An automated procedure for the correction of background due to inelastic scattering in electron diffraction patterns. By R. D. B. Fraser, T. P. Macrae, E. Suzuki and P. A. Tulloch, Division of Protein Chemistry, CSIRO, Parkville (Melbourne), Victoria 3052, Australia

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The use of electron diffraction in structural studies of fibrous polymers is complicated by the presence of an intense background associated with inelastic scattering. A method of digital processing is described which effectively removes the undesirable features of this background. The method is also applicable in low-angle X-ray diffraction studies.

Introduction

The technique of electron diffraction has considerable potential as an analytical method for the determination of the structure of fibrous polymeric materials (Vainshtein, 1964; Tulloch, 1971; Baldwin, Bradbury & McLuckie, 1973). However, both the visual assessment of photographically recorded electron diffraction patterns and the extraction of quantitative intensity data from them are complicated by the presence of an intense background associated with inelastic scattering processes (Fig. 1a). The intensity is greatest in the forward direction and decreases rapidly with scattering angle (see, for example, Burge, 1973). Because of the rapid decrease with scattering angle, reflexions are displaced from their true positions and methods of background correction based on local estimates (Langridge, Wilson, Hooper, Wilkins & Hamilton, 1960) are subject to considerable error.

With the advent of high-speed scanning microdensitometers it has become feasible to process entire diffraction patterns by digital methods (Hall & Pass, 1975; Fraser, Macrae, Miller & Rowlands, 1976), and in the present communication we describe a procedure for applying a global correction for inelastic scattering. For visual presentation a corrected optical density $D_o$ is calculated from the measured optical density $D_m$ according to the relation:

$$D_o = D_m - D_1 + c$$

where $D_1$ is an estimate of the optical density due to inelastic scattering in regions where $D_o$ is negligible and $c$ is a constant. In the absence of noise $c$ would be set equal to zero; in practice a value is chosen such that the value of $D_o$ calculated from (1) is always positive. When quantitative intensity data are required (1) must be recast in terms of intensity rather than optical density on the basis of an assumed relation between intensity and optical density for the particular emulsion in use.

Experimental procedure

Electron diffraction patterns recorded or copied on to film were scanned with a Photoscan rotating-drum microdensitometer (Optronics International Inc.) using either a $25 \times 25$ or a $50 \times 50 \mu m$ aperture and the optical density information stored on magnetic tape as 8-bit integers with a grey-scale of 0-2 or 0-3 optical density units. The optical density data from a selected area of the pattern were then converted to floating-point format and...

Fig. 1. (a) Reconstruction obtained using a Photowrite from digital optical density data collected with a Photoscan from an electron diffraction pattern of a thin section of feather rachis. The exposure used in printing has been optimized for Bragg spacings of about 6 Å. The central region of the pattern is obscured by intensity associated with inelastic scattering. By adjusting the exposure in printing, the low-angle pattern can be optimized but the high-angle pattern will no longer be visible. Each scale division corresponds to 10 raster units. (b) Reconstruction obtained after subtraction of the estimated contribution to the optical density attributable to inelastic scattering. The central, uniformly grey circular area represents the region in the original over which the optical density exceeded 3.0. An advantage of the correction procedure is that the entire density range in the print can be used to display Bragg reflexions.
grouped to construct an array in mass storage, typically of dimensions 512 x 512. A visual estimate of the position at which the undeflected electron beam had been incident on the film was refined with a two-dimensional search procedure based on the symmetry of the inelastic scatter about the forward direction. Taking this position as origin, sectors were selected which were relatively free from Bragg reflexions and the optical density integrated along arcs of constant radius spaced at intervals equal to the raster interval. In the case of the pattern shown in Fig. 1(a) a sector covering the angular range 35-45° measured clockwise from the meridian and the corresponding sectors in the other three quadrants were used. The integrated values were converted to averages by dividing by the corresponding arc length and then smoothed with respect to radius by convolution with a Gaussian function of half width equal to four raster intervals. The result for the pattern of Fig. 1(a) is shown in Fig. 2. In this instance the result was used directly as an estimate of \( D_i \) and the corrected pattern, computed from (1), was then displayed using a Photowrite film writing system (Optronics International Inc.). The result is shown in Fig. 1(b). A second example obtained with a more highly crystalline material is shown in Fig. 3.

In some cases it is impossible to find sectors in which there are no Bragg reflexions and the curve corresponding to Fig. 2 then contains peaks of optical density where reflexions have been traversed. An estimate of \( D_i \) may be obtained in these cases by fitting a polynomial to the peak-free regions and using this to extrapolate into the regions containing peaks.

**Discussion**

The procedure described here greatly improves the visual presentation of electron diffraction patterns, effectively eliminates the displacement of reflexions due to superposition on a rapidly varying background, and removes the component of the background which is cylindrically symmetric about the undeviated beam. This component is primarily due to inelastic scattering but may contain a small contribution from, for example, thermal diffuse scatter or amorphous regions in the specimen. The precision with which the background is removed is relatively unimportant since the collection of quantitative intensity data will always involve a correction for local background. With the rapidly varying component of the background removed, methods such as those used by Langridge et al. (1960) for X-ray diffraction patterns may be used with electron diffraction patterns. Although inelastic scattering is not troublesome in recording X-ray diffraction patterns there is frequently an unwanted component of intensity at low-angles which is cylindrically symmetrical about the forward direction. The procedure outlined here for electron diffraction patterns may with advantage be applied in such cases.

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Fig. 2. Estimate of cylindrically symmetrical background density in the pattern of Fig. 1(a) obtained by the method outlined in the text. The abscissa is in raster intervals. The minor inflexion in the curve at the outer edge of the pattern is due to a diffuse ring at a Bragg spacing of around 4.7 Å in the diffraction pattern.

Fig. 3. (a) Reconstruction obtained from digital optical density data collected from an electron diffraction pattern of crystalline oothecal protein from the praying mantis, *Tenodera australasiae* (Tulloch, 1976). The low-angle reflexions are overlaid by a diffuse background which rises steeply in intensity with decreasing scattering angle. (b) Reconstruction obtained after subtraction of the estimated cylindrically symmetrical component of the background. The blank central area corresponds to the region in which the optical density exceeded 3.0 in the original pattern.
The approximation of symmetric X-ray peaks by Pearson type VII distributions. By M. M. Hall Jr, Argonne National Laboratory, Argonne III 60439, USA, V. G. Veeraraghavan, School of Materials Engineering, Purdue University, West Lafayette, In 47907, USA, Herman Rubin, Mathematics Department, Purdue University, West Lafayette, In 47907, USA, and P. G. Winchell, School of Materials Engineering, Purdue University, West Lafayette, In 47907, USA

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Some symmetric X-ray diffraction peaks can be approximated in shape by Pearson type VII distributions:

$$y(x) = y_0[1 + (x - \bar{x})^2/(ma^2)]^{-m}.$$  

This distribution is Cauchy for $m = 1$, modified Lorentzian for $m = 2$, and Gaussian for $m = \infty$. Some properties of the distribution and some illustrative applications are presented.

For some purposes representation of an X-ray, crystal-dispersed diffraction peak with a simple mathematical function is convenient even if there exists no physical justification for the selection of the function. Functions proportional to a Gaussian distribution are commonly too broad near the peak and too narrow at the tails. Functions proportional to a Cauchy distribution are usually unsatisfactory in the opposite way. A distribution which can be varied from Gaussian to Cauchy and which passes through the modified Lorentzian* by selection of a parameter is the Pearson type VII distribution and the purpose of this communication is to call attention to it and show that it can be used effectively in approximating some X-ray peaks. The Pearson type VII distribution (Elderton & Johnson, 1969) is

$$y(x) = y_0[1 + (x - \bar{x})^2/(ma^2)]^{-m},$$  

$$y(\bar{x}) = y_0.$$  

Letting

$$\int_{-\infty}^{\infty} y(x) dx = I$$

sets

$$y_0 = \frac{I}{\sqrt{\pi ma}} \frac{\Gamma(m)}{\Gamma(m - \frac{1}{2})}. \tag{1c}$$

The full width at the 1/pth maximum is

$$w(y_0/p) = 2a/\sqrt{m[p^{m/2} - 1]}.$$  

Its limiting forms are

$m = 1$  

$$y(x) = y_0[1 + (x - \bar{x})^2/a^2]^{-1}, \text{ Cauchy} \tag{3a}$$

$$y_0 = I/(2\pi a). \tag{3b}$$

and

$m = \infty$  

$$y(x) = y_0 \exp \left[-(x - \bar{x})^2/a^2\right], \text{ Gaussian} \tag{4a}$$

$$y_0 = I/(4\pi a^2). \tag{4b}$$

* We are indebted to a reviewer for calling our attention to this distribution.

† This form is readily derived by expanding $(1 + m^{-1}x^2/a^2)^{-m}$ according to the binomial series and comparing the result with the expansion of the exponential.

Table 1 lists height-to-area and width ratios for several $m$ values.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$y_0an/l$</th>
<th>$w(0.9y_0)$</th>
<th>$w(0.1y_0)$</th>
<th>$w(0.5y_0)$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.000</td>
<td>0.3333</td>
<td>3.000</td>
<td>2.000</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>1.283</td>
<td>0.3520</td>
<td>2.490</td>
<td>1.877</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.414</td>
<td>0.3614</td>
<td>2.285</td>
<td>1.820</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.540</td>
<td>0.3708</td>
<td>2.107</td>
<td>1.766</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1.659</td>
<td>0.3803</td>
<td>1.954</td>
<td>1.714</td>
<td></td>
</tr>
<tr>
<td>$\infty$</td>
<td>1.772</td>
<td>0.3999</td>
<td>1.823</td>
<td>1.665</td>
<td></td>
</tr>
</tbody>
</table>

Some other properties of this distribution are as follows. Its Fourier transform is

$$\int_{-\infty}^{\infty} y_{b,m}(x) \cos(px) dx = \frac{1}{q} \left( \frac{qb}{2m} \right)^{1/2} \frac{\pi}{\Gamma(m - 1/2)} \left( \frac{qb}{m} \right)^{m} \tag{5a}$$

where $y_{b,m}(x) = [1 + m(x/b)^2]^{-m}$ and $q = |p|$. $K_m$ is a Bessel function (Watson, 1944). The above transform can be rewritten:

$$\frac{1}{q} \left( \frac{qb}{2m} \right)^{1/2} \frac{\pi}{\Gamma(m - 1/2)} \int_{-\infty}^{\infty} \exp \left( -\frac{qb}{m} \right) t^{m-1} dt, \tag{5b}$$

which is for $m$ integral

$$\frac{b}{2m} \exp \left( -\frac{qb}{m} \right) P_m \left( \frac{qb}{m} \right) \tag{5c}$$

where $P_m$ is a polynomial of degree $m - 1$.

We may obtain the Fourier transform of the convolution,

$$\int_{-\infty}^{\infty} y_{b,m}(x - x^*) \chi_{c,m}(x^*) dx^*, \tag{6}$$

as a product of the Fourier transforms of $y_{b,m}$ and $\chi_{c,m}$. If $m$ is integral, we may use the polynomial form to write this product as the Fourier transform of a linear combination of