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QUANTITATIVE METALLOGRAPHY FOR PARTICLES HAVING POLYHEDRAL SHAPES

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INTRODUCTION

The quantitative description of a metallurgical microstructure depends upon an understanding of the relationships between observations on a plane surface and the spatial structure of the constituents. One problem of quantitative metallography concerns the counting, size measurements, and shape determination of dispersed phases in alloys. For systems of dispersed particles with shapes of spheres, cylinders, ellipses, and other solids of revolution, relations have been developed connecting numbers of particles observed on a unit cross-section with number present per unit volume.[1,2,3,4] This paper shows how to develop such relations for polyhedral shaped particles dispersed in a solid and how a digital computer is of aid in the development. Double trigonometric integral equations are required, and for simple cases exact analytical solutions can be determined. A digital computer program prepared for solution of the integrals provides verification of the analytical results and permits extension to analyses of more complex polyhedral shapes.

NUMBER OF POLYHEDRAL PARTICLES PER UNIT VOLUME

For a system of particles of given shape, uniform size, and randomly oriented and dispersed within an opaque solid, the relation connecting number present per unit volume, N_V , with average number sectioned per unit area, N_S , is

$$N_S = N_V \cdot P_S \qquad (1)$$

where P_s is the probability that a single randomly oriented particle within a unit volume will be cut by a unit section. This probability equals the distance between top and bottom tangent planes, averaged over-all particle orientations. This average tangent distance may be called $\bar{D}$. The general expression for $\bar{D}$ has been shown (4) to be

$$\bar{D} = \frac{1}{4\pi} \int_{\theta=0}^{2\pi} \int_{\phi=0}^{\pi} D(\phi,\theta) \sin \phi \, d\phi \, d\theta \tag{2}$$

which involves averaging or summing over all orientations of a spherical coordinate system. It is ordinarily possible and more convenient to sum over a smaller but still representative orientation range, as the symmetry of the particle shape allows. For instance, averaging orientations within one octant requires the following form of the expression:

$$\bar{D} = \frac{2}{\pi} \int_{0}^{\pi/2} \int_{0}^{\pi/2} D(\phi,\theta) \sin \phi \, d\phi \, d\theta \tag{3}$$

The tangent plane distance $D(\phi,\theta)$ for a polyhedron is the resolved distance between top and bottom polyhedron corners for any orientation, always taken normal to the sectioning plane. The corners of the polyhedron can be assigned coordinates in a rectangular coordinate system, and if the "z" direction is taken normal to the sectioning plane, the tangent plane distance will be

$$D(\phi,\theta) = (x_2-x_1) \sin \theta \sin \phi + (y_2-y_1) \cos \theta \sin \phi + (z_2-z_1)\cos\phi \tag{4}$$

where $(x_1 y_1 z_1)$ and $(x_2 y_2 z_2)$ are the coordinates of the top and bottom corners respectively and the directions have the sign convention of Figure 1. Thus for a cubic particle of edge length "a", we have

$$D(\phi,\theta) = a[(\sin\theta + \cos\theta)\sin\phi + \cos\phi] \quad (5)$$

Substituting Equation (5) in Equation (3) and integrating gives the following result

$$\bar{D}\ (\text{cube}) = \frac{3}{2}\ a = 1.5a \quad (6)$$

Thus for a system of uniformly sized cubic particles we can determine number per unit volume from

$$N_s = N_v \cdot \frac{3}{2}\ a \quad (7)$$

A simple extension of the above analysis leads readily to following results:

Rectangular Parallelepiped $(a \neq b \neq c)$ $\quad \bar{D} = \frac{1}{2}(a+b+c)$ (8)

Rectangular Thin Plate $(a \neq b,\ c \approx 0)$ $\quad \bar{D} = \frac{1}{2}(a+b)$ (9)

Long Rod $(a,\ b \approx c \approx 0)$ $\quad \bar{D} = \frac{1}{2}(a)$ (10)

Cubes have still higher symmetry than represented in an octant of orientations, and, in fact, all orientations are present to a proportional degree within an angular range covered by the spherical triangle having as corners the poles 001, 101, and 111. This triangle is 1/48th of a sphere and has limits of $\theta = 0$ to $\pi/4$ and $\phi = 0$ to

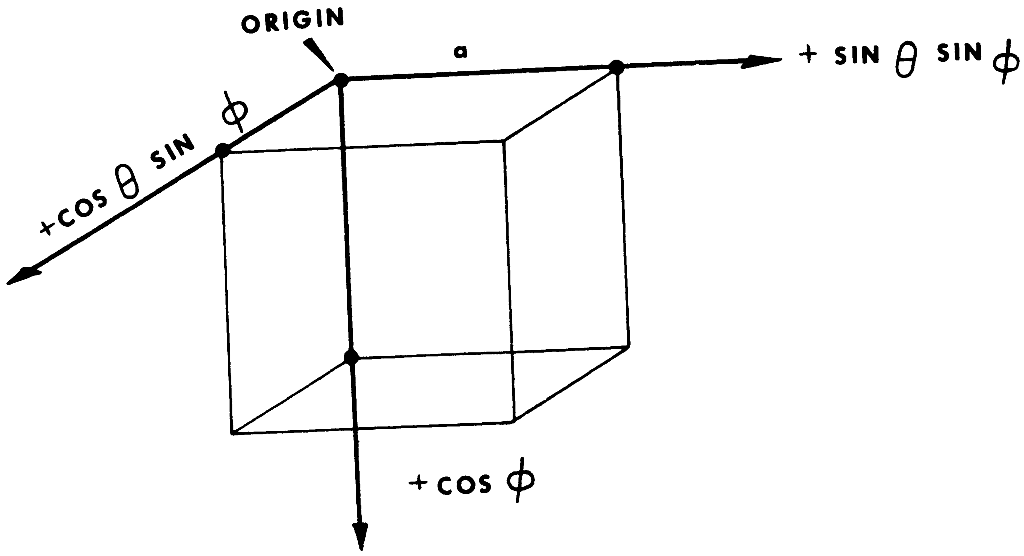

Figure 1. Cubic Coordinate Direction System.

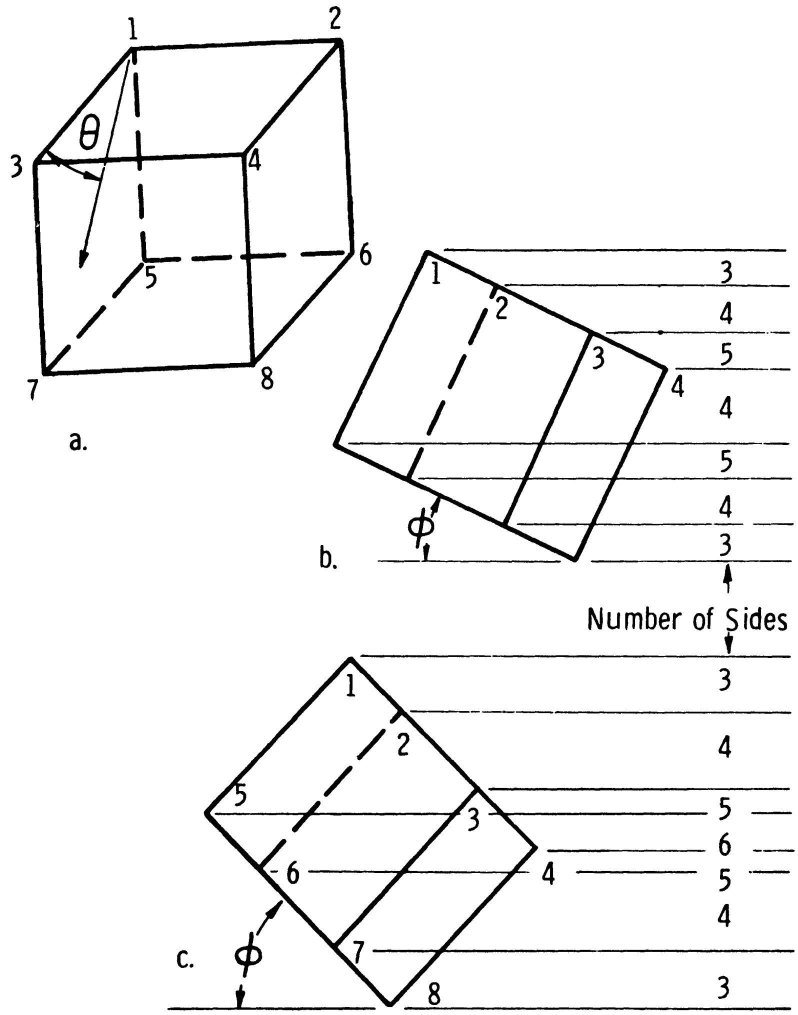

Figure 2. Projected Heights of Cubes Which Give Rise to Sections with Various Numbers of Sides.

arccot (cos Θ). Using these data in the basic Equation (2), we have

$$\bar{D}(\text{cube}) = \frac{12a}{\pi}\int_0^{\pi/4}\int_0^{\text{arccot}(\cos\Theta)}[(\sin\Theta+\cos\Theta)\sin\phi+\cos\phi]\sin\phi\, d\phi\, d\Theta \quad (11)$$

which, on integration, gives an identical result for $\bar{D}$(cube). Although the integration of Equation (11) is more difficult than the previous octant case, use of the smallest representative integration range is extremely valuable in reducing the redundancy in all but the simpliest of cases.

The sectioning probability or average tangent distance $\bar{D}$ of several other polyhedrons possessing cubic symmetry is most readily computed by determining the top and bottom corners, inserting their relative coordinates in the equation as before, and integrating over this same 1/48th spherical triangle. This has been done for the octahedron, tetrahedron, rhombic dodecahedron, and tetrakaidecahedron. In the case of the rhombic dodecahedron, this angular range must be subdivided into two smaller triangles, as two different pairs of corners become involved as top and bottom, depending on the orientation, and two integrals are required. The integral equations for all these cases can be put in the form

$$\bar{D} = A\int_C^B\int_E^D [(F\sin\Theta + G\cos\Theta)\sin\phi + H\cos\phi]\sin\phi\, d\phi\, d\Theta \quad (12)$$

In each of the present cases the relative corner distances are taken in units of "a" , which is the edge length of a cube circumscribed about the particular polyhedron. The data for the required integrals are tabulated below:

TABLE I

Data for Equation (12)

	Octahedron	Tetrahedron	Rhombic Dodecahedron 1	Rhombic Dodecahedron 2	Tetrakaidecahedron
A	$12\ a/\pi$	$12\ a/\pi$	$12\ a/\pi$	$12\ a/\pi$	$12\ a/\pi$
B	$\pi/4$	$\pi/4$	$\pi/4$	$\pi/4$	$\pi/4$
C	0	0	0	0	0
D	arccot $(\cos\theta)$	arccot $(\cos\theta)$	arccot $(\sin\theta+\cos\theta)$	arccot $(\cos\theta)$	arccot $(\cos\theta)$
E	0	0	0	arccot $(\sin\theta+\cos\theta)$	0
F	0	0	0	1/2	0
G	0	1	0	1/2	1/2
H	1	1	1	1/2	1
Answer	$\frac{a3\sqrt{2}\text{arccot}\sqrt{2}}{\pi}$	$\frac{a3\sqrt{}\arctan\sqrt{2}}{\pi}$	$a\sqrt{3}/2$		$3a/2\sqrt{2}$
$(\bar{D})$	= 0.8312a	= 1.2901a	= 0.8660a		= 1.0607a

The solutions to the integral equations arising from the data of Table I are also listed in the table. As many be seen, exact analytical solutions are obtainable, although the evaluation is sufficiently complex that a computer would be of great aid if many equations were to be solved.

SHAPES OF POLYHEDRON SECTIONS

The shapes of sections obtained from polyhedrons and their expected relative frequencies are of more than academic interest to the metallographer, because the clues to the three-dimensional structure must be obtained from the two-dimensional section. Plane sections of cubes may have three to six sides, while sections of tetrahedrons have three or four sides, octahedrons four to six sides, rhombic dodecahedrons three to nine sides, and tetrakaidecahedrons three to ten sides. An experimental determination of the relative frequencies of sections of cubes and tetrakaidecahedrons has been made by observations on wire models.[5]

It is possible by the procedure for obtaining sectioning probabilities of polyhedrons to determine analytically the relative frequencies of types of sections. Just as the tangent plane distance between top and bottom corners gives the chance that a particle will be sectioned, it is the regions between parallel planes passing through corners of the polyhedron that govern the type of section obtained. Refer, for example, to Figure 2 to see how orientation of the cube as well as location of the cut determine the section type. The average normal distances between corners over the appropriate orientation ranges give the relative frequencies of sections. Equation (12) is just the right equation to use, requiring only to determine the proper coefficients and integration limits and then to evaluate. Figure 2 for the cube shows what corners are involved for the various sections, and Equation (4) is used to get the coefficients for each pair of corners. The map of a spherical octant in Figure 3 shows the orientation ranges over which different cube sections are possible, and a series of six integral equations can be set up similar to those of Table I that will lead to the desired results.

Determination of the frequencies of section types is still easier for the octahedron and tetrahedron but becomes more complicated for the rhombic dodecahedron, which requires 18 equations, and the tetrakaidecahedron of Figure 4, which requires 204 equations and consideration of 77 separate sub-regions, as shown in Figure 5. The $\phi(\theta)$ values on the diagram which are used as integration sub-limits are most conveniently expressed as inverse cotangent functions; for example, referring to Figure 5, $\phi_{15} = \text{arccot}\,(\frac{3}{2}\cos\theta - \frac{1}{2}\sin\theta)$. The procedures for setting up the integral equations are described in more detail elsewhere.[6] Because the integral equations contain fairly complicated inverse trigonometric functions and because of the large number involved, a digital computer was utilized in their evaluation.

COMPUTER SOLUTION OF TRIGONOMETRIC INTEGRALS

The basic integral equation of the general form used to solve all sectioning problems for polyhedrons is, as given earlier,

$$\overline{D} = A \int_C^B \int_E^D [(F\sin\theta + G\cos\theta)\sin\phi + H\cos\phi]\sin\phi \, d\phi \, d\theta \qquad (12)$$

$\overline{D}$ gives the average vertical distance between two fixed points or corners,

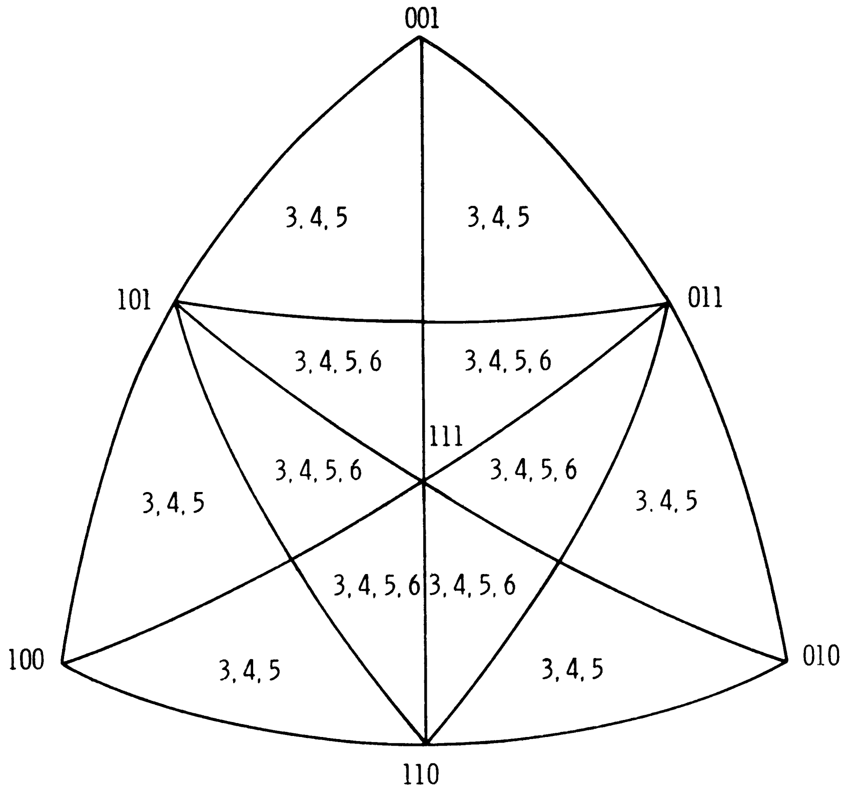

Figure 3. Spherical Octant Showing What Types of Sections Can Be Obtained on Sectioning Within the Various Angular Ranges.

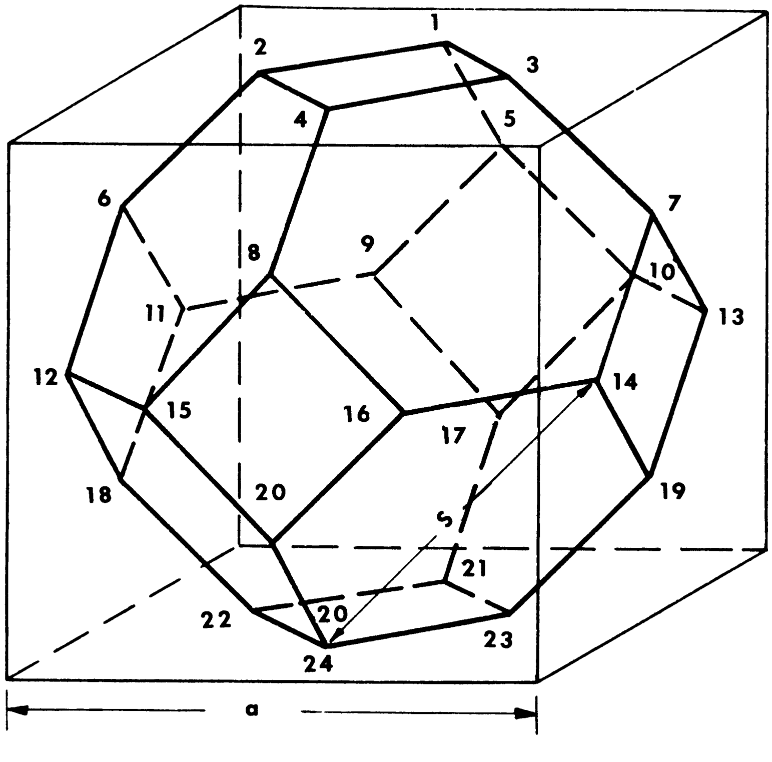

Figure 4. Tetrakaidecahedron.

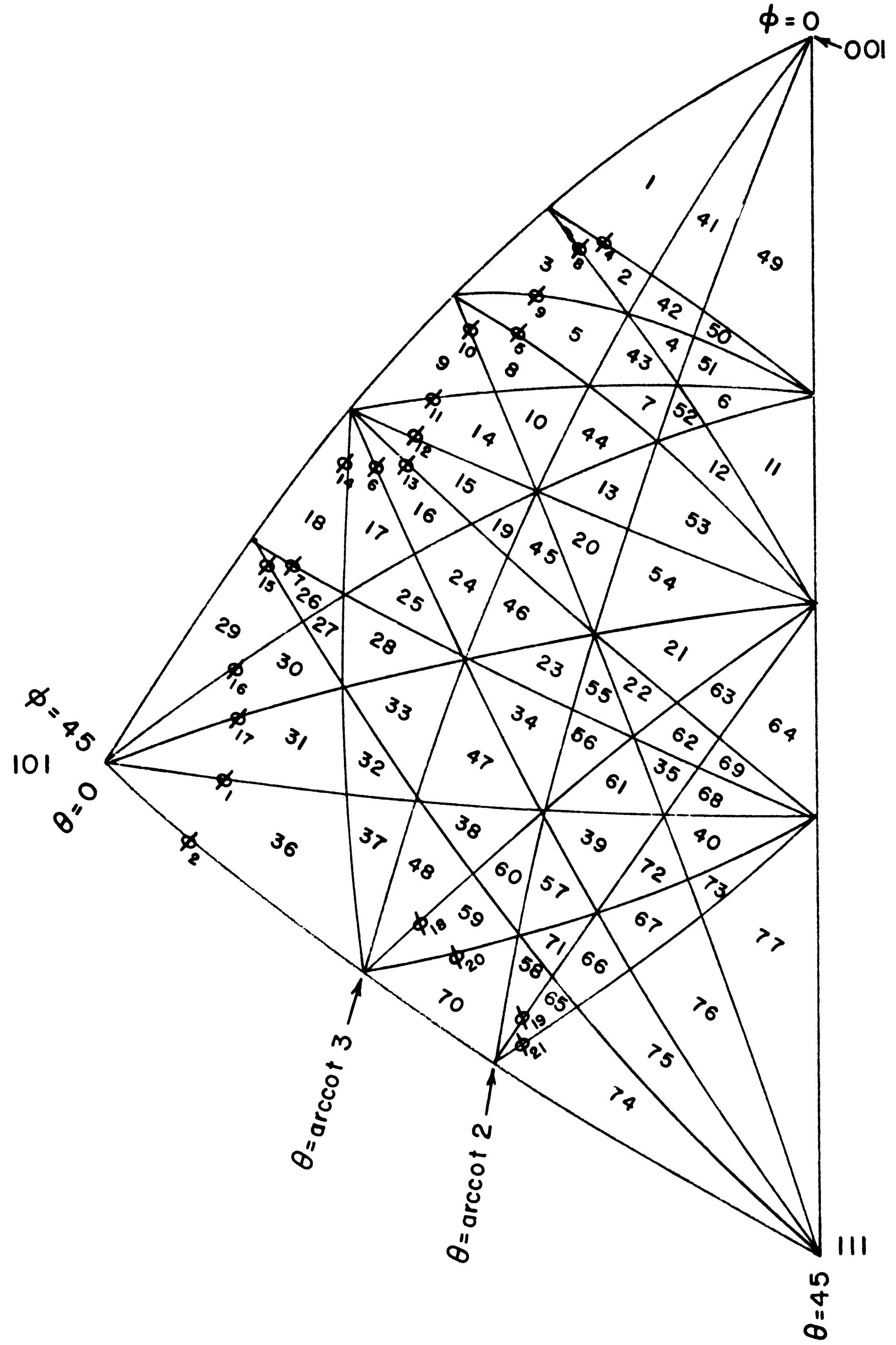

Figure 5. Spherical Triangle Showing the Seventy-seven Subsections Over Which Integration Must be Performed for the Sections of a Cubic Tetrakaidecahedron.

whose coordinates relative to each other for $\theta=0$ and $\phi=0$ are given by the coefficients F, G, and H, as their spatial orientation is changed over the ranges B to C and D to E. The coefficient A is $12a/\pi$ for orientations that are restricted to the spherical triangle represented by the 001, 101, and 111 poles, where "a" is the edge length of a cube circumscribing the polyhedron. Angles B and C are given in radians, and angles D and E are ordinarily given as inverse cotangent functions of $\sin\theta$ and $\cos\theta$. For example, $E(\theta) = \text{arccot}\,(E_1 \sin\theta + E_2 \cos\theta)$.

In order to evaluate Equation (12) for the cases described in this paper, a program was prepared for an IBM 7090 Digital Computer. The main program utilized two sub-routines, one being a Simpson's rule integration sub-routine in the computer's tape library, and the other being a sub-routine prepared to evaluate the function.

In order to evaluate this function as a single integral instead of a double integral, it was integrated once and placed in the form

$$\bar{D} = \frac{A}{2}\int_C^B [(F\sin\theta + G\cos\theta)(D-E-\sin D\cos D + \sin E\cos E) + H(\sin^2 D - \sin^2 E)\,d\theta \quad (13)$$

This is the function evaluated by the computer. A, B and C are given in the input as radians; F, G and H are numbers, either rational or irrational, positive or negative. D and E, normally being in the form $E(\theta) = \text{arccot}$ $(E_1 \sin\theta + E_2\cos\theta)$, required that D_1, D_2, E_1, and E_2 all be read into the computer.

The previously given exact analytical results for average tangent distance of various polyhedrons were used as a check on the computer programming and operation. An additional check on the computation of frequencies of polyhedron sections was that the sum of the types of sections should equal the total for the polyhedron. Thus, for the tetrakaidecahedron, 204 separate integral equations were required to total 1.0607a. When this actually occurred to within 0.000045, the results were taken as correct. The program, function sub-routine, flow diagram, and computer print-out of input data and results are available elsewhere.(6) The relative frequencies of the various types of sections of the 5 polyhedrons considered are given in Table II.

The utilization of the computer has been of very great aid in obtaining the results given in Table II, and for the frequency of tetrakaidecahedron sections the computer was virtually essential. The computer integration technique can be used in analyzing sectioning possibilities for other polyhedrons, especially when the integration limits are complicated inverse trigonometric functions, as generally is the case. The same function sub-routine should be adequate for all such problems, and the programming and evaluation would prove far easier than preparation of the input data.

TABLE II

RELATIVE FREQUENCIES OF SECTIONS (%)

Sides on Section	Polyhedron Cube	Octahed.	Tetrahed.	Rh. Dod.	Tetrakai.
3	28.0	-	71.2	4.0	7.3
4	48.7	44.8	28.8	13.4	13.4
5	18.7	-	-	16.2	11.8
6	4.6	55.2	-	29.9	31.2
7	-	-	-	19.1	18.3
8	-	-	-	16.3	13.1
9	-	-	-	1.1	3.8
10	-	-	-	-	1.1

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