MS27. Electron crystallography methods

Chairs: Alex Eggeman, Lukáš Palatinus

MS27-P1 Pair distribution function analysis of amorphous compounds using TEM electron diffraction

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It is known that in amorphous materials crystalline order exists only at short range and conventional X-Ray diffraction does not bring immediate structural information as no diffraction Bragg peaks or sharp rings are present. Pair distribution function analysis (PDF) from total scattering experiments can be used to understand the type short range order present in these types of compounds; this can be done usually with conventional Mo/Ag X-Ray diffraction (however is time consuming as it may take up to 24 hours per sample) or using Synchrotron facilities. As an alternative, PDF analysis based on electron diffraction (ED) in any transmission electron microscope (TEM) can be used to study local order. The main advantages of using ED for PDF analysis is the very quick data acquisition time (from few msec to 2-3 minutes per ED pattern) and possibility of probing small nm size areas.

In this work two different types of samples were studied: 1) a metallic glass material with composition Pd42.5Ni7.5Cu30P20 to understand possible non-homogeneity in the material by scanning different areas of the sample 2) Honduras Opal amorphous sample to understand local ordering.

Data were collected using a 120 kV Zeiss Libra TEM microscope with 2k x 2k TMS CCD camera. Since it is important for reliable PDF analysis to have good quality data at high Q range, in order to increase the dynamic range of the experimental ED data and to increase counting statistics, several ED patterns were collected from the same area and were further summed up. PDF patterns were obtained after normalization and Fourier transformation using the software PDFGetEGui.

For the amorphous glass Pd42.5Ni7.5Cu30P20 sample, after collecting several ED PDF patterns at different positions intervals (every 200 nm) a change of individual PDF peak positions was observed, which could be possibly ascribed to inhomogeneity of the sample.

For the Honduras Opal mineral sample, ED PDF analysis reveals clearly the existence of short range order (up to 7 Å). Distances (which correspond to different atom bondings) of main PDF peak positions are very close to characteristic interatomic distances of SiO_2 structure.

For both cases structure modeling is underway to fully describe the structural environment in short range.

References:

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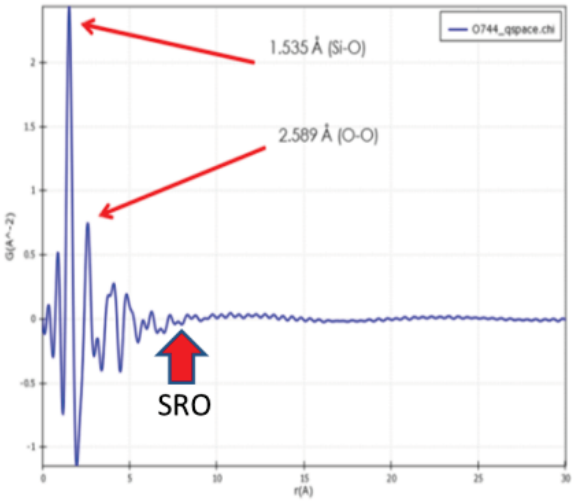

Figure 1. Pair distribution function as obtained from honduras opal data

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