Invited Lecture

Structural characterization with electron Pair Distribution Function data

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Over the past decade, Bragg peak electron diffraction (3D ED / MicroED) has rightfully took its place in the arsenal of structure analysis methods [1]. It is only natural that the analysis of total electron scattering also finds its way into the line-up of structure characterization techniques [2].

Similar to X-rays, electrons can be used for atomic pair distribution function (PDF) analysis. Technically, different ranges of scattering vectors can easily be accessed by adjusting the effective camera length in a TEM, and electrons can be focused down to a very small probe. This provides a unique opportunity to study tiny volumes of materials. Electron PDF (ePDF) analysis becomes particularly useful for small amounts of material, special sample geometries — such as thin films, often exhibiting texture, or inhomogeneous samples — where spatial information is necessary.

The same formalism used for X-ray PDF analysis applies to ePDF. The specialties are given by considerations for background formation mainly through inelastic scattering and the multiple scattering of electrons.

Applications of ePDF analysis can generally be categorized into three areas: (i) classical PDF analysis of amorphous or poorly crystalline materials, (ii) PDF data analysis of thin films, which often exhibit texture effects, and (iii) mapping of inhomogeneous samples with a small probe.

This presentation will discuss the technical aspects of electron diffraction data collection and processing for ePDF analysis, highlighting the benefits and addressing the challenges of using electron diffraction.

[1] Gemmi, M., Mugnaioli, E., Gorelik, T. E., Kolb, U., Palatinus, L., Boullay, P., Hovmöller, S. & Abrahams, J. P. (2019). ACS Cent. Sci. 5, 1315.

[2] Gorelik, T. E., Neder, N., Terban, M. W., Lee, Z., Mu, X., Jung, C., Jacob, T., Kaiser, U., (2019). Acta Cryst. B75, 532.