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Numerical modeling of crystal shapes in thin sections: Estimation of crystal habit and true size

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ABSTRACT

Although the size and shape of crystals in thin sections have been measured in a number of studies, it has not been possible so far to calculate from these data the true, three-dimensional shape and size of the crystals. A numerical model, based on orthogonal solids, has been developed to attack this problem. This model shows that crystal habit can be calculated from width to length ratio distributions for most crystals in massive rocks and for all crystals in laminated or lineated rocks. Variations in the habit of minerals can reveal aspects of the physicochemical conditions of crystallization.

The same model has also been used to develop the equations necessary to transform two-dimensional crystal size distributions into true crystal size distributions. Corrections for the cut effect and the intersection probability effect both require a knowledge of the crystal habit.

INTRODUCTION

Although most quantitative studies of igneous rocks concentrate on whole rock and mineral chemistry, recently there has been a growing interest in quantification of the textures of igneous rocks. Most work has been confined to the study of crystal size distributions (see review by Cashman, 1990), with a little work on crystal habit and orientation (Higgins, 1991) and none on the spatial arrangement of crystals. All these studies have been limited by the lack of knowledge of stereological effects, measurements are generally made in two dimensions on thin sections, but crystals, and textures, are three dimensional. An exact solution to this problem is only possible for spherical objects, and empirical methods must be used for other shapes. Earlier stereological studies were confined to spheres and equidimensional objects (see reviews in Cashman and Marsh, 1988; Cashman, 1990; Royet, 1991), but the numerical model presented here can be applied to any orthogonal solid. The particular stereological problems addressed here are the determination of crystal habit and the extraction of three-dimensional crystal size distributions from two-dimensional measurements of crystals in thin sections.

Crystal habit

The study of crystal habit has a long history. In 1669 Nicolaus Steno (1968), well known for his law concerning the constancy of interfacial angles, proposed that the external form of a crystal depends on the growth rates of the different faces. Since that time the factors controlling growth rate anisotropy, such as temperature and chemical potential gradient, have become better known (see recent reviews in Sunagawa, 1987a). These studies imply that observations of the actual habits of crystals can reveal something about their chemical and physical environment of formation.

Many studies of the habits of silicate minerals have been concerned with the forms developed during rapid cooling, such as those seen in some experimental products and volcanic rocks (see for example Lofgren, 1980). Relatively little work has been done on the habits of the generally larger crystals in plutonic rocks or the more euhedral forms in some volcanic rocks (see the review in Sunagawa, 1987b). Crystal habit is easily measured if a rock can be disaggregated, but that is not usually practicable. Generally, only two-dimensional slices through a rock are available, in the form of thin sections.

If a sufficient number of crystals are observed in thin section, then those with special orientations, for example, those intersected parallel to their crystallographic axes, can be distinguished and their dimensions used to establish the habit and true size of the crystals. However, this technique has several limitations: crystals with suitable orientations must be available, and they must be known to be representative of the whole population. A different approach is presented in this paper. It will be shown that statistical analysis of crystal shapes and sizes in thin sections can be used to establish the habits of most crystals and their true sizes.

Crystal size distributions

Recently, there has been a resurgence of interest in crystal size distributions in igneous rocks (see review by Cashman, 1990). Such studies can provide important information on the kinetics of crystallization, such as nucleation and growth rates. In this way they can complement information from chemical and isotopic studies on the environment of crystallization of the component minerals in a rock.

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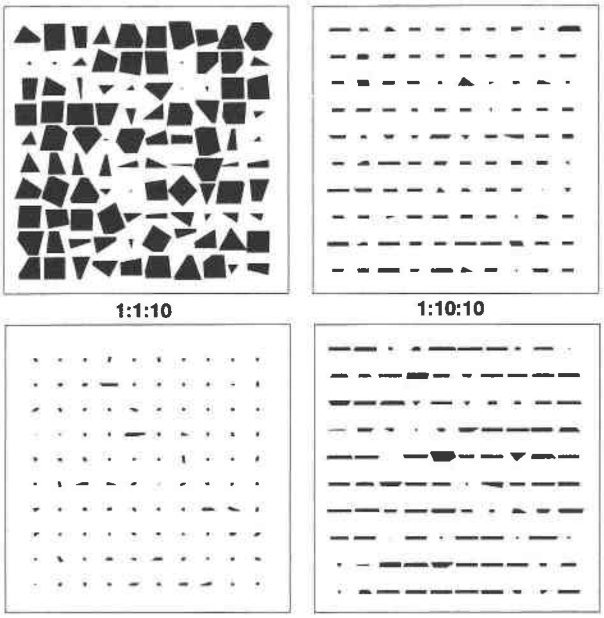

Fig. 1. Intersection shapes of 100 randomly oriented and positioned planes with four orthogonal solids of different aspect ratios (shortest : intermediate : longest). In each case the L parameter of the solid (1 or 10) is approximately equal to the spacing between the figures.

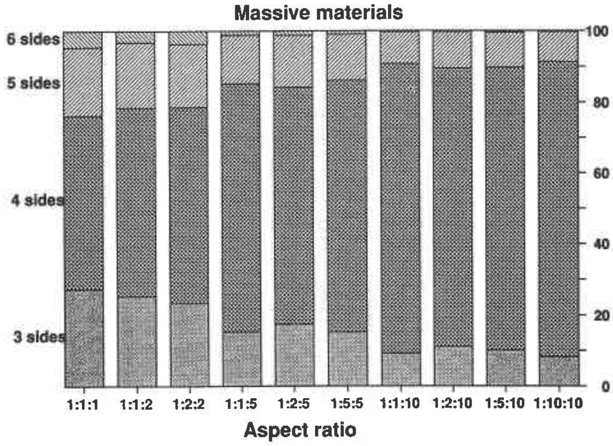

Fig. 2. Distribution of intersection shapes for different aspect ratios of orthogonal solids.

For want of suitable stereological studies, it has frequently been assumed that the modal crystal length observed in thin section approaches the true length of the crystal (e.g., Cashman and Marsh, 1988). Cashman (1990) suggested that the crystal width may be a better measure of crystal size. Others have suggested that crystal area may be a better measure than length. Clearly it is important to be able to relate all these measurements to a single crystal-size distribution, where size is the true length of the crystals. Other parameters, such as area and volume, can be calculated from the crystal habit and true length.

Numerical modeling

Isotropic materials

A numerical model has been constructed to simulate the variations in apparent two-dimensional grain shape and size in isotropic materials for various different grain shapes of uniform size. This model is a development of that described by Naslund et al. (1986). In an isotropic material any plane intersects crystals with every orientation. From the frame of reference of the crystals, the intersection can be considered to be that of randomly oriented and positioned planes. This is the frame of reference used in the model. The simplified crystal used in these calculations has the form of an orthogonal solid, with dimensions S = shortest dimension, I = intermediate dimension, and L = longest dimension.

A randomly oriented plane was produced as follows: randomly distributed points were generated with *X, Y,* and *Z* coordinates between -1 and $+1$, until one point fell inside a sphere of radius 1 centered on the origin. The point was projected from the origin onto the surface of the sphere, and the resulting *X, Y,* and *Z* coordinates were used as the direction cosines of the equation of the plane. The addition of a randomly distributed number between -1 and $+1$ determined the position of the plane. Such planes were produced until one cut the solid, when the number of sides and the area, length, and width of the intersection were calculated. Typical intersection shapes are shown in Figure 1 for four shapes of orthogonal solid. Trials for 50000 planes were conducted for S = 1, for I and L = 1, 2, 5, and 10, and for unconstrained and constrained orientations of the planes. The program is written in Pascal, and a copy is available from the author.

The intersection of a plane with an orthogonal solid can produce three-, four-, five-, and six-sided figures (Fig. 2). The most common figure has four sides, and the least common six. Three-sided figures are generally smaller, in contrast to five- and six-sided figures, which are among the largest. The proportions of different shapes are most strongly dictated by the length of the longest dimension (L) of the aspect ratio.

Distributions of intersection lengths are complex, with two or three peaks (Fig. 3A): the mode (highest peak) is at a length equal to the intermediate dimension, I, of the crystal, and there are subsidiary peaks at L and $\sqrt{L^2 + I^2}$. Distributions of intersection widths are slightly simpler than those of lengths (Fig. 3B): the mode is at S, and the peak is strongly asymmetric, with few narrower intersections and a long tail to wider intersections. There is a small subsidiary peak at I. Distributions of intersection areas show two to four peaks (Fig. 3C). All habits show a narrow peak close to zero. This is not an artifact but reflects a real concentration of intersections of small area, at the corners of the crystal. The most important peak is at $S \cdot I$, with subsidiary peaks at $S \cdot L$ and, for high values of I, at I/2. Width to length ratio distributions have one or two peaks (Fig. 3D). The main peak for prisms (in

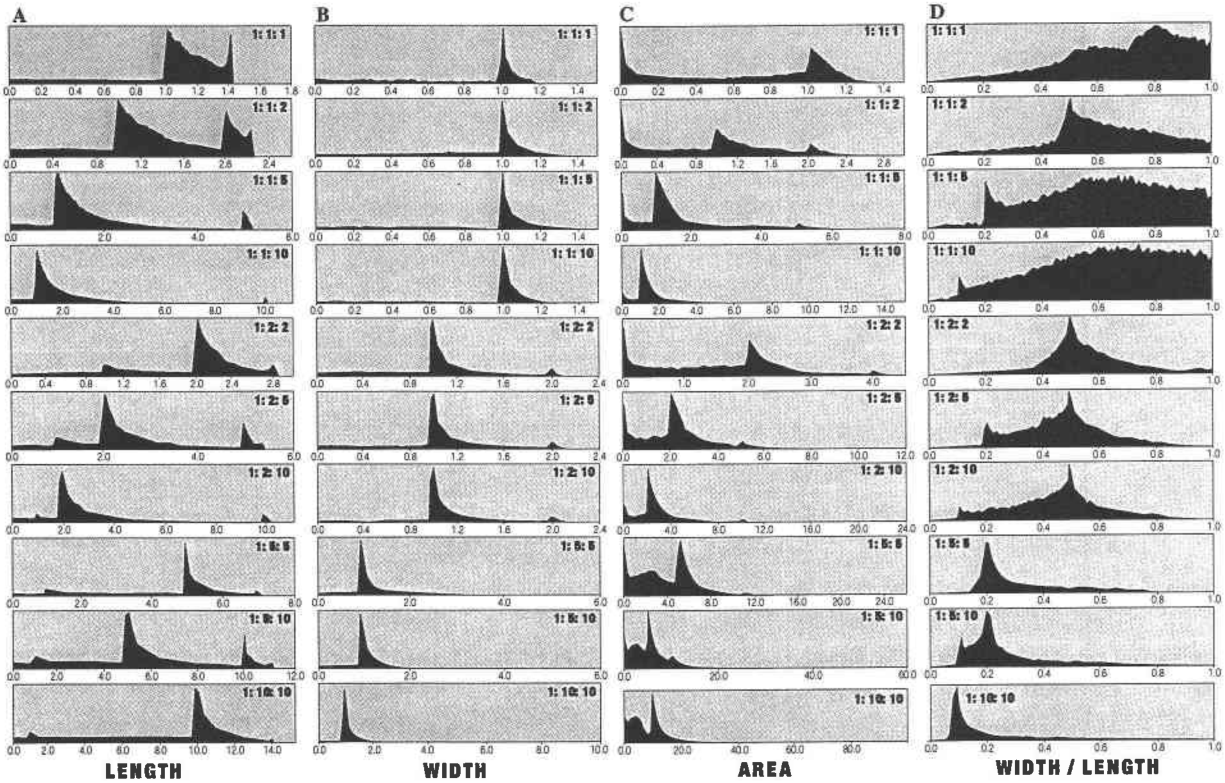

Fig. 3. Frequency vs. (A) intersection lengths, (B) intersection widths, (C) intersection areas, and (D) intersection width to length ratios for orthogonal solids with different aspect ratios. The distribution of the intersection planes is isotropic.

which I = L) is usually broad and in the region 0.5–1.0. For other aspect ratios the main peak is at S/I and is sharp. There is a subsidiary peak at S/L, but it is generally small.

The results of this model can also be revealed in a qualitative way by an examination of the intersection shapes (Fig. 1). The cube (1:1:1) has few square intersections, but most intersections are equidimensional. However, most of the intersections with the prisms (1:1:10) are almost square, and few are elongated. Most intersections with the tablets (1:5:10 and 1:10:10) are elongated, and few show the face of the tablet. Therefore, almost square outlines in a thin section indicates the presence of prismatic crystals, whereas elongated outlines indicate tabular crystals.

Linear and laminar fabrics

The alignment of nonequant crystals gives linear or laminar fabrics or both. The numerical model for these materials is similar to that for the isotropic materials described above, except that variation in the orientation of the planes of intersection is constrained. In contrast to isotropic materials, the orientation of the section with respect to the fabric is important. Two orientations are considered here: parallel and normal to the lamination or the lineation. For both linear and planar fabrics, the constraints on the orientations of the intersection planes in sections normal to the fabric are different from those in sections parallel to the fabric. It is assumed that all crystals are perfectly aligned, and hence the fabric is developed to the maximum extent. All intersections have four sides.

Crystals in rocks with a laminar fabric are aligned with their short axes pointing in the same direction. Sections normal to the lamination have modal lengths, areas, width to length ratios, and overall data shapes similar to those of isotropic materials with crystals of the same habit (Table 1). In contrast, sections parallel to the lamination are

Table 1. Equations relating modal values and invariant values of different parameters to the crystal dimensions

Fabric	Length	Width	Area	Width/ length
Isotropic	I	S	S·I	I/S
Laminar (normal)	I	S	S·I	I/S
Laminar (parallel)	L*	I*	I·L*	L/I*
Linear (normal)	I*	S*	S·I*	I/S*
Linear (parallel)	L	I	S·L	L/S
Laminated and linear (normal)	I*	S*	S·I*	I/S*
Laminated and linear (parallel)	L*	I*	I·L*	L/I*

Note: S = shortest, I = intermediate, L = longest.
* Denotes invariant values.

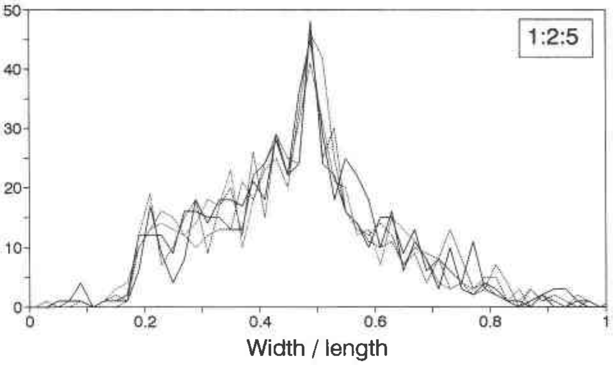

Fig. 4. Frequency vs. width to length ratios for five series of 500 planes cutting an orthogonal solid of dimensions 1:2:5.

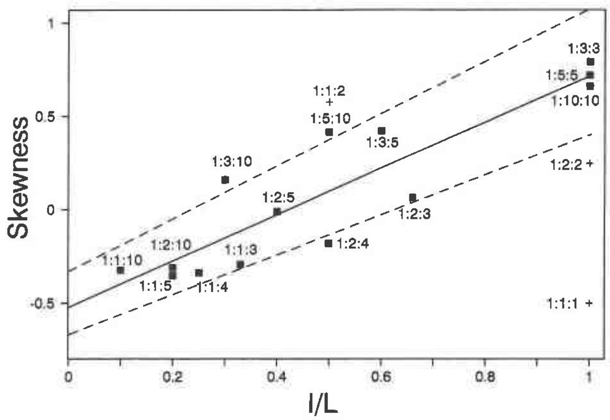

Fig. 5. Skewness (mean-mode/standard deviation) vs. I/L parameters for different habits. There is a strong correlation for tabular and prismatic habits (squares), but nearly equidimensional figures depart from the line (+). The solid line is a regression of the data excluding the nearly equidimensional data. Dashed lines are standard errors.

invariant, in that they have single values of length, area, and width to length, different from those of the normal section (Table 1).

Crystals in rocks with a linear fabric are aligned with their long axes pointing in the same direction. Sections normal to the lineation are invariant and have length, area, and width to length values similar to the modal values of isotropic materials with crystals of the same shape (Table 1). In sections parallel to the lineation, length is invariant, but the area and width to length ratio are variable (Table 1).

Crystals in rocks with a linear-laminar fabric are all aligned in the same direction. This is the simplest case of all. Sections parallel to the lamination and normal to the lineation and lamination give invariant values of length, area, and width to length ratios. These values are equal to modal or invariant values of a material that has only a laminar fabric (Table 1).

Differences between the model and crystals

This model is for orthogonal blocks, but crystals rarely correspond to this shape. The greatest difference is for the edges and corners: sharp for the model and rounded, or multifaceted, for the crystals. This difference shows up as a reduced number of small intersections, that is, short intersections with small areas, in the crystals. The peak near zero in the area distributions (Fig. 3C) is unlikely to exist in nature.

The sharpness of most of the peaks in the synthetic data (Fig. 3A–3D; length, width, area, and width to length) is also unlikely to be observed in crystals, partly because of the more irregular nature of crystals and partly because of the much smaller number of observations, which necessitates broader data intervals. However, distributions of width to length ratios for only 500 trials show that the position of the peaks and form of the curves can be determined readily from this small number of observations (Fig. 4).

The invariant values for sections parallel to the lamination or lineation are unlikely to be observed, as the alignment of crystals is never perfect, and crystal habit is never perfectly uniform. Instead there is a spread in the data, and the shape of the data distribution changes with the degree of lamination from the invariant value to that of the isotropic material.

Determination of crystal habit

The model presented above is for blocks of uniform size. The determination of crystal habit (S, I, and L parameters) for this special case will first be discussed, and then the arguments will be extended to the more realistic case of varying crystal sizes.

For isotropic (massive) materials, a broad peak at large ratios of width to length indicates that the crystals have a prismatic habit (i.e., S = I), whereas tabular crystals produce sharp peaks at S/I. Therefore, in both cases the I parameter can be determined.

The L parameter can, in theory, be determined from the subsidiary peak at I/L, but this peak is small and is unlikely to be observed in natural distributions. Another approach is to use the skewness of the distributions, where skewness = (mean mode)/(standard deviation).

There is a correlation between the skewness and I/L for most solids, except for solids that are almost equidimensional (Fig. 5). Hence the skewness generally can be used to estimate the L parameter, even if the precision is not very good. However, it is best to confirm L values by the examination of hand specimens or specially oriented crystals in thin section.

All three parameters of crystal habit (S, I, and L) can be determined in lineated and laminated materials from the mode of the width to length data in the sections normal and parallel to the fabric, using the relationships in Table 1.

In most natural materials crystal sizes vary, and it is always possible that habit varies with size. It is pertinent, then, to ask how such variations can be determined. Ex-

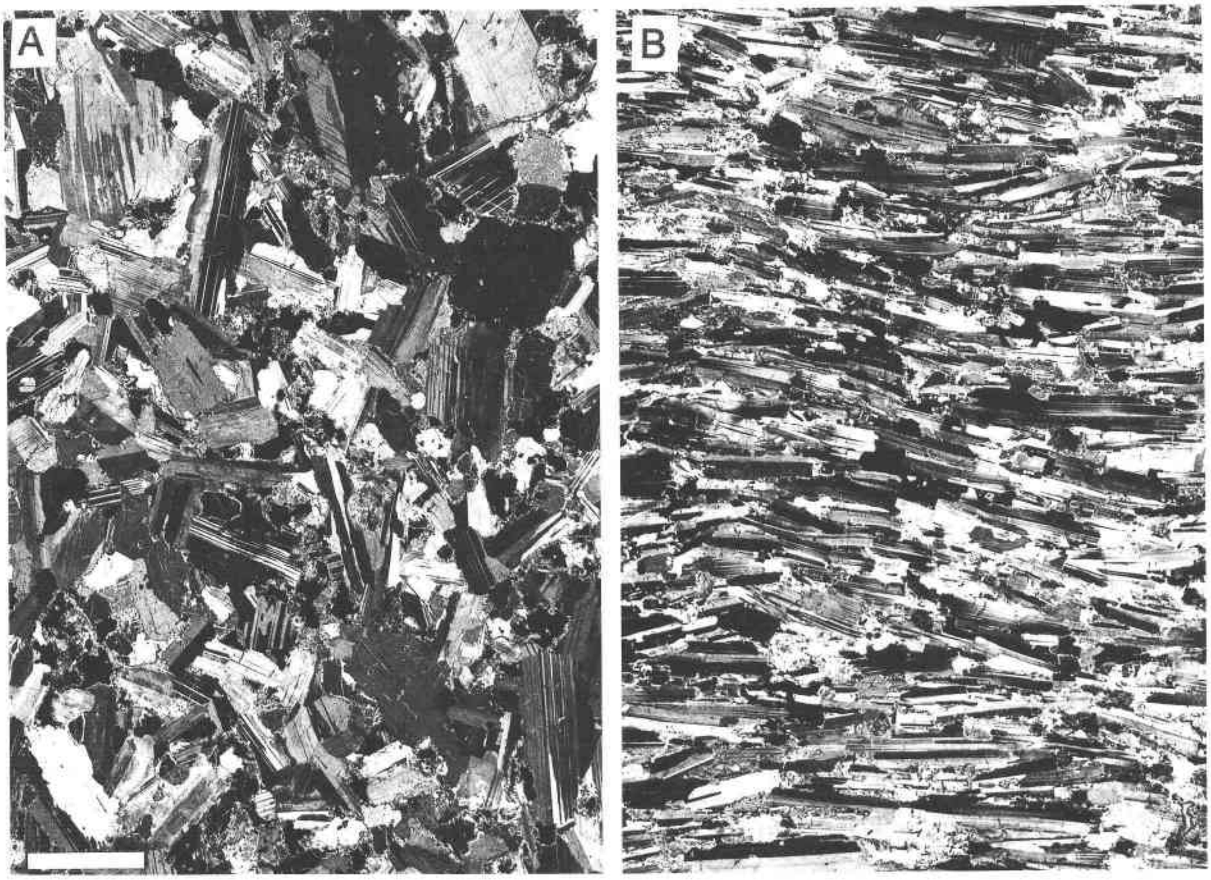

Fig. 6. (A) Massive and (B) laminated anorthosite from the Sept Iles mafic intrusion. Maximum field of view is 7 cm. Scale bar is 1 cm.

amination of the distributions of intersections (Fig. 3) shows that there are few short or narrow intersections for all the shapes considered here. Therefore, most of the width to length ratios used to determine the crystal habit are contributed by the larger intersections with a relatively limited range in intersection size. Hence, in a population of crystals with different true sizes, the width to length distribution of each class of intersection lengths (or areas etc.) will reflect the habit of the corresponding class of crystals. That is, the habit of crystals in each true size class can be determined more or less independently from the variations in the width to length ratios, subject to the limitations described above.

Plagioclase habit

Compositionally similar massive (isotropic) and laminar anorthosite (Fig. 6) occur together in the upper part of the Sept Iles mafic intrusion (Higgins and Doig, 1981). Higgins (1991) described these rocks and used intuitive arguments to determine the difference in habit between plagioclase grains in these two facies. Data on the shapes of plagioclase grains (Higgins, 1991) from the massive and laminar anorthosite have been replotted in Figure 7, together with theoretical values from the numerical model presented above.

The massive anorthosite has a broad peak centered at a width to length ratio of 0.5, which gives I/S = 2 (Table 1). The skewness of the width to length distribution is −0.07, indicating an I/L value of 0.4 (Fig. 5) and hence an L value of 5. The width to length distribution for an orthogonal solid with dimensions 1:2:5 broadly follows the data for the massive anorthosite (Fig. 7A).

Data from a cut section of the laminar anorthosite normal to the lamination have a broad peak with a mode at 0.2–0.25 (Fig. 7B). Application of the model gives I/S = 5 or 4. The section parallel to the lamination has a broad peak, with a mode at about 0.6. The numerical model presented here implies that if the crystals were perfectly aligned, then only a single value of width to length would be present. The crystals are not perfectly aligned in this rock, and that contributes to the observed broad peak. This value gives I/L = 1.7, and hence an overall aspect ratio of 1:5:8 or 1:4:7. The two different width to length distributions are shown in Figure 7B: the fit is much better for 1:5:8 than for 1:4:7.

The difference in plagioclase habit between the massive

(1:2:5) and laminated (1:5:8) anorthosite is probably related to the effects of magma movement (stirring) during the production of the lamination in the following way. In a stationary magma, slow rates of chemical diffusion lead to the production of a chemical boundary layer adjacent to the crystal face depleted in the crystal components and enriched in the rejected components. It is the chemical potential adjacent to the crystal face that controls the rates of growth of the different faces and hence the habit of the crystal. Movement of magma mechanically removes material from the chemical boundary layer and replaces it with fresh material less depleted in crystal components. This changes the chemical potential near the crystal face and hence the growth rate and crystal habit. Those faces with the fastest growth rates are most strongly affected by this process, as they are those most depleted in the crystal components. For example, stirring of the magma during the production of the lamination doubled the growth rates of the I and L dimensions, relative to the S dimension.

A change in plagioclase size and habit has also been observed in basalts from the 1984 Mauna Loa eruption (Cashman, 1990). The modal width to length ratio varies from 0.33 to 0.13, implying a change in S/I from 1:3 to 1:8. Unfortunately the data are insufficient to assess the variation in the L parameter. The variation in S/I was interpreted by Cashman (1990) as reflecting changing conditions of crystallization with time, specifically an approach to equilibrium. However, it could also be related to the increased stirring of the magma as the eruption proceeds. It is interesting to note that the change in the I parameter is of the same magnitude as the difference between the plagioclase in massive and laminated anorthosite at Sept Iles.

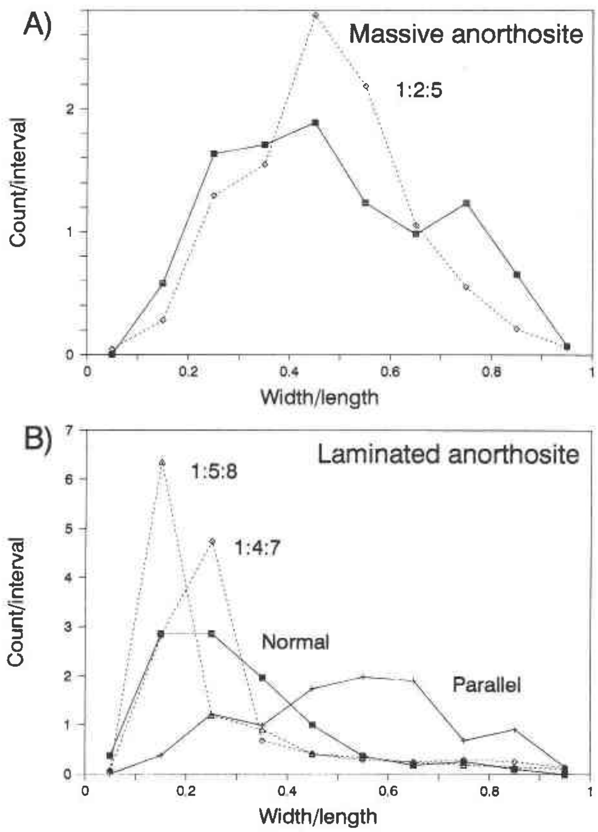

Fig. 7. Width to length distributions for massive and laminar anorthosite from the Sept Iles intrusion are shown in solid lines (Higgins, 1991), model distributions in broken lines. The vertical axis is abundance normalized for the interval width and number of data points. (A) Massive anorthosite compared with results from a model with dimensions 1:2:5. (B) Sections of laminar anorthosite normal and parallel to the lamination. The models are for sections normal to lamination with dimensions 1:4:7 and 1:5:8. The model predicts an invariant value for the section parallel to the lamination.

Corrections of crystal size distributions

The conversion of apparently two-dimensional size distributions to true three-dimensional size distributions is a complex stereological problem (see review by Royet, 1991). There are two separate sectioning problems: the cut effect, which has been developed in the model above, and the intersection probability effect, which will be discussed later.

The cut effect concerns the reduction in intersection sizes produced when the intersection plane does not pass directly through the center of the crystal, parallel to the longest axis. The model presented here shows that the mode of the crystal length in thin sections of isotropic materials is equal to the I dimension. For sections normal to the fabric of laminated or lineated materials, the mode of crystal length is also equal to I, whereas in sections parallel to the fabric the modal length is equal to the true length L.

Cashman (1990) suggested that intersection widths might be less variable than intersection lengths. The results of this model confirm that, especially for prismatic crystals. However, the advantages of width measurement must be balanced against the greater errors associated with the smaller sizes to be measured.

Crystal size distributions (Cashman and Marsh, 1988; Marsh, 1988; Cashman, 1990) can be corrected for the cut effect in two ways. The simplest is to assume that all observed crystals have the same length as that of the modal value. Then all that is necessary is to multiply the crystal size distributions by correction factors derived from Table 1. A more complex correction can be made using the calculated distribution of intersection lengths for a crystal of a particular habit, such as those in Figure 3A. These corrections are applied stepwise to the length intervals. The added complexity of this procedure and the possible introduction of further errors is probably not justified by the precision of measurement in most studies.

The intersection probability effect concerns the likelihood that a random plane would intersect a crystal. For spheres of uniform size this effect is related to size, by

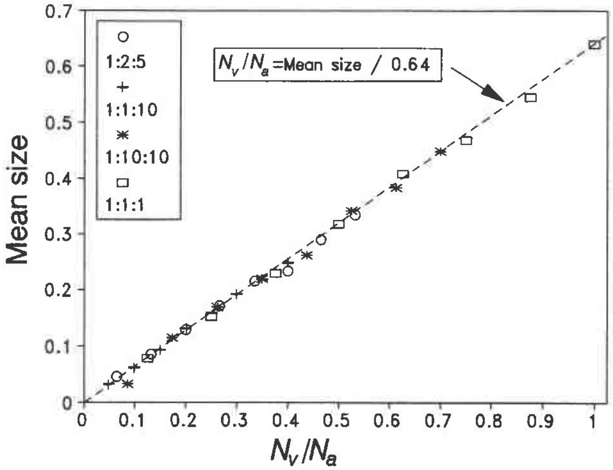

Fig. 8. Number per unit volume (N_V) multiplied by the mean size [(S + I + L)/3] vs. number per unit area (N_a) for various sizes and shapes of orthogonal solids. The dashed line is a regression of the data. It has a slope of 1.56 (1/0.64).

means of the relation $N_V = N_a/D$ where N_V is the number of crystals per unit volume, N_a is the number of crystals per unit area, and D is the diameter.

The computer program used above to investigate the cut effect also gives values for N_V and N_a, shown in Figure 8 for orthogonal solids of different sizes and shapes. These data indicate that for orthogonal solids the equation must be modified to $N_V = N_a/(0.64\ D')$ where D′ = mean size = (S + I + L)/3 and 0.64 is a shape constant. This equation must be applied separately to each size interval of the crystal size distribution. It has been shown above that in most situations the modal length is equal to the I dimension. The mean size (D′) for the interval can then be calculated from the midpoint of the interval and the crystal habit (values of S, I, and L). This correction is applied in addition to that for the cut effect.

Conclusions

Numerical modeling presented here shows that for an orthogonal crystal the distribution of width to length ratios of the intersections can be used to establish the crystal habit of the solid, except for almost equidimensional crystals in isotropic materials. The model also illustrates that cubic crystals rarely produce square intersections, but instead they are produced commonly by prismatic crystals. Tabular crystals commonly yield elongated intersections.

Once the crystal habit has been determined, then distribution of crystal lengths, widths, or areas in thin section can be partly corrected for stereological effects and transformed into three-dimensional crystal size distributions. Among other uses, the true growth rates of the different faces of crystals can be determined from such data.

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