

ePDF mapping: a new tool for nanometer scale analysis of amorphous materials

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Understanding material properties requires insight into atomic structure. While traditional diffraction methods rely on sharp Bragg peaks, they fail for nanocrystalline and amorphous materials due to the absence of long-range order. In such cases, Pair Distribution Function (PDF) analysis—via X-rays (xPDF), neutrons (nPDF), or electrons (ePDF)—offers critical local structural information.

Electron PDF in a Transmission Electron Microscope (TEM) provides unique advantages over xPDF, enabling nanoscale analysis with minimal sample quantity and rapid data acquisition—milliseconds versus hours in laboratory X-ray setups [1]. Conventionally, ePDF data is acquired manually using SAED or NBD, recording one pattern at a time.

We have developed a user-friendly tool that processes both single-pattern data and datasets from Scanning Precession Electron Diffraction (SPED) or 4D-STEM. In these techniques, a focused electron probe (1–10 nm) scans the sample with fine step sizes (1–3 nm), achieving spatial resolutions down to ~1 nm depending on the system. ePDFs are automatically calculated at each scan point, and the software generates correlation maps and analyzes peak positions, widths, and intensities across the scanned area—enabling detection of local structural changes [2–4].

This method can be applied to study semiconductors, glasses, catalysts, amorphous dispersions, and polymers. In a recent study, ePDF mapping revealed two amorphous layers in a semiconductor: a Si₃N₄ layer (yellow pixels, Fig. 1) with a first peak at 1.65 Å, and a SiO₂ layer (green pixels, Fig. 1) with a slightly shorter-than-expected first peak at 1.56 Å - likely due to carbon incorporation during fabrication.

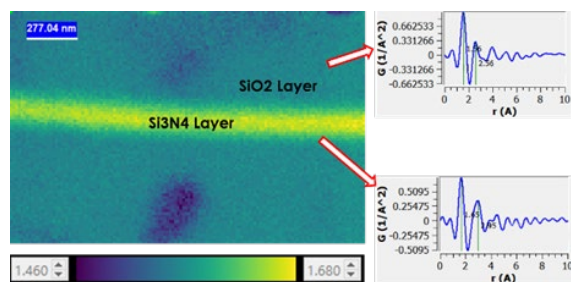


Figure 1. Left - Color map showing the variation of peak positions (Å) in the scanned area, highlighting layers of Si₃N₄ and SiO₂. Right: Representative ePDF (blue curve) from these layers, with vertical green lines indicating the first two peak positions and their numerical values—1.56 and 2.56 Å for the SiO₂ layer, and 1.65 and 2.95 Å for the Si₃N₄ layer—in the experimental ePDF.

In summary, ePDF mapping enables high-resolution, local structural analysis of amorphous materials by extracting pair distribution functions from SPED or 4D-STEM data—revealing nanoscale variations that traditional techniques cannot detect.

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