

## EVALUATION BY COMPUTER SIMULATION OF CERTAIN ERRORS IN THE THREE DIMENSIONAL TEXTURE ANALYSIS

M. HUMBERT, F. WAGNER, and R. BARO

*Laboratoire de Métallurgie Structurale,  
Faculté des Sciences - 57000 Metz, France*

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**Abstract:** The influence of certain experimental errors in pole-figure determination on the accuracy of calculated coefficients of the orientation distribution function has been analyzed.

### INTRODUCTION

The orientation distribution function (O.D.F.) introduced by Bunge<sup>1</sup> and Roe<sup>2</sup> gives a complete representation of the texture. This function [written  $f(g)$ ], developed on the basis of the generalized spherical harmonics, is achieved from several pole figures which are themselves developed on the basis of simple spherical harmonics. Indeed, as Bunge shows, the relations between the simple and the generalized harmonics lead to the following systems of equations:

$$\frac{4\pi}{2\ell + 1} \sum_{\mu=1}^{M(\ell)} C_{\ell}^{\mu\nu} k_{\ell}^{\mu*}(h_i) = F_{\ell}^{\nu}(h_i) \quad (1)$$

which allow the expression of the coefficients  $C_{\ell}^{\mu\nu}$  of the O.D.F. in terms of the coefficients  $F_{\ell}^{\nu}$  of the pole figures.

The measurement of the pole figure involves experimental errors which influence the determination of the  $F_{\ell}^{\nu}$  coefficients, and therefore the calculation of the  $C_{\ell}^{\mu\nu}$  coefficients.

In his works, Bunge<sup>3,4</sup> estimates the errors of the coefficients  $F_{\ell}^{\nu}$  and  $C_{\ell}^{\mu\nu}$  without dissociating the influence of their origins. To obtain the most exact O.D.F., it is of course necessary to minimize each of the experimental errors.

The present investigation was undertaken to examine by computer-simulating the influence of some experimental errors on the calculation of the coefficients of the pole figure. We studied more particularly the influence of:

- the partition of the pole sphere;
- the statistical fluctuations;
- the partial overlap of the zones of the pole sphere.

#### PARTITION OF THE POLE SPHERE

The pole figure  $P_{hi}(y)$  is the distribution, on the pole sphere, of the density of the normals to the lattice planes  $\{hkl\}$ .

The properties of the simple spherical harmonics allow us to calculate the coefficients  $F_{\ell}^{\nu}$  of the development of the pole figure by the integral

$$F_{\ell}^{\nu} = \oint P_{hi}(y) \dot{k}_{\ell}^{\nu*}(y) dy \quad (2)$$

Experimentally, the pole density distribution function is known in a set of discrete values  $\bar{P}(p,k)$  proportional to the mean pole densities in the solid angle  $A(p,k)$

$$\text{with } A(p,k) = \int_{(p-1)\Delta\phi}^{p\Delta\phi} \int_{(k-1)\Delta\beta}^{k\Delta\beta} \sin\phi \, d\phi \, d\beta$$

And relation (2) takes the following form:

$$F_{\ell}^{\nu'} = \sum_{p,k} \bar{P}(p,k) \int_{(p-1)\Delta\phi}^{p\Delta\phi} \int_{(k-1)\Delta\beta}^{k\Delta\beta} \dot{k}_{\ell}^{\nu*}(\phi,\beta) \sin\phi \, d\phi \, d\beta \quad (3)$$

The accuracy of the measurement of the pole figures, as well as of the calculation of  $F_{\ell}^{\nu}$  coefficients, depends on the dimensions of the solid angles. This is the reason why we computer-simulated the influence of the partition of the pole sphere on the determination of the  $F_{\ell}^{\nu}$  coefficients.

Starting from a set of  $F_{\ell}^{\nu}$  coefficients, it is easy to calculate the mean pole density in the area of the solid angle  $A(p,k)$  whatever the partition of the pole sphere.

$$\bar{P}(p,k) = \sum_{\ell,\nu} F_{\ell}^{\nu} \int_{(p-1)\Delta\phi}^{p\Delta\phi} \int_{(k-1)\Delta\beta}^{k\Delta\beta} \dot{k}_{\ell}^{\nu}(\phi,\beta) \sin\phi \, d\phi \, d\beta / A(p,k)$$

Then we calculate the  $F_{\ell}^{\nu'}$  coefficients with relation (3) and we define the ratio

$$\frac{\Delta F_{\ell}^{\nu}}{F_{\ell}^{\nu}} = \frac{|F_{\ell}^{\nu'} - F_{\ell}^{\nu}|}{|F_{\ell}^{\nu}|}$$

The coefficients  $F_{\ell}^{\nu}$ , called theoretical coefficients, are the basis of the calculation performed in this simulation. It is important not to choose these coefficients arbitrarily. In order to give them a significant role, we identify these coefficients, purposely limited to rank  $\ell$  equal 22, with the corresponding coefficients of a real pole figure.

Several partitions of the pole sphere, which correspond to solid angles such as  $\Delta\phi$  taking the values  $2^{\circ}$ ,  $3^{\circ}$  and  $5^{\circ}$ , and  $\Delta\beta$  being kept constant at  $5^{\circ}$ , were examined.

The following results may be observed regardless of the nature and texture of the specimens.

For  $\nu = 0$  and for a given  $\Delta\phi$  the ratio  $\Delta F_{\ell}^{\nu}/F_{\ell}^{\nu}$  rapidly increases with  $\ell$ . The increase of  $\Delta\phi$  causes a significant increase in the slope of these different curves as shown in Figure 1. For a given  $\Delta\phi$  and a fixed rank  $\ell$ , the values of

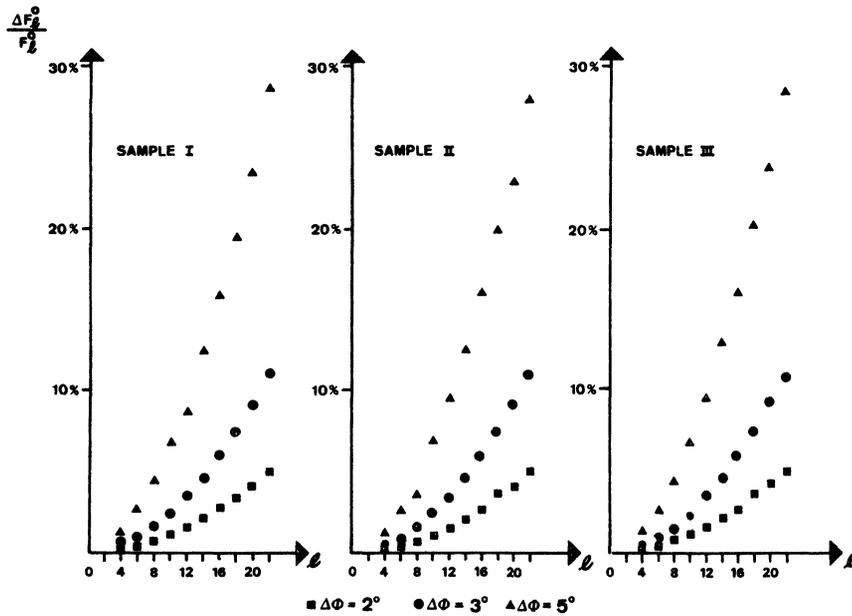


Figure 1. Relative variations of coefficients  $F_{\ell}^{\nu}$  with  $\Delta\phi$ .

the ratio  $\Delta F_{\ell}^{\nu}/F_{\ell}^{\nu}$  spread around a mean distribution curve which grows steadily with  $\nu$  (Figure 2). An increase of  $\Delta\phi$  leads to a significant increase of the level of the ratio  $\Delta F_{\ell}^{\nu}/F_{\ell}^{\nu}$ .

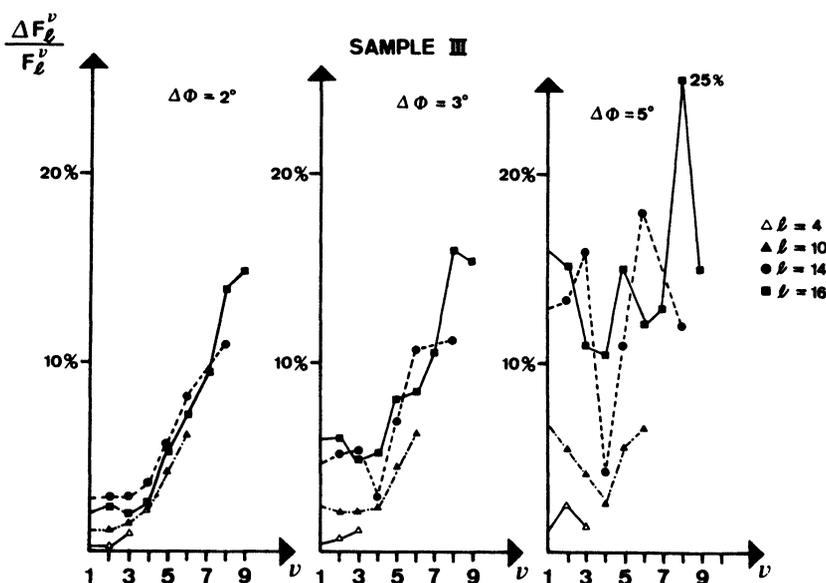


Figure 2. Relative variations of coefficients  $F_{\ell}^{\nu}$  versus  $\nu$  and  $\Delta\phi$ . (The index  $\nu$  counts the linearly independent coefficients  $1 \leq \nu \leq \ell/2 + 1$ .)

These results show that the partition of the pole sphere has a sensitive influence on the  $F_{\ell}^{\nu}$  coefficients. Indeed, the relative errors increase rapidly with  $\Delta\phi$  especially when  $\ell$  and  $\nu$  are high, so that from certain values on up, the determination of the  $F_{\ell}^{\nu}$  no longer produces meaningful results. If we want to develop the pole figure to a given rank  $\ell$  we have to choose a partition of the pole sphere so that the errors do not rise beyond a certain level.

In practice, as shown in our figures, if we want to obtain a reasonable precision of the  $F_{\ell}^{\nu}$  coefficients up to the rank  $\ell$  equal to 22--the limit generally used in the case of a texture which does not present very sharp orientations--the partition will have to be chosen so that  $\Delta\phi$  be noticeably lower than  $5^{\circ}$ .

#### STATISTICAL FLUCTUATIONS

When one measures a pole figure the recorded counting rate undergoes statistical errors. The influence of these statistical errors on  $F_{\ell}^{\nu}$  were calculated by computer simulation. The total recorded number of pulses  $N$  is proportional to the density of the planes  $\{hkl\}$  in Bragg reflexion and the counting error is  $\sqrt{N}$ . We used the following simulation scheme:

$$F_{\ell}^{\nu} \begin{cases} \rightarrow \bar{P}(p,k) \rightarrow F_{\ell}^{\nu'} \\ \rightarrow \bar{P}(p,k) + \varepsilon[\bar{P}(p,k)] \rightarrow F_{\ell}^{\nu''} \end{cases} \Delta F_{\ell}^{\nu} = |F_{\ell}^{\nu'} - F_{\ell}^{\nu''}|$$

Starting from a set of the theoretical coefficients  $F_{\ell}^{\nu}$ , which have been chosen as shown in the previous paragraph, we calculate, on the one hand, the mean densities in a partition such as  $\Delta\phi = \Delta\beta = 5^{\circ}$ , and then the  $F_{\ell}^{\nu'}$  coefficients, and on the other hand, the mean densities with the statistical error of the counting and finally the corresponding  $F_{\ell}^{\nu''}$  coefficients.

The statistical counting error was assumed to be in the form of  $\varepsilon[\bar{P}(p,k)] = k \cdot \varepsilon_a(p,k) \cdot \sqrt{N(p,k)}$  where  $N(p,k)$  is the counting in the solid angle  $A(p,k)$  while  $\varepsilon_a(p,k)$  is a random value between -1 and +1, and  $k$  is a proportionality factor.

The recording counting  $N(p,k)$  remained lower than 1400 impulses. The computer simulation was performed for several pole figures corresponding to samples of different textures.

Figure 3 shows the absolute errors  $\Delta F_{\ell}^{\nu}$  corresponding to one of the samples. Whatever the pole figure we examined, we obtained results of this type. It may be noticed, indeed,

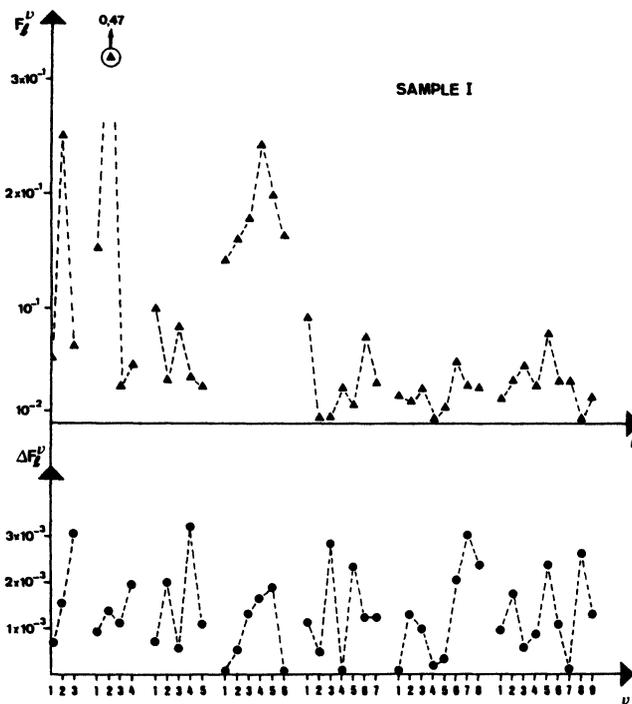


Figure 3. Coefficients  $F_{\ell}^{\nu}$  and their absolute errors in the case of statistical fluctuations of counting.

that the absolute errors  $\Delta F_{\ell}^{\nu}$  are low in comparison with the norm coefficients  $F_{\ell}^{\nu}$  equal to 1.\* For example in the case of sample I all the absolute errors are below 0.0035.

Figures 3 and 4 (kindly suggested by Bunge) clearly show that the  $\Delta F_{\ell}^{\nu}$  are independent of  $\ell$  and  $\nu$  as well as of  $F_{\ell}^{\nu}$  values.

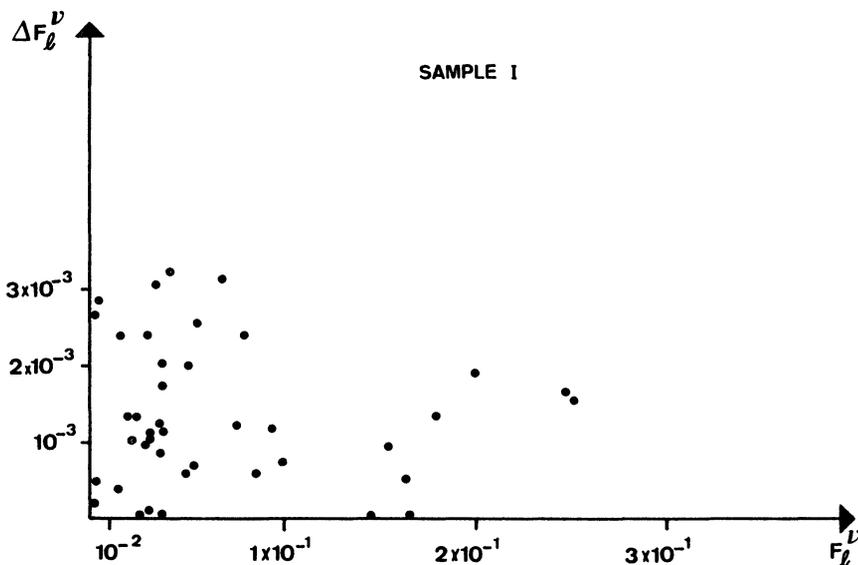


Figure 4. Random dependence between the values of the errors  $\Delta F_{\ell}^{\nu}$  and the absolute values  $F_{\ell}^{\nu}$  in the case of statistical fluctuations.

For each rank  $\ell$ , the mean value of the absolute errors occurring in the case of statistical fluctuations is almost constant as shown in Figure 3. So the relative precision of the low-value coefficients  $F_{\ell}^{\nu}$  (for instance in high rank  $\ell$ ) is not as good as in the case of high-value coefficients  $F_{\ell}^{\nu}$ .

So statistical fluctuations give rise to errors, which can be made negligible in comparison with other errors by increasing counting time, or by performing measurements with sufficiently high constant impulse number.

#### OVERLAPPING OF THE EXPLORED ZONE

The setting of the texture goniometer<sup>5,6</sup> as well as of the horizontal slits of the counter determines the width  $\Delta\phi$  of pole sphere zones as shown by the following relation:

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\*This normalization convention deviates from that one used in reference 3.

$$\Delta\phi = \frac{H}{2R \sin \theta}$$

where  $H$  is the aperture of the horizontal slits;  $R$  is the distance between sample and counter; and  $\theta$  is the Bragg angle. If the aperture  $H$  is too wide the zones overlap, and the measurement of the pole density becomes erroneous.

This type of error was computer-simulated in the case of a 5% overlap which should be of the amount of the usual experimental error. The simulating scheme used was as follows:

$$F_{\ell}^{\nu} \begin{cases} \rightarrow \bar{P}(p,k) \longrightarrow F_{\ell}^{\nu'} \\ \rightarrow \bar{P}(p,k) + \Delta\bar{P}(p,k) \longrightarrow F_{\ell}^{\nu''} \end{cases} \left. \vphantom{F_{\ell}^{\nu}} \right\} \Delta F = |F_{\ell}^{\nu'} - F_{\ell}^{\nu''}|$$

The analysis, which was again applied to several pole figures corresponding to samples of different nature and texture, led to the following general results:

$$\text{the coefficient } F_0^0 = \sum_{p,k} \int_{A(p,k)} P(p,k) dy$$

which is the norm of the density distribution function, grows quite logically, inasmuch as the same intensity is collected twice by overlapping. The growth of the  $F_0^0$  coefficient disappears by normalizing the pole figure to unity.

Figure 5 represents the  $\Delta F_{\ell}^{\nu}$  errors corresponding to sample I in the case of a 5% overlapping. One may observe that, for each rank  $\ell$ , the errors  $\Delta F_{\ell}^{\nu}$  are decreasing with  $\nu$ . Furthermore, the errors are all less than a certain value (0.008 in the case of sample I). We obtain this type of results for pole figures of all kinds.

Figure 6 shows the level of the mean errors (over  $\nu$  in each degree  $\ell$ ) due to the overlapping of the explored zones in comparison with the errors occurring in the sphere partition (the highest) and in the statistical fluctuations (the lowest). This result leads us to draw the same conclusion as in the previous section, and to dwell on the fact that this type of errors must be more severely corrected to improve the precision of the  $F_{\ell}^{\nu}$  coefficients by taking the greatest care in the setting of the goniometer and the counter.

In Figure 7, the absolute values of  $F_{\ell}^{\nu}$  and of  $\Delta F_{\ell}^{\nu}$  are plotted as a function of the rank  $\ell$ , where  $\Delta F_{\ell}^{\nu}$  represents the sum of the various errors examined. It is shown that the magnitude of the error  $\Delta F_{\ell}^{\nu}$  is almost as great as the value of  $F_{\ell}^{\nu}$  calculated at high ranks of  $\ell$  values.

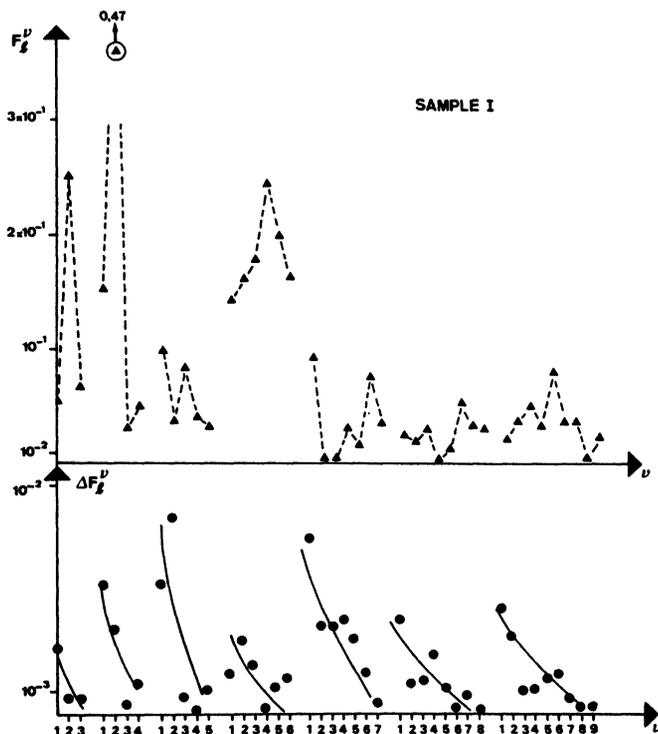


Figure 5. Coefficients  $F_{\ell}^{\nu}$  and their absolute errors in the case of a 5% overlap of the zones ( $\Delta\phi = 5^{\circ}$ ,  $\Delta\beta = 5^{\circ}$ ).

#### CONCLUSION

In order to obtain a better precision, one is tempted to develop the O.D.F. with rank  $\ell$  as high as possible. Only the number of the pole figures seems to limit the serial development.

However, this work shows that experimental errors are the cause of important errors in the calculation of  $F_{\ell}^{\nu}$  coefficients. If the latter, which only represent an intermediate stage in the determination of the O.D.F. present a high error the calculation of the  $C_{\ell}^{\mu\nu}$  coefficients is no longer of much significance.

Practically, various precautions such as increasing the counting rate, setting the apparatus with great care and partitioning the pole sphere with  $\Delta\phi$  lower than five degrees are necessary in order to obtain meaningful coefficients, especially when the rank  $\ell$  is to be higher than or equal to 22.

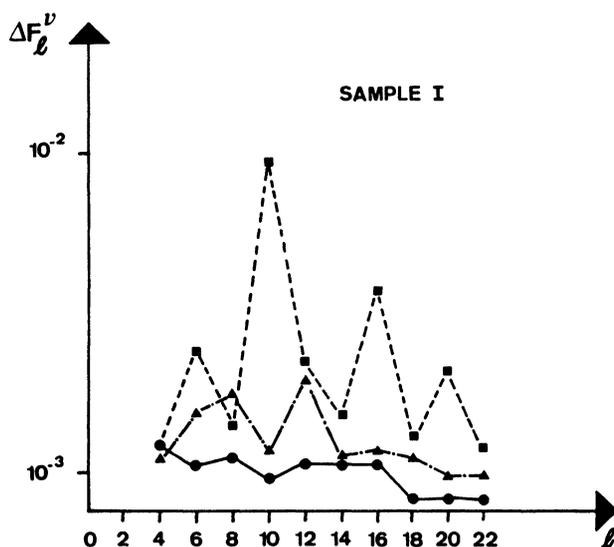


Figure 6. Comparison between different errors occurring: In partition of the pole sphere ( $\Delta\phi = 5^\circ$ ,  $\Delta\beta = 5^\circ$ ) (■); in statistical fluctuations (●); in overlapping of the explored zones (▲).

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## SAMPLE 1

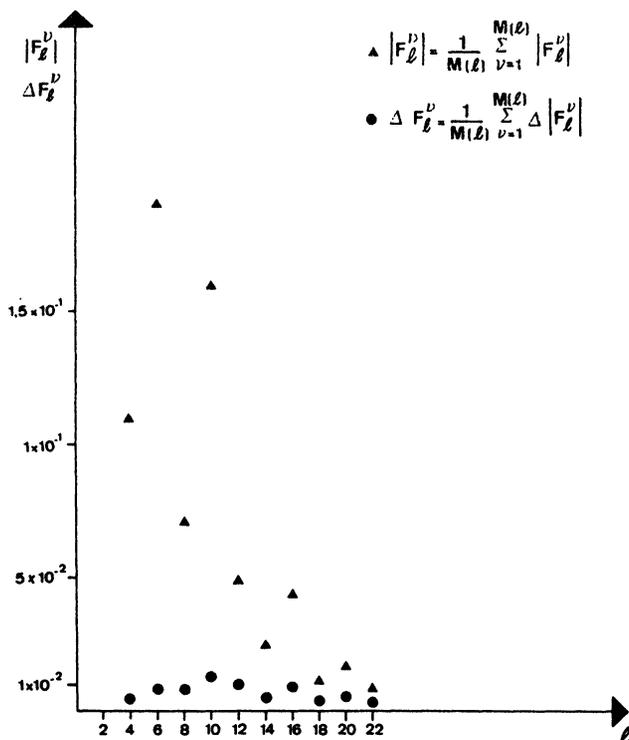


Figure 7. Average sum over  $\nu$  of the coefficients  $F_l^\nu$  and of the errors  $\Delta F_l^\nu$  stemming from: the partition of the pole sphere in the case  $\Delta\phi = 5^\circ$ ; the statistical fluctuation (maximum number of pulse: 1400 in an area); the 5% overlap of each zone of the pole sphere.