical properties of metallic glasses at an atomic level. In addition we developed the dynamic PDF method that describes the local atomic dynamics, using inelastic neutron scattering [3]. For too long a time crystallographers enjoyed living in the reciprocal space where only professionals can go. However, we live in real space, and our intuition works best in real space. I hope soon all x-ray users start thinking both in reciprocal and real spaces.

- [1] “*Underneath the Bragg Peaks: Structural Analysis of Complex Materials*”, T. Egami and S. J. L. Billinge (Pergamon Press, Elsevier Ltd., Oxford, 2003).
- [2] Y. Suzuki, J. Haimovich and T. Egami, *Phys. Rev. B* **35**, 2162 (1987).
- [3] W. Dmowski, S. B. Vakhrushev, I.-K. Jeong, M. P. Hehlen, F. Trouw and T. Egami, *Phys. Rev. Lett.*, **100**, 137602 (2008).