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STATISTICAL CHARACTERISTICS OF SELECTED POLYHEDRA

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ABSTRACT

An analysis is given of the properties of model structures consisting of known polyhedra. The conditions of using the Monte Carlo method which reduce to a minimum the errors of simulation one- and two-dimensional parameters of polyhedra are examined. Characteristics of parameters, which are most frequently analysed in real structures, obtained as a result of the analysis of four selected polyhedra (cube, Kelvin's tetraidecahedron, pentagonal and rhombic dodecahedrons) are presented.

Keywords: Polyhedron, computer simulation, random plane section, random plane angles, stereology.

INTRODUCTION

The most frequently measured parameters of the images of metal and alloy structures, using quantitative instruments, are: area of section, A, chord length L, perimeter L_p and tangent diameters in two vertical directions (Feret's diameters: horizontal D_h ,vertical D_v). On the basis of these parameters, derivatives describing grain shape are calculated: $F_D=D_v/D_h$, $F_B=4\pi A/L_p^2$. Size distributions of the plane angles measured at the grain section vertices provide an important information about the structure but this measurement is not frequently applied because it is time consuming when made manually. However it is possible to measure these angles using quantitative instruments (Adrian et al. 1986, Oldmixon et al. 1988). The reconstruction of the size distribution of three-dimensional grain parameters, using the results obtained by measuring the above mentioned parameters, is possible only in systems of well defined grain shapes. Different polyhedra may be considered as grain models, e.g. Kelvin's tetraidecahedron, rhombic or pentagonal dodecahedrons. For some phases a cube model is appropriate. In order to obtain the size distribution of the parameters on sections of polyhedra, a physical model was first tested (Hull and Houk 1953). Computer developments have produced the possibility of mathematical simulations of polyhedra sections using the Monte Carlo method (e.g. Naumowich at al 1980, Malinski at al. 1986,Adrian 1986, Warren 1987). Warren 1987 presents a comprehensive review of the earlier literature on the mathematical simulations of polyhedra sections. To obtain the size distributions of some parameters, analytical methods can be used (e.g.Itoh 1970, Sukiasian 1982, Miles 1987, Butler and Reeds 1987, Reeds and Butler 1987,Socha 1988). The Monte Carlo method has the advantage over the analytical method in that it enables information about characteristics of such parameters to be obtained, which is difficult (or impossible) to derive by the analytical method because of the complexity of the calculations. Thus the Monte Carlo Method is a useful "skeleton-key" permitting solutions of the problems which are difficult to solve using the "key"" - analytical method. However its shortcoming is the imperfection of applied mathematical random-numbers generators, in fact called "pseudorandom". This is the reason for the occurrence of systematic errors. Increasing the number of sections in order to reduce these errors may not give the expected results because of the well known fact that mathematical random number generators show periodicity. The accuracy of the analysis can however be estimated because it is possible to calculate mean values of some parameters of the sections of a model using the relationships between them and the polyhedron dimensions.

The aim of this work was to find the method for obtaining the characteristics of polyhedron parameters (mean values x, standard deviation s(x),size distributions, coefficients of variation v=s(x)/x with minimal errors. This method was then used for analysing four polyhedra: cube, Kelvin's tetraidecahedron, rhombic and pentagonal dodecahedrons The characteristics of 10 parameters of the section of polyhedra were studied.

THEORETICAL PROPERTIES OF THE ANALYSED POLYHEDRA

Comprehensive but incomplete specifications of the theoretical parameters for a series of solids is given by Underwood (1970). Using known stereological relationships between the dimensions of polyhedra and one- or two- dimensional parameters, these parameters were derived and are listed in table 1. The nomenclature of Underwood (1970) is used: V, S, H' - volume, surface and mean length of polyhedron, $\overline{M}$, M_v - mean and per volume unit polyhedron curvature, $\overline{A}$, $\overline{L}$, $\overline{d}$ - mean values of area, chord length and tangent diameter, β - dihedral angle. Kelvin's tetraidecahedron has two dihedral angles β_1, β_2 and therefore the mean dihedral angle $\overline{\beta}$ was calculated. Mean perimeter $\overline{L}_p$ which is not mentioned in table 1 can be calculated using the equation: $\overline{L}_p = \pi\overline{d}$.

Note: In tables 1-3 the notifications **C**, **T**, **RD** and **PD** mean cube, Kelvin's tetraidecahedron, rhombic and pentagonal dodecahedrons respectively.

Table 1.

Theoretical properties of the analysed polyhedra
(a-edge of polyhedron, $W=1+2\sqrt{3}$ and $K=tg^2(54^o)tg(\beta/2))$.

Param.	C	T	RD	PD
V	a^3	$8\sqrt{2}\ a^3$	$16a^3/(3\sqrt{3})$	$2.5\ K\ a^3$
S	$6a^2$	$6Wa^2$	$8\sqrt{2}\ a^2$	$15\ tg(54^o)a^2$
H'	1.5 a	3a	2a	$7.5(\pi-\beta)a/\pi$
$\overline{A}$	$2a^2/3$	$8\sqrt{2}\ a^2/3$	$8a^2/(3\sqrt{3})$	$\pi Ka^2/(3(\pi-\beta))$
$\overline{L}$	2a/3	$16\sqrt{2}\ a/(3W)$	$4\sqrt{2}\ a/(3\sqrt{3})$	$2\ tg(54^o)tg(\beta/2)a/3$
$\overline{M}$	$3\pi a$	$6\pi a$	$4\pi a$	$15(\pi-\beta)a$
M_v	$3\pi/a^2$	$3\pi/(4\sqrt{2}\ a^2)$	$3\sqrt{3}\ \pi/(4a^2)$	$6(\pi-\beta)/(Ka^2)$
$\overline{d}$	a	0.5Wa	$\sqrt{2}\ a$	$\pi tg(54^o)a/(2(\pi-\beta))$
β	$\pi/2$	$\overline{\beta}=2\pi/3$ $\beta_1=\arccos(1/3)$ $\beta_2=\arccos(1/\sqrt{3})$	$2\pi/3$	$2\ \arcsin(1/(2\sin(36^o)))$

METHOD OF CALCULATION

The analysis was made on isolated solids with constant dimensions. The equations of the faces and edges of the polyhedron were defined by the coordinate system. For generating the random secant planes and lines, two types of random-number generators were used: multiplicative and additive generators (Zielinski, 1970). The equation of a plane had the form:

$$x \sqrt{1-\varphi_i^2} \cos(2\pi\psi_i) + y \sqrt{1-\varphi_i^2} \sin(2\pi\psi_i) + z\varphi_i = l_{max}\gamma_i \tag{1}$$

where: l_{max} is the maximum distance from the coordinate origin to the surface of the analysed solid, φ_i, ψ_i, γ_i are the random numbers. The secant plane π_1 was created by generating three numbers φ_1, ψ_1 and γ_1 in the intervals (-1,1), (-1,1), (0,1) respectively using three independent multiplicative generators. The coordinates of the intersection points of π_1 with the edges of the polyhedron were obtained by the simultanous solution of the equation for π_1 with the equations for the abutting edges. Only the points belonging to the polyhedron surface were taken into account. The intersection points were ordered following the contour. From the polygon the following parameters were calculated: A, L_p, F_B, maximum diameter D (maximum distance between two vertices), number of the polygon sides N_s and plane angles α at each vertex. Using the next three independent multiplicative generators the plane π_2 described by three number φ_2, ψ_2 and γ_2 was created. The edge of the intersection π_1 and π_2 was the axis of the polygon projection for the D_v calculation. The second axis for obtaining D_h occurred in π_1 and was perpendicular to the first axis. The shape coefficient F_D was calculated. The random secant line for finding the chord length L was obtained from the system of the equations for planes π_3 and π_4, defined by six random numbers, generated using three additive (φ_4, ψ_4, γ_3) and three multiplicative (φ_3, ψ_3, γ_4) generators. A simultaneous solution of the system of equations for the secant line and the adjoining face of the polyhedron enabled the coordinates of the intersection points to be found, thus permitting calculations of the chord length L, lying inside the polyhedron. Parameters A, D, L_p, D_v, D_h, L, F_B have been normalised with respect to their maximum values. For each polyhedron 250,000 active sections and chords lying inside the solid were used. The numbers of all sections (n_{AC}) and lines (n_{LC}) were stored. In the range of 250,000 active sections and chords starting from 100,000, the optimum characteristics of the analysed polyhedron were sought. The optimum characteristics are regarded to be the mean values, coefficients of variation and size distributions of all the parameters obtained for such a number of sections, (n_{AO}), Feret' diameters, (n_{DO}), and chords, (n_{LO}), so that appropriate errors are minimised. As the optimum criteria, three errors were calculated for each section and chord using the theoretical mean values of parameters listed in table 1:

$$\Delta_1 = (\Delta A)^2 + (\Delta L_p)^2 + (\Delta\alpha)^2 \qquad (2)$$

$$\Delta_2 = (\Delta D_v)^2 + (\Delta D_h)^2 \qquad (3)$$

$$\Delta_3 = |\Delta L| \qquad (4)$$

where: ΔX is the relative error (in %) of parameter X ($\Delta X = 100*(X_m - X_t)/X_t$), where X_m and X_t are measured and theoretical values of parameter X. The optimum characteristics of A, D, L_p, F_B, α, and N_s were found on the basis of Δ_1 being a minimum, D_v, D_h and F_D - using Δ_2 and L - using Δ_3. The numbers for n_{AC}, n_{LC}, n_{AO}, n_{LO}, n_{DO} are listed in table 2.

Table 2.

Numbers of total sections, lines (n_{AC}, n_{LC}) and optimum sections, tangent diameters, chord length (n_{AD}, n_{DO}, n_{LO}) for analysed polyhedra.

Number	C	T	P D	R D
n_{AC}	288,660	263,542	265,098	288,667
n_{AO}	120,683	246,187	225,463	162,875
n_{LC}	636,949	475,290	484,417	599,588
n_{LO}	142,952	180,634	204,188	102,744
n_{DO}	212,995	120,752	151,764	106,726

RESULTS AND DISCUSSION

Fig. 1 shows the dependence of the relative errors ΔA, $\Delta\alpha$, ΔL_p and Δ_1 for Kelvin's tetraidecahedron calculated for every 1000 active sections and chords as a function of the number of sections. A similiar dependence was observed for other errors (ΔD_v or ΔD_h, Δ_2, ΔL) of the polyhedra which were studied. Presented errors oscilate around 0 but it has to be noted that analysed errors ΔA, ΔL_p, $\Delta\alpha$ do not reach 0 at the same section number. Therefore we cannot use just one type of error to find the optimum characteristics of all the parameters. The function $\Delta_1 = f(N)$ shows that with an increasing number of sections the sum squares of errors generally tends to 0 but the assumption of a definite number of sections does not

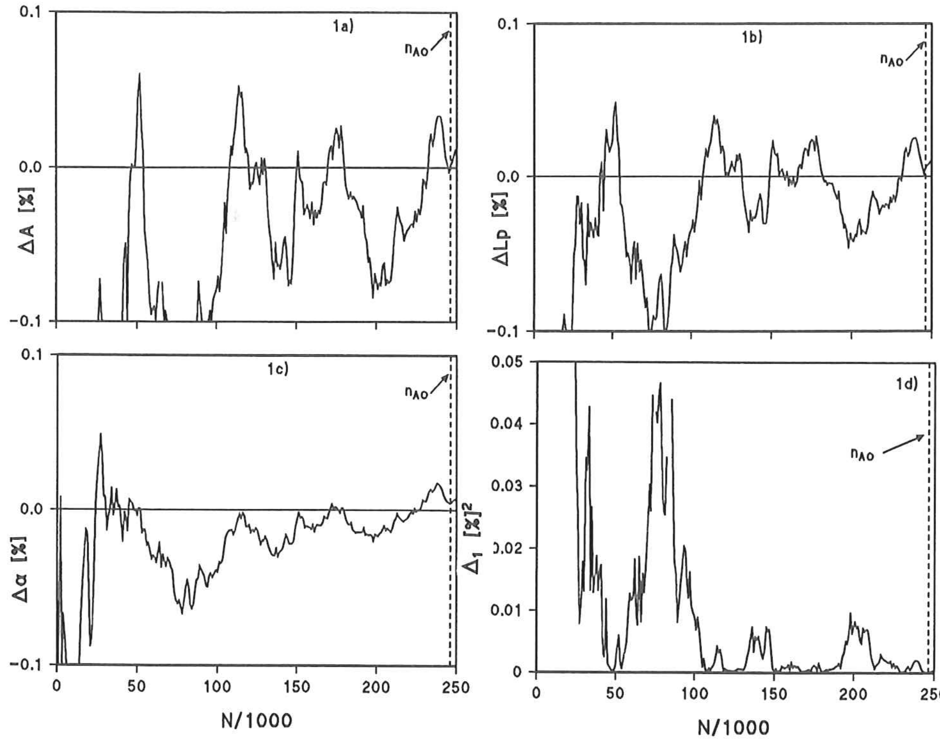

Fig. 1. Dependence of errors of area of section ΔA, plane angle Δα, perimeter ΔL_p and Δ_1 as a function of the number of sections of Kelvin's tetraidecahedron. **Note:** n_{AO} =246,187.

secure a minimum in the errors even if this number is as large as 200,000. The way to find the characteristics of the optimum parameters is correct for the case where several interconnected parameters are generated. Optimum characteristics tend to be ideal when the errors of all the parameters tend to 0 but when only one parameter is generated (e.g. chord length L) this may give incorrect results and an increasing number of analysed elements leads to an improvement in accuracy of the analysis.

The results of the analysis are presented in tables 3,4 and in figures 2-9. Table 3 contains frequency distributions of the polygon sides A comparison of the frequency distributions of the polygon sides for a cube with the data obtained by Sukiasian (1982) using the analytical method, has shown that differences do not exceed 0.1%.

Table 3.

Frequency distributions (in %) of polygon sides N_s for analysed polyhedra.

N_s	C	T	PD	RD
3	27.9783	7.2502	9.2463	4.020
4	48.6340	13.4032	13.0070	13.3925
5	18.7856	11.8134	19.1131	16.1584
6	4.6021	31.2194	29.8146	29.9708
7	–	18.2300	19.6884	19.0152
8	–	13.1526	7.5046	16.3340
9	–	3.8475	0.8094	1.1082
10	–	1.0837	0.8165	–

In table 4 the mean values of the parameters X, coefficients of variation v, and relative errors ΔX are given. These errors do not exceed $2*10^{-2}$%. As can be seen from table 4 the mean section for a cube is square ($\alpha = 90^o$, $N_s = 4$). The mean sections for Kelvin's tetraidecahedron and the rhombic dodecahedron are identical - regular hexagon ($\alpha = 120^o$, $N_s = 6$).

Table 4.

Mean values X, coefficients of variation v, relative errors X obtained with use of minimum errors criterion.

Par.	Cube			Kelvin's tetraidecahedron		
	X	v	¦ΔX¦	X	v	¦ΔX¦
A	0.47140	0.64187	$1.88*10^{-5}$	0.53874	0.53187	$1.76*10^{-5}$
D	0.66975	0.36163	-	0.76339	0.29104	-
L_p	0.65067	0.38782	$3.37*10^{-5}$	0.72615	0.32341	$2.02*10^{-5}$
L	0.38490	0.58820	$1.69*10^{-8}$	0.53429	0.47176	$2.20*10^{-8}$
D_v	0.57746	0.40962	$1.92*10^{-4}$	0.70597	0.32992	$1.93*10^{-4}$
D_h	0.57725	0.40976	$1.40*10^{-4}$	0.70577	0.33068	$1.00*10^{-4}$
F_B	0.66942	0.21487	-	0.81177	0.17476	-
F_D	1.06115	0.46312	-	1.03119	0.31264	-
α [^{o}]	90.0026	0.27332	$2.90*10^{-5}$	120.0042	0.19239	$3.52*10^{-5}$
N_s	4.00012	0.2018	-	6.00042	0.26534	-

Table 4. - continue.

	Rhombic dodecahedron			Pentagonal dodecahedron		
A	0.54433	0.56457	$3.98*10^{-6}$	0.57568	0.53760	$6.93*10^{-5}$
D	0.67578	0.33457	-	0.75153	0.29803	-
L_p	0.68017	0.35992	$8.15*10^{-6}$	0.74484	0.32964	$5.15*10^{-5}$
L	0.47131	0.47805	$1.93*10^{-4}$	0.52977	0.47402	$2.01*10^{-11}$
D_v	0.61235	0.36842	$4.21*10^{-5}$	0.69679	0.33592	$1.84*10^{-7}$
D_h	0.61234	0.36782	$4.55*10^{-5}$	0.69679	0.33566	$5.40*10^{-8}$
F_B	0.81493	0.15638	-	0.80971	0.17914	-
F_D	1.02478	0.37341	-	1.02831	0.31300	-
α [°]	120.0002	0.18322	$1.53*10^{-6}$	116.5668	0.19331	$1.48*10^{-8}$
N_s	6.00002	0.23584	-	5.67526	0.25768	-

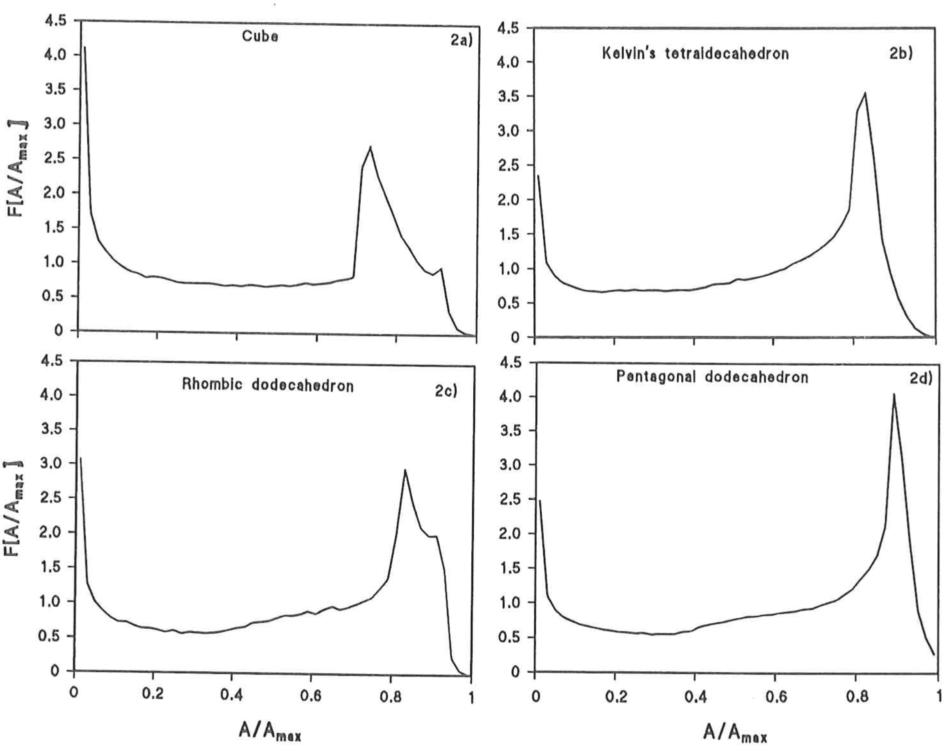

Fig. 2. Frequency distributions of area of section, A.

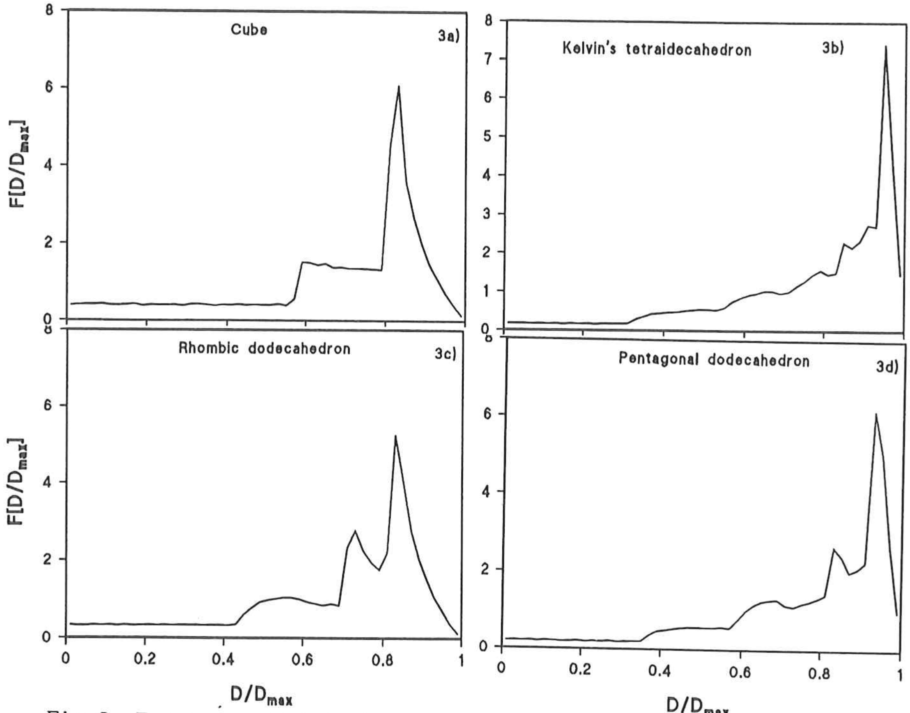

Fig. 3. Frequency distributions of maximum diameter D_{max}.

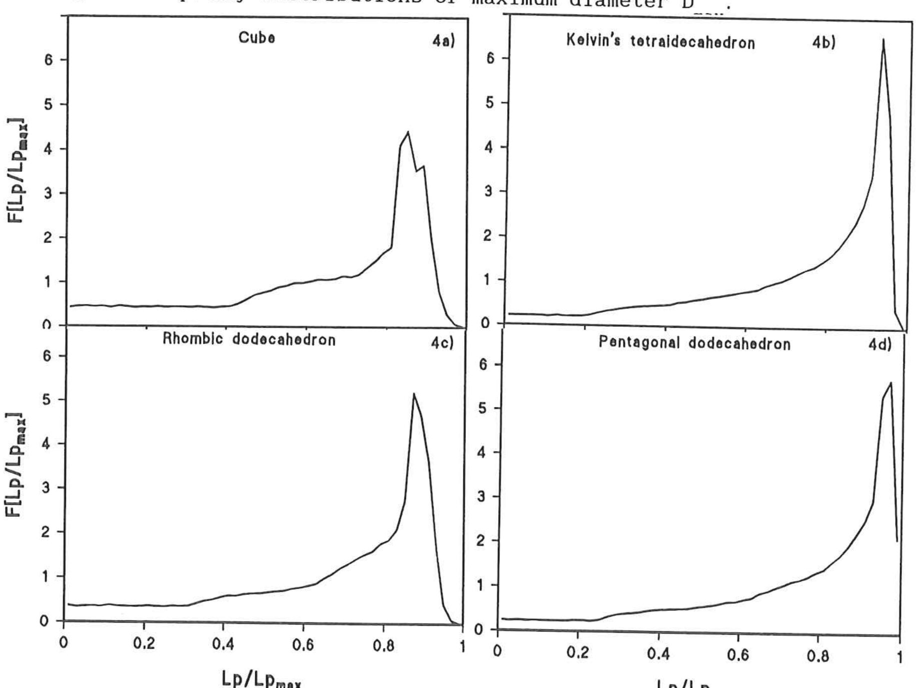

Fig. 4. Frequency distributions of perimeter of section L_p.

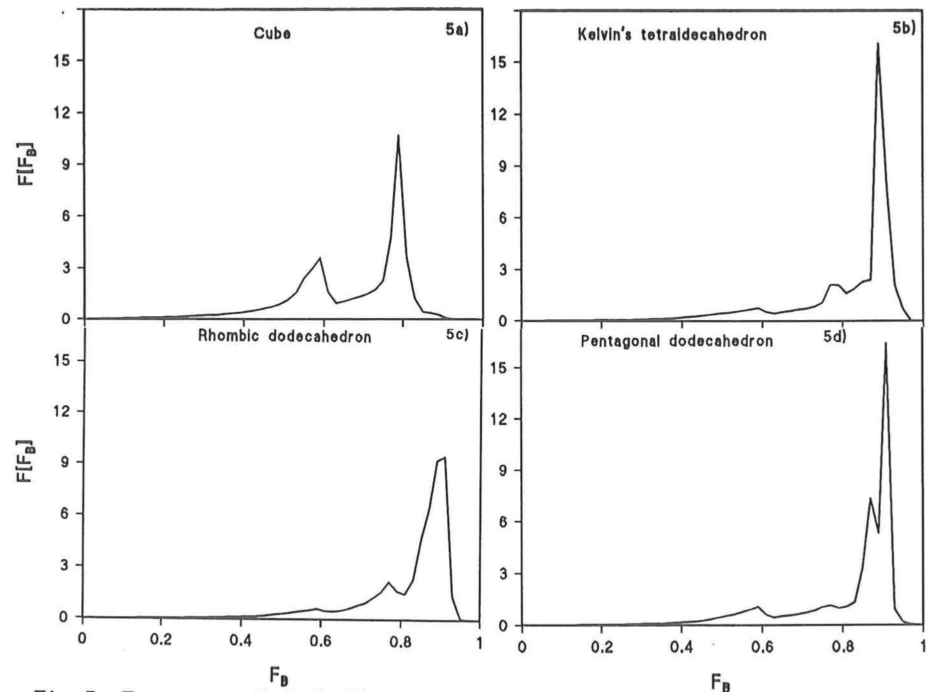

Fig. 5. Frequency distributions of shape coefficient F_B.

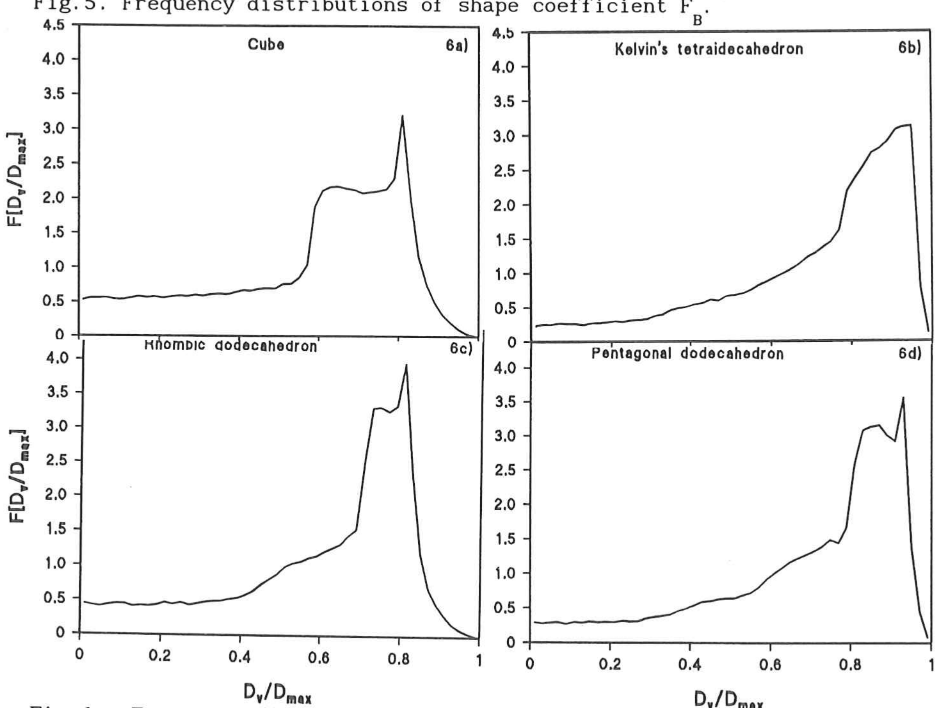

Fig. 6. Frequency distributions of tangent diameter D_v.

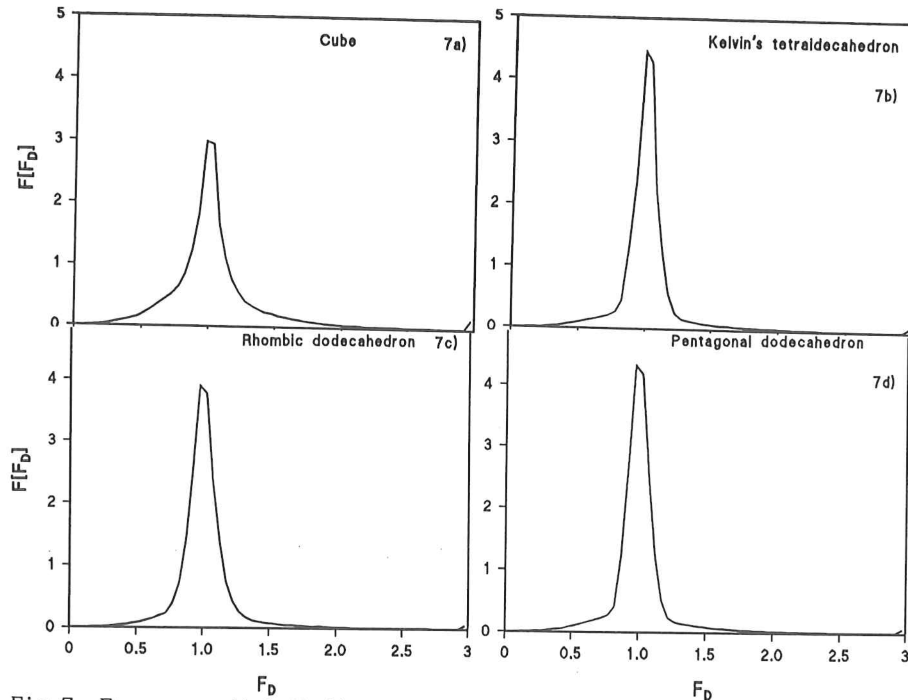

Fig. 7. Frequency distributions of shape coefficient F_D .

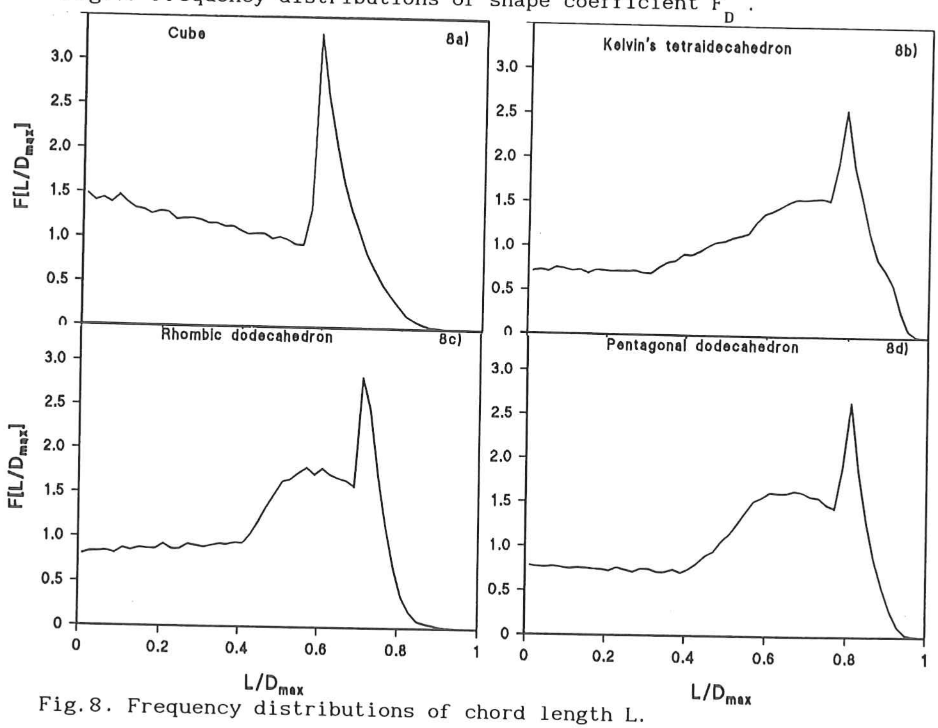

Fig. 8. Frequency distributions of chord length L.

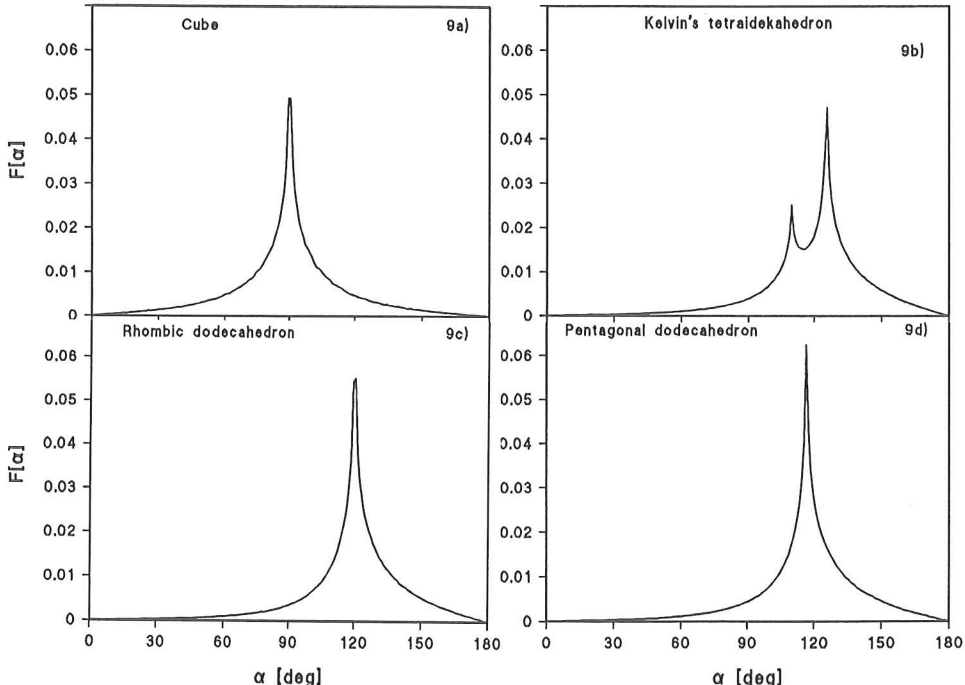

Fig. 9. Frequency distributions of plane angles α .

Coefficients of variation for these parameters enable these polyhedra to be differentiated. It is worth mentioning that the mean values for the coefficients of shape F_D for all polyhedra exceed a value of 1. Size distributions of F_D are similiar for all polyhedra but different frequencies at modal values make it possible to distinguish between them. For polyhedra which are assumed as grain models of monophased structures, the shape of the size distribution for some parameters (A, D, F_B α, D_v or D_h) makes it possible to distinguish between these polyhedral shapes. They can be used in practice to identify the shape of the grains in homogenous structures. The most useful seems to be the size distribution of plane angles (fig. 9), showing singularities at angles equal to dihedral angles of polyhedra.

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