Refinements in the Collection of Energy Filtered Diffraction Patterns from Disordered Materials

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Despite the fact that disordered materials are much more prevalent than their crystalline counterparts, our understanding of their structure is less significantly developed. This is an unsatisfactory situation as it can impede the use of disordered materials in new devices which makes it difficult to optimise their properties when designing new materials. Hence it is vital that we continue to refine techniques that accurately measure aspects of the structure of disordered materials at high spatial resolution.

Energy filtered electron diffraction (EFED) performed using a transmission electron microscope (TEM) can be employed to determine the radial distribution function (g(r)) from disordered materials at high spatial resolutions [1]. A critical step in the collection of EFED patterns is the measurement of the elastically scattered electron intensity, since g(r) is derived using kinematical scattering theory [2] which assumes elastic interactions. Cockayne and McKenzie (1988) [3] devised an experimental procedure for the collection of EFED patterns of polycrystalline and amorphous thin films by scanning the diffraction pattern over the entrance aperture of an electron energy loss spectrometer (EELS) and filtering out the in-elastically scattered electrons. However, these procedures only collect information along a line through the centre of the diffraction pattern. The development of large dynamic range CCD cameras has improved the efficiency with which EFED patterns can be collected. The advantage of using two-dimensional detectors is that entire segments of an EFED pattern can be collected. For isotropic materials this means that azimuthal averaging can be used to obtain high quality data. Such averaging ameliorates the effects of noise in the data which allows scattering data to be collected at higher scattering angles. In this paper, a detailed description of our method for the collection of EFED patterns will be presented [5]. The method combines advances in data analysis with energy filtering to extend the performance of the technique.

Fig. 1 shows the structure factor (S(k)) for glassy carbon collected using our new method by splicing together three segments of a diffraction pattern. Scattering data with a good signal to noise ratio has been collected to $k \approx 35 \, \text{Å}^{-1}$, where $k = 4\pi\sin(\theta)/\lambda$. This angular range is a considerable improvement for electrons [4] and compares favorably with other scattering methods. Also shown in Fig. 1, for comparison, is x-ray and neutron scattering data from the same sample. The different methods agree, although the electron data extends over a much larger range of k.

Fig. 2 shows the radial distribution function g(r) for several disordered materials, which are well characterized and all show good agreement with previous work. These include glassy carbon (calculated by Fourier inversion of the S(k) shown in from Fig. 1), tetrahedral amorphous carbon (ta-
C) and hydrogenated amorphous silicon (a-Si:H). One of the major sources of error associated with Fourier inversion of S(k) arises from the limited range over which the data is collected (i.e. truncation of S(k) at small k). This causes large oscillations in g(r) at small r. To reduce these artifacts, damping functions can be applied to S(k), however, this decreases the resolution of g(r). For the results shown in Fig. 2, damping factors were not used, since the S(k) data was collected over a large range of scattering angles.

FIG. 1. Comparison of S(k) for glassy carbon collected using EFED with the S(k) measured using neutron and x-ray diffraction from the same sample. The inset shows an enlarged region of the data at low k.

FIG. 2. The radial distribution function (g(r)) for glassy carbon (a), tetrahedral amorphous carbon (b) and hydrogenated amorphous silicon (c).

References