Chord intercepts in a two-dimensional cell growth model

Part 2 *Chord intercepts of the grains*

G. E. W. SCHULZE, L. O. SCHWAN*, R. WILLERS‡
*Abteilung Werkstoffwissenschaft, *Lehrstuhl Festkörperspektroskopie, und ‡Rechenzentrum, des Instituts für Physik der Kondensierten Materie der Universität Düsseldorf, West Germany*

The microstructure of a two-dimensional cell growth model at each fraction transformed along Rosiwal's line is characterized. Rosiwal's line cut grains and yields chord intercepts. By the use of probability theory we derive the mean number of chord intercepts per unit length as well as the dependence of the distribution density of the length of these chord intercepts on the fraction transformed. Furthermore, other quantities are derived which appear along and around Rosiwal's line.

1. Introduction

Fig. 1 shows a cut through the investigated microstructure, in which half of the area is occupied by β-grains (spherulites). It has been formed by the following process: nuclei (points) are Poisson-distributed within the plane of a supercooled amorphous α-material. Out of these nuclei, β-grains start to grow instantaneously, circularly and at a constant rate. Where two grains touch, growth stops and a straight grain boundary is formed. In the present paper, we define the unit length by stating that the "mean point density of the nuclei within the plane" amounts to one. Furthermore, we define the unit time by stating that the radial growth rate also amounts to one.

Therefore, after time t, the radius, R, of the free growing grains is given by $t = R$, and the fraction transformed, F, is given by Avrami's relation [1]

$$F = 1 - \exp(-\pi t^2) \qquad (1)$$

Later the corresponding values from Table I will be required.

In order to characterize this microstructure, we place arbitrarily a straight line (Rosival's traverse) into the plane. This line yields chord intercepts of different lengths, of the grains and of the amorphous regions, as shown in Fig. 1.

The distribution of the length a of the α-chord intercepts at a time t has been derived by the use of probability theory in Part 1 of the present series [1]. In the present paper we solve this problem for the length b of the β-chord intercepts. But first we derive simpler quantities with respect to Rosiwal's line from the assumptions above.

2. Probabilities $q_i(Y; R)$

2.1. Definitions and assumptions

We extend the classification of the chord intercepts to their associated nuclei, as given in Fig. 1. This means that a nucleus of type i yields a chord intercept of type i, and vice versa. A nucleus which yields no associated chord intercept on Rosiwal's line is called "ineffective". Of course all nuclei with a distance $Y > R$ are ineffective, but ineffective nuclei may also exist for $0 < Y \leqslant R$, as shown in Fig. 1.

In the following we suppose that a nucleus, N, with a distance Y exists. The probability that N is of type i ($i = 1, 2, 3$) or is ineffective at a given R is named by $q_i(Y; R)$ or $q_{\text{ineff}}(Y; R)$, respectively. Therefore, it is true that

$$1 = \sum_{i=1}^{3} q_i(Y; R) + q_{\text{ineff}}(Y; R) \qquad (2)$$

Furthermore, we identify Rosiwal's line with the x-axis, and the y-axis may run through the nucleus N.

2.2. Calculation of $q_1(Y; R)$

The nucleus N(0, Y) is of type 1 at R, if the length b of its chord intercept in Fig. 2 amounts to

$$b = 2(R^2 - Y^2)^{1/2} \quad \text{for } 0 \leqslant Y \leqslant R \qquad (3)$$

This is realized if the eight-shaped area, S, with included boundary in Fig. 3 contains no nucleus except N(0, Y). The probability $q_1(Y; R)$ to obtain no nucleus within the area S – if the nuclei are Poisson-distributed with a mean density of one – follows from Poisson's formula [2]

$$q_1(Y; R) = \exp(-S) \qquad (4)$$

According to Fig. 3 we have

$$S = S_L + S_R \qquad (5)$$

TABLE I

F	0.25	0.5	0.75	1.0
R	0.3026	0.4697	0.6643	∞

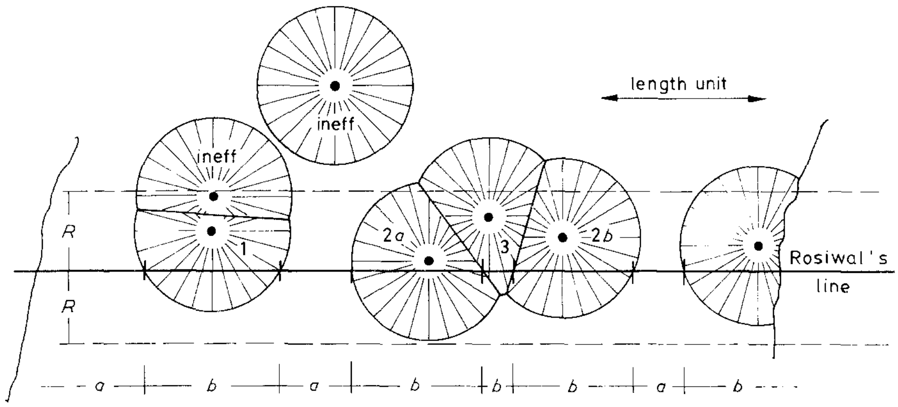

Figure 1 Part of the two-dimensional cell model during transformation at $F = 1/2$. Along the R line chord intercepts exist of grains with different lengths b and of amorphous regions with different lengths a. The chord intercepts of grains are classified into four types: type 1, limited on both sides by amorphous regions; type 2a, limited on the left-hand side by an amorphous region, on the right by a grain; type 2b, limited on the left-hand side by a grain, on the right by an amorphous region; type 3, limited on both sides by grains.

and

$$S_L = S_R = \pi R^2 - R^2\{\arcsin(Y/R) - Y/R[1 - (Y/R)^2]^{1/2}\} \quad \text{for } 0 \leqslant Y \leqslant R \tag{6}$$

Fig. 4 shows $q_1(Y; R)$ for four different values of R.

2.3. Calculation of $q_{2a}(Y; R)$

The nucleus N is of type 2a, if the coordinate x_r of the right boundary of its chord intercept lies between x_L and x_R. This is realized if the circle, S_{circle}, around x_L with radius R in Fig. 5 contains no nucleus, but the rest, S_{rest}, of the eight-shaped area contains one or more nuclei. The latter case can also be expressed by "S_{rest} contains not no nuclei" and its probability amounts to $1 - \exp(-S_{rest})$. Therefore, we have

$$\begin{aligned} q_{2a}(Y; R) &= \exp(-S_{circle})[1 - \exp(-S_{rest})] \\ &= \exp(-S_{circle}) - \exp[-(S_{circle} + S_{rest})] \\ &= \exp(-\pi R^2) - q_1(Y; R). \end{aligned} \tag{7}$$

Analogously we obtain $q_{2b}(Y; R)$. Furthermore, we have

$$\begin{aligned} q_2(Y, R) &= q_{2a}(Y; R) + q_{2b}(Y; R) \\ &= 2q_{2a}(Y; R) \end{aligned} \tag{8}$$

Later we need

$$\begin{aligned} q_{1+2a}(R) &= q_1(Y; R) + q_{2a}(Y; R) \\ &= \exp(-\pi R^2) \\ &= 1 - F \end{aligned} \tag{9}$$

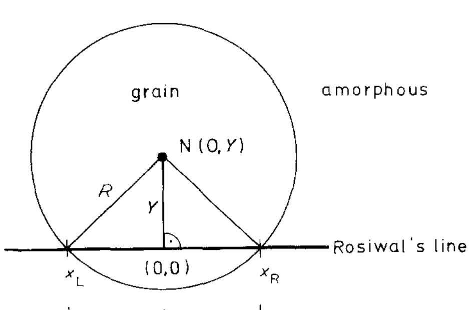

Figure 2 Nucleus N(0, Y) is of type 1, because its chord intercept with length b borders an amorphous phase at x_L and x_R.

Fig. 4 shows $q_2(Y; R)$ and $q_{1+2a}(R)$ for different values of F.

2.4. Calculation of $q_3(Y; R)$

The nucleus, N, is of type 3 for $x_L \leqslant x_l \leqslant x_r \leqslant x_R$, where x_l and x_r represent the coordinates of the left and right boundary of the associated chord intercept with a length $b = x_r - x_l$. A right boundary at $x_r \leqslant x_R$ exists, if a nucleus is arranged within S_r according to Fig. 6. A left boundary at x_l ($x_L < x_l < x_r$) exists, if

(i) the circle around x_r and its included area, S_M, contain no nucleus;

(ii) the area S_l has to contain at least one nucleus. S_M and S_l depend on x_r, and x_r depends on the position of the neighbouring nucleus N_r of the right side. If the right boundary lies between x_r and $x_r + dx_r$, the right nucleus, N_r, has to be arranged within a crescent-shaped differential area element dS, as shown in Fig. 6.

The probability that dS contains at least one nucleus is given by

$$1 - \exp(-dS) \tag{10}$$

This equals dS for small values.

In order to include all possibilities, which lead to nuclei of type 3, we have to integrate over S_r of Fig. 6

$$q_3(Y; R) = \int_{S_{rest}} \exp(-S_M)[1 - \exp(-S_l)]\, dS \tag{11}$$

$q_3(Y; R)$ is obtained by numerical integration and given in Fig. 4 for different values of F. Fig. 4 shows also

$$q_{eff}(Y; R) = \sum_{i=1}^{3} q_i(Y; R). \tag{12}$$

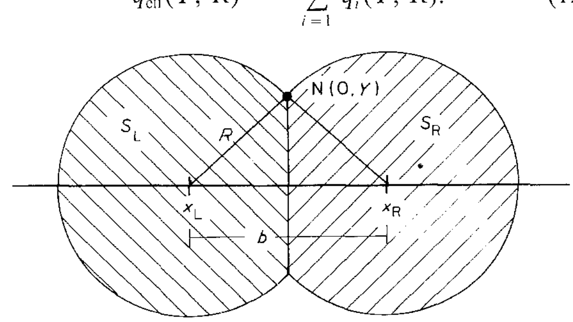

Figure 3 The state as in Fig. 2. Construction of the area which contains N as the only nucleus.

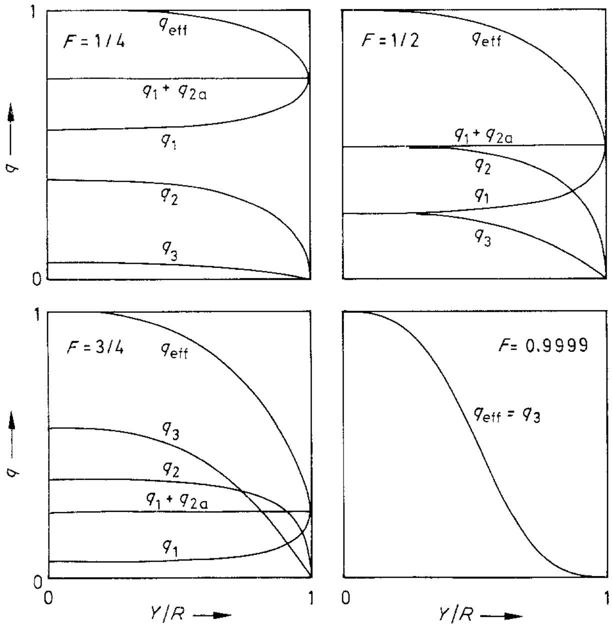

Figure 4 Mean point densities $q_i(Y;\ R)$ of the nuclei of type i at a distance Y from Rosiwal's line and at a state R. Note, that $q_{\text{ineff}} = 1 - q_{\text{eff}}$.

Its complement to one yields $q_{\text{ineff}}(Y;\ R)$. $q_{\text{eff}}(Y;\ R)$ for $R \to \infty$ has been given in [3].

3. Consequences of the $q_i(Y;\ R)$

3.1. Mean numbers $N_i(R)$

In another interpretation, $q_i(Y;\ R)$ represents the mean point density of nuclei of type i at distance Y and at state R, because the total mean point density of nuclei is supposed to be one in the whole area. The mean number $N_i(R)$ of chord intercepts of type i per length unit on Rosiwal's line at R is computed by

$$N_i(R) = 2\int_{Y=0}^{R}\int_{x=x_0}^{x_0+1} q_i(Y;\ R)\,\mathrm{d}x\,\mathrm{d}Y \qquad (13)$$

The region of integration is a band with a unit length and a width of $2R$. Fig. 7 shows $N_i(F)$ and $N_{\text{eff}}(F)$ with

$$N_{\text{eff}} = \sum_{i=1}^{3} N_i(F) \qquad \text{for } 0 \leqslant F \leqslant 1 \qquad (14)$$

Fig. 14 shows the "number fractions"

$$W_i(F) = N_i(F)/N_{\text{eff}}(F) \qquad (15)$$

The mean number of $N_{\text{mov}}(R)$ of all moving boundaries per unit length along the R line at R amounts to

$$N_{\text{mov}}(R) = 2N_1(R) + N_{2\text{a}}(R) + N_{2\text{b}}(R) \quad (16)$$

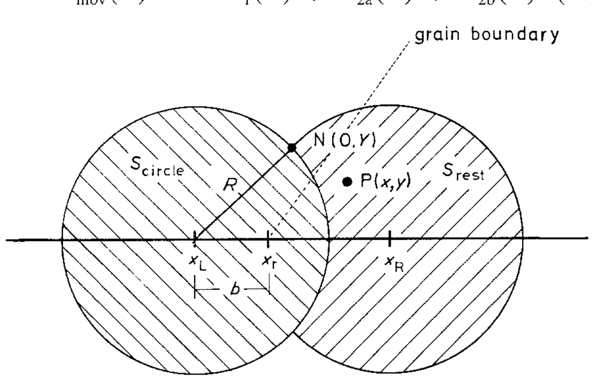

Figure 5 Construction of the areas used for calculation of type 2a. The grain boundary between N and P is dotted.

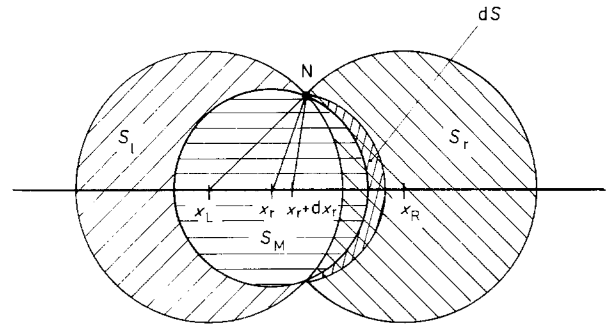

Figure 6 Construction of the areas used for calculation of type 3. All four circles hit nucleus N. The neighbouring nucleus of the right side is arranged in the differential area element, dS, within S_r.

because each chord intercept of type 1 has two moving boundaries. A short calculation yields

$$N_{\text{mov}}(R) = 4R\exp(-\pi R^2) \qquad (17)$$

The mean number, $N_{\text{fix}}(R)$, of fixed boundaries per unit length along Rosiwal's line at R amounts to

$$N_{\text{fix}}(R) = N_{2\text{a}}(R) + N_3(R) \qquad (18)$$

Finally, we obtain

$$N_{\text{total}}(R) = N_{\text{mov}}(R) + N_{\text{fix}}(R) \qquad (19)$$

$N_{\text{mov}}(F)$, $N_{\text{fix}}(F)$, and $N_{\text{total}}(F)$ are shown in Fig. 8.

3.2. Rate, v, along Rosiwal's line

The rate, v, of the moving boundary of a growing chord intercept along Rosiwal's line is investigated in the left direction only. From Fig. 9 we obtain

$$x^2 = R^2 - Y^2 \qquad (20)$$

For a fixed Y the differentiation with respect to time t gives

$$\dot{x} = v = \frac{R/\dot{R}}{(R^2 - Y^2)^{1/2}} = \frac{1}{[1-(Y/R)^2]^{1/2}} \qquad (21)$$

with the supposed $\dot{R} = 1$. Therefore, the range of v-distribution is $1 \leqslant v < \infty$.

If we resolve this equation for Y and differentiate

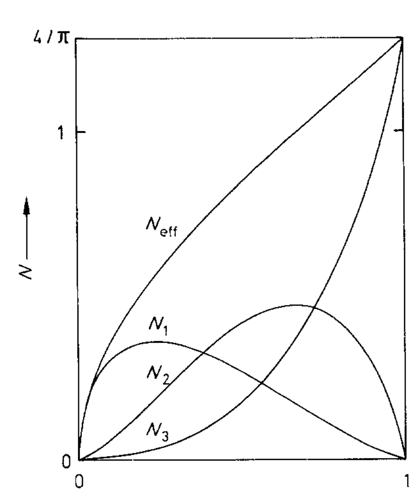

Figure 7 Mean number of chord intercepts at F per unit length on Rosiwal's line.

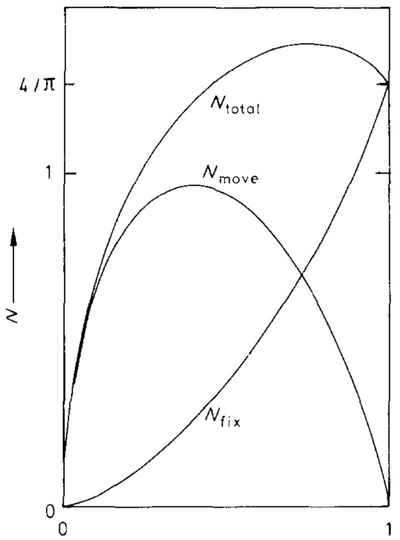

Figure 8 Mean number of boundaries at F per unit length on Rosiwal's line.

with respect to v by a fixed R, we obtain

$$dY = \frac{R\,dv}{v^2(v^2 - 1)^{1/2}} \tag{22}$$

The mean density of such nuclei, whose chord intercepts grow at R to chord intercepts of grains from the assumed distribution of the left side, is given by $q_{1+2a}(R)$ in Equation 9. Because this density is constant within the band with a width of $2R$ around Rosiwal's line we obtain

$$q_{1+2a}(R)\,dY = q_{1+2a}(R)R\frac{dv}{v^2(v^2 - 1)^{1/2}} \tag{23}$$

Integration of the left-hand side of this equation from $Y = 0$ to R gives $q_{1+2a}(R)R$. Therefore, the normalized distribution density of the rates in one direction along Rosiwal's line is given by

$$w(v) = \frac{1}{v^2(v^2 - 1)^{1/2}} \quad \text{for } 1 \leqslant v \leqslant \infty, \tag{24}$$

This is true at each R during the whole process of growth. The mean rate of all growing boundaries in one direction amounts to $v = \pi/2$. Fig. 10 shows $w(v)$.

4. Unnormalized distribution densities $n_i(b; R)$

4.1. Definition

$n_i(b; R)\,db$ represents the mean number of chord intercepts of type i per unit length upon the R line with lengths between b and $b + db$ at R. Of course we obtain

$$N_i(R) = \int_{b=0}^{2R} n_i(b; R)\,db \tag{25}$$

In the following we derive $n_i(b; R)$.

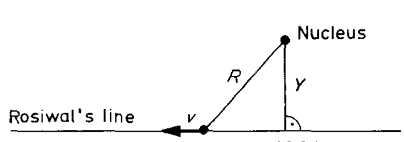

Figure 9 Figure computing of the rate $v(Y, R)$ of the moving boundary along Rosiwal's line.

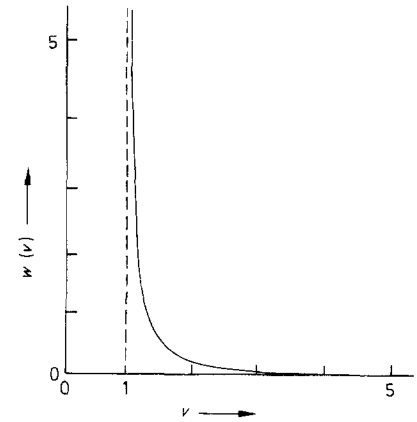

Figure 10 Distribution density $w(v)$ of the rate v of the moving boundary along Rosiwal's line at each R.

4.2. Calculation of $n_1(b; R)$

A simple relation exists between Y and b for chord intercepts of type 1, given in Equation 3. From this we obtain

$$\begin{aligned} q_1(Y; R)\,dY &= q_1(b; R)\left\{\frac{-b}{4[R^2 - (b/2)^2]^{1/2}}\right\}db \\ &= \tfrac{1}{2}n_1(b; R)\,db \end{aligned} \tag{26}$$

and therefore

$$n_1(b; R) = \exp[-(S_L(b; R) + S_R(b; R)] \times \frac{b}{2[R^2 - (b/2)^2]^{1/2}} \quad \text{for } 0 \leqslant b \leqslant 2R \tag{27}$$

4.3. Calculation of $n_{2a}(b; R)$

Analogously to $q_{2a}(Y, R)$ we now calculate the probability $q_{2a}(b; Y; R)\,db$ where, in addition, the chord intercept takes on a length between b and $b + db$. We use Fig. 11 and obtain

$$q_{2a}(b; Y; R)\,db = \exp(-S_L)\exp(-S_R)\,dS_R \tag{28}$$

For a given R and b the distance Y runs between zero and $[R^2 - (b/2)^2]^{1/2}$. For all possible Y values we obtain

$$\begin{aligned} n_{2a}(b; R) &= 2\int_{Y=0}^{[R^2-(b/2)^2]^{1/2}} q_{2a}(b; Y; R)\,dY \\ &= 2\int_{Y=0}^{[R^2-(b/2)^2]^{1/2}} \exp(-(S_L + S_R))\frac{\partial S_R}{\partial b}\,dY \end{aligned} \tag{29}$$

4.4. Calculation of $n_3(b; R)$

$q_3(b; x_1; y; R)\,db\,dx_1$ represents the probability, that the nucleus N at R is of type 3 and that, in addition,

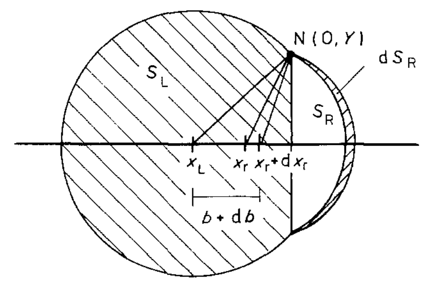

Figure 11 Construction of the areas used for calculation of $q_{2a}(b; R)$.

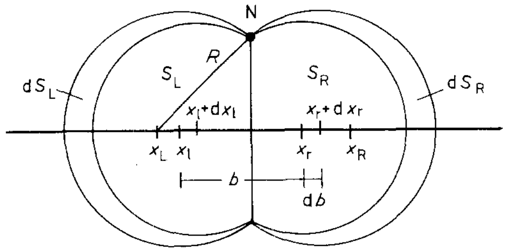

Figure 12 Construction of the areas used for calculation of $q_3(b; R)$. dS_L and dS_R are differential area elements.

the left boundary is arranged between x_l and $x_l + dx_l$ and that the length of the chord intercept lies between b and $b + db$. By use of Fig. 12 we obtain

$$q_3(b; x_l; Y; R)\, db\, dx_l = dS_l \exp(-(S_L + S_R))\, dS_R \quad (30)$$

or

$$q_3(b; x_l; Y; R) = \exp[-(S_L + S_R)] \frac{\partial S_l}{\partial x_l}\frac{\partial S_R}{\partial b} \quad (31)$$

Fig. 12 shows

$$-(R^2 - Y^2)^{1/2} \leqslant x_l \leqslant (R^2 - Y^2)^{1/2} - b \quad (32)$$

and

$$x_r = x_l + b \quad (33)$$

First we integrate with respect to x_l

$$q_3(b; Y; R) = \int_{x_l=-(R^2-Y^2)^{1/2}}^{(R^2-Y^2-b)^{1/2}} \exp[-(S_L + S_R)] \times \left\{\frac{\partial S_l}{\partial x_l}\frac{\partial S_r}{\partial b}\right\} dx_l \quad (34)$$

and then with respect to Y

$$n_3(b; R) = 2\int_{Y=0}^{[R^2-(b/2)^2]^{1/2}} q_3(b; Y; R)\, dY \quad (35)$$

5. Consequences of the $n_i(b; R)$

5.1. Distribution of the length b

The (normalized) distribution density $B_i'(b; R)$ of the length b of all chord intercepts of type i at R along Rosiwal's line is given by

$$B_i'(b; R) = \frac{n_i(b; R)}{N_i(R)}. \quad (36)$$

For the chord intercepts of all three types we obtain the distribution density at R

$$B'(b; R) = \frac{1}{N_{\text{eff}}(R)} \sum_{i=1}^{3} n_i(b; R) \quad (37)$$

$B'(b; R)$ and its summands $n_i(b; R)/N_{\text{eff}}(R)$ are shown in Fig. 13 for some values of R. Another deviation of $B'(b; R)$ for $R = \infty$ has been given by [3]. The cumulative distribution function $B(b; R)$ of chord intercepts of all types follows by

$$B(b; R) = \int_{b'=0}^{b} B'(b'; R)\, db' \qquad \text{for } 0 \leqslant b \leqslant 2R \quad (38)$$

5.2. Mean lengths $\bar{b}(R)$ of chord intercepts

The mean length $\bar{b}_i(R)$ of all chord intercepts of type i at R is defined by

$$\bar{b}_i(R) = \int_{b=0}^{2R} bB_i'(b; R)\, db \quad (39)$$

Furthermore, we have

$$\bar{b}(R) = \int_{b=0}^{2R} bB'(b; R)\, db \quad (40)$$

5.3. Mean length fractions $F_i(R)$

The fraction transformed, $F(R)$, also represents the mean transformed length per unit length upon Rosiwal's line at R. This transformed mean length is composed by the lengths $F_i(R)$ of the three types according to

$$F(R) = \sum_{i=1}^{3} F_i(R) \quad (41)$$

with

$$F_i(R) = N_i(R)\bar{b}_i \quad (42)$$

The length fraction $D_i(F)$ with respect to the transformed length is given by

$$D_i(F) = \frac{F_i(F)}{F} \quad (43)$$

and is shown in Fig. 14.

6. Conclusion

Geometric aspects of the microstructure of the

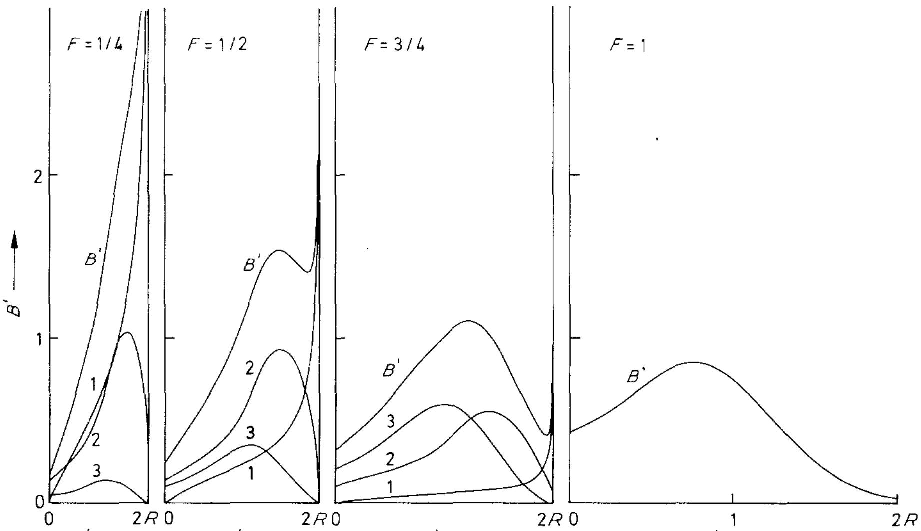

Figure 13 Distribution density $B'(b; F)$ of the length b of the chord intercepts and the fractions of the three types.

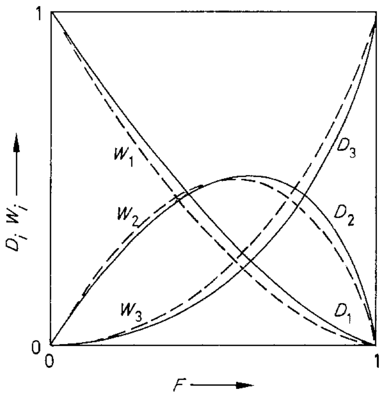

Figure 14 $D_i(F)$ is the fraction of length of type i related to the transformed length at F. $W_i(F)$ (dotted) is the number of chord intercepts of type i related to the number of all chord intercepts at F.

growing two-dimensional cell model can be characterized by use of probability theory. In doing so we obtain results about the area around Rosiwal's line (as shown by $q_i(Y; R)$) as well as on Rosiwal's line (as shown by N_i, W_i, D_i, B_i', B', N_{eff}). All these results prove quantitatively the following trends.

1. Chord intercepts of type 1 dominate for small F, but their influence decreases with growing F.

2. Chord intercepts of type 2 dominate for F about 0.5, running from zero through a maximum to zero.

3. Chord intercepts of type 3 dominate for large F, increasing with F. At $F = 1$ type 3 exists only. This special case has been treated in [3].

Two invariants of the growing system are found:

1. The distribution density $w(v)$ of the rate $v(>0)$ is independent of F and the mean value is $v = \pi/2$.

2. The mean nucleus density $q_{1+2a}(F)$ is independent of Y and amounts to $1 - F$.

A numerical simulation with 10^9 nuclei around Rosiwal's line has been done, proving the results above. A correspondence between the results derived and the experimental results obtained on foil of isotactic polypropylene will be given in Part 4 of this series.

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