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FIGS. 1-5, MARCH, 1970

AN EXACT METHOD FOR CHARACTERIZATION OF GRAIN SHAPE[1]

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ABSTRACT

Grain shape may be described as precisely as needed by Fourier series expansion of the radius about the center of mass utilizing coordinates of peripheral points. Empirical results of grains from typical samples indicate that the series contains, in partitioned form, a large amount of geologically interesting information. Consequently, previous subjective evaluations of the worth of shape variations in the solution of geologic problems are justified. The shape variable is amenable to semiquantitative graphical evaluation or may be used as data for multivariate analytical schemes. Illustrative examples show that the shape variables easily discriminate grain differences arising from geographic, stratigraphic, and process factors.

INTRODUCTION

The lack of general utility of grain-shape data for the solution of geologic problems is not a reflection of current or past disinterest in grain-shape as an important diagnostic criterion. General reasons for the value of shape data can be found in beginning texts in sedimentology—petrology (Spock, 1953, Pettijohn, 1957, Bayly, 1968). In addition, measurement schemes designed to quantify shape characteristics have appeared regularly (ref. cited in: Krumbein and Pettijohn, 1938; Pettijohn, 1957; Lees, 1964; Griffiths, 1967.) However, few, if any, subsequent researchers have successfully used shape statistics as a basic parameter.

Part of this failure to exploit a widely recognized primary petrologic variable might be ascribed to the relatively few numbers of petrologists engaged in "grain petrology." However, much resides with conceptual or operational problems associated with the aforementioned measurement schemes.

A fundamental problem in shape quantification lies in the difficulty of developing a variable that unambiguously treats (and separates) shape characteristics of different magnitude. A generally accepted method is to separate the "shape-variable" into two parts: gross shape (sphericity) and relatively smaller-scale directional changes of the grain surface (roundness or angularity). Both qualities have long been observed and noted qualitatively. In addition, Wadell (1933) has shown these qualities to be logically independent (e.g. one can produce a series of shapes that demonstrate that change in one does not affect the value of the other).

"Sphericity" is usually expressed as a set of ratios of a unique set of axial measurements (from Zinng, 1935 in Pettijohn, 1957) and is usually obtained with operational ease; whereas "roundness" and its ilk involves a potentially large number of complex operations on each single grain (Krumbein and Pettijohn, 1938; Lees, 1964).

Acceptance of these two shape variables involves concomitant acceptance of certain underlying assumptions on the nature of natural shape variation. Orthogonal axial measurements are most effective for shapes of regular symmetry and decrease in value as grain shape departs from this condition. Use of two separate, conceptually independent variables to describe a single shape seems to imply that real shape variation is composed of distinctly-scaled "shape-quanta." Both assumptions are *a priori* and can only be evaluated by empirical tests. Indeed, at this stage, it may be safer to assume *a priori*, that shape characteristics operate over a continuum, and may not be strongly controlled by symmetry laws.

In addition to "theoretical" problems, dichotomous shape variables possess the unfortunate intrinsic property that precision of estimate is either arbitrarily fixed in the case of sphericity or, with roundness, is a variable out of direct control of the investigator. A more desireable measurement scheme would allow the investigator to set a level of precision (by stipulating the number of measurements or measurement arrays per grain) consonant with his resources and interests.

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Griffiths (1967, p. 110) has outlined a measurement technique that leaves the number of measurements per grain to the choice of the investigator and, at the same time, attacks the problem of irregular geometry. His solution yields a stochastic picture of shape—composed of a nested set of means and variances. Grain shape is thereby analyzed by mathematical "dismemberment" of the grain and a subsequent synthesis of partially ordered fragments by analysis of variance techniques. This approach, attractive from both theoretical and operational viewpoints, may well be the nucleus of a well-accepted shape measurement scheme.

Described below is yet another shape describing technique. It shares with Griffith's method, a sensitivity to irregular shapes and operational simplicity as well as an implicit requirement for modern data-processing facilities. A major difference is that this method yields a mathematical model of the grain that will regenerate the grain shape as precisely as required. In addition, by representing grain shape as a linear equation with an indefinite number of terms, with each term representing the contribution of a known shape component, shape and changes in shape can be readily analyzed or monitored. Although values of the terms of the shape equation can be used as an end result in shape analysis, they should prove to be most valuable as a source of data for further analysis.

METHOD

Shape properties of sand grains from a variety of deposits are used to illustrate the nature and utility of the method for analyzing variation of twodimensional maximum-projection-area grain-shape. Generalization of the scheme to three-dimensional grain shape is relatively straightforward both analytically and operationally and will be described in a later paper.

Grain shape is estimated by an expansion of the periphery radius as a function of angle about the grain's center of gravity by a Fourier series. The radius is therefore given by:

$$R(\theta) = R_0 + \sum_{n=1}^{\infty} R_n \cos (n\theta - \phi_n) \qquad (1)$$

where θ is the polar angle measured from an arbitrary reference line. The first term in the series, R_0, is equivalent to the average radius of the grain in the plane of interest. For the remainder of the terms, n is the harmonic order, R_n is the harmonic amplitude, and ϕ_n is the phase angle. As an illustrative example, several harmonic figures are shown in figure 1. Observe that the n'th harmonic contributes as a figure with n "bumps." That is, the "zeroth" harmonic is a centered circle with an area equal to the total area, the first harmonic is an offset circle, the second is a figure eight, and the third is a trefoil. The center of gravity of the shape is chosen as the origin of the radius expansion to simplify interpretation of the generated series.

Coordinates of points on the periphery of the grain are necessary for expansion. At least twice the number of points must be known as the number of the highest desired harmonic. The initial origin of the periphery points may be arbitrary. That is, the coordinates of points on the grain margin may possess any origin—external or internal to the grain—because later in the analysis a transformation will place the origin at the grain center.

Digitization of the periphery can be done by projecting the grain on a grid and recording the intercepts manually or using an automatic "digitizer" that determines coordinates and punches them directly on data cards.

Essentially the method of analysis commences by calculating from the rectangular periphery coordinates the center of gravity of the grain. Once the center of gravity is known, the periphery points are converted to polar coordinates and therefrom the two Fourier coefficients for each harmonic are calculated.

CENTER OF GRAVITY DETERMINATION

Let the grain be represented by an ordered set of L points counterclockwise about its periphery as shown in fig. 2. If a straight line approximation between the points is used, the equation for the j'th segment existing between point j and $j+1$ is

$$Y_j(X) = \frac{(Y_{j+1} - Y_j)X + (X_{j+1})(Y_j) - (X_j)(Y_{j+1})}{X_{j+1} - X_j} \qquad (2)$$

The area of the j'th trapezoid, bounded by the segment and axis, is for counter-clockwise rotation

$$\begin{aligned} A_j &= -\int_{X=X_j}^{X_{j+1}} \int_{Y=0}^{Y_j(X)} dY dX \\ &= \frac{(Y_{j+1} + Y_j)(X_j - X_{j+1})}{2} \end{aligned} \qquad (3)$$

The first moment about the X-axis for the j'th trapezoid is

$$\begin{aligned} My_j &= -\int_{X=X_j}^{X_{j+1}} \int_{Y=0}^{Y_j(X)} Y\, dY\, dX \\ &= \frac{(Y_{j+1}^2 + (Y_{j+1})(Y_j) + Y_j^2)(X_j - X_{j+1})}{6} \end{aligned} \qquad (4a)$$

If equation (1) is solved for X rather than Y, then in a similar fashion, the first moment about the Y-axis is

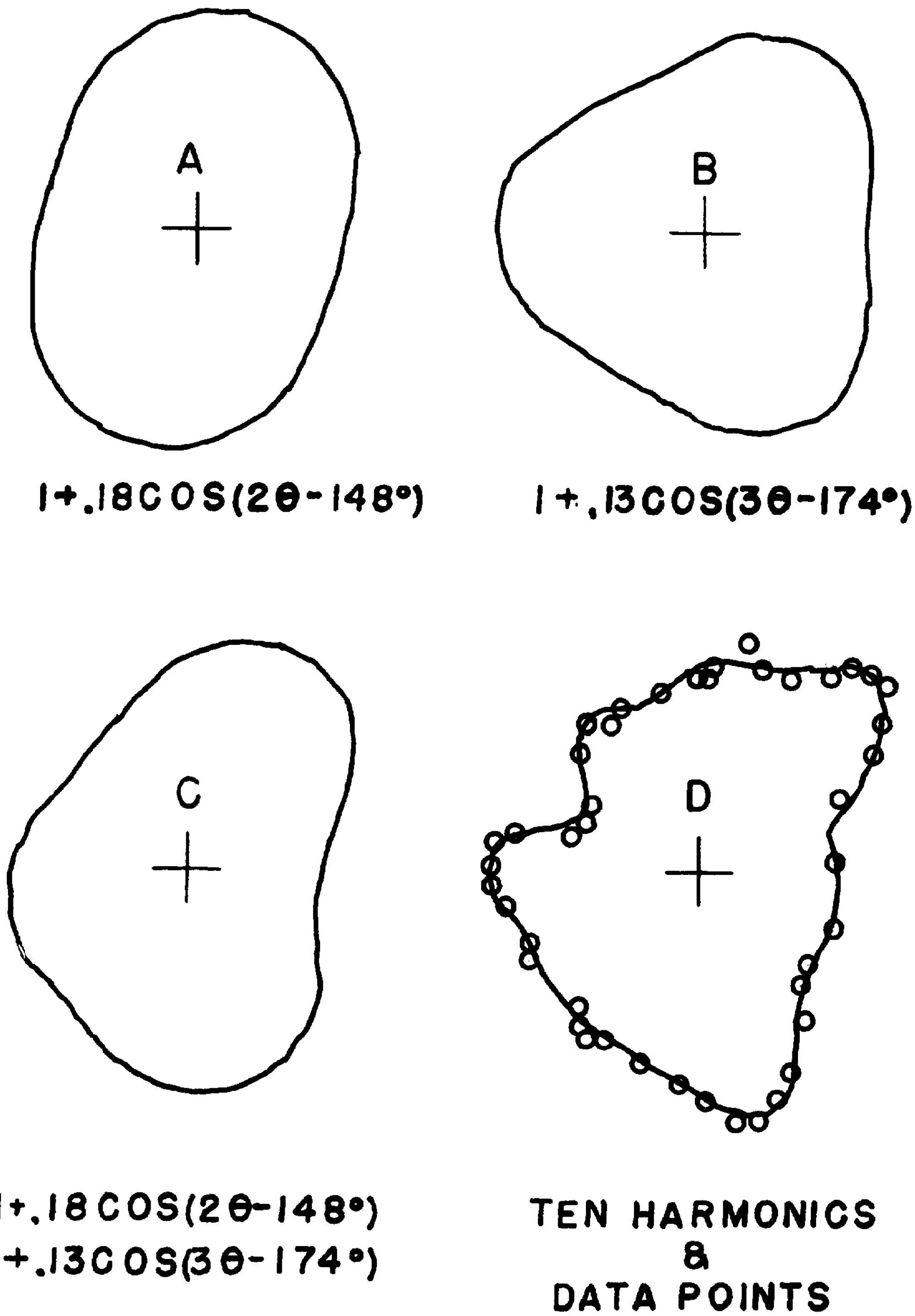

FIG. 1.—Harmonic contributions to shape.

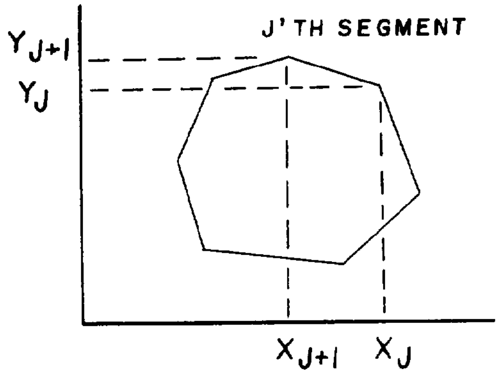

FIG. 2.—Coordinate system.

$$Mx_j = -\int_{Y=Y_j}^{Y_{j+1}} \int_{X=0}^{X_j(Y)} X\,dX\,dY = \frac{(X_{j+1}^2 + (X_{j+1})(X_j) + X_j^2)(Y_j - Y_{j+1})}{6} \tag{4b}$$

The coordinate of the grain centroid is given by dividing the appropriate total moment by the total area. Therefore, because of the ordering of the points and the sign convention

$$\overline{Y} = \frac{\sum_{j=1}^{L} My_j}{\sum_{j=1}^{L} A_j} \tag{5a}$$

$$\overline{X} = \frac{\sum_{j=1}^{L} Mx_j}{\sum_{j=1}^{L} A_j} \tag{5b}$$

Each point on the periphery may be expressed in polar coordinates about the center of gravity as

$$R_j = \sqrt{(Y_j - \overline{Y})^2 + (X_j - \overline{X})^2} \tag{6a}$$

$$\theta_j = \mathrm{Tan}^{-1} \frac{Y_j - \overline{Y}}{X_j - \overline{X}} \tag{6b}$$

For the purpose of evaluation, it is convenient to transform the Fourier series of equation (1) to the form

$$R(\theta) = R_0 + \sum_{n=1}^{\infty} A_n \cos n\theta + \sum_{n=1}^{\infty} B_n \sin n\theta \tag{7}$$

wherein the transformations are

$$A_n = R_n \cos \phi_n \tag{8a}$$

$$B_n = R_n \sin \phi_n \tag{8b}$$

Utilizing the orthoganality properties of sine and cosine, the Fourier coefficients may be evaluated as

$$R_0 = \frac{1}{2\pi} \int_0^{2\pi} R(\theta)d\theta = \frac{1}{2\pi} \sum_{j=1}^{L} \int_{\theta_j}^{\theta_{j+1}} R_j(\theta)d\theta \tag{9a}$$

$$A_n = \frac{1}{\pi} \int_0^{2\pi} R(\theta) \cos n\theta d\theta = \frac{1}{\pi} \sum_{j=1}^{L} \int_{\theta_j}^{\theta_{j+1}} R_j(\theta) \cos n\theta d\theta \tag{9b}$$

$$B_n = \frac{1}{\pi} \int_0^{2\pi} R(\theta) \sin n\theta d\theta = \frac{1}{\pi} \sum_{j=1}^{L} \int_{\theta_j}^{\theta_{j+1}} R_j(\theta) \sin n\theta d\theta \tag{9c}$$

where $R_j(\theta)$ is the polar coordinate equation for the j'th segment. Assuming the radius to be a linear function of angle between the periphery points, then

$$R_j(\theta) = \frac{(R_{j+1} - R_j)\theta + (R_j)(\theta_{j+1}) - (R_{j+1})(\theta_j)}{\theta_{j+1} - \theta_j} \tag{10}$$

Corroboratively, substituting equation (10) into equations (9) yields for the Fourier coefficients:

$$R_0 = \frac{1}{4\pi} \sum_{j=1}^{L} (R_{j+1} + R_j)(\theta_{j+1} - \theta_j) \tag{11a}$$

$$A_n = \frac{1}{\pi} \sum_{j=1}^{L} \left[\frac{(R_{j+1} - R_j)(\cos n\theta_{j+1} - \cos n\theta_j)}{(\theta_{j+1} - \theta_j)n^2} + \frac{R_{j+1} \sin n\theta_{j+1} - R_j \sin n\theta_j}{n} \right] \tag{11b}$$

$$B_n = \frac{1}{\pi} \sum_{j=1}^{L} \left[\frac{(R_{j+1} - R_j)(\sin n\theta_{j+1} - \sin n\theta_j)}{(\theta_{j+1} - \theta_j)n^2} - \frac{R_{j+1} \cos n\theta_{j+1} - R_j \cos n\theta_j}{n} \right] \tag{11c}$$

The computational effort required to describe a grain in this manner is minimal. For a typical grain with 40 peripheral points, about 1.5 seconds of CDC 3600 computer time are required to obtain the first ten harmonics.

LIMITATIONS OF METHOD

Regardless of the grain configuration, the method presented correctly locates the center of gravity within limitations of numerical accuracy. However, a Fourier series is only useful in expanding a single valued function. Therefore embayments, if present, must be of such a shape or be represented by a set of peripheral points such that a radius drawn from the grain center of gravity will intersect only one peripheral point.

Whether this weakness will severly impair the method cannot be known without extensive empirical results. To date, however, Fourier estimates of maximum projection area shapes of several thousand sand grains taken from a variety of recent and ancient deposits have not been greatly affected by the presence of double-valued functions.

The computer program developed for this analysis rejects points which would cause bivaluedness and indicates this on the printed output. Inspection of those grains so labelled indicates that a significant number were manifestations of obvious coding errors; others, although correctly coded, could be modified without loss of shape data by slightly shifting points. A few possessed truly double valued points that could not be shifted without introducing gross error into the empirical grain outline. These were excluded from the results. If this inability to describe such deeply and complexly embayed grains proves serious in practice, then a more complex analysis must be undertaken. Figure 1 illustrates the relationships between shapes resulting from various components of the Fourier series with the actual profile of the grain the series approximates. Figure 1a represents the combination of the "zeroth" harmonic (the figures are always "normalized" such that the coefficient of this, the centered circle, is unity) and the second harmonic—a "figure eight." The coefficient ".18" weights the relative contribution of this harmonic, and the offset angle

$$\left(\alpha = \frac{\phi_n}{n} = 74°\right)$$

orients the harmonic with respect to the coordinate system.

Figure 1b illustrates the combination of the centered circle with the third harmonic for the same grain; and 1c illustrates the combination of the three orders. The grain outline in figure 1d is that generated by a Fourier series of ten harmonics. Centers of the small circles surrounding the figure represent actual points on the periphery of the original grain. The "fit" of the computed shape to the empirically determined peripheral points can be improved from that represented by figure 1d by simply adding more terms to the series assuming enough peripheral points are present. An important result of this is that, if as assumed, grain shape carries information, then *all* that information must reside somewhere within the shape equation, since the shape may be described mathematically as precisely as desired.

EXAMPLES

Although the shape equation may be used directly in a semiquantitative fashion, it should have greatest utility as a source of data for further analysis. Analysis of shape variation, whatever the technique, falls into two general categories: discrimination and monitoring. Discrimination involves determination of differences

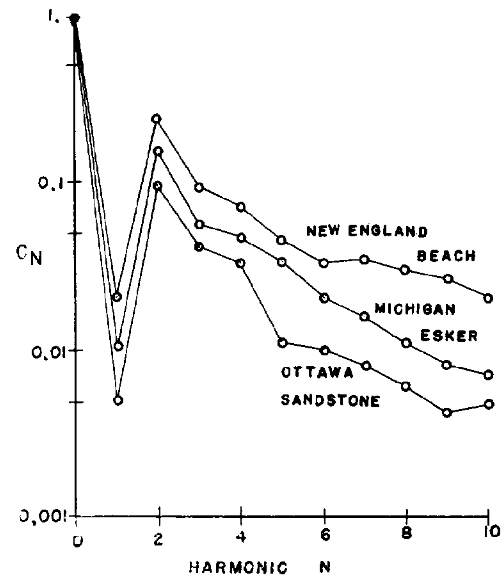

FIG. 3.—Mean amplitude spectra of quartz from three sands.

between categories that are, or might be, distinctly different; whereas monitoring concerns determination (of at least the existance) of continuous functional relationships between shape and other variables such as time or space. Examples of the utility of Fourier shape data for these purposes are described below. Weighting coefficients of the series (the "Fourier amplitude spectrum") are the variables used. Although the other variable in the shape equation-phase angle—may be an important vehicle of information, its usefulness is just now being evaluated; analysis being complicated by the usual problems associated with analysis of vectorial data. The information carrying properties of phase angle variation, and the relationships between phase angle, weighting coefficient, and mineralogy will be reported in a later paper.

Discrimination

The amplitude spectrum may be displayed for subjective evaluation by plotting amplitude coefficients against appropriate harmonic numbers. Figure 3 illustrates the mean differences in shape between grains from three samples: sand from a Michigan esker, a New England beach, and the Ottawa Sandstone (a "St. Peter-type" orthoquartizite).

Each plotted coefficient represents the mean values of a sample of twenty six grains for the esker, fourteen from the beach, and thirty-three from the Ottawa Sandstone. Inspection of the figure indicates distinct differences in the shape equations for the three samples. Amplitudes are consistently greater, order for order, for the complexly sculpted grains of the New England beach sample than those from the other samples. The Michigan esker occupies a consistent intermediate position; and values of the Ottawa Sandstone manifest a relatively simple shape by the relatively low position of the coefficients.

A discriminant function was used as a general test for the validity of the mean separations of this graphic display. Coefficients for the first ten harmonics were used as independent variables. The result more than supports the differences displayed in figure 3. On a grain-by-grain basis, the function misclassified only nine grains from a total of seventy three. The probability that differences between all ten means could result from chance variation is much less than .0005 as evaluated by Mahalonobis' D of 136.2 with twenty degrees of freedom.

Monitoring

Analysis of shape variation of quartz grains from samples taken from a soil profile represents a crude example of the potential of the method for "monitoring." The profile, genetically related to underlying gneissose bedrock, is located on an arête adjacent to Juneau, Alaska. The sampled soil is developed on a small elevated knoll on the ridge. The total possible drainage area is less than 2 square meters. Significant changes in shape between the three samples (taken from the "*A*", "*B*", and "*C*" horizons) should indicate a relationship between quartz grain shape and pedogenesis with resulting geochemical implications. This may be manifest as a continuous functional relationship between grain shape and relative position in the soil profile. (Representative grains are shown in figure 4.)

Results of discriminant analysis indicate significant differences between samples (probability of random result less than 0.0005). These results indicate the grains are more complexly sculptured higher in the soil profile. Consistency of grains within a sample are indicated by the low amount of misclassification (four of forty one).

Roughness Coefficient

A quantative index of differences between amplitude spectra (figure 5) of the three samples may be obtained by determination of the average squared deviation of the grain perimeter from a circle of equal area (which in fact is the "zeroth" harmonic). This "roughness coefficient" may be defined as

$$P^2 = \overline{R^2(\theta)} - \overline{R(\theta)}^2 = \frac{1}{2\pi}\int_0^{2\pi} R^2(\theta)d\theta - \left[\frac{1}{2\pi}\int_0^{2\pi} R(\theta)d\theta\right]^2 \qquad (12a)$$

Upon substitution of equation (7), equation (12) becomes upon utilizing the identities of (8):

$$P = \sqrt{1/2\sum_{n=1}^{\infty}(A_n^2 + B_n^2)} = \sqrt{1/2\sum_{n=1}^{\infty} C_n^2} \qquad (12b)$$

Thus the roughness coefficient is simply the square root of one-half the sum of the squared Fourier coefficients.

It is also convenient to consider a modified roughness coefficient spanning a selected range of harmonics rather than all of them. Therefore,

$$P_{jk} = \sqrt{1/2\sum_{n=j}^{k} C_n^2} \qquad (13)$$

Associated P values for the soil profile samples are tabulated in Table 1.

TABLE 1.—*Roughness coefficients for Alaskan profile*

Profile	P_{1-20}	P_{1-10}	P_{11-20}
A	0.123	0.121	0.017
B	0.121	0.120	0.009
C	0.118	0.117	0.011

Subscripts indicate harmonic orders used to calculate P.

Both the amplitude spectra of figure 5 and Table 1 are potentially misleading to the casual observer. At first glance figure 5 suggests that the descending order of roughness is A-C-B while column one of Table 1 suggests A-B-C. Because the magnitude of the Fourier coefficient decreases greatly with increasing harmonic number, the first few coefficients account for the bulk of roughness coefficient but occupy only a small space on the harmonic number axis.

The modified roughness coefficient which arbitrarily utilizes the first ten harmonics indicates that the grains of profile *C* are more circular than the grains of the *A* and *B* profiles. The roughness coefficient utilizing the eleventh through twentieth harmonic indicates that the *B* and *C* level grains are relatively smooth while those of the *A* level are more textured.

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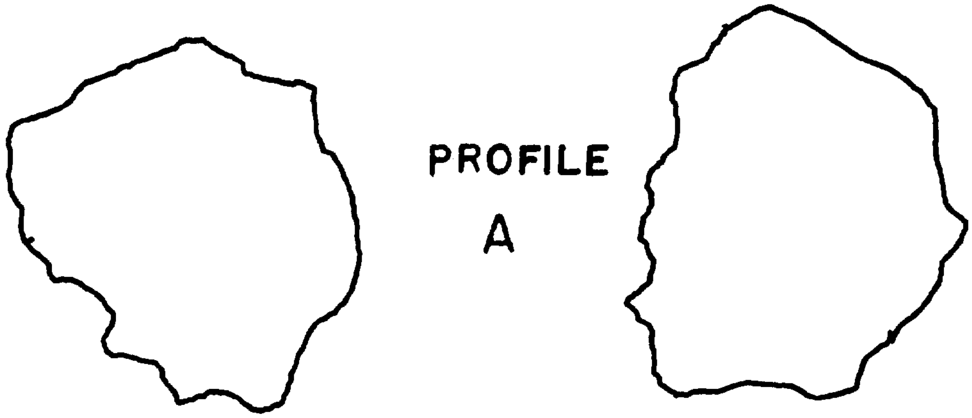
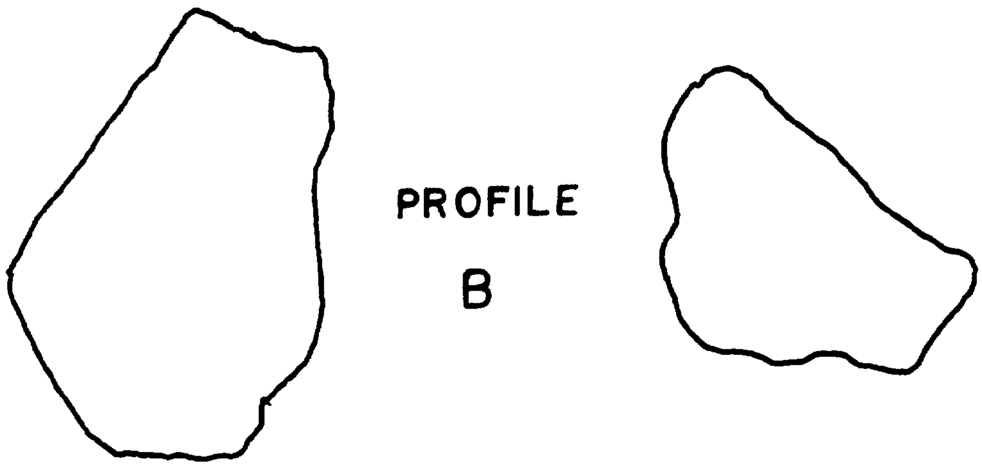
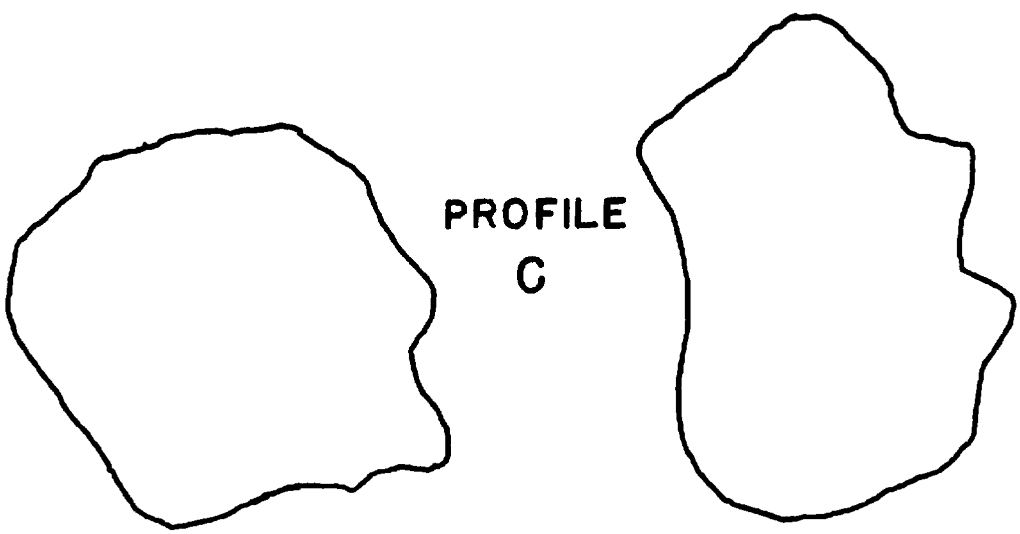
FIG. 4.—Representative quartz grains from Alaksan profile.



PROFILE A



PROFILE B



PROFILE C

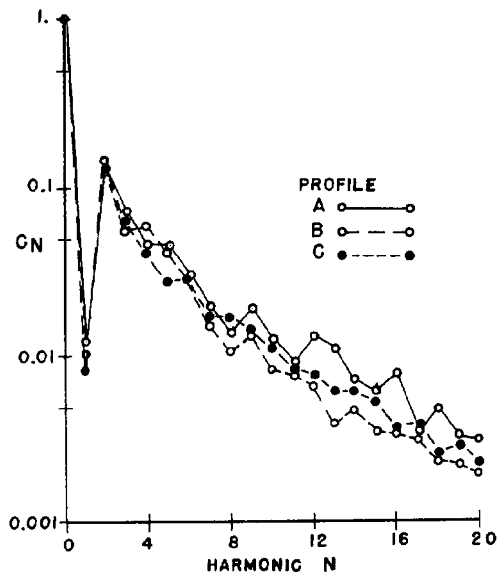


FIG. 5.—Mean amplitude spectra of quartz grains from Alaskan soil profile.

In particular the grains of the C profile are round and smooth and those of the B profile are likened to simple polygons. The shape of the *A* profile grains may be derived from *C* polygons by formation of cusps on the originally fairly straight edges.

Uniform scatter of roughness coefficient values plotted against grain area for the soil samples indicates no relationship whatever between these manifestations of shape and size. Further investigation into the presence of other size-shape relationships are underway.

SUMMARY

The technique described above yields a shape equation that estimates, and can reproduce, two dimensional grain shapes as precisely as needed. A choice of the precision of estimate as well as analytical procedures may be governed by the requisites of a given problem. Input data consists of position coordinates of peripheral points whose total controls the maximum number of valid harmonics generated for a given grain. Analysis of the output can range from direct or indirect uses of the amplitude spectrum, such as a simple graphic display or multivariate analysis, to use of index numbers such as the roughness coefficient which summarize shape variation in a succint manner.

Empirical results indicate that much information is carried by shape characteristics of quartz grains. In fact, results indicate that monomineralic grain shape variation, estimated and partitioned by the Fourier series, may contain amounts of geologically interesting information of similar magnitude as that contained in size or compositional variation. This shape information is distributed across a wide enough spectrum of shape variation so that only modest precision is needed to reveal it. Thus ten harmonics probably represent a degree of "overkill" with regard to solution of many geological problems, although higher orders doubtless carry additional information.

Although the worth of this technique for analysis of detrital sediments has been demonstrated, the authors believe it has equal or greater value for the study of phases that have crystallized *in situ*. Shape variation should thus serve to clarify geochemical aspects of diagenesis. Similarly, insights concerning geochemical-thermodynamic backgrounds of igneous and metamorphic rocks should be gained from this sort of textural analysis.

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