applied to amorphous NiNb alloy, allowing an estimate of the foil thickness, and thereafter improved the fit to the PDF obtained from Ag-anode X-ray scattering experiments (Ankele *et al.*, 2005).

Alternatively, the wavelength dependence of the multiple-scattering term can be used. A set of diffraction patterns of a glassy carbon film was collected from the same sample (apparently having the same thickness) using different wavelengths (Petersen *et al.*, 2005). These patterns were then processed in order to retrieve the single-scattering profile of tetrahedral amorphous carbon, which showed an improved fit to the reduced scattering function obtained with neutrons (Petersen *et al.*, 2005). This method can be applied to materials for which significant multiple scattering is expected and the thickness of the foil cannot be determined *a priori*. For very thin films the contribution of the multiple scattering is very low and, therefore, often neglected.

The PDF of elemental materials arising from only one contributing atomic scattering function can be directly interpreted in terms of coordination numbers and allows conclusions to be drawn about the local structure. PDF analysis of amorphous silicon prepared by deposition showed the existence of voids in the structure (Moss & Graczyk, 1969) which anneal on progressive heating. PDF investigation of amorphous carbon films prepared by arc plasma deposition showed that the material mainly consists of tetrahedrally coordinated carbon rather than having a graphitic structure (McKenzie *et al.*, 1991).

For ZrNi and ZrCu metallic glasses, partial PDFs were obtained by reverse Monte Carlo simulation (McGreevy & Pusztai, 1988) and fitted to the experimentally obtained electron scattering data. The analysis of the polyhedral statistics showed that the average coordination number of Cu was 11, while for Ni it was less than 10 (Hirata *et al.*, 2007). Study of amorphous FeB alloys (Hirata *et al.*, 2006) and $Fe_{90}Zr_7B_3$ (Hirotsu *et al.*, 2003) by PDF analysis allowed detection of nanoscale phase separation resulting in the formation of a mixture of different clusters.

Nanocrystals can be efficiently analysed by electron PDF analysis, giving information complementary to TEM imaging. The electron PDF of detonation nanodiamonds (DND) was used to estimate the average domain size (Zhang, 2011). Studies of phase separation in AgCu alloys showed the complex behaviour of the material with variation of temperature (Chen & Zuo, 2007). In the first stage, the nanodomains of the two terminal phases (Ag- and Cu-rich) are built; in the second stage, dewetting of the thin film and formation of large Ag and Cu grains occur. A comparison of electron PDFs from nanocrystalline, partially ordered and amorphous parts of silica glasses (Kovács Kis *et al.*, 2006) allowed the estimation of the degree of order developed by changing the connectivity and orientation of the undistorted SiO_4 tetrahedra. Indirect detection of hydrogen atoms was performed from a modified distribution of atomic distances in soot samples using electron PDF analysis (Kis *et al.*, 2006).

With an increase in the particle size the deviations from the kinematical scattering become severe. Nevertheless, the electron PDF calculated for 100 nm Au crystals reproduced the simulated data quite well: the peak positions and relative amplitudes were not significantly modified (Abeykoon *et al.*, 2012).

2.4.8. Summary

Powder electron diffraction can be used for materials structural characterization, just as is routinely done using X-rays and neutrons. The specific characteristics of electron scattering result in both benefits and drawbacks to using electron diffraction data. Strong scattering of electrons allows collection of a sufficient signal from nanovolumes of material, thus offering the possibility of studying small amounts of material and thin films. The opportunity to couple the diffraction information with imaging gives the unique possibility of performing a structural study on the nanoscale in a controlled way. The strong interaction of electrons with matter leads to dynamical-scattering effects that result in deviation of the electron diffraction intensities from the kinematical model. Since the amount of the dynamical-scattering component in a powder sample is difficult to quantify, the quantitative use of electron diffraction intensity data is limited. For large crystals, the dynamical treatment of electron diffraction data is efficiently done in CBED analysis, providing exclusive information about the structure. For nanocrystalline or amorphous materials, an increasing number of sets of experimental data show that quantitative structure information can be obtained using electron powder diffraction. This encourages further applications of different kinds of electron diffraction data, giving new perspectives for the quantitative use of electron diffraction in general.

APPENDIX A2.4.1
Computer programs for electron powder diffraction

CHECKCELL is a graphical powder-pattern indexing helper and space-group-assignment program that links into the *CRYSFIRE* powder indexing suite. More information and the program are available at http://www.ccp14.ac.uk/tutorial/lmgp/achekcelld.htm.

CRYSFIRE is a powder-pattern indexing system for DOS/Windows for unit-cell parameter determination from powder data (free for academic use). More information and the program are available at http://www.ccp14.ac.uk/tutorial/crys/.

ELD is a commercial program for calibrating and integrating two-dimensional electron diffraction patterns. The program is commercially available from Calidris, Sweden. More information is available from http://www.calidris-em.com/eld.php.

Electron diffraction pattern atlas. The website of Professor Jean-Paul Morniroli (http://electron-diffraction.fr/) provides an atlas of electron diffraction patterns that can be used to identify the space group of a crystal from observation of a few typical PED and CBED zone-axis patterns.

FIT2D is a general-purpose image and diffraction processing program, designed for use with synchrotron data, that integrates pre-selected sections of either one-dimensional or two-dimensional data. Corrections for geometrical distortion and for nonlinearity of intensity are included. It is available both for the Windows operating system (and DOS window) and for Macintosh OSX. The program is freely available for academic users. More information and the program are available at http://www.esrf.eu/computing/scientific/FIT2D/.

JEMS is a popular suite of simulation routines for a variety of platforms, mainly used for simulating high-resolution TEM (HRTEM), CBED, PED and SAED patterns. Simulation of powder diffraction rings is also included. The student version is free of charge. A licence is available from the author: http://www.jems-saas.ch/.

PCED is a program for the simulation of polycrystalline electron diffraction patterns (Li, 2010). A licence file is needed to unlock the program for loading input data files. More information is available at http://www.unl.edu/ncmn-cfem/xzli/.