An improved single-line method for the wide-angle X-ray scattering profile analysis of polymers

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A modified single-line technique for determining separately the size and lattice distortion parameters of the crystalline regions by wide-angle X-ray scattering (WAXS) of typical polymer materials is proposed. The efficiency of the method is demonstrated by model calculations. Furthermore, the improved single-line treatment is applied to experimentally gained WAXS profiles of polyethylene, for which, for comparison, a standard two-line profile analysis was also applied. Two alternative single-line methods presented in the literature for the investigation of metal WAXS profiles are taken into consideration.

(Keywords: wide-angle X-ray scattering; polymers; crystallite size; lattice distortions; single-line methods)

INTRODUCTION

The wide-angle X-ray scattering (WAXS) of polymer materials provides a lot of information about the microstructure of the investigated samples, for instance about size and lattice distortions of crystallites. These structural parameters can be obtained by analysing the peak profiles of the WAXS pattern. There are many methods allowing the separation of size and disorder effects in the diffraction patterns of polymers. These are variance methods[1-3], linewidth methods[4-6] and methods based on the Fourier analysis of WAXS reflection profiles[7-9]. All these treatments were originally developed for metals and demand the experimental availability of two or more orders of a certain reflection.

Unfortunately, with most polymer samples, higher orders of a WAXS reflection cannot be measured with reasonable accuracy or only one order is available at all. Therefore, it is mostly impossible to use multiple-line techniques for WAXS profile analysis of polymers. Hence, size and strain parameters have to be determined by a single-line method. In this respect various approaches have been suggested in the literature[10]. Up to now there is no known single-line technique based on the variance of WAXS reflection line profiles[10,11]. Single-line treatments concerning the linewidth generally demand very special assumptions about the individual lineshapes relating to the contribution to line broadening associated with crystallite size and lattice distortions[10,12].

Therefore we will deal only with single-line methods in the Fourier space. Delhez, de Keijser and Mittemeijer[10] discussed some of these techniques. They demonstrated that most of these methods are unreliable even for the investigation of metal reflections.

But the technique of Mignot and Rondot[13] provided acceptable results for special metal samples. This technique will be considered in more detail in this paper. Our own investigations, however, showed that the application of the Mignot and Rondot method to typical polymer WAXS reflections does not result in unique values. Therefore, we will propose an improved modified single-line treatment for determining relevant microstructural parameters of polymers from the Fourier analysis of WAXS peak profiles. The efficiency of this treatment will be tested by model calculations. Furthermore, the suggested method will be applied to WAXS profiles of some polyethylene (PE) samples. In this connection the results of the single-line method will be compared with the results of a standard two-line analysis for confirming the efficiency of the method proposed.

THE SINGLE-LINE METHOD OF MIGNOT AND RONDOT

Every (*hkl*) WAXS reflection of a real polycrystalline material is a convolution of one profile broadened only by the finite coherence length of the crystallites comprising the sample and of another one broadened only by the displacement disorder incorporated in the individual crystallites of the sample. Then in a Fourier analysis of the profiles, which are assumed to be nearly symmetrical, the following relation is valid for the real normalized Fourier cosine coefficients A_n, A_n^s and A_n^d for the whole profile, only the size-broadened profile and only the distortion-broadened profile, respectively[9,14]:

$$A_n = A^s{}_n A^d{}_n \tag{1}$$

After Bertaut[7] and Warren and Averbach[8,9,15] the size coefficient A_n^s is a function of the 'number-average' number N_3 of cells per column in the Warren and Averbach column model of crystallites. This model assumes the crystallites to be composed of columns of cells having an average height d_{hkl} (see *Figure 1*) with

$$d_{hkl} = \lambda/4(\sin\theta_2 - \sin\theta_{\max,hkl})$$

where $\theta_{\max,hkl}$ is the position of the maximum intensity of the reflection and θ_2 is the upper profile truncation angle

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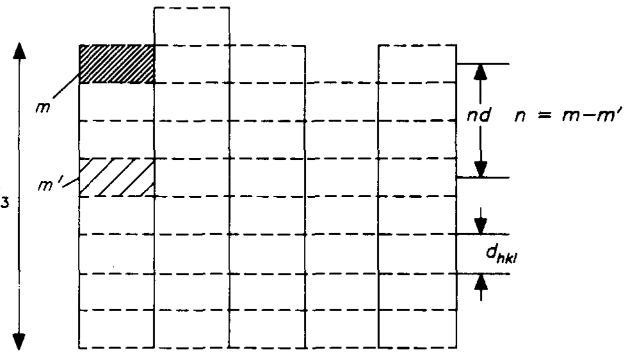

Figure 1 The column cell model for a given set of reflecting lattice planes of a crystallite; d_{hkl} is the average height of one cell; N_3 is the average number of cells per column

chosen for the Fourier analysis. The exact relation for the coefficient A_n^d is[8]:

$$A_n^d = \langle \cos 2\pi r Z_n \rangle \qquad (2)$$

in which r is the order of the reflection and Z_n is the lattice distortion variable. In an ideal crystallite the distance between the nth neighbours in the same column is always nd_{hkl}, whereas in a real crystallite the deviation from this ideal value is given by $Z_n d_{hkl}$. The angle brackets in equation (2) denote the average of pairs of nth neighbours in the sample area under the X-ray beam. Single-line profile analysis methods require special assumptions concerning the form of the functions $A^s{}_n(N_3)$ and $A_n^d(r,Z_n)$. Mignot and Rondot[13], as originally Gangulee[16], used the following expressions:

$$A_n^s = 1 - n/N_3 \qquad (3)$$

$$A_n^d = 1 - 2\pi^2 r^2 \langle Z_n^2 \rangle = 1 - 2\pi^2 r^2 n^2 \langle e_n^2 \rangle = 1 - 2\pi^2 r^2 n C_1 \qquad (4)$$

with $\langle e_n^2 \rangle = \langle Z_n^2 \rangle / n^2$ is the mean-squared strain variable for which the experimentally verified approximation $\langle e_n^2 \rangle = C_1/n$ is further used. The relation (3) is the assumption used preferentially in the literature for A_n^s. Extended model calculations by Delhez *et al.*[10] showed that this approximation for not too high n values ($n \lesssim 10$) holds precisely for a lot of column length distributions of practical importance. Formula (4) simply results from the usual Taylor series expansion for the cosine term in equation (2). Combining (3) and (4) results in

$$A_n = A_n^s A_n^d = 1 - (1/N_3 + 2\pi^2 r^2 C_1)n + 2\pi^2 r^2 C_1 n^2/N_3 \qquad (5)$$

Mignot and Rondot then make a curve fitting with the polynomial $p(n) = a_0 + a_1 n + a_2 n^2$. By comparison of coefficients it is then possible to obtain N_3 and C_1:

$$1/N_3^{\pm} = -a_1 \pm (a_1^2/4 - a_2)^{1/2} \qquad (6)$$

$$C_1^{\pm} = N_3 \pm a_2/2\pi^2 r^2 \qquad (7)$$

The method described above was developed for application to polycrystalline metals. Having investigated the examples of Mignot and Rondot we were able to find that the condition $a_2 \ll a_1$ was always fulfilled. This resulted in N_3^+ being of the order of magnitude of 10^2, a physically reasonable value, and in N_3^- being of the order of magnitude of 10^5, a physically unreasonable one. This means that in the case of most polycrystalline metallic samples the Mignot and Rondot treatment secures unique results. The application of the method to usual polymer conditions however showed that in this case the relation $a_2 \ll a_1$ is no longer realized. Therefore, one cannot decide which value, N_3^+ or N_3^-, is the physically relevant one if complex values do not result from formula (6). Thus, the Mignot and Rondot technique cannot be used for the WAXS profile analysis of most polymer materials.

It should be mentioned that there are also critical comments concerning this method in a paper by Nandi *et al.*[17] In the same paper a simple single-line method of analysing the Fourier coefficients of a WAXS peak is proposed. It is assumed that for small Fourier orders n the Fourier cosine coefficients are mainly determined by the particle-size-dependent coefficients $A^s{}_n$. Then the approximation (3) can be used for determining the averaged column length N_3 from the initial slope of a plot of A_n *versus* n (using hook effect corrected for uninfluenced values). The authors compared the results of their technique with a two-line method for some metallic samples with small lattice distortions $\langle Z_1^2 \rangle^{1/2} \times 100 < 1\%$. Applying this treatment to samples with non-zero lattice distortions, the authors found errors in the N_3 determination between 6% and 17%.

In this paper we only deal with single-line methods which are easily applicable to all sufficiently accurately measurable and resolvable WAXS reflections of investigated samples. But additionally two papers of Windle[18,19] should be mentioned, which report a very careful and extensive analysis concerning parameters of crystallite size, the distribution of crystallite sizes, the shape function and the degree of paracrystalline order for the [002] direction of special PE samples. This analysis was based on the interpretation of subsidiary maxima of the WAXS intensity distribution of the (002) peak.

AN IMPROVED SINGLE-LINE METHOD FOR POLYMERS

Since the Mignot and Rondot method usually proved inappropriate for investigating polymers, the assumptions for the strain and/or size dependence of the Fourier coefficients A_n^s and A_n^d, respectively, has to be changed. The assumption for the size-dependent coefficients was found to be very useful. Therefore, we were looking for another relation for the strain-dependent coefficients. Delhez *et al.*[10], after a critical survey of single-line techniques, proposed that perhaps a formulation initially presented by Eastabrook and Wilson[20] could profitably be applied. But they made no further use of this proposal for establishing a single-line treatment. Eastabrook and Wilson, also not in connection with single-line methods, expanded the mean-square strain variable in a Taylor series:

$$\langle e_n^2 \rangle = \langle e^2 \rangle + \langle ee' \rangle n + \ldots \qquad (8)$$

From the usual expansion of the distortion coefficient $A_n^d = 1 - 2\pi^2 r^2 n^2 \langle e_n^2 \rangle$ and equation (8) it then follows:

$$A_n^d = 1 - 2\pi^2 r^2 n^2 \langle e^2 \rangle - 2\pi^2 r^2 n^3 \langle ee' \rangle + \ldots \qquad (9)$$

with $\langle e^2 \rangle = \langle e_0^2 \rangle$ and e' being the second derivative of the displacement variable Z at the position of the mth unit cell in a particular column of the Warren and Averbach column model. We felt it to be advantageous to combine the relation (9) with the assumption (3) for the size coefficients A^s_n. Then

$$A_n = A^s_n A^d_n = 1 - n/N_3 - 2\pi^2 r^2 \langle e^2\rangle n^2 + (2\pi^2 r^2 \langle e^2\rangle /N_3 - 2\pi^2 r^2 \langle ee'\rangle)n^3 \qquad (10)$$

or, if unnormalized Fourier cosine coefficients $\bar{A}_n$ are used:

$$\bar{A}_n = \bar{A}_0[1 - n/N_3 - 2\pi^2 r^2 \langle e^2\rangle n^2 + (2\pi^2 r^2 \langle e^2\rangle /N_3 - 2\pi^2 r^2 \langle ee'\rangle)n^3] \qquad (11)$$

Then fitting a third-order polynomial

$$p(n) = a_0 + an + bn^2 + cn^3 \qquad (12)$$

to the experimentally gained $\bar{A}_n = f(n)$ curve leads to:

$$\bar{A}_0 = a_0 \qquad (13)$$

$$N_3 = -a_0/a \qquad (14)$$

$$\langle e^2\rangle = -b/(2\pi^2 r^2 a_0) \qquad (15)$$

$$\langle ee'\rangle = \langle e^2\rangle /N_3 - c/(2\pi^2 r^2 a_0) \qquad (16)$$

The microstructural parameters obtained by the single-line technique just proposed have now to be checked for possible errors resulting from this pure technique itself, and from the treatment of experimentally gained data (e.g. background—and hook effect—correction). This is done in the following two sections.

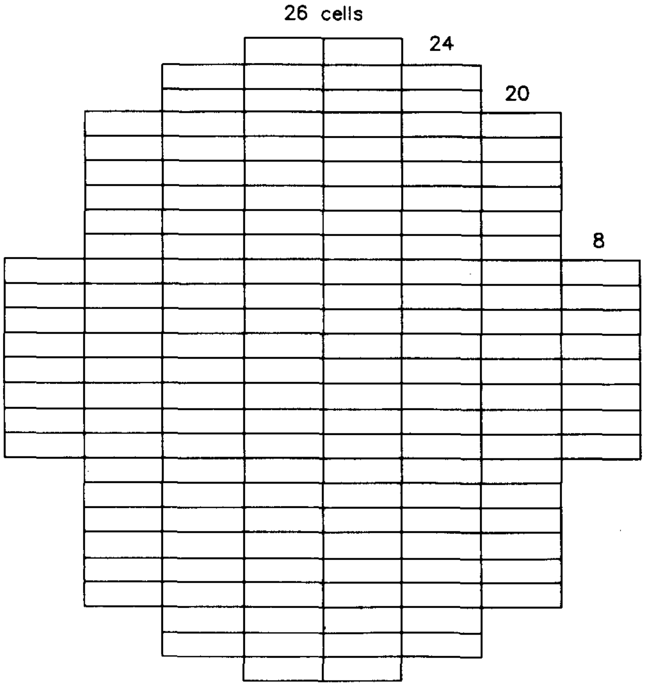

Figure 2 Cross section of an inhomogeneous column cell model composed of roughly circle-shaped layers

MODEL CALCULATIONS

For checking the efficiency of the method proposed above, extended model calculations using the column cell model of Warren and Averbach were performed. As an example we take here two basic column cell configurations typical for the situation perpendicular to the (*hk*0) and (00*l*) lattice planes in fibre-textured orthorhombically crystallized material (i.e. materials with cylindrically shaped crystallites). Here for reflecting (00*l*) lattice planes the attached column cell model is roughly composed of columns of equal length while the column cell model for reflecting (*hk*0) lattice planes consists of circle-shaped layers of equal radius (cf. *Figure 2*). At first we deal with model samples containing only one kind of crystallite composed of identical columns in the column cell model. Values typical for polymers (cf. ref. 3) were chosen for the size N_3 and the averaged $\langle Z_1^2\rangle$ distortion quantity of the basic column.

If all first neighbour distortions Z_1 are given for a column of cells then all higher neighbour distortions Z_n and hence all $\langle \cos 2\pi r Z_n\rangle$ values needed for the A^d_n calculation can be obtained. We considered a 26 cells long basic column with higher distortions of $\varepsilon^t_1 = \langle Z_1^2\rangle^{1/2} \times 100 = 2.94\%$ (cf. *Table 1*, column a), a 26 cells long basic column with medium distortions of $\varepsilon^t_1 = 1.92\%$ (cf. *Table 1*, column b), and a 24 cells long basic column with rather small distortions of $\varepsilon^t_1 = 1.35\%$ (cf. *Table 1*, column c). Symmetrical distortion distributions $P_n(Z_n)$ were chosen in all examples.

Talbe 1 Arbitrarily chosen first neighbour displacement configurations for the column cell models used in the theoretical calculations

Number of distance	Z_1						
	a	b	c	d	e	f	g
1	0	0	0	0	0.01	0.01	0.01
2	0	0.01	0	0	0.01	0.02	0.03
3	0.01	0.01	0.01	0.01	0.02	0.01	0.01
4	0.01	0.02	0.01	0.01	0.03	0	0
5	0.02	0.03	0.02	0.02	0.04	−0.01	−0.01
6	0.04	0.04	0.03	0.03	0.03	−0.02	−0.03
7	0.08	0.03	0.02	0.02	0.02	−0.01	−0.01
8	0.04	0.02	0.01	0.01	0.01		
9	0.02	0.01	0.01	0.01	0.01		
10	0.01	0.01	0	0	0		
11	0.01	0	0	−0.01	−0.01		
12	0	0	0	−0.01	−0.01		
13	0	0	0	−0.02	−0.02		
14	0	0	0	−0.03	−0.03		
15	−0.01	0	−0.01	−0.02	−0.04		
16	−0.01	−0.01	−0.01	−0.01	−0.03		
17	−0.02	−0.01	−0.02	−0.01	−0.02		
18	−0.04	−0.02	−0.03	0	−0.01		
19	−0.08	−0.03	−0.02	0	−0.01		
20	−0.04	−0.04	−0.01				
21	−0.02	−0.03	−0.01				
22	−0.01	−0.02	0				
23	−0.01	−0.01	0				
24	0	−0.01					
25	0	0					
Number of cells	26	26	24	20	20	8	8
$\varepsilon^t_1 = \langle Z_1^2\rangle^{1/2} \times 100$ (%)	2.94	1.92	1.35	1.49	2.20	1.31	1.77

Table 2 Comparison between the assumed theoretical size and distortion parameters and the parameters obtained from a single-line fit procedure according to equations (10)–(16) for equal length column samples with:

$$\Delta N_3 = [(N_3 - N_3^t)/N_3^t] \times 100$$

$$\Delta \varepsilon_1 = [(\varepsilon_1 - \varepsilon_1^t)/\varepsilon_1^t] \times 100$$

$$\langle Z_1^2 \rangle = \langle e^2 \rangle + 1 \langle ee' \rangle$$

Theoretical values		Values from single-line technique				
N_3^t	ε_1^t (%)	N_3	ΔN_3 (%)	ε_1 (%)	$\Delta \varepsilon_1$ (%)	$N_3^{N\,a}$
24	1.351	24.0	0.0	1.337	−1.0	17.6
26	1.918	26.1	0.4	1.941	1.2	14.2
26	2.939	25.4	−2.3	2.842	3.3	11.3

[a] N_3^N is the averaged crystalline particle size after Nandi *et al.*[17]

Using the relation $A_n^d = \langle \cos 2\pi r Z_n \rangle$ we calculated the distortion-dependent Fourier cosine coefficients. According to Warren[9] the particle-size-dependent Fourier cosine coefficients A_n^s can be obtained from the column length distribution p_i of the sample by:

$$A_n^s = (1/N_3) \sum_{i=1}^{n} (i-n) p_i \qquad (17)$$

with

$$\sum_{i=1}^{\infty} p_i = 1 \qquad (18)$$

In each case considered here only one p_i value is a non-zero one ($p_{24} = 1$ and $p_{26} = 1$, respectively). It should be noticed that then the approximation (3) is a completely accurate representation of the particle-size-dependent Fourier cosine coefficients A_n^s. From A_n^s and A_n^d the Fourier cosine coefficients A_n were obtained. These coefficients were treated by the modified single-line method proposed here (equations (10)–(16)). The results are represented in *Table 2*.

It is seen that, probably at least with samples having a first neighbour root mean square (r.m.s.) displacement not much greater than 3–4% and the special column length distribution chosen here, the single-line technique provides reasonable results. It should be mentioned that the use of the single-line method for a 26 cells long model sample with $\varepsilon_1^t = 6.4\%$ led to an unacceptable result (e.g. the averaged column length was determined to be 20.4). On the other hand the single-line treatment according to Nandi *et al.*[17] was found to result in unsatisfactory values for the averaged column length at least with samples with $\varepsilon_1 \gtrsim 1\%$. This means that probably the Nandi method will not be suitable for typical polymer samples (that means $\varepsilon_1 \approx 1$–4%, $N_3 \approx 10$–30).

Secondly, we considered samples consisting of only one kind of crystallite involving non-identical columns in the column cell model for a certain set of reflecting lattice planes. We chose the column cell model I of layers with a roughly circle-shaped column length distribution (cf. *Figure 2*). The theoretical averaged column length for this sample is $N_3^t = 19.5$. The particle-size-dependent Fourier cosine coefficients A_n^s were calculated using equations (17) and (18) (here $p_i = 0$ except $p_8 = 0.25, p_{20} = 0.25, p_{24} = 0.25$ and $p_{26} = 0.25$). The A_n^s values obey precisely the approximation (3) as long as the Fourier index does not exceed 8. (In general, the approximation (3) for A_n^s will be very good as long as the sample involves no considerable amount of cells with lengths smaller than the Fourier order n for which A_n^s is determined.)

In obtaining the lattice-distortion-dependent Fourier cosine coefficients A_n^d we chose the first neighbour displacements in *Table 1*, column a, for the 26 cells long columns (with $\varepsilon_1^t = 2.94\%$); in *Table 1*, column c, for the 24 cells long columns (with $\varepsilon_1^t = 1.35\%$); in *Table 1*, column e, for the 20 cells long columns (with $\varepsilon_1^t = 2.20\%$); and in *Table 1*, column g, for the 8 cells long columns (with $\varepsilon_1^t = 1.77\%$). From this starting point we calculated the values of $A_n^d = \langle \cos 2\pi r Z_n \rangle$ (with $r = 1$), $\langle Z_n^2 \rangle$ and $\langle e_n^2 \rangle = \langle Z_n^2 \rangle / n^2$ of every single type of column and then we took the mean values for the whole crystallites according to Warren[9]. Further, a column cell model II as in *Figure 2* but with 26 cells long columns indicated in *Table 1*, column b, (with $\varepsilon_1^t = 1.92\%$), 24 cells long columns in *Table 1*, column c (with $\varepsilon_1^t = 1.35\%$), 20 cells long columns in *Table 1*, column d (with $\varepsilon_1^t = 1.35\%$) and 8 cells long columns in *Table 1*, column f (with $\varepsilon_1^t = 1.31\%$) was taken into consideration.

Table 3 shows that the single-line method discussed above provides reasonable results with samples containing equal crystallites composed of different columns for a certain set of lattice planes at least if the r.m.s. displacement for first neighbours will not exceed 3% by too much. This result is easily generalized for samples consisting of different types of crystallites each of which is composed of a certain *Figure 2* type or a certain equal length column cell model for the reflecting lattice planes under investigations. Further extended model calculations with different column cell distributions confirm that the error of microstructural parameters obtained by this single-line treatment will not be greater than ±5% if the r.m.s. displacement is not greater than 3%.

TREATMENT OF PRACTICAL EXAMPLES

In the previous part of the paper the errors of N_3 and $\langle Z_1^2 \rangle$ values obtained from the proposed modified single-line technique were related only to the truncation errors of the series (8) and (9) and the usual Taylor series expansion for $A_n^d \approx 1 - 2\pi^2 r^2 \langle Z_n^2 \rangle$. In this case therefore the fit of the polynomial (12) to the Fourier coefficients $A_0, \ldots, A_3$ is always the best fit since here we have the Fourier interval (n_1, n_2) with the smallest upper bound possible for this fitting procedure. If we otherwise have to treat Fourier cosine coefficients based on experimentally measured WAXS profiles, we will find another source of errors in the single-line technique. It is the so-called hook

Table 3 Comparison between the assumed theoretical size and distortion parameters and the parameters obtained from a single-line fit procedure according to equations (10)–(16) for samples composed of unequal columns (see *Figure 2*)

Theoretical values			Values from single-line technique				
Number of model	N_3^t	ε_1^t (%)	N_3	ΔN_3 (%)	ε_1 (%)	$\Delta \varepsilon_1$ (%)	N_3^N
1	19.5	2.242	19.5	0.0	2.221	−1.9	12.1
2	19.5	1.594	19.6	0.5	1.617	1.4	14.2

Table 4 Comparison between the results of the proposed single-line method and a standard two-line profile analysis technique after Warren[9] for (*hk*0) WAXS peaks of PE samples with $L_{hkl}=N_3 d_{hkl}$

Sample	Reflection	L_{hkl} (nm)	ε_1 (%)	Remarks
PE band (hot stretched)	(110)	6.6	2.4	single-line
	(110)/(220)	6.7	2.7	two-line
	(200)	7.1	1.5	single-line
	(200)/(400)	6.9	1.4	two-line
PE extrudate[a]	(200)	13.6	0.9	single-line
	(200)/(400)	12.9	0.9	two-line

[a] The (220) peak was not resolvable from the (201) peak in the case of the PE extrudate

effect at small n values resulting mainly from the practically always necessary truncation of the investigated reflex profile and errors in the background subtraction from the WAXS pattern. Therefore, using the proposed single-line technique the physically most relevant fit interval (n_1,n_2) has to be found where the combined influence of both errors discussed above is minimized. In this connection experimental conditions should be chosen in such a manner that this interval is as near as possible to (0,3), where the treatment of the theoretical examples results in the smallest errors of the determined size and lattice distortion parameters. This means that the hook effect has to be reduced as much as possible. One possibility is provided by the hook effect correction procedures of Warren[9] or Rothman and Cohen[21]. But the negative curvature of A_n at low n does not only result from the hook effect but, to a smaller extent, also from lattice distortions (cf. also ref. 10). Therefore, if we treat the hook effect using the procedures of Warren or Rothman and Cohen we will neglect the part of the effect related to the sample material. For that reason, we take the following procedure for determining the physically most relevant fitting interval.

By appropriately choosing the truncation angle of the measured WAXS profile we keep the interval of negative curvature of the A_n values so small that only the positions of A_0 and A_1 are influenced. Then the hook effect should mainly affect the magnitude of A_0 (cf. also ref. 9) while we assume the position of A_1 to be mainly determined by the lattice distortions present in the investigated material. Therefore only the position of A_0 is corrected linearly using the magnitudes of A_1 and A_2.

After this correction it is possible that a small error remains. By fitting the third-order polynomial (12) to the corrected A_n values it is therefore necessary to choose the physically most relevant fit interval (n_1, n_2) as discussed above. For this reason we apply the fit procedure according to equations (12)–(16) to the intervals $(n_1, n_2)=(0,3)$, (0,4), (1,4), (0,5), . . . and take the first of these intervals providing physically reasonable results (that means for instance: $N_3>0$, $\langle e^2\rangle<0$ and $N_3\geq N_3^{\mathrm{N}}$) as the physically most relevant one.

By treating a lot of practical examples we found that it was always sufficient to consider the fit intervals (0,3), (0,4) and (1,4). In the single-line technique used here, a four-parameter fit polynomial is fitted to four or five A_n values. This means that the fit error will be zero or nearly zero in all cases. Consequently, here the fit error cannot be used for searching for the physically most relevant set of fit parameters.)

Investigations concerning the reliability of results achieved by the help of the procedure discussed above for repeatedly measured and analysed (including background and hook effect corrections) WAXS peaks showed that at least for accurately enough measurable WAXS reflections of highly oriented, highly crystalline ($\omega_c \geq 50\%$) polymer samples the crystallite size and lattice distortion parameters can be well reproduced. In this case the fluctuations of the determined parameters are not much higher than $\pm 5\%$ concerning the respective average values.

To obtain some feeling about the full deviation of the structural parameters calculated using the proposed single-line method from their genuine values, it is useful to compare the results of the single-line treatment for special samples with the respective results of a two-line technique after Warren[9]. Such results are given in *Table 4* for some WAXS reflections of special PE samples for which it was possible to analyse the higher-order peaks (220) and (400) too. An acceptable coincidence between the results of both methods was found. This is a further indication for the applicability of the single-line method proposed here to polymer WAXS reflections.

CONCLUSIONS

The separate determination of crystallite size and lattice distortion parameters from WAXS patterns of polymers is important in investigating the microstructure of polymer materials. But these materials scarcely show more than one evaluable order of (*hkl*) reflections. Therefore, the separation of size and disorder effects of WAXS patterns has to be achieved by using single-line techniques demanding special assumptions about the nature of the effect of crystallite size and lattice distortions on the WAXS reflections. Techniques based on the investigation of the coefficients of the Fourier analysis of the investigated WAXS profiles proved to be suitable. But it is presumably impossible to apply the single-line methods of Mignot and Rondot[13] or Nandi *et al.*[17], which have been established for metal research, to WAXS reflections of typical polymer samples. On the other hand, as revealed by model calculation, and comparison with results of standard two-line techniques, the single-line treatment proposed here appears to be more appropriate for many polymer materials if the r.m.s. strain ε_1 of the samples does not exceed 3–4%.

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