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IT-9-P-2158 Multiple scattering in amorphous structures

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Electron diffraction is a convenient technique to study the structure of materials with the advantage of high spatial resolution compared to X-ray diffraction. This fact has recently also increased interest in measuring the pair-distribution function (PDF) of amorphous materials by electron diffraction.[1] However, electrons are likely to scatter multiple times on their path through the sample, due to their strong interaction with matter. Thus, understanding the effect of multiple scattering (MS) on extracting PDFs from electron diffraction is crucial for the quantitative interpretation.

It is generally accepted that for materials possessing a 3-dimensionally isotropic structure subsequent scattering events along the electron path are independent from one another. It implies that MS can be accounted for by a simple convolution.[2] The single-scattering signal should thus be extractable from a diffraction pattern containing the contribution from MS electrons by deconvolution.[3] In our study of amorphous MgF2,[4] we found that the PDF extracted from the deconvolved diffraction pattern does not differ significantly from the PDF extracted from the original experimental data in peak shape and positions, even though there has been a significant amount of MS.

In order to investigate this similarity between the original and the deconvolved data, we used the QSTEM package [5] for simulating a dynamical diffraction pattern of an amorphous structure [6] and extracted the PDF from it. The first multislice simulation (figure 1c) was done to simulate a diffraction pattern from a small model (figure 1a) obtained by molecular dynamics simulation, mimicking single scattering because of the very thin specimen. Another simulation (figure 1d) was done to simulate the diffraction pattern from a supercell being constructed by vertically stacking the original model 20 times (figure 1b), mimicking a 20 times thicker specimen. Figure 2 shows that, except for a reduction in peak height at low frequencies, the diffraction pattern containing MS agrees rather well with the kinematical one. The PDFs (figure 2d) extracted from the MS data and the kinematic data also show no difference in peak shape or position. We finally conclude that, apart from a reduction in peak height, MS has no significant effect on the PDF. Therefore, deconvolution is not necessary in case that correct retrieval of coordination numbers is not important.

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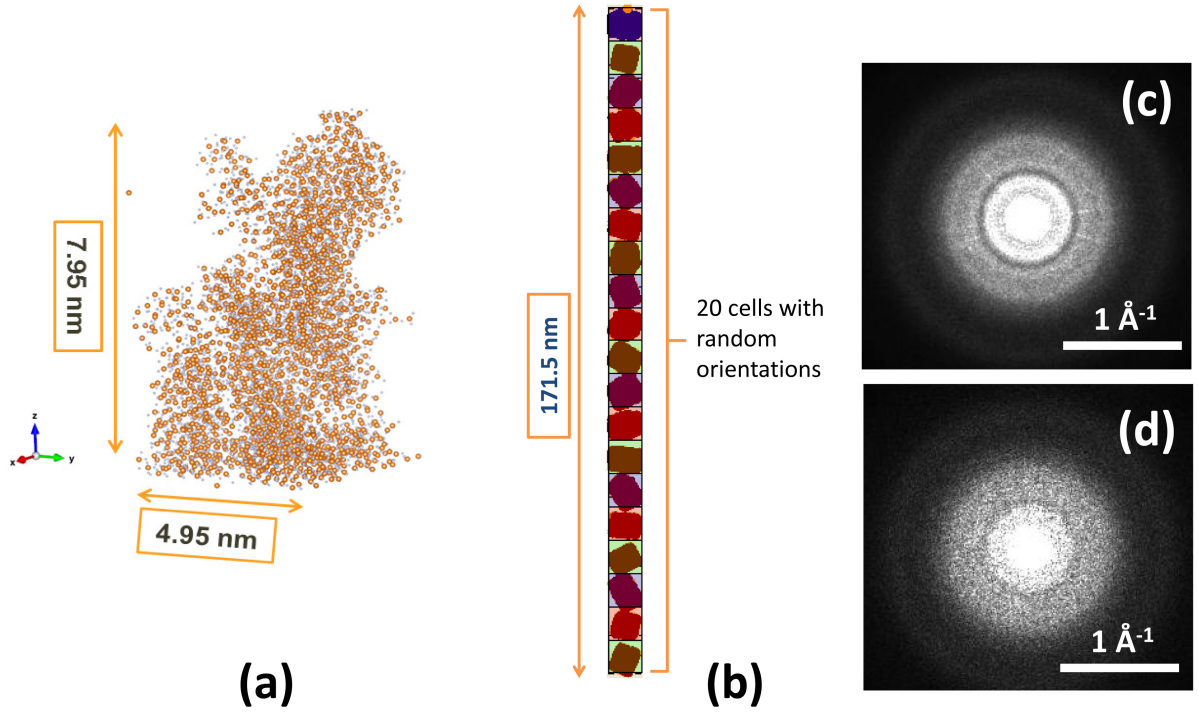

Fig. 1: Figure 1. (a) A MgF_2 cell containing 6150 atoms. (b) Supercell constructed by stacking 20 randomly orientated single cells (shown in a) to mimic the thick material for the dynamical diffraction simulation. (c) Simulated diffraction pattern from the single cell of the model shown in a. (d) Simulated diffraction pattern from the supercell shown in b.

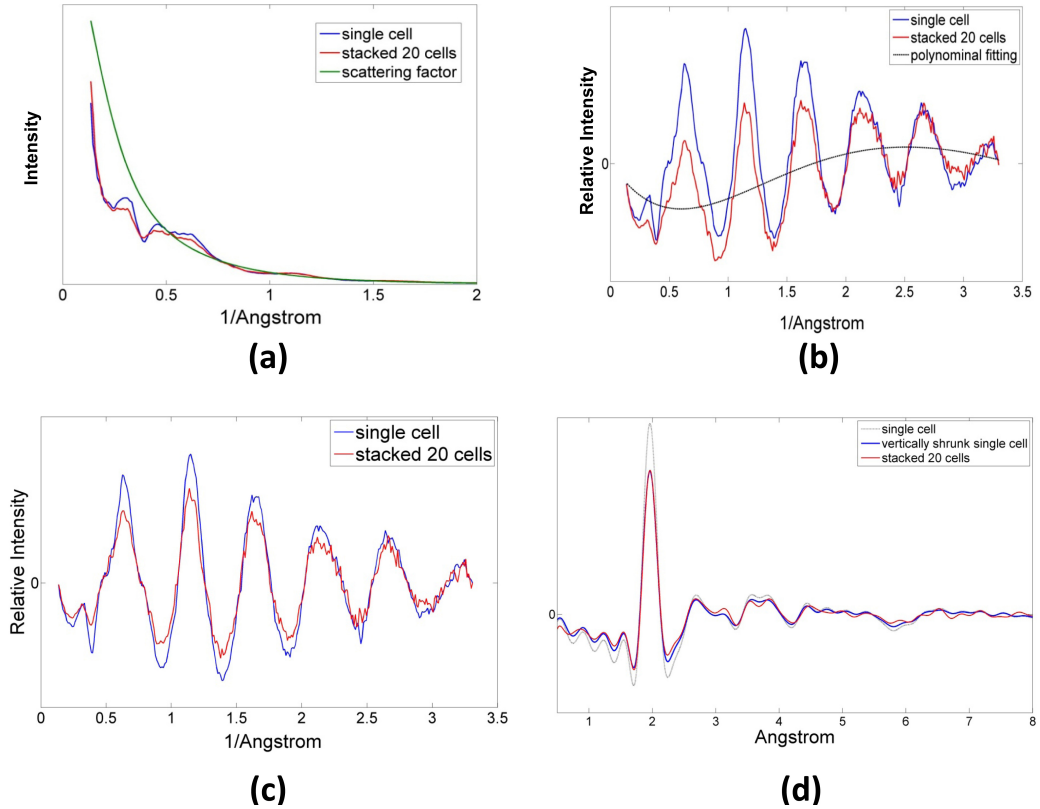

Fig. 2: Figure 2. (a) Profiles of simulated diffraction patterns; (b) structure factors extracted from a; the black dotted line is a 4th-order polynomial function fitted to the red curve; (c) same as (b) but the polynomial has been subtracted from the red curve (d) PDFs obtained by Fourier sine transform of the structure factors in b.