Automated grain shape analysis

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Abstract—A computer programme is used to identify grain boundaries from an image digitized using a transmitted light, *X–Y* recording microdensitometer. For each grain the following parameters are computed: area, length of the long dimension and the width at right angles to it, the location of the center of gravity, perimeter length and the orientation of the long axis. The shape of each grain is described using regular geometric shapes: the enveloping rectangle, the area ellipse and the best-fit ellipse. The data for the individual grains are averaged to yield descriptive parameters for the aggregate.

INTRODUCTION

MANY qualitative descriptions of mineral textures are available but quantified analyses of textural parameters such as grain shape, size and orientation are few, probably because of the difficulty of obtaining adequate data. Barrett (1980) has described three independent properties to define shape, namely form, roundness and surface texture. The present study deals only with form in two dimensions.

Recent analyses of shape parameters have employed Fourier analysis (Ehrlich & Weinburg 1970) or image analysis (Ehrlich *et al.* 1984, Fabbri 1984, Serra 1982). The method used here is based on image analysis using data obtained by an *X–Y* recording microdensitometer from a photomicrograph. A computer programme recognizes the individual grains and eliminates grains which are not completely within the area of the photomicrograph. For each grain the programme also fits regular shapes, rectangles and ellipses to the irregular grain boundaries.

The data obtained for the individual grains are combined and averages for the aggregate are computed. In particular, average ellipses and rectangles are fitted to the data which summarize size, aspect ratio and orientation of the long axes of the grains in the aggregate. The methods are illustrated by a study of pyrrhotite in a specimen from the Calloway mine, Tennessee.

SHAPE ANALYSIS

Although, it is possible to work directly with photographic images of the specimen, in the present study it was decided to use tracings (Fig. 1). The quantification of the image is accomplished by digitization, using an Optronics International Photoscan system P-1000. The density data are measured using a 200 μm aperture placed on a square raster with a spacing of 200 μm; the data are recorded on magnetic tape. A computer programme reads the data from the magnetic tape, identifies the grain boundaries and calculates and stores parameters such as the area, center of gravity, long dimen-

sion and the width at right angles to it, aspect ratio, the length of the perimeter and the angle of inclination of the long dimension of the grain relative to a selected reference direction. Each grain can be drawn on a Calcomp plotter (Fig. 2) for comparison with the acetate tracing (Fig. 1) to verify which grains were analysed.

Once the parameters of all the grains in the aggregate have been measured and recorded any two-dimensional method of shape analysis can be used. The method used here derives a regular geometric form from certain parameters of the irregular grain, thereby transforming the irregular grain into a regular shape which is easy to visualize and from which it is possible to calculate an average.

Two of the geometric shapes frequently used by geologists to describe the form of grains are the rectangle and the ellipse. A rectangle is calculated for every grain in Fig. 2. The long and short dimensions of the rectangles for each grain are shown in Fig. 3. The short axis is calculated to be the maximum perpendicular distance of peripheral points from the long axis.

A best-fit ellipse (Craig *et al.* 1982) is calculated using eigenvalues to derive the ellipse which passes through the grain boundary in such a way that the sum of the squares of the distance between each point on the boundary and the ellipse is minimized. This procedure yields the aspect ratio (long axis vs short axis) and the orientation of the long axis of the ellipse. A scale factor is calculated to permit the best-fit ellipse for each grain in the aggregate to be drawn (cf. Figs. 2 and 4). The scale factor is defined as $a/\pi \cdot \sqrt{R}$, where a is the area and R is the ratio of the eigenvalues.

Figure 5 shows ellipses calculated for each grain of the aggregate shown in Fig. 2 in which the area of the grain is preserved. These 'area ellipses' are calculated using the observed area and long axis of the grain to derive the short axis, $2b$, from the formula $b = A/\pi a$, where A is the area of an ellipse and a is one half of the long axis.

In Fig. 6 the stippled grain from the aggregate shown in Fig. 2 is illustrated surrounded by the rectangle, by the best-fit ellipse and by the area ellipse. Comparison of the shapes shown in Fig. 6 illustrates that the rectangle does not maintain the area of the grain, as do both the area
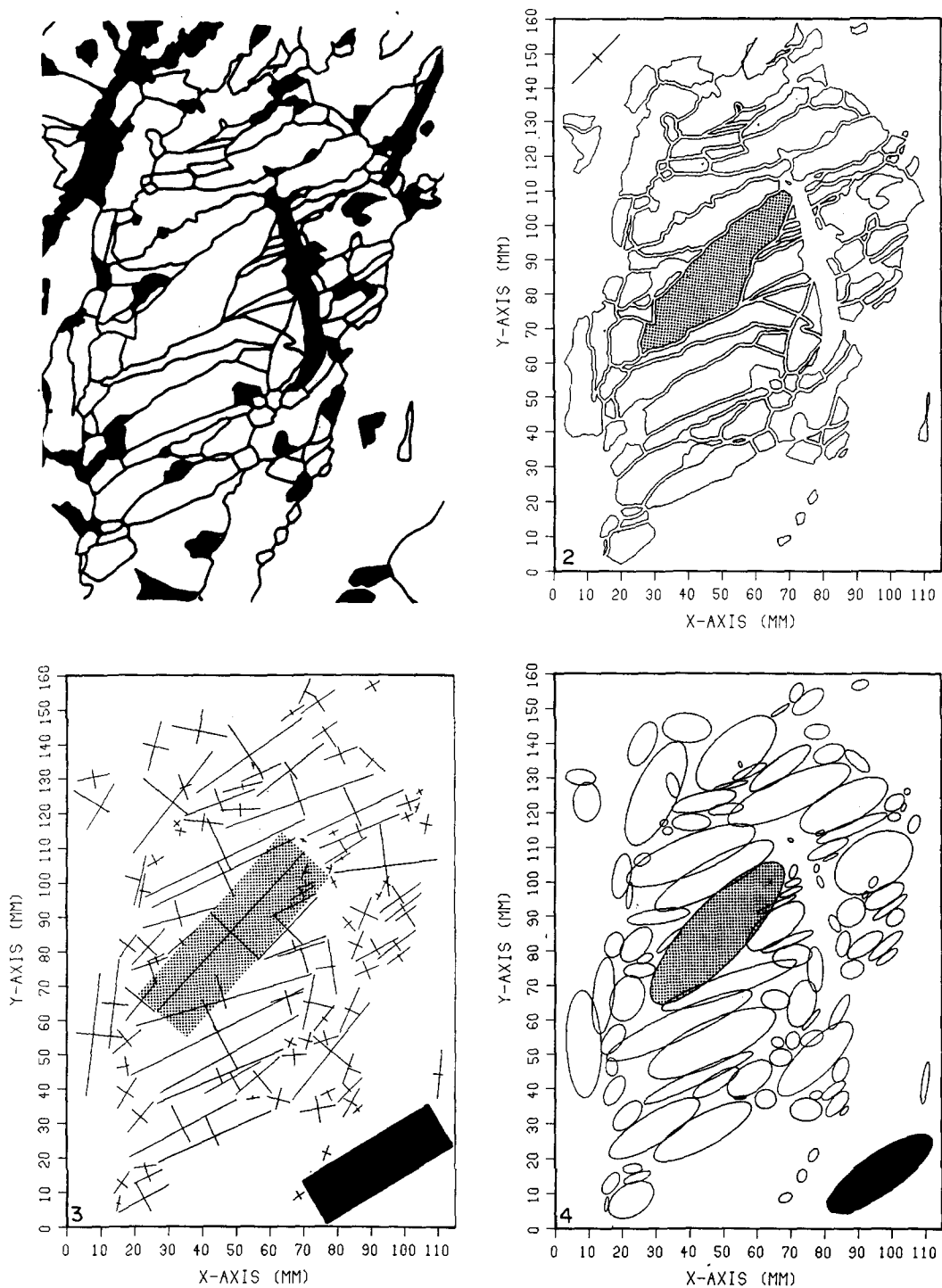
Fig. 1. A tracing of the grain boundaries, prepared originally on transparent acetate. The short dimension corresponds to 0.45 mm on the specimen, which is pyrrhotite.

Fig. 2. The grain boundaries identified automatically and drawn by the computer programme. Note that grains which are not entirely within the image area have been eliminated. The stippled grain is used as an example in Fig. 6. The short dimension of the figure corresponds to 0.45 mm on the specimen. The orientation of the schistosity in the specimen is indicated in the upper left hand corner.

Fig. 3. The computer-drawn long and short axes of the rectangles which enclose the grains shown in Fig. 2. The stippled rectangle is used as an example in Fig. 6. The average rectangle is indicated in black (see text). The short dimension of the figure corresponds to 0.45 mm on the specimen.

Fig. 4. The computer-drawn best-fit ellipses corresponding to the grains shown in Fig. 2. The stippled ellipse is used as an example in Fig. 6. The average best-fit ellipse is indicated in black (see text). The short dimension of the figure corresponds to 0.45 mm on the specimen.
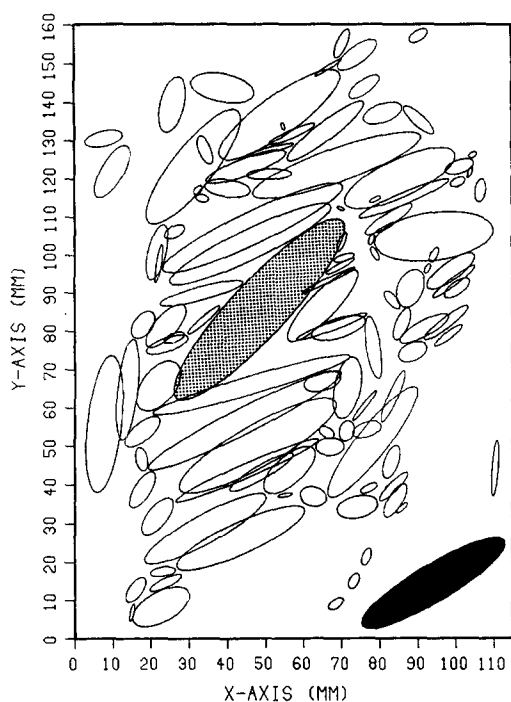
Fig. 5. The computer-drawn area ellipses corresponding to the grains shown in Fig. 2. The stippled ellipse is used as an example in Fig. 6. The average area ellipse is indicated in black (see text). The short dimension of the figure corresponds to 0.45 mm on the specimen.

ellipse and the scaled best-fit ellipse. Also the area ellipse, because it preserves the observed long axis of the grain, emphasizes the elongation, which is the dimension commonly observed subjectively.

STATISTICAL ANALYSIS

Once the size and shape parameters have been obtained for each grain in an aggregate the total sample can be described statistically. The individual parameters for each grain, such as aspect ratio, long axis, short axis, area and perimeter length, can be averaged and average shapes can be derived. Thus, the average rectangle, average area ellipse and average best-fit ellipse are calculated for the same aggregate shown in Fig. 2 and are illustrated in black in the Figs. 3, 4 and 5.

However, the mean orientation of the long axes presents a problem since non-directional observations cannot be averaged using the vector method (Mardia 1972). The method used here to analyse the orientation of the two-dimensional long axes is in some respects similar to the rotational vector procedure used by Mark (1971) for three-dimensional data.

To determine the mean orientation angle, the values between 0 and 180° are selected and averaged. The orientations are measured from the scan direction of the microdensitometer, the long dimensions of Figs. 2–5. For a second iteration the values within 90° of the computed mean are selected and a new mean orientation is calculated. This procedure is continued until a final computed mean is obtained which does not vary significantly from the previously computed mean orientation. The standard deviation of the data around the final computed mean orientation is determined.

The process outlined above is repeated using the orientation angles in the range 90–270° and a second mean orientation and associated standard deviation are determined.

Where the distribution of orientation angles is unimodal the two calculated average orientations converge on a single value. This is illustrated by the data from Fig. 2 which yield the two identical average orientations, 128.2 ± 30.42 and 308.2 ± 30.42, although numerically they are 180° apart.

For comparison with the iterative method described above a method proposed by Krumbein (1939) was used and similar results are obtained (127.33 ± 35.29 and 37.33 ± 69.81; the latter mean would be rejected because of the larger associated standard deviation). A method based on eigenvalues (Mark 1973, Shimamoto & Ikeda 1976, Woodcock 1977) could have been used for the comparison but this reduces to the method used by Krumbein (1939) when applied to two-dimensional data.

The two methods for calculating an average orientation were tested using a set of uniform orientation angles at 5° intervals. The values calculated by the iterative method developed here failed to converge (the means were 87.0 ± 53.36; 4.71 ± 51.72), which is to be expected for a uniform distribution which has no mean
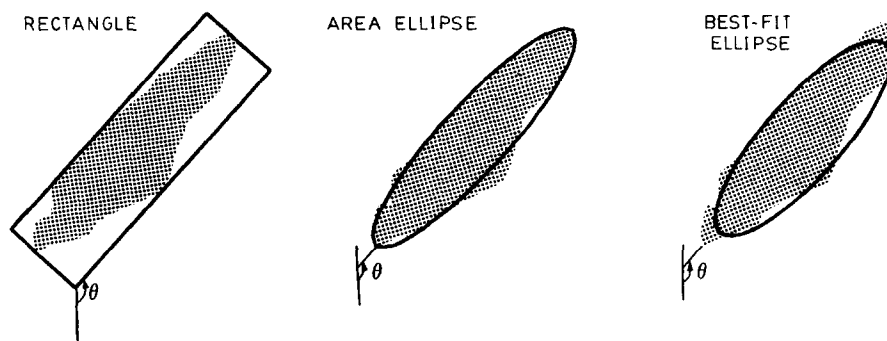

Fig. 6. The stippled grain from Fig. 2 with each of the derived regular shapes used to describe it: the rectangle, the area ellipse and the best-fit ellipse. The long axis of both the rectangle and the area ellipse is 63.8 mm and for the best-fit ellipse it is 54.78 mm. The short axis for the rectangle is 18.84 mm, for the area ellipse it is 14.52 mm and for the best-fit ellipse it is 16.91. The aspect ratio for the rectangle is 3.39:1, for the area ellipse 4.39:1 and for the best-fit ellipse 3.24:1. The orientation angle, θ, for both the rectangle and the area ellipse is 136.6° and for the best-fit ellipse it is 136.2°. This angle is measured from the long dimension of the figure which is the scan direction of the microdensitometer.

orientation. The method of Krumbein (1939) yielded means of 15.0 ± 51.23 and 105.0 ± 56.4; standard deviations above 50° are considered to indicate an approach to a uniform distribution (Curray 1956). The two methods were also tested using a set of random numbers which were generated using a pseudo-random number generator. The results are similar to those obtained for the uniformly distributed data (100.34 ± 49.8 and 328.9 ± 51.02 by the iterative method; 26.6 ± 54.69 and 116.61 ± 49.75 by the Krumbein method). Again the means calculated by the iterative method failed to converge and the standard deviations calculated by both methods are large.

The standard deviations associated with the mean orientation angles calculated from the data for the aggregate illustrated in Fig. 2 are significantly less than those obtained from the uniform and random data, and are indicative of the preferred orientation of the long axes of the grains in this sample.

DISCUSSION

The automated image analysis system described here analyses grains of any shape. From the parameters obtained for each grain, a description of the form of each grain can be derived by calculating the enveloping rectangle, the best-fit ellipse and the area ellipse. Rectangles and ellipses are commonly used by geologists to obtain the data necessary for grain shape analysis but it has been shown that the ellipse may be the better shape to use since it preserves the area of the grain. Siddans (1976) has demonstrated the need to obtain such data automatically for shape analyses used in strain determination. Siddans digitized ellipsoidal markers and found

that errors increased rapidly with the departure from ellipticity; however, this may be alleviated by fitting the ellipses as described here and obtaining averages.

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