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Crystal Powder Statistics. IV. Calculation of the Line Profile Using the Sampling-Line Method

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Abstract

The sampling-line method is a convenient procedure for evaluating the line profile of a polycrystalline sample. To deal with size-broadening effects only, the method is applied to Bernoullian and Gaussian samples; the line profile is given by a Lorentzian function in the first case and by a similar function in the second case. For *any real* polycrystalline sample the intensity decreases as s^{-2} for large $|s| = |S - S_{hkl}|$. For a given average thickness the apparent crystallite size is up to 2 times larger than for samples consisting of crystals with the same size and shape.

Introduction

The influence of crystal size distributions on diffraction profiles is an important subject at present, in that an accurate knowledge of the line shape is required for the structural refinement *via* powder analysis, such as the Rietveld method (*e.g.* Albinati & Willis, 1982).

Following previous studies on the subject (Allegra, Bassi & Meille, 1978; Allegra & Ronca, 1978, 1979), in the present paper we will propose a general mathematical treatment for simple statistical distributions. A few examples of line profiles thus obtained will be compared with well-known results from single crystals (see, in particular, Wilson, 1949), with the purpose of providing simple guidelines for the characterization of the sample statistics.

We shall confine our attention to those crystal size distributions that may be factorized into terms each depending on a single crystallite thickness. In other words, if the crystals are bound by n sets of planes and $d_i (i = 1, \ldots, n)$ is the distance between two consecutive parallel planes of the ith set for the general crystal, we have

$$p(d_1 d_2 \ldots d_n) = p(d_1)\, p(d_2) \ldots p(d_n), \qquad (1)$$

where the p's are normalized probability density functions. The theory will be applied to the Bernoullian and Gaussian distributions, already considered in previous papers. For the former case (Allegra, Bassi & Meille, 1978), the present treatment may be viewed as an extension of the results to the general model with any number of boundary planes. For the Gaussian distribution, an error contained in the former approach (Allegra & Ronca, 1978) was pointed out later (Allegra & Ronca, 1979), but its consequences on the results were not amended, so that they are only correct for particular classes of reflections; the procedure given in this paper leads to the general result.

The method of the sampling line

Stokes & Wilson (1944) showed that the size-dependent line profile is uniquely related with the probability distribution of the lengths of the intra-crystalline chords parallel to $\mathbf{S}_0 = \mathbf{S}(hkl)$ ($S = |\mathbf{S}| = 2 \sin\theta/\lambda$; a chord is defined as any segment having both ends on the crystal surface). Indicating by T the general chord length and by $p(T)$ its area probability density, we derive the general expression of the line profile for any polycrystalline specimen from that proposed for identical crystals (*cf.* Wilson, 1949, ch.IV, equation 5) as

$$\mathcal{I}(s) = \mathcal{N}/V \int_0^\infty p(T) \frac{\sin^2(\pi T s)}{(\pi s)^2}\, \mathrm{d}T/\langle T \rangle, \qquad (2)$$

where s is the difference $S - S_0$ between the general value of S and that corresponding to the hkl point in

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reciprocal space, V is the volume of the unit cell, $\mathcal{N}$ is the total number of diffracting unit cells and $\langle T \rangle$ is the average value of T. The above expression is normalized as follows

$$\int_{-\infty}^{+\infty} \mathcal{F}(s)\, ds = \mathcal{N}/V. \tag{3}$$

The quantity $p(T)\, dT$ may be defined as the probability of finding a chord length between T and $T + dT$ when picking a crystal at random and randomly sellecting a point on its area projected along $\mathbf{S}_0$.

The approach followed in the present paper exploits the statistical independence between the different crystal thicknesses d_i, implicit in (1). In particular, under such circumstances the polycrystalline sample may be generated by cleaving an infinite three-dimensional crystal through three or more sets of parallel planes, with a suitable statistical distribution of interplanar spacings. As an example, in the Bernoullian case the spatial distribution of the parallel planes within a given set is completely random, so that the probability density of their general interplanar distance d is given by

$$p(d) = L^{-1} \exp(-d/L) \tag{4}$$

where L is the average value of d. In the Gaussian case the corresponding probability is given by

$$p(d) = 2(\pi L)^{-1} \exp(-d^2/\pi L^2). \tag{5}$$

A Gaussian distribution as above might arise if all the crystals nucleated at the same time and their growth occurred *via* reversible steps (Allegra & Ronca, 1978). Another possible example could be represented by a Gaussian distribution with a non-zero average, *i.e.*

$$p(d) \propto \exp[-(d - L)^2/2\sigma^2], \tag{6}$$

which may occur if the crystals display minor differences in size among themselves (σ^2 and L respectively are the variance and the average of the distribution, $\sigma \ll L$). In the present context we will confine our attention to the distributions given by (4) and (5).

Let us consider any straight line s through the infinite crystal, parallel to $\mathbf{S}_0$. In view of the lack of correlation between different plane sets, there can be no spatial regularity among their intersections. Consequently, no matter where s is placed, the segments intercepted by the planes on s will represent a general statistical sample of the intracrystalline chords; for this reason s will be designated henceforth as the *sampling line* (see Fig. 1). It is shown in the Appendix that the probability distribution of the chord lengths on the sampling line [*i.e.* $p(T)$] may be obtained from the interplanar statistics of the different plane sets. Then the line profile is evaluated through (2).

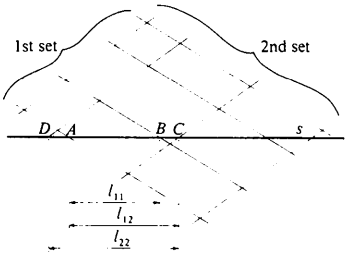

Fig. 1. Two-dimensional sketch showing two sets of parallel cleavage planes crossed by the sampling line s (see text).

The general result may be expressed in terms of the relative probability P_k that the planes of the kth set intersect the sampling line, as well as of the conditional probability density $\bar{p}_{ki}(l_{ki})$ that after any such intersection a chord length l_{ki} is terminated by a plane of the ith set. We have (see Wilson & Zsoldos, 1966)

$$P_k = L_{ks}^{-1} / \sum_k L_{ks}^{-1}, \tag{7}$$

where L_{ks} is the average segment length intercepted on s by two consecutive planes belonging to the kth set, and is related to the average interplanar distance L_k by

$$L_{ks} = L_k / \cos(\widehat{\mathbf{a}_k^* \mathbf{S}_0}) = L_k a_k^* S_0 / |\mathbf{a}_k^* . \mathbf{S}_0|. \tag{8}$$

In (8), $\mathbf{a}_k^*$ is any (reciprocal) vector othogonal to the planes of the kth set. As for $\bar{p}_{ki}$, if $k = i$ we have

$$\bar{p}_{kk}(y) = p(y; L_{ks}), \tag{9}$$

where the right-hand side is given by the appropriate interplanar probability [*i.e.* (4)–(6)] in which the average value L is replaced by L_{ks}. If $k \neq i$, it is shown in the Appendix that

$$\bar{p}_{ki}(y) = L_{is}^{-1} \int_y^\infty \bar{p}_{ii}(z)\, dz. \tag{10}$$

The probability density for the chord length T may now be obtained as [see (*A*5) and (*A*7)]

$$p(T) = \sum_k \sum_i P_k \bar{p}_{ki}(T) \left[\prod_{j \neq i} \int_T^\infty \bar{p}_{kj}(y)\, dy \right], \tag{11}$$

and the line profile is given by (2).

The Bernoullian case

It should be anticipated that this case might be treated by an extension of the kinetic theory proposed by Wilson (1943, 1949) and Wilson & Zsoldos (1966) for the crystals containing planar boundaries ('mistakes') between different domains. We will show in the following how the problem may be tackled through the sampling-line approach.

From (4) and (9), we have

$$\bar{p}_{kk}(y) = L_{ks}^{-1} \exp(-y/L_{ks}), \tag{12}$$

and from (10)

$$\bar{p}_{ki}(y) = L_{is}^{-1} \exp(-y/L_{is}) = \bar{p}_{ii}(y). \quad (13)$$

It should be noted that the last equality merely says that the probability of finding an intersection point on s with a plane of the ith set is always the same no matter where we choose the point from which the probability is evaluated, in agreement with the random character of the Bernoullian distribution. From (11), (12) and (13) we get

$$p(T) = L_s^{-1} \exp(-T/L_s) \quad (14)$$

where

$$L_s^{-1} = \sum_k L_{ks}^{-1} \quad (15)$$

and from (2) the line profile reduces to

$$\mathcal{J}(s) = \frac{2\mathcal{N}}{V} \frac{L_s}{1 + (2\pi L_s s)^2}, \quad (16)$$

showing that the Lorentzian shape is a general property of the Bernoullian powder samples, no matter how many sets of boundary planes there are.

As an example, the line profile already given for the general sample of parallelepiped crystals (Allegra, Bassi & Meille, 1978, equations 19 and 19′) may be easily obtained with the present approach, and L_s is identified with $S_0/Q(hkl)$. However, it should be stressed that (16) applies to any number of boundary plane sets.

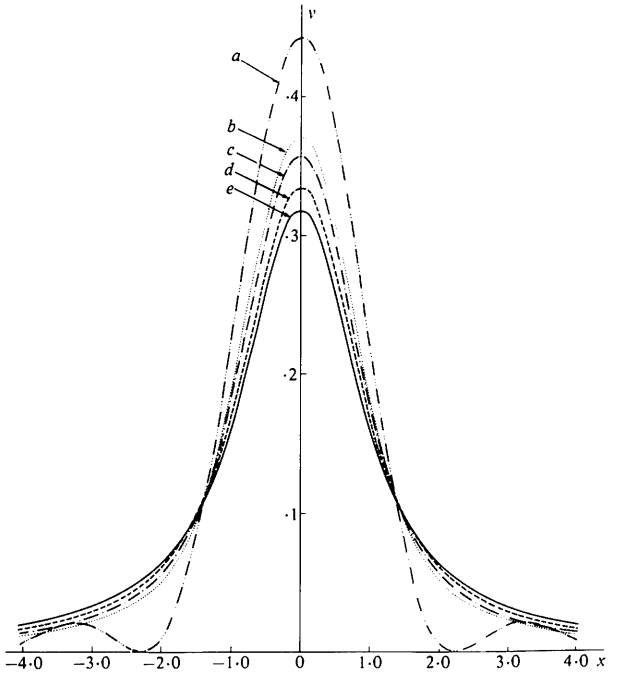

Fig. 2. Five different line profiles normalized to a unit area and to a half-peak half-width also equal to unity: (*a*) from identical cubic crystals, *h*00 reflection; (*b*) from identical cubic crystals, *hhh* reflection; (*c*) from a Gaussian distribution, crystals with cubic cell and three equivalent edges, *h*00 reflection; (*d*) from a Gaussian distribution as in point (*c*), *hhh* reflection; (*e*) from a Bernoullian distribution, any reflection [Lorentzian or Cauchy function, see (16)].

The Gaussian case

We will give in the following the full expression of $p(T)$ in the case of the three sets of boundary planes. First of all, taking $\bar{p}_{kk}(y)$ from (5), where $L = L_{ks}$ [see (8)] we get

$$\bar{p}_{ik}(y) = L_{ks}^{-1} \operatorname{erfc}(y/\sqrt{\pi} L_{ks}), \quad (17)$$

where $\operatorname{erfc}(y) = 1 - \operatorname{erf}(y) = 1 - 2/\sqrt{\pi} \int_0^y \exp(-t^2)\,dt$. From (7)–(11)

$$\begin{aligned} p(T) = 2\left(\sum_{i=1}^{3} L_{is}^{-1}\right)^{-1} \Bigg(& \pi^{-1}\left(\sum_{i=1}^{3} L_{is}^{-2}\right) \exp\left(-\frac{T^2}{\pi} \sum_{i=1}^{3} L_{is}^{-2}\right) \\ & - 3T \prod_{i=1}^{3} L_{is}^{-1} \operatorname{erfc}\left(\frac{T}{\sqrt{\pi} L_{is}}\right) \\ & + \Bigg[(L_{2s} L_{3s})^{-1} (T^2/\pi L_{1s}^2 + 1) \exp\left(-\frac{T^2}{\pi L_{1s}^2}\right) \\ & \times \operatorname{erfc}\left(\frac{T}{\sqrt{\pi} L_{2s}}\right) \operatorname{erfc}\left(\frac{T}{\sqrt{\pi} L_{3s}}\right) \\ & + (\text{two more terms obtained } \textit{via} \text{ cyclic index permutation}) \Bigg] \\ & - \pi^{-1} T \Bigg\{ L_{1s}^{-1} (L_{2s}^{-2} + L_{3s}^{-2}) \operatorname{erfc}\left(\frac{T}{\sqrt{\pi} L_{1s}}\right) \\ & \times \exp\left[-\frac{T^2}{\pi} (L_{2s}^{-2} + L_{3s}^{-2})\right] \\ & + (\text{two more terms obtained } \textit{via} \text{ cyclic index permutation}) \Bigg\} \Bigg). \end{aligned} \quad (18)$$

The line profile may now be evaluated through the application of (2), although the general analytical expression would be very complicated. Numerical computation is necessary. It should be remarked that if the reciprocal vector $\mathbf{S}_0$ of the reflection under consideration is parallel to one or two of the boundary plane sets, the corresponding L_{ks}'s go to infinity and the above expression simplifies [*i.e.* $L_{ks}^{-1} \to 0$, $\exp(-x^2/L_{ks}) \to 0$, $\operatorname{erfc}(x/L_{ks}) \to 1$]. In particular, this arises if the crystal faces are parallel to the unit-cell vectors. If a crystal edge is parallel to $\mathbf{S}_0$, there is one non-zero index only and the result already given by Allegra & Ronca (1978) is correct. [The probabilities of unit-cell termination (α,β,γ) adopted by Allegra & Ronca (1978) for the Gaussian crystal distribution are easily related with the average interplanar distances L, see equation (5), through $L_1 = (\sqrt{\pi} a a^*)^{-1}$ *etc.*]

Fig. 2 shows the line profiles for the Bernoullian [from (16)] and the Gaussian distributions [from (18)

and (2)]; for the latter case both the $h00$ and the hhh reflections are taken into consideration (crystals with a cubic cell and three statistically equivalent edges). For the sake of comparison, the $h00$ and hhh profiles from identical crystals with a cubic shape are also reported with the same normalization, the corresponding equations being [see Wilson (1949), Ch.IV, equation (26), normalization coefficients altered to fit present equation (2)]

$$\mathscr{I}_{h00}(s) = \frac{\mathscr{N}L}{V}\frac{\sin^2\psi_1}{\psi_1^2}; \quad \mathscr{I}_{hhh}(s) = \frac{\mathscr{N}L}{V}\frac{3\sqrt{3}}{2}\frac{\psi_2^2 - \sin^2\psi_2}{\psi_2^4}, \tag{19}$$

where L is the crystal edge length and $\psi_1 = \pi Ls$, $\psi_2 = \sqrt{3}\pi Ls$.

Discussion of the results

From inspection of Fig. 2 it is apparent that the profiles display considerable similarities among themselves with the only exception of the $h00$ reflection from identical crystals. In particular, unlike the other curves that show a smooth decrease for large $|s|$, the $h00$ profile contains a characteristic sequence of decreasing ripples in the tail region. The reason for this behaviour is related to the discontinuous character of the function $p(T)$ in this case. In fact, as may be seen from (2), in the limit of large $|s|$ the T values for which the integral gives a non-negligible contribution are such that $T|s| \gg 1$, with the consequence that $\sin^2(\pi Ts)$ may be replaced by its average value 1/2 as long as $p(T)$ is a reasonably continuous function. Consequently, considering that $\int_0^\infty p(T)\,\mathrm{d}T = 1$ and remembering (3), we have

$$\lim_{|s|\to\infty} \mathscr{I}(s) = \frac{1}{2\pi^2 s^2\langle T\rangle}\int_{-\infty}^{+\infty}\mathscr{I}(s)\,\mathrm{d}s = \text{constant}/s^2, \tag{20}$$

which suggests a possible experimental determination of $\langle T\rangle$. Unlike the other cases, for an $h00$ reflection from identical crystals $p(T)$ is highly discontinuous insofar as it reduces to a δ peak for $T = L$, the length of the crystal edge. As an additional comment, it seems worth pointing out that the s^{-2} intensity decrease at large $|s|$ would not be altered by a possible convolution of the intrinsic line shape with a more quickly vanishing function, such as the Gaussian. This may be easily shown for the Voigt function, *i.e.* a convolution of a Gaussian with a Lorentzian. Such a function may be evaluated as the transform of the product of a Gaussian and a simple exponential, *i.e.*

$$\begin{aligned}\mathscr{I}(s) &\propto \int_{-\infty}^{+\infty}\exp(-\xi^2/2\bar{x}^2 - |\xi|/\bar{y} + 2\pi i s\xi)\,\mathrm{d}\xi \\ &= 2\,\mathrm{Re}\int_0^\infty \exp(-\xi^2/2\bar{x}^2 - \xi/\bar{y} + 2\pi i s\xi)\,\mathrm{d}\xi \\ &= \sqrt{2\pi}\bar{x}\,\mathrm{Re}[w(z)],\end{aligned} \tag{21}$$

where

$$\begin{cases} w(z) = \exp(-z^2)\,\mathrm{erfc}(-iz) \\ z = \sqrt{2}\pi\bar{x}s + i\bar{x}/(\sqrt{2}\bar{y}), \end{cases} \tag{22}$$

and Re stands for the real part. For $|s| \to \infty$, it is possible to see that $\mathscr{I}(s) \propto \bar{s}^2$ [Abramowitz & Stegun (1965), *cf.* asymptotic expansions of $w(z)$ for large $|z|$, p. 328].

The asymptotic behaviour expressed by both (20) and Fig. 2 suggests a practical criterion to construct realistic line shapes for polycrystalline samples. Namely, whenever $|s| \gtrsim 2s_{1/2}$, $s_{1/2}$ being the half-width at half-peak-height, the s^{-2} law may be fairly safely assumed; as an approximate measure of the error involved, if the intensity value at $x = s/s_{1/2} = 2$ is made to be 100 for curves (*b*)–(*e*) in Fig. 2, the largest difference between them for $x > 2$ would be less than six units. The unphysical character of the Gaussian line shape, implying virtual disappearance of the intensity for $x > 2{\cdot}5$, should be stressed once again (Allegra & Ronca, 1978).

Table 1 summarizes the main conclusions of this analysis. The table shows few parameters and statistics corresponding to the profiles reported in Fig. 2. Following Lanford & Wilson (1978), three different definitions of the apparent crystal thickness are considered, their relationships being expressed in terms

Table 1. *Intensity ratios and apparent crystal thickness for different samples*

$\varepsilon_\beta = \langle T_v\rangle = \langle T^2\rangle/\langle T\rangle$; $\varepsilon_k = \langle T\rangle$; $\varepsilon_w = 0{\cdot}443/s_{1/2} = 0{\cdot}886\lambda/[\cos\theta.\Delta(2\theta)]$; T = crystal thickness along $\mathbf{S}_0$; L = edge of cubic crystals; $s_{1/2}$ = half-peak half-width in units: $S = 2\sin\theta/\lambda$; $\Delta(2\theta)$ = half-peak full-width in $2\theta°$.

Sample (*cf.* Fig. 2)	$\mathscr{I}(0)/\mathscr{I}(1{\cdot}5s_{1/2})$	$\mathscr{I}(0)/\mathscr{I}(2s_{1/2})$	$\varepsilon_k/\varepsilon_\beta$	$\varepsilon_w/\varepsilon_\beta$
(*a*) Identical cubic crystal, $h00$ reflection	5·76	>60	1	1
(*b*) Identical cubic crystal, hhh reflection	4·10	7·57	0·667	1·196
(*c*) Gaussian distribution, cubic crystal, $h00$ reflection	3·69	6·39	0·637	1·244
(*d*) Gaussian distribution, cubic crystal, hhh reflection	3·45	5·45	0·553	1·320
(*e*) Bernoullian distribution, any reflection	3·25	5·00	0·500	1·392

of the volume, or weight, average thickness $\langle T_v \rangle = \langle T^2 \rangle / \langle T \rangle$ $(= \varepsilon_\beta)$, which is perhaps the most meaningful parameter in many cases. In view of the s^{-2} dependence at large $|s|$ common to all but the anomalous $h00$ profile for identical crystals, information on the size distribution should best be derivable from analysis of the profile within the range $s_{1/2} < s < 2s_{1/2}$, wherein the peak-to-general intensity ratios are the lowest for the Bernoullian case. It may be observed that the ratios $\varepsilon_k/\varepsilon_\beta$ and $\varepsilon_w/\varepsilon_\beta$ both appear to be well correlated with the above intensity ratios, as has been checked by us on yet another statistical model not reported in Table 1, *i.e.* cubic crystals with identical shapes and a number probability distribution $\propto \exp(-L \times \text{constant})$. The extreme values of the parameters displayed by the Bernoullian statistics are produced because it represents the most randomized model. In physical reality, complete randomness in the placements of the boundary planes should be more or less unfavoured to the extent that it leads to a relatively large surface energy [compare, for example, the overall crystal volume distribution in the Bernoullian with that in the Gaussian case, given by Allegra & Ronca (1978), showing for the former a much larger percentage of crystals below the average size]. In conclusion, comparison of the actual intensity ratios with the figures reported in Table 1 should allow the reader to get an approximate index of the departure from full randomness (*i.e.* the Bernoullian distribution) in terms of the ratio $\varepsilon_w/\varepsilon_\beta$, whence the volume average thickness may be obtained from the half-peak width $2s_{1/2}$ and the definition $\varepsilon_w = 0{\cdot}443/s_{1/2}$.

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APPENDIX

Let us refer to Fig. 1, where a two-dimensional example is shown, with two sets of cleavage planes. We shall confine our attention at first to the chords having their left end on planes belonging to set 1 (see point A). We will first obtain the conditional probability $\bar{p}_{12}(l_{12})$ for the segment length l_{12} between point A and the next intersection C of the sampling line with a plane of set 2 (l_{12} is *not* a chord, in general). Let us remark that for point A to be comprised within the segment $\overline{DC} = l_{22}$, $\overline{AC}$ must be shorter than or equal to $\overline{DC}$; consequently,

$$\bar{p}_{12}(l_{12}) \propto \int_{l_{12}}^{\infty} \bar{p}_{22}(l_{22})\, \mathrm{d}l_{22}. \qquad (A1)$$

Generalizing the above result $(1, 2 \rightarrow k, i)$ with the normalizing condition $\int_0^\infty \bar{p}_{ki}(y)\, \mathrm{d}y = 1$, after integration by parts we get

$$\bar{p}_{ki}(y) = \int_y^\infty \bar{p}_{ii}(z)\, \mathrm{d}z / L_{is}, \qquad (A2)$$

where

$$L_{is} = \langle l_{ii} \rangle = \int_0^\infty z\, \bar{p}_{ii}(z)\, \mathrm{d}z, \qquad (A3)$$

and the actual value of L_{is} is given by (8). [It should be pointed out that $\bar{p}_{ki}(y)$ is independent of k.] The next step will be to define the joint conditional probability $\bar{p}_k(l_{k1}, l_{k2}, \ldots, l_{kk}, \ldots)$ that an intersection with the kth plane set (see point A in Fig. 1, $k = 1$) is followed by an intersection with the ith set at a distance l_{ki}. In view of the statistical independence between different sets, we have

$$\bar{p}_k(l_{k1}, l_{k2}, \ldots) = \prod_j \bar{p}_{kj}(l_{kj}). \qquad (A4)$$

The probability $\bar{p}_k(T)$ of having a chord length T starting from an intersection with the kth set is given by

$$p_k(T) = \sum_j \left\{ \bar{p}_{kj}(T) \prod_{l \neq j} \int_T^\infty \bar{p}_{kl}(y)\, \mathrm{d}y \right\}, \qquad (A5)$$

since a segment l_{kj} may be a chord if and only if it is shorter than all the other segments starting from the same intersection. Integrating by parts and making use of $(A2)$, we may reduce the above integrals to $(k \neq i)$

$$\int_T^\infty \bar{p}_{kl}(y)\, \mathrm{d}y = L_{is}^{-1} \int_T^\infty (y - T)\, \bar{p}_{ii}(y)\, \mathrm{d}y, \qquad (A6)$$

so that $(A5)$ may be formally expressed in terms of the basic probabilities $\bar{p}_{ii}(y)$ and their simple integrals. The overall probability $p(T)$ of having a chord length T, no matter what the plane set producing the first intersection point, is

$$p(T) = \sum_k P_k \bar{p}_k(T), \qquad (A7)$$

where P_k is the relative probability of having an intersection with the kth plane set [see (7)], and remembering $(A5)$, from $(A7)$ we finally obtain (11).

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