STANISŁAW RABIEJ[*)], MAŁGORZATA RABIEJ

University of Bielsko-Biała
ul. Willowa 2, 43-300 Bielsko-Biała, Poland

Determination of the parameters of lamellar structure of semicrystalline polymers using a computer program SAXSDAT

Summary — A computer program SAXDAT for the analysis of small angle X-ray scattering (SAXS) curves of semicrystalline polymers is described. The program is based on a lamellar stack model of polymer structure. In the program, the parameters of stacks can be determined from one-dimensional correlation function calculated as a Fourier transform of intensity distribution or by model calculations which consist in fitting of a theoretical intensity distribution function to the experimental curve. The program can be applied to single curves as well as to big sets of curves obtained from time resolved experiments. Both point and slit collimation recording systems are acceptable.
Keywords: small angle X-ray scattering, correlation function, semicrystalline polymers, lamellar structure, computer program.

WYZNACZANIE PARAMETRÓW STRUKTURY LAMELARNEJ POLIMERÓW SEMIKRYSTA-LICZNYCH ZA POMOCĄ PROGRAMU KOMPUTEROWEGO SAXSDAT
Streszczenie — W pracy opisano możliwości opracowanego przez autorów programu komputerowego SAXSDAT przeznaczonego do analizy krzywych małokątowego rozpraszania promieniowania rentgenowskiego (SAXS) otrzymanych podczas badań polimerów semikrystalicznych. Algorytmy programu wykorzystują zależności znane z teorii rozpraszania promieniowania rentgenowskiego przez polimery semikrystaliczne, opracowane przy założeniu lamelarnego modelu ich struktury wewnętrznej. Program może być stosowany do analizy pojedynczych krzywych SAXS otrzymanych w eksperymentach statycznych, przy użyciu klasycznych kamer małokątowych typu kamera Kratky'ego, jak też do wieloelementowych zbiorów krzywych otrzymywanych w eksperymentach dynamicznych prowadzonych z zastosowaniem promieniowania synchrotronowego. Jego istotną zaletą jest to, że może być używany do opracowania krzywych zarejestrowanych przy użyciu zarówno punktowego jak i szczelinowego systemu kolimacji wiązki pierwotnej. Jednym z głównych zadań programu jest wyznaczenie tzw. jednowymiarowej funkcji korelacyjnej charakteryzującej strukturę warstwowych domen wypełniających objętość polimeru. Na podstawie przebiegu tej funkcji, obliczane są wszystkie parametry charakteryzujące strukturę tych domen: grubość lamel krystalicznych i warstw amorficznych, wielki okres, objętościowy stopień krystaliczności domen, grubość obszaru przejściowego na granicy faz, inwariant idealny i rzeczywisty.
Słowa kluczowe: małokątowe rozpraszanie rentgenowskie, funkcja korelacyjna, polimery semikrystaliczne, struktura lamelarna, program komputerowy.

From the point of view of the small angle X-ray scattering (SAXS) method, semicrystalline polymers can be considered as periodic, condensed systems composed of two types of regions of different electron density — crystalline lamellae and amorphous layers, with a diffuse transition layer between them. Alternating crystalline and amorphous layers form characteristic stacks which can be clearly distinguished inside spherulites filling the polymer volume. Of course, the structure of stacks is not perfect: the layers are not ideally parallel, they may be curved or undulated and their orientation in space changes continuously. However, because the lateral dimensions of stacks are much bigger than the wavelength of X-rays, the scattering from such specific, layered structures can be described using a model in which the layers are of infinite size and they are perfectly parallel to one another. Thanks to this fact, the scattered intensity is completely determined by the electron density variations occurring in only one direction — perpendicularly to the layers.

The theory of small angle scattering from semicrystalline polymers was elaborated mostly by Hosemann [1, 2], Vonk [3—9], Ruland [10—16], Blundell

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[*)] Corresponding author; e-mail: stanislaw.rabiej@ath.bielsko.pl

[17—19] and Strobl [20—25]. Application of this theory to the analysis of SAXS curves, makes possible determination of several important parameters of stacks, such as the thicknesses of amorphous layers and crystalline lamellae, long period, volume fraction crystallinity, thickness of the transition layer. In some cases, one can determine not only the average values but also standard deviations of long period and of the thicknesses of crystalline and amorphous layers. Another important parameter is an invariant which characterizes the average square of electron density fluctuation in the polymer volume. Particularly interesting and instructive is observation of the changes of these parameters which occur during phase transformations of investigated polymer, for instance during melting or crystallization. Such possibilities are offered by dynamic time resolved experiments which are performed using synchrotron radiation. As the ranges of crystallization and melting temperatures of polymers are broad, the total number of diffraction curves recorded during such processes can reach several hundreds for one sample. Employing the SAXS method in combination with the method of wide angle X-ray diffraction, we can obtain a comprehensive picture of the internal structure of polymer at different levels of molecular organization. However, the analysis of SAXS curves is rather complicated and needs an advanced numerical processing.

A computer program SAXSDAT [26], presented in this work is designed for a comprehensive analysis of the SAXS curves of semicrystalline polymers. It can be used both for the elaboration of single curves, recorded in static experiments using classical laboratory SAXS cameras, as well as for big sets of curves, obtained in dynamic time resolved experiments, performed with the synchrotron radiation. Both point and slit collimation recording systems are acceptable.

ONE-DIMENSIONAL CORRELATION FUNCTION

In the theory of SAXS for semicrystalline polymers, elaborated by the authors mentioned above, polymer volume is considered as a pseudo two phase system. As it is shown in Figure 1 this system is represented by an isotropic arrangement of randomly oriented stacks which are composed of lamellar crystals and amorphous layers.

Stacks are characterized by the average values of crystal thickness, amorphous layer thickness and long period, which is the sum of these two thicknesses. The thicknesses of lamellae and amorphous layers, statistically fluctuate independently of one another. The fluctuations are described by distribution functions $H(C)$ and $h(A)$ and standard deviations. Statistically, the structure of all stacks is the same. Electron density distribution in the stacks can be described by a correlation function. Because of the specific character of electron density variations, it is a one-dimensional correlation function $K_1(x)$, defined in the direction perpendicular to the surface of the crystalline lamellae and amorphous layers [24].
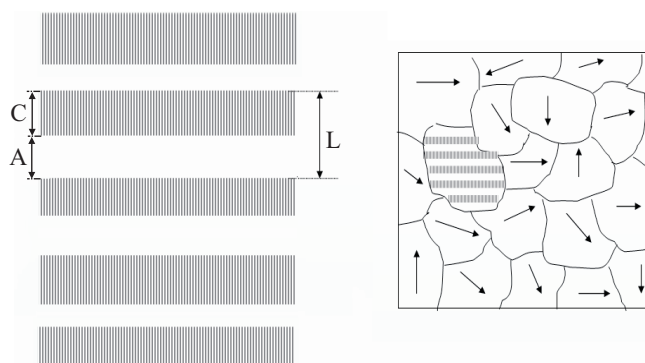

Fig. 1. Scheme of a stack and a model of polymer structure assumed in the SAXS method (symbols C, A and L stand for the thickness of crystalline lamella, amorphous layer and long period, respectively; the arrows indicate random orientation of stacks in the polymer volume)

$$K_1(x) = \langle \eta(x')\eta(x' + x) \rangle = \langle [\rho(x') - \langle\rho\rangle][\rho(x' + x) - \langle\rho\rangle] \rangle \quad (1)$$

This function presents an averaged over the polymer volume product of electron density fluctuations $\eta(x')$ and $\eta(x' + x)$, at two points located on a line perpendicular to the layers, with the distance x between them. $\rho(x')$ and $\rho(x + x')$ in eq. (1) are electron densities, $\langle\rho\rangle$ is an average electron density of a stack, and the brackets $\langle \rangle$ stand for an average value. A detailed analysis of the one dimensional correlation function and its properties has been presented by Strobl [24]. Figure 2 presents the plot of such a function for an ideal case in which the thicknesses of crystalline lamellae C and amorphous layers A are constant in the polymer volume and the borders between the phases are sharp. In his example, the thickness of crystal-
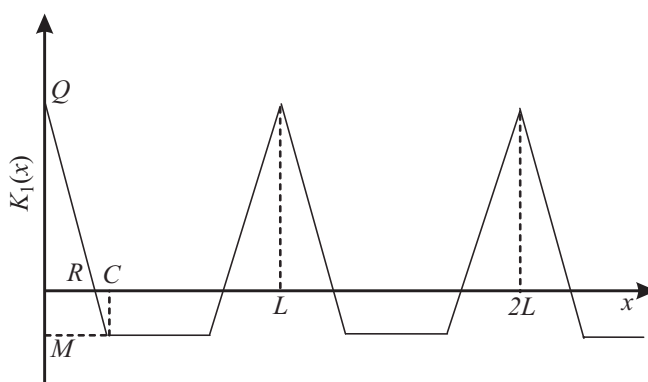

Fig. 2. Plot of the one-dimensional correlation function for the ideal lamellar structure

line lamellae C is smaller than the thickness of amorphous layers (volume crystallinity <0.5). The first triangle in this plot is called a self correlation triangle. It can be shown [24], that the coordinates of the characteristic points of this triangle are connected with the parameters of stacks:

$$Q = K_1(0) = (\Delta\rho)^2\varphi(1 - \varphi) \tag{2}$$

$$M = K_1(C) = -\varphi^2(\Delta\rho)^2 \tag{3}$$

$$R = C(1 - \varphi) \tag{4}$$

where: $\Delta\rho = \rho_1 - \rho_2$ — *the difference in electron densities between crystalline and amorphous phase; φ, $(1 - \varphi)$ — volume fractions of crystalline and amorphous phases, respectively ($\varphi = C/L$); $Q = K_1(0)$ — so called invariant, the average square of electron density fluctuations in the polymer.*

In the case of real stacks, both the thickness of crystalline lamellae as well as that one of amorphous layers, and consequently the long period, show a certain distribution. Moreover, the boundaries between the phases are not sharp, but the electron density varies smoothly between ρ_1 and ρ_2. As a result, the plot of the correlation function changes considerably. However, the coordinates of the self correlation triangle are still closely connected to the parameters of stacks. In Figure 3 we can see, that
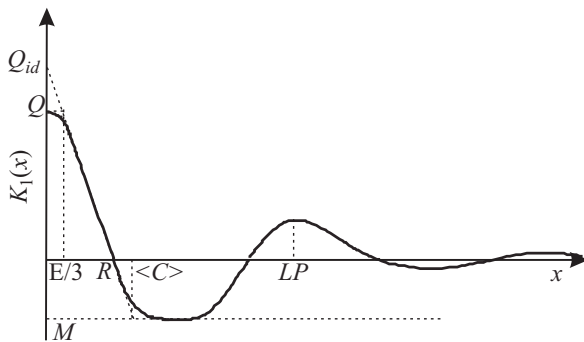

Fig. 3. Plot of the one-dimensional correlation function for the real lamellar structure

the plot of the correlation function, in the frames of the self correlation triangle, is not linear any more. Due to the distribution of lamellar thicknesses, the plot is curved near the flat minimum level. But the value of the minimum, still remains the same as in the ideal structure: $M = -\varphi^2(\Delta\rho)^2$. The presence of a transition layer between the phases causes that invariant is smaller now than in the ideal structure. As a consequence, the value of the correlation function at $x = 0$ decreases and the plot is curved in this region. Assuming that the lamellar surfaces in the stacks are flat and parallel, it can be proved that:

$$K_1(0) = Q = (\Delta\rho)^2\left[\varphi(1 - \varphi) - \frac{E}{3\langle L\rangle}\right] \tag{5}$$

where: *E — the thickness of the transition layer, $\langle L\rangle$ — the number average value of the long period.*

The central part of this fragment of the plot is still linear, and it is described by:

$$K_1(x) = (\Delta\rho)^2\left[\varphi(1 - \varphi) - \frac{x}{\langle L\rangle}\right] \tag{6}$$

The extension of this linear fragment to $x = 0$, gives the invariant — Q_{id} which corresponds to an ideal structure

with sharp phase boundaries. Extrapolating the linear fragment to the intersection with the level of minimum of the correlation function we obtain the average thickness of lamellae $\langle C\rangle$. On the other hand, the intersection of this fragment with the x axis occurs at:

$$R = \langle C\rangle(1 - \varphi) \tag{7}$$

where: $\varphi = \langle C\rangle/\langle L\rangle$.

Location of the second maximum of the correlation function corresponds to the most probable value of the long period — LP, however in most cases, when the distribution of long period is not very broad, one can assume that $LP \approx \langle L\rangle$.

Summarizing, the coordinates of characteristic points which can be read out in the plot of the correlation function, contain information on the most important parameters of stacks *i.e.* the average long period $\langle L\rangle$ and the average thicknesses of crystalline lamellae $\langle C\rangle$ and amorphous layers $\langle A\rangle$. Moreover, one can determine the thickness E of transition layer between the phases as well as the ideal Q_{id} and real Q invariants.

All these parameters of investigated polymer sample can be determined experimentally using the SAXS method. As it is well known from the fundamental law of the scattering theory, the intensity distribution is a Fourier transform of the correlation function related to the structure of the scattering object. So, the correlation function can be calculated by an inverse Fourier transform of the intensity distribution, which in this case takes a shape of [24]:

$$K_1(x) = \int_0^\infty 4\pi s^2 I(s)\cos(2\pi s x)ds \tag{8}$$

where: $s = 2\sin\theta/\lambda$, 2θ — *the scattering angle, λ — the wavelength, $I(s)$ — the intensity function.*

STRUCTURE OF THE SAXSDAT PROGRAM

Calculation of the correlation function and determination of the parameters of stacks is one of the main aims of the SAXSDAT program. However, the Fourier transform given by eq. (8) is calculated only in one of the last modules of the program. At first, several introductory steps must be performed. The structure of the program is shown in Figure 4. As it has already been mentioned above, the program can be used for the elaboration of single curves $I(s)$, recorded in static experiments with classical SAXS cameras, as well as for big sets of curves, obtained in dynamic, time resolved experiments.

Introductory data elaboration

In the first module of the program, designed for the introductory data elaboration, the experimental curves can be prepared for the main calculations and corrected for different distortions. The module, whose window is presented in Figure 5, offers all computational tools, necessary to this aim. Using these tools we can perform dif-
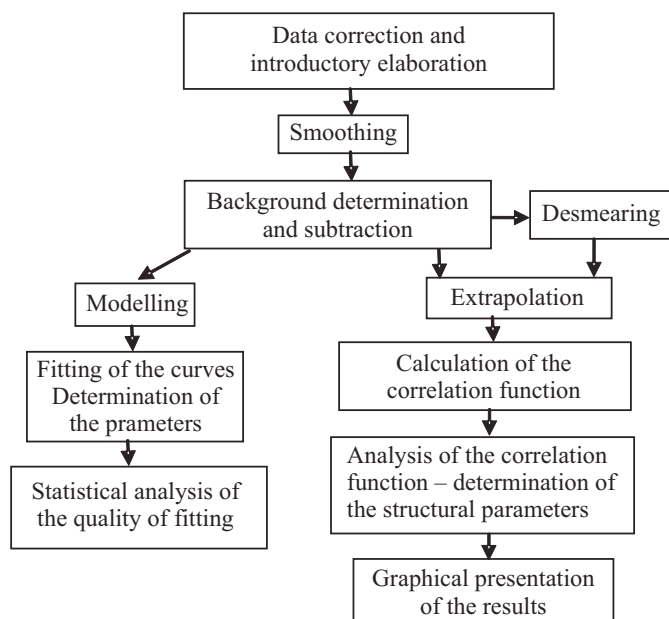
Fig. 4. Structure of the SAXSDAT program

ferent mathematical operations on the experimental curves $I(s)$: multiplication, division, subtraction, addition, averaging of chosen subsets of curves, integration in a chosen range and so on. Among other actions, in this module we can remove a diffuse scattering which is not related to the polymer structure, we can perform calibration of the detector, scaling and normalization of the curves, corrections for the variable intensity of the

primary beam, Lorentz correction and elimination of the experimental noises.

In the second module, the window of which is presented in Figure 6, the corrected scattering curves can be smoothed. Smoothing is a very important step in the elaboration of SAXS data. To this aim, the program offers three different methods: cubic B splines, Hermite's polynomials and Savitzky-Golay filters. For a given curve (Fig. 6), we can use one chosen method or we can combine these three methods, using different method at different fragments of the same curve. Moreover, the smoothing degree of different fragments can be controlled by choosing appropriate values of the smoothing parameters.

Background subtraction and extrapolation of the curves

The next important module is designed for subtraction of the background intensity which is not related to the polymer structure but is caused by thermal density fluctuations inside crystalline and amorphous phases. Besides, in this module the scattering curves can be extrapolated towards small and large scattering angles. As we can see in eq. (8), the integration limits in the Fourier transform, stretch from zero to infinity, while the experimental curves are recorded only in a limited angular range. This is why extrapolation is necessary. To extrapolate a curve we have to know the function describing it at large angles. Generally, experimental intensity $I_{exp}(s)$ is a sum of two components:
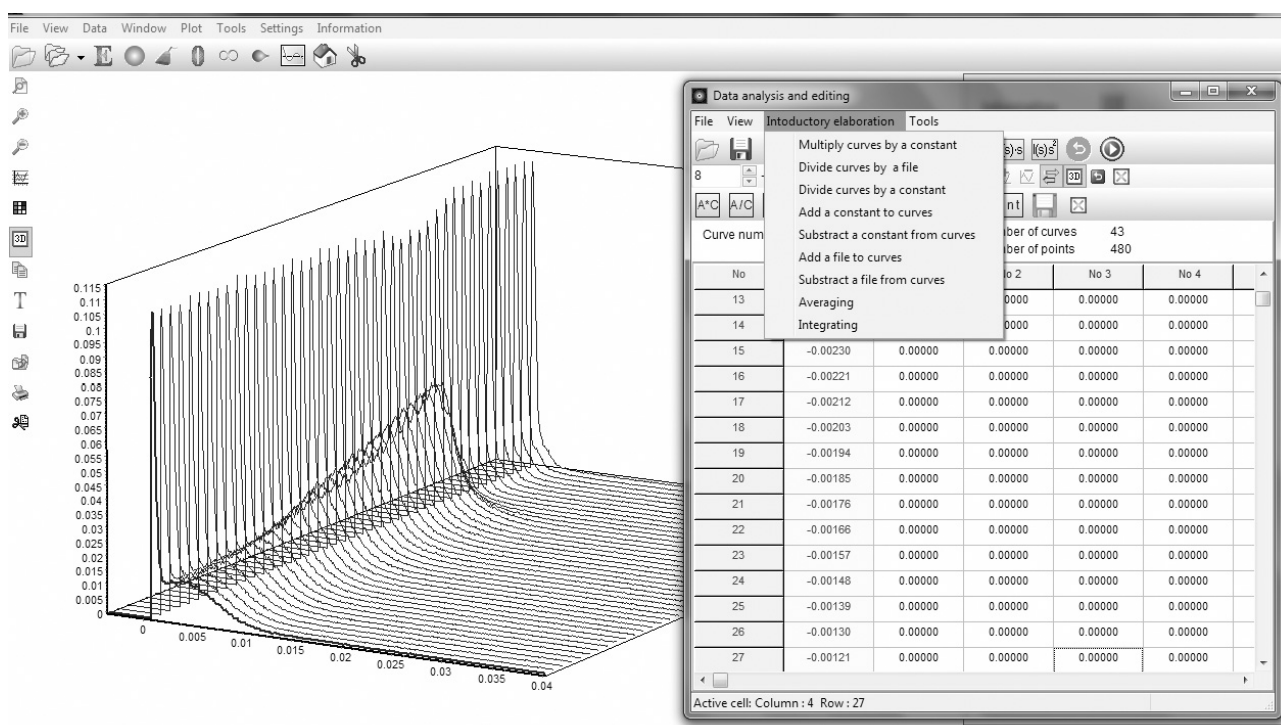

Fig. 5. Window of the SAXSDAT program showing a set of curves subjected to the introductory elaboration procedure (the curves were recorded during melting of polyethylene sample in a dynamic, time resolved experiment)
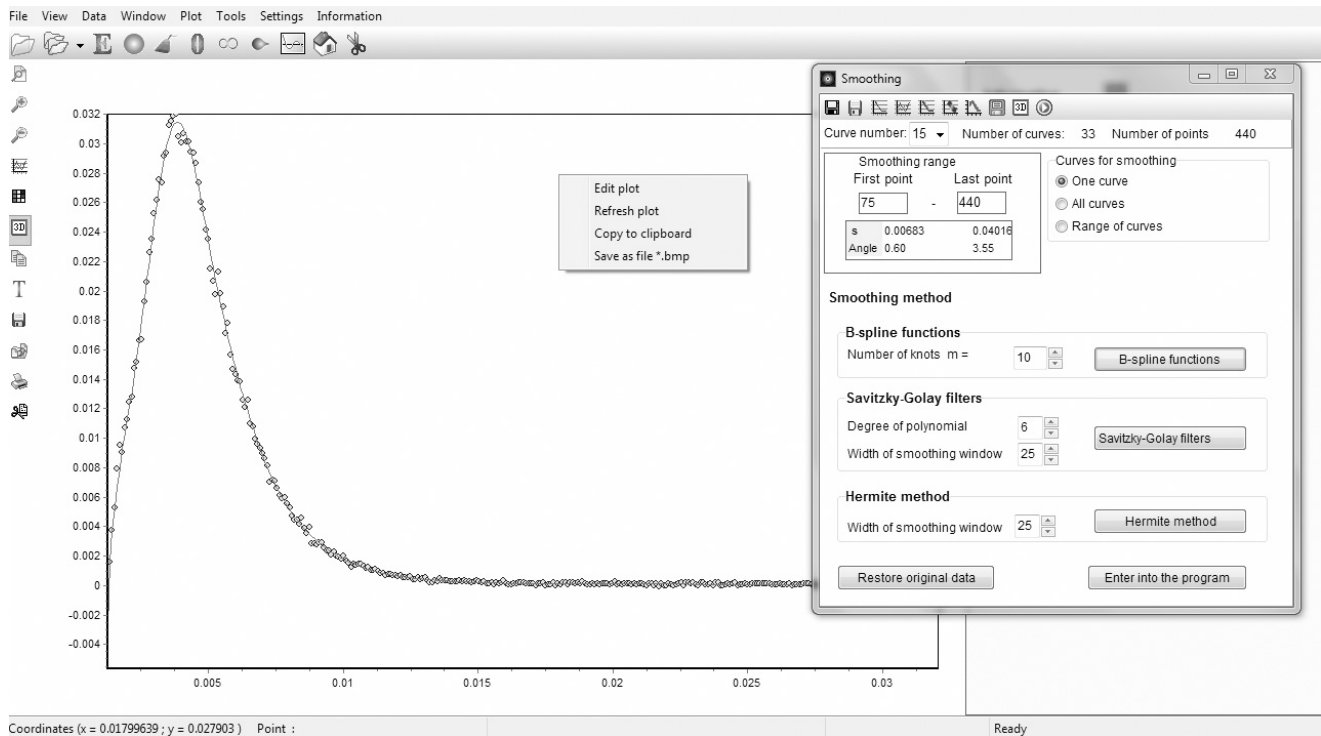
Fig. 6. Window of the SAXSDAT program showing a scattering curve subjected to the smoothing procedure

$$I_{\exp}(s) = I(s) + I_B(s) \qquad (9)$$

where: $I(s)$ — *intensity related to the polymer structure,* $I_B(s)$ — *a background intensity.*

The background can be described by two empirical approximations. According to Vonk and other authors [6, 27, 28]:

$$I_B(s) = B + Ds^n \qquad (10)$$

where: B, D — *constants, $n = 2$, 4 — an even integer.*

Ruland [16] proposed an exponential function to this aim:

$$I_B(s) = Be^{Gs^2} \qquad (11)$$

where: B, G — *constants.*

At large scattering angles, the intensity $I(s)$ is a product of two components. The first one represents Porod's law, according to which, intensity falls off as the reciprocal fourth power of the scattering vector s. The second component is related to a diffuse transition layer between the crystalline and amorphous phases [11, 29]:

$$\lim_{s \to \infty} I(s) = \frac{k}{s^4} \cdot e^{-(2\pi\sigma s)^2} \qquad (12)$$

where: k, σ — *constants.*

At small angles, the background intensity $I_B(s)$ is much smaller than the intensity $I(s)$, and can be omitted. But at large angles it influences considerably the shape of scattering curve, causing so called positive deviations from the Porod's law. For this reason, the background intensity must be thoroughly subtracted from the experimental curve.

In the SAXSDAT program, subtraction is performed in four steps. In the first step, the experimental curve is presented in an appropriate system of coordinates in which the "tail" of this curve at large angles has a linear shape. Then, the unknown background parameters are estimated using the linear regression method. As it results from equations (9)—(12), at very large angles, where the intensity $I(s)$ can be omitted being much smaller than $I_B(s)$, the following approximations hold:

$$I_{\exp}(s) \approx I_B(s) = B + Ds^n \qquad (13)$$

or

$$I_{\exp}(s) \approx I_B(s) = Be^{Gs^2} \qquad (14)$$

So the required plots are: $I_{\exp}(s)$ versus s^n, or $\ln I_{\exp}(s)$ versus s^2. Using the linear regression method, parameters B and D or B and G can be obtained from slopes and intercepts of obtained lines. In the second step, the background $I_B(s)$, estimated in that way, is subtracted from the experimental curve $I_{\exp}(s)$. At large angles, the resultant curve is given by:

$$[I_{\exp}(s) - I_B(s)] = \frac{k}{s^4} \cdot e^{-(2\pi\sigma s)^2} \qquad (15)$$

In the third step, unknown parameters k and σ are computed using the plot of: $\ln\{[I_{\exp}(s) - I_B(s)] \cdot s^4\}$ versus s^2. This plot is linear at large angles, so using linear regression method, parameters k and σ can be computed from the intercept and slope of the obtained line. In the last step, all parameters estimated by the two graphical methods presented above, are refined by best fitting of the theoretical function describing the curve at large angles, to the experimental one $I_{\exp}(s)$. A classical optimiza-
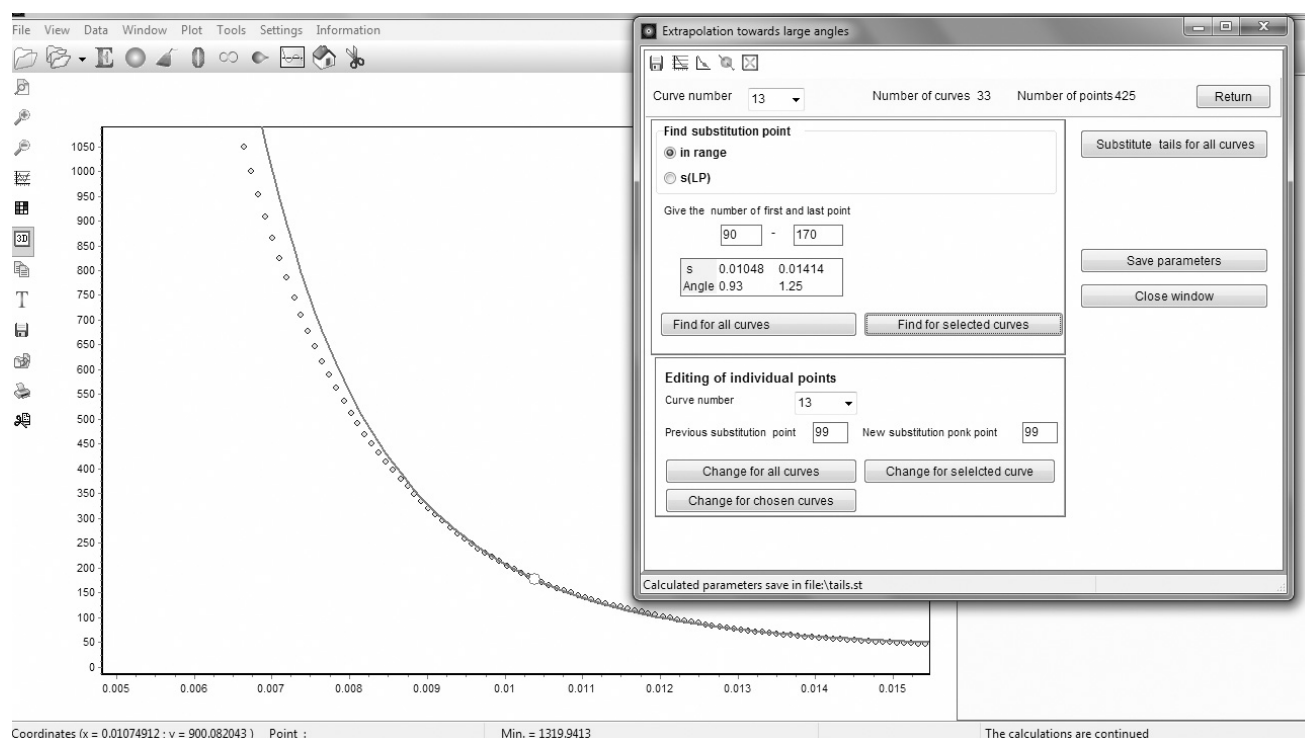
Fig. 7. Window of the SAXSDAT program showing the substitution of the tail of a scattering curve with the best fitted theoretical function (the point of a smooth substitution is found by the program)

tion procedure of Rosenbrock is used to this aim. The parameters found from the graphical methods serve as starting values in this procedure. Theoretical function may be given by:

$$F(s) = \frac{k}{s^4} \cdot e^{-(2\pi\sigma s)^2} + B + Cs^n \qquad (16)$$

or

$$F(s) = \frac{k}{s^4} \cdot e^{-(2\pi\sigma s)^2} + Be^{Gs^2} \qquad (17)$$

depending on the version of background approximation.

Apart from these two functions, SAXSDAT program offers three other ones which can be used to describe experimental curves at large angles:

$$F(s) = \frac{k}{s^4} \cdot e^{-(2\pi\sigma s)^2} + B \qquad (18)$$

$$\widetilde{F}(s) \approx \frac{k''}{s^3} \exp\left[-38\,(\sigma s)^{1.81}\right] + B' + D' \cdot s^n \qquad (19)$$

$$\widetilde{F}(s) \approx \frac{k''}{s^3} \exp\left[-38\,(\sigma s)^{1.81}\right] + B' \cdot s^{G's^2} \qquad (20)$$

Eq. (18) is suitable for curves with a constant level of background which is typical when curves are recorded in a relatively narrow angular range. Two remaining functions given by eqs. (19) and (20), are used for curves recorded with slit collimation systems. They may be used when the infinite-slit-length assumption is valid [29]. The unknown parameters of these functions are found in the program in the same way as it was described above *i.e.* by combining graphical methods and best fitting of the theoretical function to the experimental one.

Finally, when the shape of experimental curve at large angles is established, the tail of this curve is substituted with the theoretical function, what is presented in Figure 7. The point of a smooth substitution is found by the program. Next, the background is subtracted and the curve can be extrapolated towards a desired large angle at which intensity values is negligibly small.

After this stage, the user can pass to another module in which the scattering curve can be extrapolated towards the zero angle. In this case, four different functions are available: a combination of Gauss and Cauchy functions, Pearson function, Guinier function and a constant function. As it results from eq. (8), the shape of the scattering curve near the zero angle influences the correlation function only to a very limited degree. For this reason, the constant function is most frequently used.

Calculation of the correlation function

When all introductory steps are performed, the one-dimensional correlation function can be calculated. As it is shown in Figure 8, based on their shape the following parameters of stacks are found: average long period, average thickness of crystalline lamellae and amorphous layers, volume fractions of these two phases in stacks, real and ideal invariant, thickness of the transition layer between the phases. In the program, the parameters of stacks can be calculated in two ways. The first method
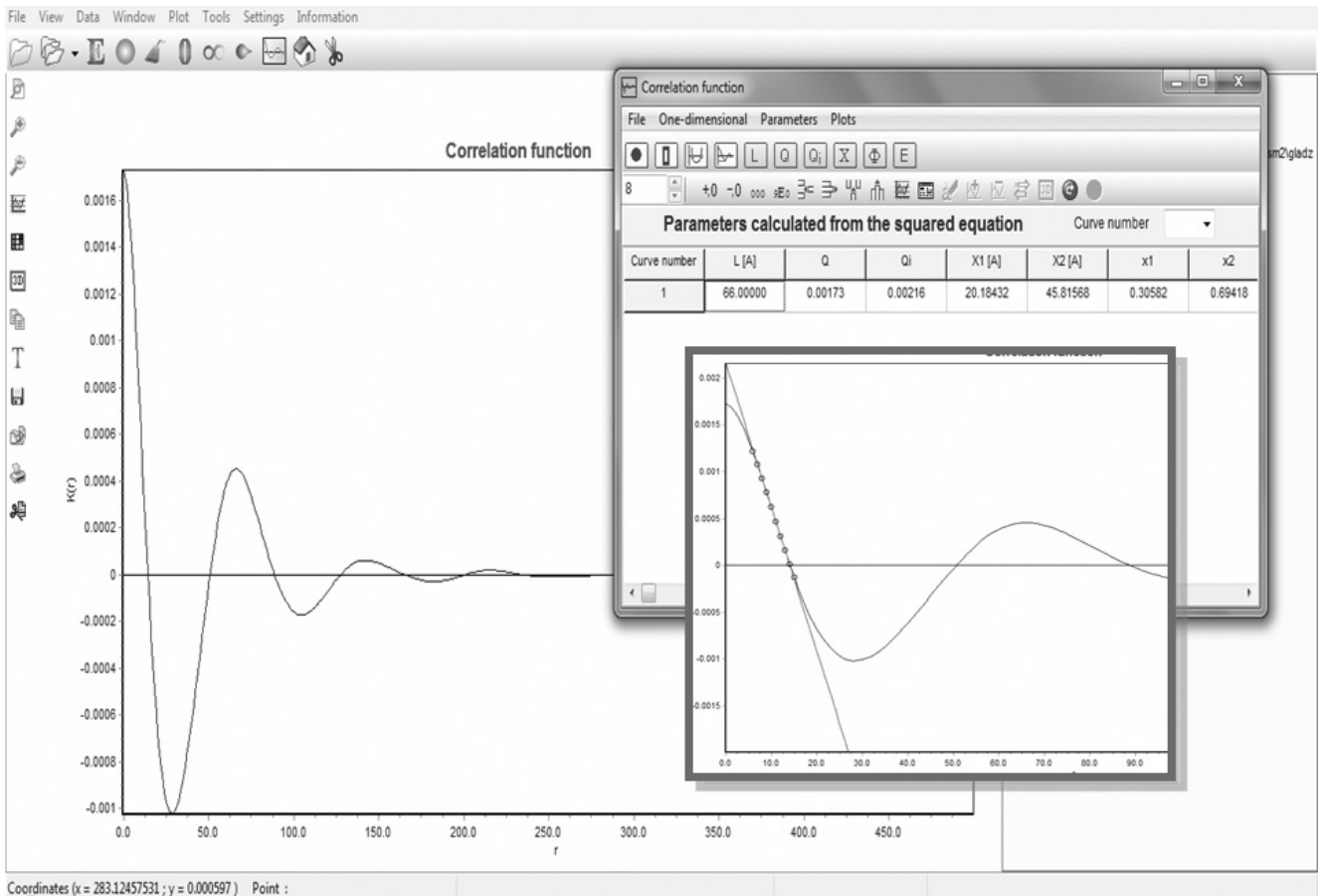
Fig. 8. Windows of the SAXSDAT program showing the calculated correlation function and the table with parameters determined from its shape

uses the coordinates of the points *M*, *Q* and ⟨*C*⟩ (see Fig. 3). The second one uses the points *R* and *LP*. When a big set of curves from a time resolved experiment is analyzed, the program prepares a tabular presentation of obtained results and the plots showing changes of investigated parameters as functions of a given operand.

In the case of scattering curves recorded with a slit collimation system, for which the infinite-slit-length assumption is valid, the program can calculate the correlation function directly from a "smeared" curve $\tilde{I}(s)$ using the Fourier-Bessel transform [9, 30]:

$$K_1(x) = 2\pi \int_0^\infty s\tilde{I}(s) \cdot \left[B_o(2\pi sx) - 2\pi sx \cdot B_1(2\pi sx) \right] d \qquad (21)$$

where: B_n — *a Bessel function of order n*.

But at first, the background at large angles has to be determined and subtracted [functions given by eqs. (19) and (20)] and the curves should be extrapolated, similarly as in the case of those recorded with point collimation system.

Desmearing

In the case of slit collimation systems, which scheme is presented in Figure 9, the intensity $\tilde{I}(x)$ measured at a given point *M* in the plane of registration is the sum of in-

tensities *I(z)* from different points of the sample, scattered at different angles relative to the primary beam [9]:

$$\tilde{I}(x) = \int_{-\infty}^\infty W(y)I(z)dy = \int_{-\infty}^\infty W(y)I\left(\sqrt{x^2 + y^2}\right)dy \qquad (22)$$

where: *W(y)* — *so called slit-length weighting function*.

Hence, the use of slit collimation system leads to a considerable distortions of the recorded intensity distributions — so called "smearing effect" is observed. If we want to reconstruct the intensity distributions which
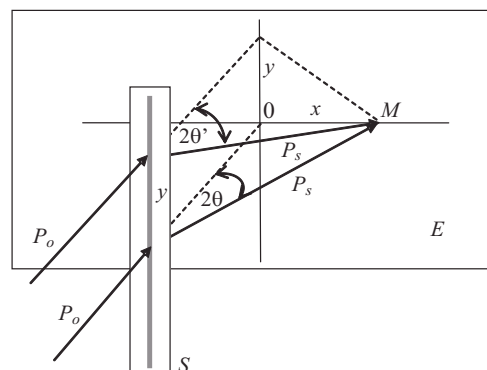

Fig. 9. Recording of the scattered radiation with a slit collimation system

would have been obtained with point collimation, we have to perform a "desmearing" procedure.

An alternative approach may be applied when the approximation of infinite-slit-length can be accepted. Such an approximation is valid, when the weighting function $W(y)$ is constant over the entire range of observable small angle scattering. In such cases, we can analyze smeared curves $\tilde{I}(s)$ using analytical expressions that have been modified to take the collimation smearing effect into account [3—16, 29].

If the approximation of infinite-slit-length is not valid, the desmearing procedure is necessary. When $W(y)$ and $\tilde{I}(s)$ functions are known, the intensity $I(x)$ can be recovered from eq. (22) with numerical methods. The weighting function $W(y)$ can be determined experimentally by measuring the primary beam intensity distribution along the slit direction. It is also possible to calculate $W(y)$ from the knowledge of the detailed geometry of the slit collimation system and the camera [31—33].

Several numerical procedures have been devised for performing the slit desmearing process. In the SAXSD program, the procedure elaborated by Singh *et al.* [33] has been implemented. This is a direct (*i.e.* not iterative) procedure in which the integral given by eq. (22) is digitized into a sum:

$$\tilde{I}(x_i) \cong \Delta_o W_o I(x_i) + \sum_{j=1}^{n} \Delta_j \cdot \left[W(y_j) + W(-y_j) \right] \cdot I\left(x_{\sqrt{i^2 + j^2}} \right) \quad (23)$$

where: Δ_j — *the step of measurement*.

In this formula, the intensities $I(x_k)$ with the indices k which are not integral numbers, are expressed by linear interpolation between the intensities related to the nearest integer ones.

So, eq. (23) can be transformed into:

$$\tilde{I}(x_i) \cong \sum_{j=i}^{n} A_{ij} I(x_j) \quad (24)$$

where: A_{ij} — *the elements completely determined by the weighting function* $W(y)$.

In the procedure of Singh, the unknown intensities $I(x_j)$ are found not by inversion of the matrix **A**, as it occurs in many other procedures, but by the method of simple back substitution. This is an important advantage, because the process of inversion is numerically unstable in dealing with real data. To use the module of desmearing, the weighting function has to be entered into the SAXSDAT program as a set. Before desmearing, the background at large angles has to be subtracted using graphical methods. Besides, a smeared curve should be thoroughly smoothed. Random errors and noises should be eliminated to the most possible extent since they give rise to artificial details in the desmeared curve. After desmearing, we can calculate the correlation function using the module of the program described above.

Modelling

Apart from the method based on the correlation function analysis, the program offers another one in which the parameters of stacks can be determined by model calculations. The calculations consists in fitting of a theoretical function, which describes the intensity scattered by a stack, to the experimental SAXS curve. The calculations
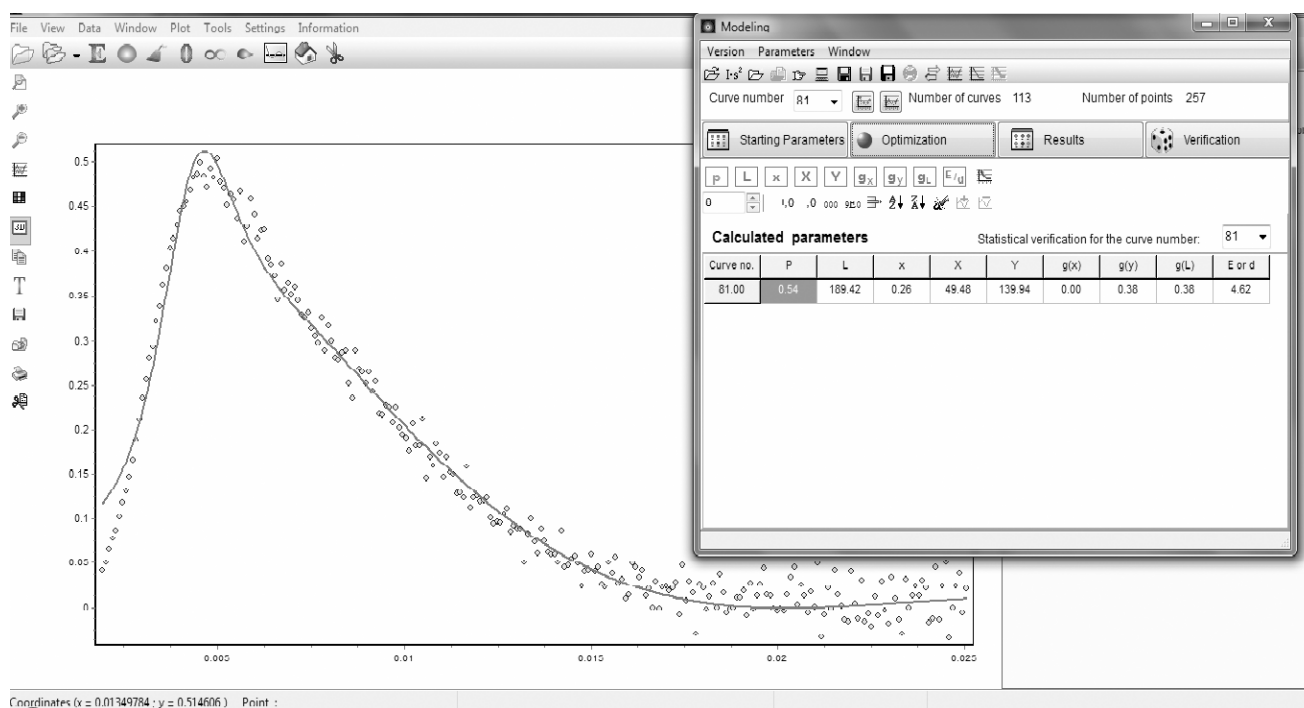

Fig. 10. *Windows of the SAXSDAT program showing the experimental one-dimensional scattering function $I_1(s) = I(s) \cdot s^2$ and the best fitted theoretical function calculated for the assumed model of stacks (calculated parameters of the stacks are shown in the table)*

are performed using relationships derived by Hosemann [2] and modified by Blundell [18, 19]. It is assumed that the distribution functions of the thicknesses of crystalline and amorphous layers in stacks are Gauss functions. Besides, in accordance with Blundell [18, 19], it is assumed, that the reduced standard deviations of these two functions are the same.

In the calculations, five independent parameters of the theoretical function are optimized, according to the best least squared fit: P — scaling parameter (dependent on the primary beam intensity), X — average thickness of one of the layers (crystalline or amorphous), g — reduced standard deviation of the thickness, x — volume fraction of this phase, and E or σ — parameters representing the thickness of the transition layer.

When the volume fraction of one of the phases is low ($x \leq 0.2$), we can use a simplified form of the theoretical function, in which standard deviation of this phase is assumed to be negligibly small. Appropriate window of the SAXSDAT program is shown in Figure 10. The curves can be fitted using four different optimization procedures: two classical procedures of Rosenbrock and Powell, generic algorithm and a hybrid system which combines the genetic algorithm with the procedure of Rosenbrock. Before fitting, the background at large angles has to be subtracted using graphical methods described above. Besides, using Lorentz correction, the experimental curves has to be transformed into so called one-dimensional scattering functions $I_1(s) = I(s) \cdot s^2$.

It should be noted that real structures not always can be described correctly by a relatively simple model of stacks used in the program.

In the last module of the program, the quality of fitting can be checked using several statistic tests.

CONCLUDING REMARKS

The SAXSDAT program makes possible a comprehensive analysis of SAXS curves of semicrystalline polymer. The possibility of simultaneous elaboration of big sets of curves obtained in dynamic, time resolved experiments is one of its important advantages. Moreover, it can be employed both for curves recorded with a point collimation system as well as for "smeared" curves recorded with a slit collimation systems. The latter case occurs in most laboratories equipped with classical Kratky cameras. SAXSDAT gives to the user several computational tools useful in the introductory data elaboration — background subtraction, smoothing and correction for different distortions. It is equipped with an easy to use interface and offers several graphical possibilities, enabling the user to prepare various kinds of plots and graphical presentation of the results.

The program (Polish version) is available from the website: www.ath.bielsko.pl/~stanislaw.rabiej/saxsdat/)

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