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A Technique for the Simulation of Hardmetal Microstructures

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ABSTRACT

A computer simulation technique has been developed that allows images of hardmetal microstructures to be synthesised using assumed grain size distributions. The technique produces structures based on random slicing and subsequent tessellation of slices taken from truncated tetragonal prisms of WC. The method was also used to examine the consequences of changes in grain size distribution on the image appearance. It was found that inaccuracies in the measurement of small intercept lengths had a marked effect on the distribution shape but less so on the appearance of the simulated structure and that a three dimensional lognormal size distribution did not produce a lognormal distribution in two dimensions. These structures can also be used to provide reference images for the validation of microstructural measurement techniques.

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INTRODUCTION

The mechanical properties of hardmetals, like many other engineering materials, are strongly influenced by their grain size [1]. However, for hardmetals there is no standard method for measuring the size of the WC grains or their distribution. Lack of reference methods for this purpose is hindering a fundamental understanding of the link between grain size, distribution and mechanical properties. In particular a knowledge of how measurements in two dimensions are related to a three dimensional shape distribution is vital if the question of how uniformity (or non-uniformity) of structure relates to strength and toughness. In the present work this operation has been examined initially by the development of a computer simulation method for producing two-dimensional images from a three dimensional shape distribution.

To characterise a given microstructure it is necessary to reduce the information content of a typical micrograph of the material to a limited number of parameters. In the measurement of hardmetal microstructures a cross-section of the material is first produced, and after polishing and etching a quantitative metallographic technique is used to produce a mean value for grain size either by point or area counting or by linear intercept techniques. In particular the linear intercept technique is popular because it produces size distribution information. It is often found that the measured intercept distribution is lognormal in form, which gives a straight line when plotted on lognormal probability paper. An alternative is the measurement of the sectional grain area; however, this is not common or well developed.

In order to assess the effectiveness of the linear intercept of area measurement technique and their relevance to three dimensional structures a method of producing images of hardmetal structures simulated by computer was developed. This procedure used an assumed distribution combined with information about the three dimensional WC grain shape to produce images that were simulated sections through the hardmetal structure. These were compared with and shown to be similar in appearance to those produced using standard metallographic preparation techniques.

WC crystals develop the shape of a tetragonal prism (with truncated corners) when allowed to grow unconstrained. However, little is yet known about what is the correct aspect ratio for these crystals in 3-D structures, whether the aspect ratio has single or distributed values or how the 3-D shapes are modified by constraint in a real multiparticle structures.

The technique adopted was based on the random slicing and subsequent tessellation of slices taken from truncated tetragonal prisms of WC. The assumption that this process represents a true random slicing of a sintered WC/Co structure cannot be justified mathematically. However, a simulation of 3-D structures of two phase materials is computationally difficult with current computing systems and very time consuming. Consequently the 2-D approach was examined as a first step in gaining confidence in simulation methods. Also the 2-D sections of tessellated images were very effective in demonstrating the effects of differences in distribution width and shape.

2 SIMULATION TECHNIQUE

2.1 *Truncated Tetragonal Prism*

For the purposes of the simulation the structure of a typical hardmetal was assumed to be made up of many crystals of WC bonded in a cobalt matrix. The crystals are assumed to be in the form of a truncated tetragonal prism (TTP), Fig 1. The dimensions can be adjusted as required, but the values chosen for the majority of this work are shown in Fig 1, with the height of the TTP arbitrarily chosen to have the value 3 based on observations of the 3-D shape of WC crystals observed growing on the internal surfaces of small closed pores in WC/Co hardmetals. In real structures the WC grains will not be fully formed TTP crystals

because of constraints imposed on the growing crystals by their neighbours. However as a first step in the simulation exercise perfect TTP crystals were used for simplicity.

Initially, a large number of random TTP sections were generated. The sections so produced were studied by randomly rotating a single TTP which was sliced with a plane that was produced perpendicular to the z-axis and at a random distance from the origin. Therefore a distribution of different shapes were generated. An example of some randomly generated sections derived from individual TTP crystals are shown in Fig 2. These can be compared with real sections, shown in Fig 2b taken using a scanning electron micrograph.

Randomly oriented lines were used to cut the TTP to produce a distribution of intercept line lengths, Figs 3a and 3b. The frequency distribution was found to be in good agreement with that computed by Wasen and Warren [2]. The effect of the number of generated intercepts on the uncertainty associated with the data can be clearly seen when comparing Figs 3a and 3b, which were calculated from 10,000 and 3,000,000 intercepts respectively. The two peaks in the distribution are correlated with the maximum line intercepts corresponding to the basal and pyramidal planes. A cumulative distribution for Fig 3b, with thickness 3.0, is shown in Fig 3c, together with cumulative distributions for other values of thickness.

2.2 *TTP Assemblies*

A fundamental assumption was made that packing TTPs in three dimensional space and then slicing the agglomeration was equivalent to slicing one TTP at random and then producing a tessellation of sections in two dimensional space. This assumption does not have mathematical rigour but it was considered a reasonable first approximation since it is difficult to compute the effects of cooperative packing of TTPs in three dimensional space.

A large number of sections were required to achieve a packing density of sections close to that required by experimental observation. Therefore a technique was used that tessellated 500 two dimensional sections of TTPs that had previously been generated as described above. Fig 4 shows the flow diagram required to produce a simulated image.

The first step in the simulation procedure was to choose the number of sections required. The sections were then picked at random from the pool of 500 precalculated polygonal TTP sections. A lognormal distribution of 3-D TTPs was assumed so the sizes of the sections to be placed were calculated by scaling the vertices of the chosen polygonal TTP section by a lognormal probability density function with appropriate mean and variance. The sections were then sorted by area and a number of the largest sections were placed in order of decreasing size as predetermined seeds. The seeds were placed at random positions in a two dimensional box with random orientation and were removed and placed again if they intersected the box boundaries or any other previously placed section.

To improve the efficiency of the simulation a positioning algorithm was used which placed the sections in order of decreasing area. Each new section was placed so that it touched a previously placed section along one edge, which mimics features observed in the microstructures of real materials.

After placing the seeds the remaining sections were placed by choosing a point at random on the computer screen. If there was no TTP section at this point then another point was picked until the point was inside a TTP section. Then a line was constructed in one of four perpendicular directions, chosen at random, and starting at the point and ending at the periphery of the placed section. A point was then chosen on the periphery of the TTP section to be placed, in a similar fashion and the new section rotated in such a manner so that the points on the edges coincided and touching edges were parallel.

Because of rounding error sometimes a small gap appeared between faces, further modifications of the software will be needed to be done to remove this artefact. However, it has been ignored for the purpose of illustrating the principles used to compute the images. In fact, sometimes the phenomenon is observed in real structures, but at a much lower frequency than in the simulations.

The boundary of the new section was drawn and if this line did not intersect a previously placed section then the interior of the section was filled with a unique colour. If, in the process of filling the section or during construction of its boundary, a previously placed section was intersected then the section was erased and a new position sought at random as described above.

This process was continued until a place could be found to locate the TTP section. If after 100,000 attempts the TTP section could still not be placed then it was discarded and the simulation continued with an attempt to place the next section in the distribution. This process continued until all the TTP sections were placed. The successfully placed particles typically accounted for 80% - 85% of the total area of the image which is similar to a micrograph of a WC/10 wt% Co hardmetal. Additionally a cutoff on minimum size was imposed so that small sections that were a few square pixels in size would not be placed because rounding errors caused inaccurate rendering of the shape.

Since each TTP section was drawn in a different colour a false colour image was easily constructed with sections colour coded according to size. Other software routines were written that allowed the sections to be coloured with random shades of grey and with light or dark boundaries in order to simulate optical or electron micrographs.

The software for these algorithms were developed at the NPL and were written in Parallel C to run on a transputer network.

3 RESULTS AND DISCUSSION

3.1 Microstructure Measurements

The microstructure of a 6 wt% Co/WC hardmetal (code D1 - supplied by Marshalls Hardmetals Ltd) was analysed using both a linear intercept and area measurement technique. Typical micrographs of the material are shown in Figs 5 and 6.

A lognormal distribution $f[x]$ is defined as:

$$f[x] = \frac{1}{x\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(x) - \ln(\mu))^2}{2\sigma^2} \right]$$

with $F[x]$ the cumulative lognormal distribution defined as:

$$F[x] = \frac{\int_0^x \frac{1}{y\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(y) - \ln(\mu))^2}{2\sigma^2} \right] dy}{\int_0^\infty \frac{1}{y\sigma\sqrt{2\pi}} \exp \left[-\frac{(\ln(y) - \ln(\mu))^2}{2\sigma^2} \right] dy}$$

The lognormal distribution parameters, μ, σ (the geometric mean and standard deviation) can be ascertained by plotting the measured linear intercept data on lognormal probability axes, Fig 7 with a $\log_{10}$ abscissa. The straight line is a linear regression fit and it can be seen that a lognormal distribution is a good approximation to the measured distribution of intercepts of WC grain sizes. If the measured area distribution data is plotted on lognormal probability

axes then it can be seen that the area data are also well described by a lognormal distribution, Fig 8. This implies that the three dimensional shapes of the WC particles in the hardmetal are probably not lognormally distributed [3] but by how much remains to be assessed since as yet no direct measurements of 3-D shape distributions in WC/Co have been made. In the absence of this information the current exercise assumed 3-D lognormal distributions for ease of calculation.

Table 1

Lognormal distribution parameters derived from
two different measurement techniques

Technique	μ	σ
Linear intercept μm	1.08	0.27
Area μm^2	1.25	0.20

3.2 Simulations

The simulated images shown in Figs 9 and 10 were formed using the linear intercept lognormal distribution parameters obtained from these measurements. Five seeds were chosen and the image was scaled such that approximately 500 sections fitted into the field of view. The packing density for this image was 84% and it took 2,317,516 different attempts at placing sections to produce the image. For the intercept distribution simulation each section was shaded at random over a certain range of grey to produce an image, Fig 9, which was analogous to an optical micrograph. With a change of background to represent the contrast typical of the cobalt regions and edge enhancement to mimic features seen in scanning electron micrographs then an image could be formed which simulated a scanning electron micrograph, Fig 10.

The packing density is an adjustable parameter that can be set at the start of the simulation procedure. It is intended to be analogous to the amount of cobalt present in the hardmetal. Clearly as this parameter was increased towards 100% then it became increasingly more difficult to place sections since there was less free space available for the TTP sections. Generally it was found that a packing density of 70-85% was a reasonable compromise between realism of simulation and run time. This packing density covers a reasonable range of volume fractions for typical hardmetals. For example, a 12 wt% Co/WC hardmetal contains about 20% Co by volume.

While the simulation is running the placement of sections on the screen can be seen and the number of failed attempts to place the sections is displayed. For a typical simulation there may be a total of over 2 million failed attempts to place the 500 sections. This averages at about 4000 attempts per section placed. However, the number of failed attempts per section varied with the number of sections already placed and also the form of the sectional distribution. Initially it was very low, since there was plenty of empty space around each placed TTP section. But as the screen became increasingly filled with TTP sections then the number of failed placement attempts rose dramatically. It was only when a large number of sections had been placed that the number of failed placement attempts decreased. This was solely due to the nature of the shape of the distribution and the fact that the sections were placed in order of decreasing size. A graph of section number versus number of placement attempts is shown in Fig 11. Fig 12 shows how the filled area varied with the number of sections placed.

If more than 100,000 attempts were required to place a TTP section then the placement of the section was abandoned and the next section was placed instead. In a typical simulation there may be 1-2% of the sections unplaced, however, this did not appreciably change the distribution, since the unplaced sections tended to come from the centre of the distribution, where there were many similar sized sections.

Although the lognormal distribution of three dimensional particle sizes used for the simulation produced realistic images, it was found that this did not result in an intercept length distribution which was similar to the experimentally measured intercept length distribution. As is shown in Fig 13 there was a notable deviation at small intercept lengths. This effect has also been noted in measurement studies of TiB_2 cermet microstructures [4,5]. This may be because the real distribution of three dimensional particle sizes is not lognormal. Alternatively, rounding of the edges of the TTP and particle/particle contiguity effectively apply a cut-off in the intercept distribution, Fig 13, line 2 [6]. There is also the possibility that real structures contain a collection of different TPP crystal shapes, rather than just one shape. This would clearly affect the final intercept distribution.

The deviation of the simulated linear intercept distribution from the experimentally observed lognormal distribution at small values of intercept length could not be seen in simulated images. This is because of an additional weighting of the section sizes that occurs when the image is observed and interpreted by a human observer. It is not the number of sections of a given size that is noticed but a function of the total area of the sections. This means that large sections tend to dominate the images by virtue of their perceived area, whilst small particles are fairly insignificant. Therefore the deviations from a lognormal distribution at small section sizes is not noticed when looking at a simulated image, since it is the distribution behaviour of large sections that dominates. This can be seen in Fig 14 where an additional weighting has been applied to an intercept length distribution. The weighting was chosen to be proportional to the area of the particle. The graph of perceived frequency versus intercept length, Fig 14, showed that visually the differences between a simulated and real image were quite small.

3.3 *Shape and Distribution Effects*

The simulation technique is very convenient for examining a number of additional input parameters such as the shape and size distribution of the TTPs. Fig 15 shows the effect of varying the height, and also the shape of the TTP on typical simulated images. Fig 16 shows the effect of bimodal three dimensional particle distributions similar to those seen by Friederich et al [7].

4 CONCLUSIONS

A computer simulation technique has been developed for simulating hardmetal microstructures using a pragmatic approach based on observations of real hardmetal micrographs. The technique can be used as a tool for the interpretation of grain size distribution measurement data and to study the consequences of changes in the three dimensional size distribution on the two dimensional measurements of the WC distribution. In particular it was shown that a three dimensional lognormal distribution of crystal sizes with an aspect ratio of 3:1 (edge length:thickness) did not result in a lognormal distribution of intercepts in two dimensions. Furthermore, uncertainties involved with measurements of small intercept lengths can have a marked effect on the measured number distribution of intercepts but that these differences are not easily noticeable by eye in a simulated image.

The images were developed based on the assumption that 2-D tessellations were realistic in modelling distributions of 3-D sections. The latter approach would have more mathematical validity but at present is not cost effective in computing time. Additional work would be

helpful by investigating experimentally what forms of 3-D number and shape distributions would result in a lognormally distributed intercept distribution.

The technique also has potential as a source of reference images for calibrating standard measurement methods for many types of engineering materials. This simulation procedure clearly can provide one of the basic building blocks required to develop a fully integrated and validated measurement standard for grain size.

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6 ACKNOWLEDGEMENTS

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LIST OF CAPTIONS

- Figure 1 A schematic diagram of a truncated trigonal prism.
- Figure 2 a) Some typical sections of randomly sliced TTPs, b) real sections observed by scanning electron microscopy.
- Figure 3 a) A histogram of number intercepts of a given length versus length for 10,000 intercepts in a TTP of arbitrary thickness 3.0, b) as a) but with 3,000,000 intercepts, c) cumulative number distribution for b) (including data for additional thicknesses, 0.5-4.5).
- Figure 4 A flow diagram showing the processes required to place each new TTP.
- Figure 5 An optical micrograph of hardmetal D1 at a magnification of x1633.3.
- Figure 6 A scanning electron micrograph of hardmetal D1 at a magnification of x3000.
- Figure 7 A lognormal probability plot of intercept frequency data
- Figure 8 A lognormal probability plot of area frequency data.
- Figure 9 A simulation using the linear intercept lognormal distribution parameters measured from the D1 sample but with the particles shaded at random to mimic an optical micrograph.
- Figure 10 A simulated scanning electron micrograph derived from Fig 9.
- Figure 11 A graph of section number versus number of placement attempts.
- Figure 12 The variation of filled area with number of sections placed.
- Figure 13 A lognormal probability plot of intercept length frequency data. Line 1 (black circles) is the data that is used in a simulation and is simply a lognormal distribution of particle sizes combined with a linear intercept distribution for a TTP, as in Fig 3a,b. Line 2 (squares) is similar to line 1, but the linear intercept distribution has been modified by imposing a cut-off at small intercepts. Line 3 (triangles) is a lognormal distribution of 2D linear intercept sizes.
- Figure 14 A plot of perceived frequency versus intercept length. The perceived frequency is the actual frequency of a particular intercept length multiplied by the area of a particle that would just contain that intercept.
- Figure 15 a) A simulated image as Fig 10 but with height = 0.75, ie half the thickness of the original TTP, b) as Fig 10 but with the height = 6, ie twice the thickness of the original TTP.
- Figure 16 A simulated scanning electron micrograph generated using a bimodal distribution with 96% by number with $\mu = 1$ and 4% by number with $\mu = 5$ and a) $\sigma = 0.001$ and b) $\sigma = 0.3$.

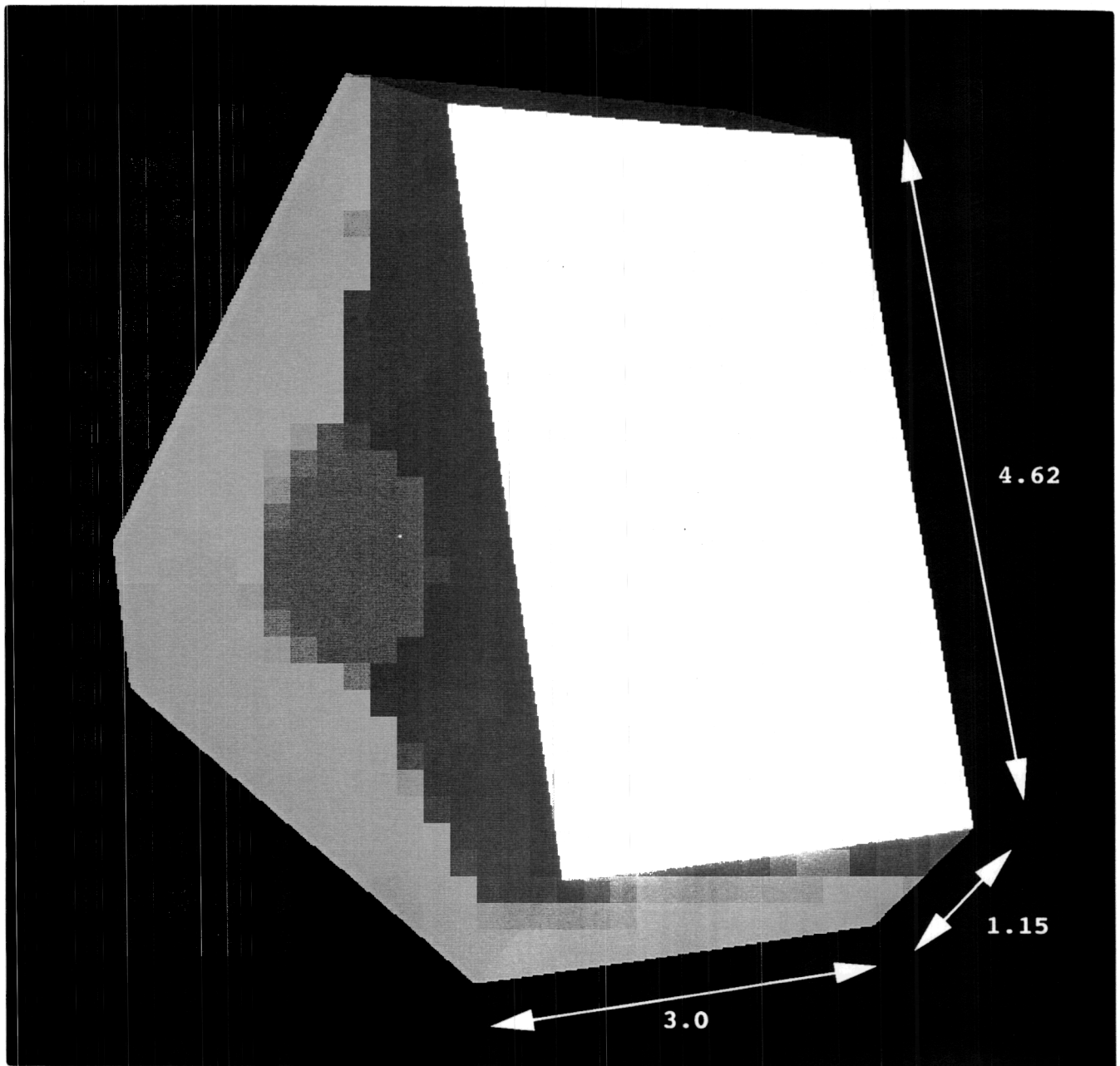


Figure 1 A schematic diagram of a truncated trigonal prism.

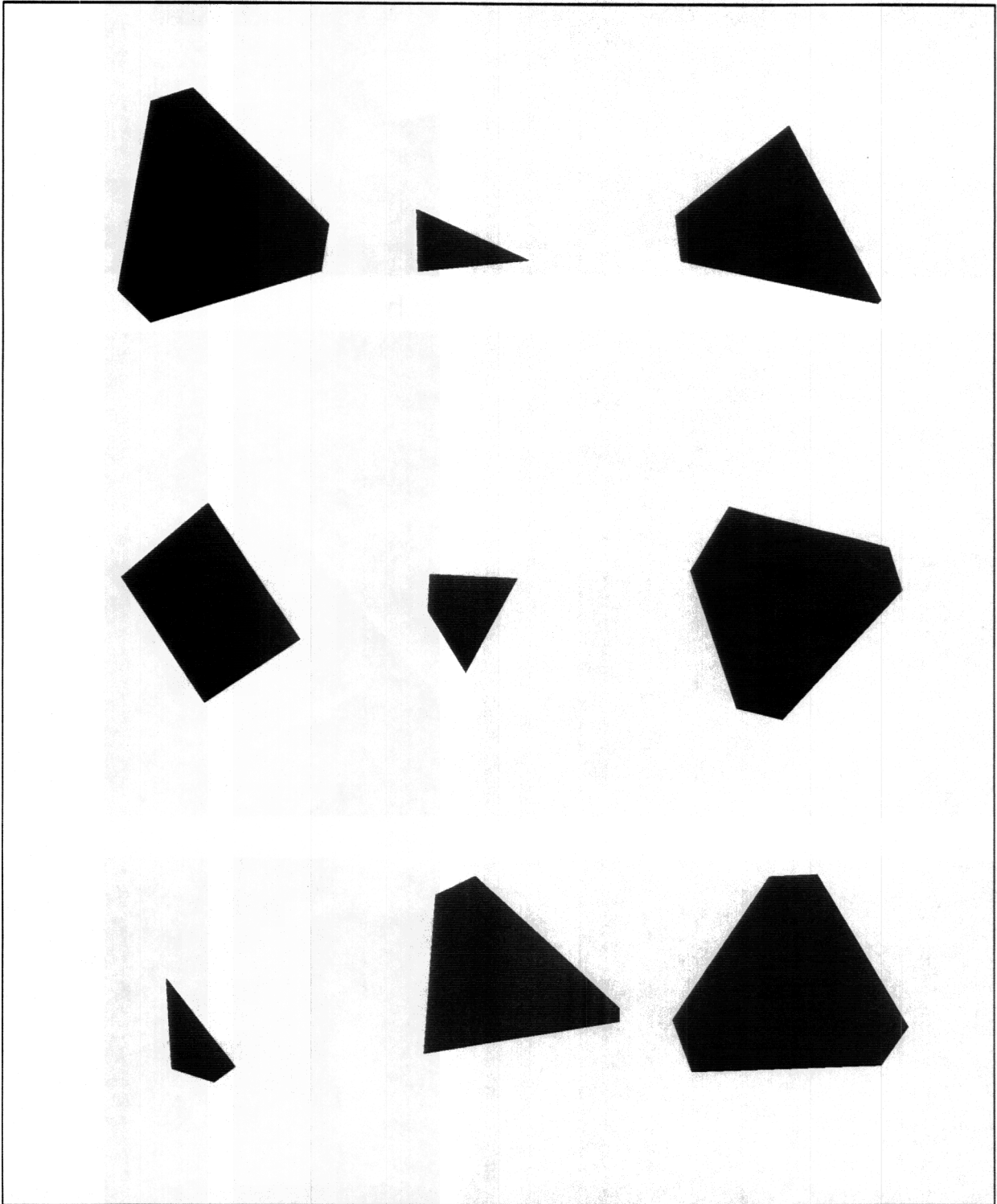


Figure 2a

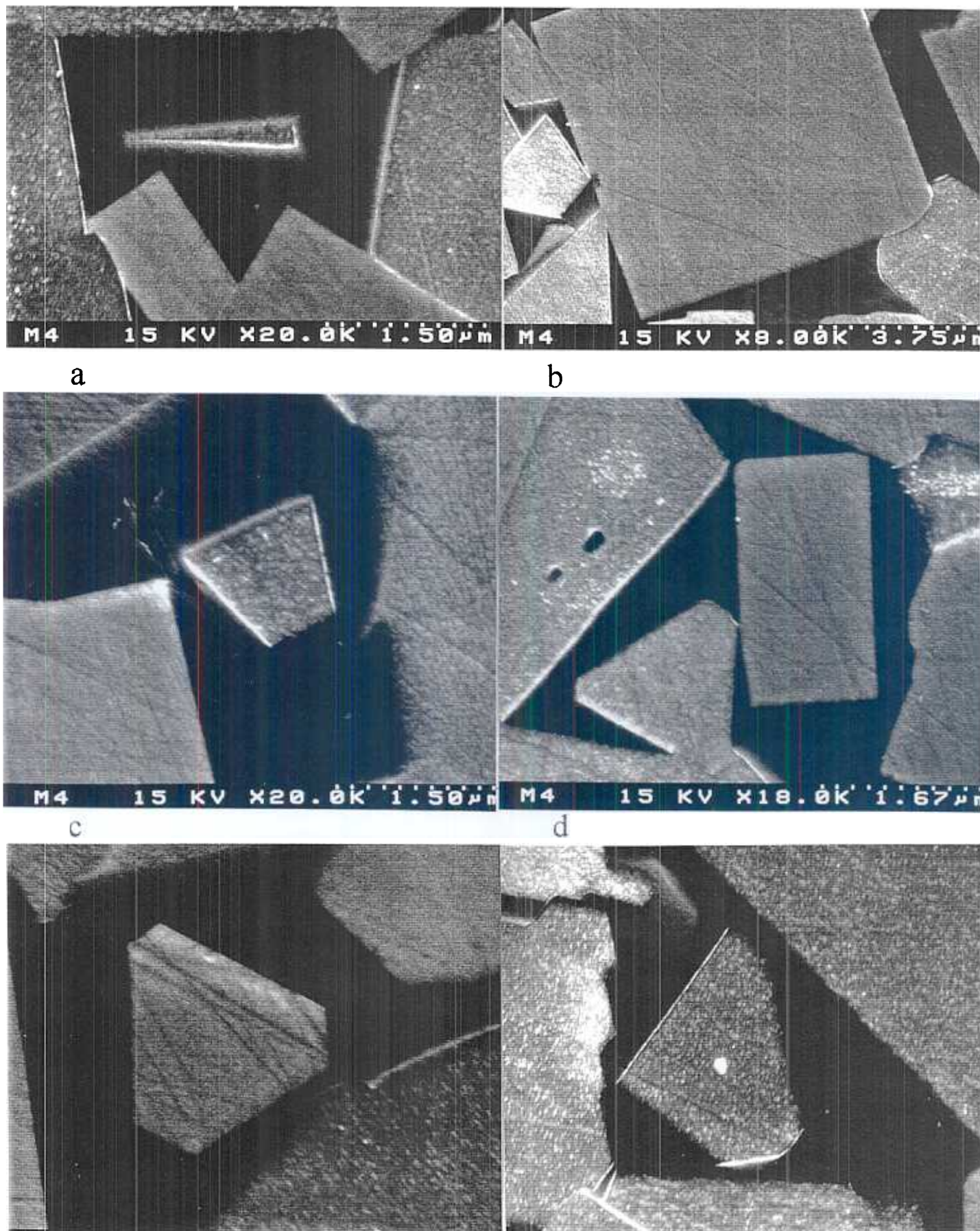


Figure 2b

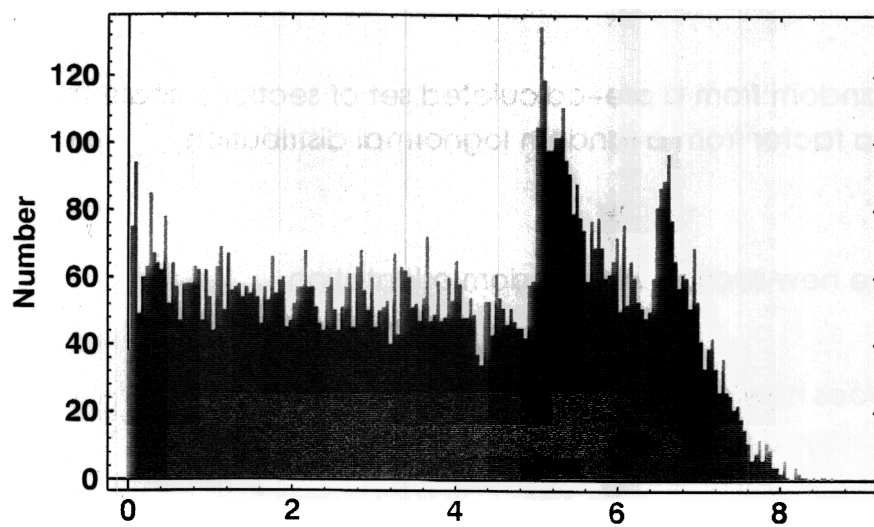


Figure 3a

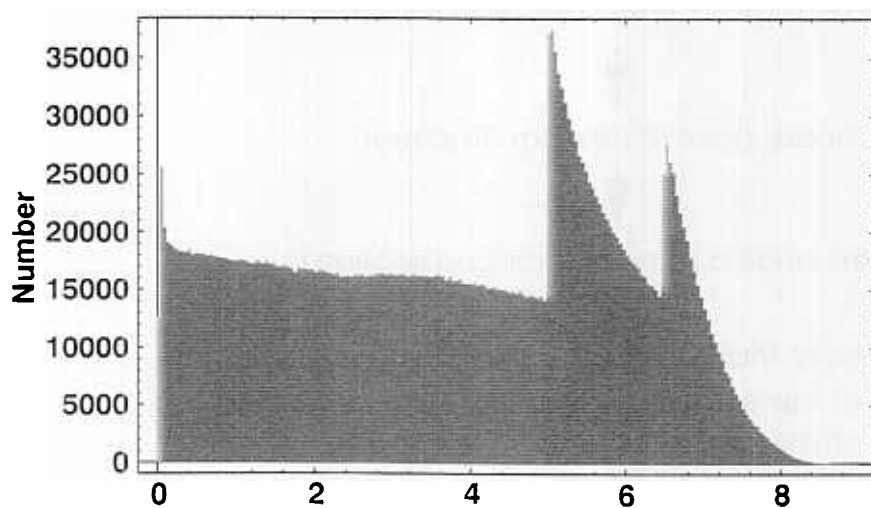


Figure 3b

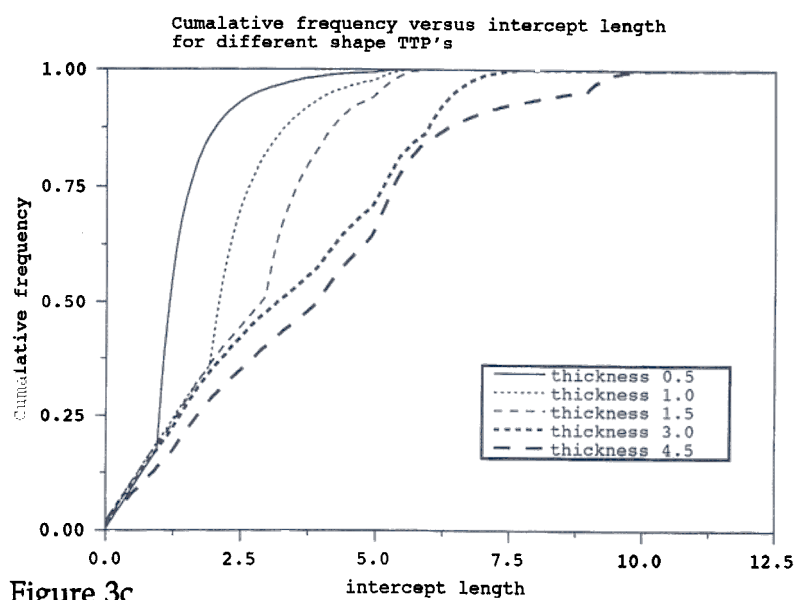


Figure 3c

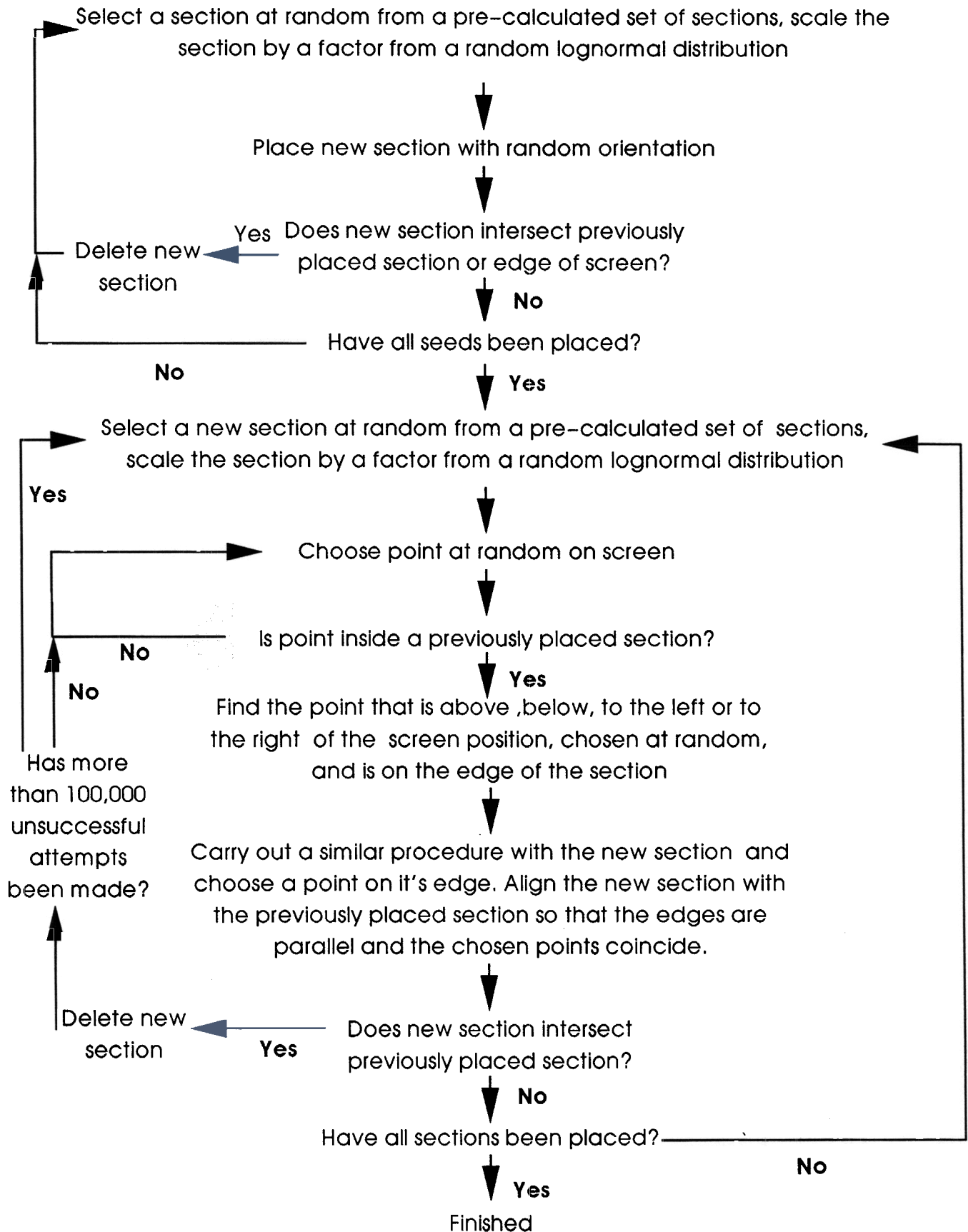


Figure 4

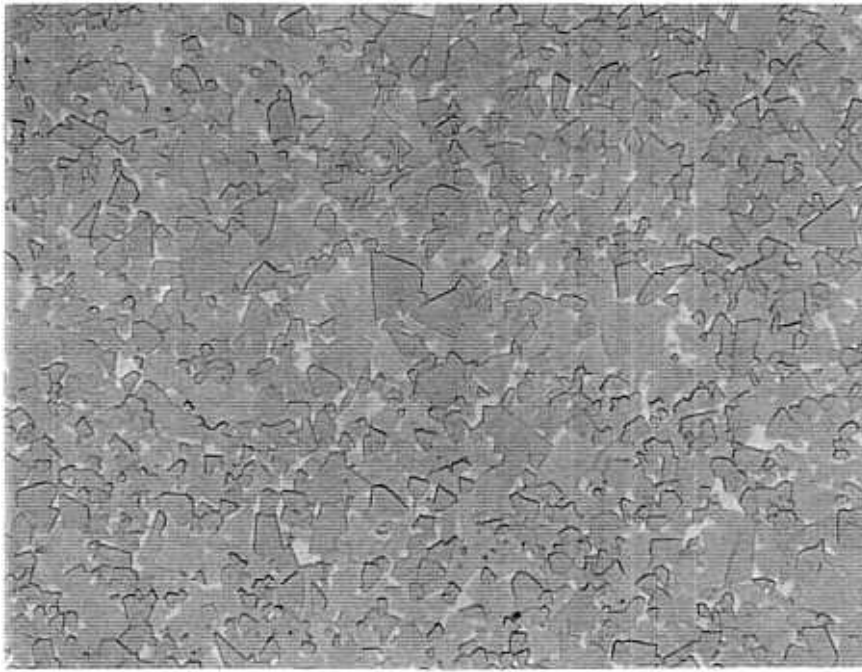


Figure 5

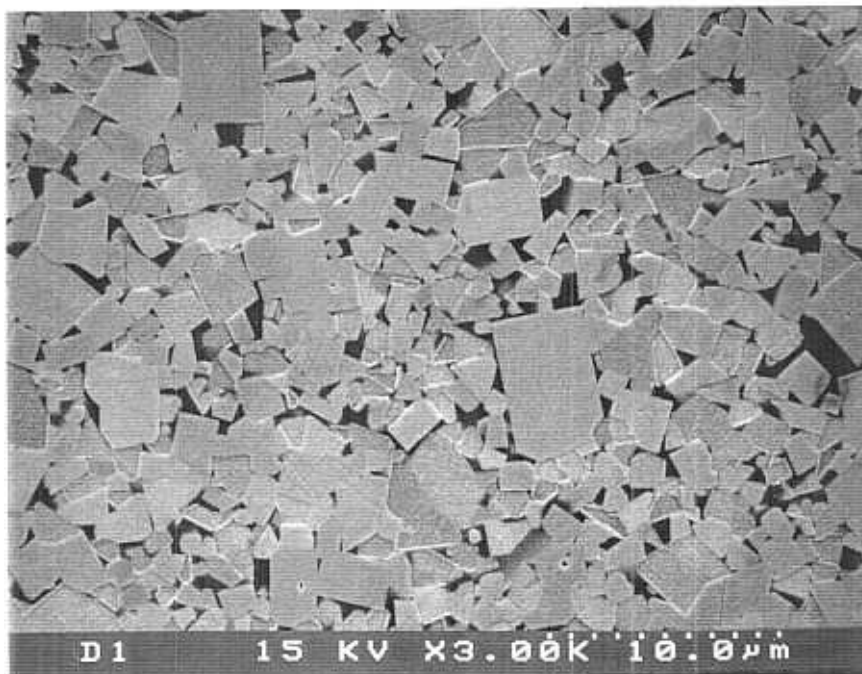


Figure 6

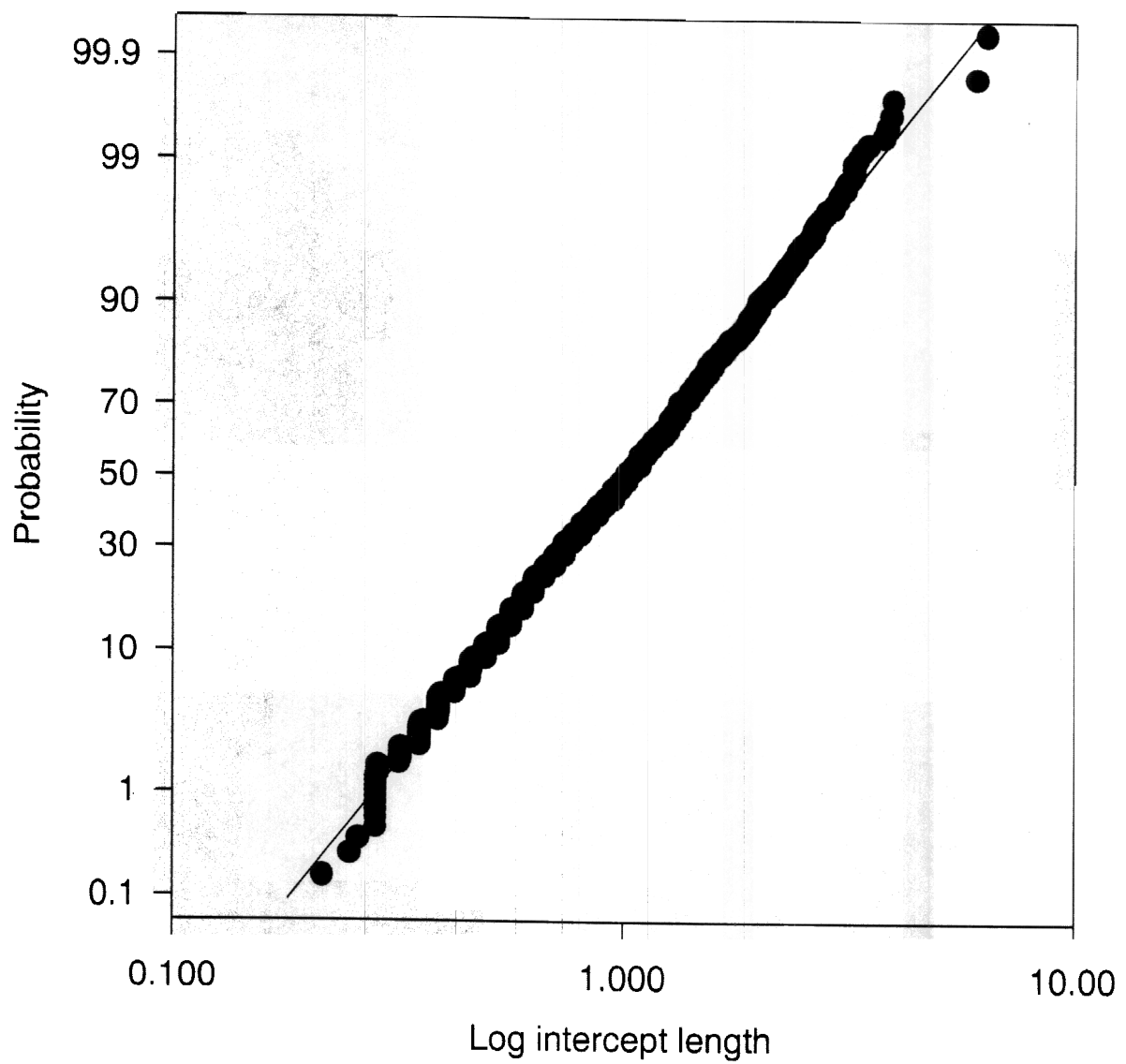


Figure 7

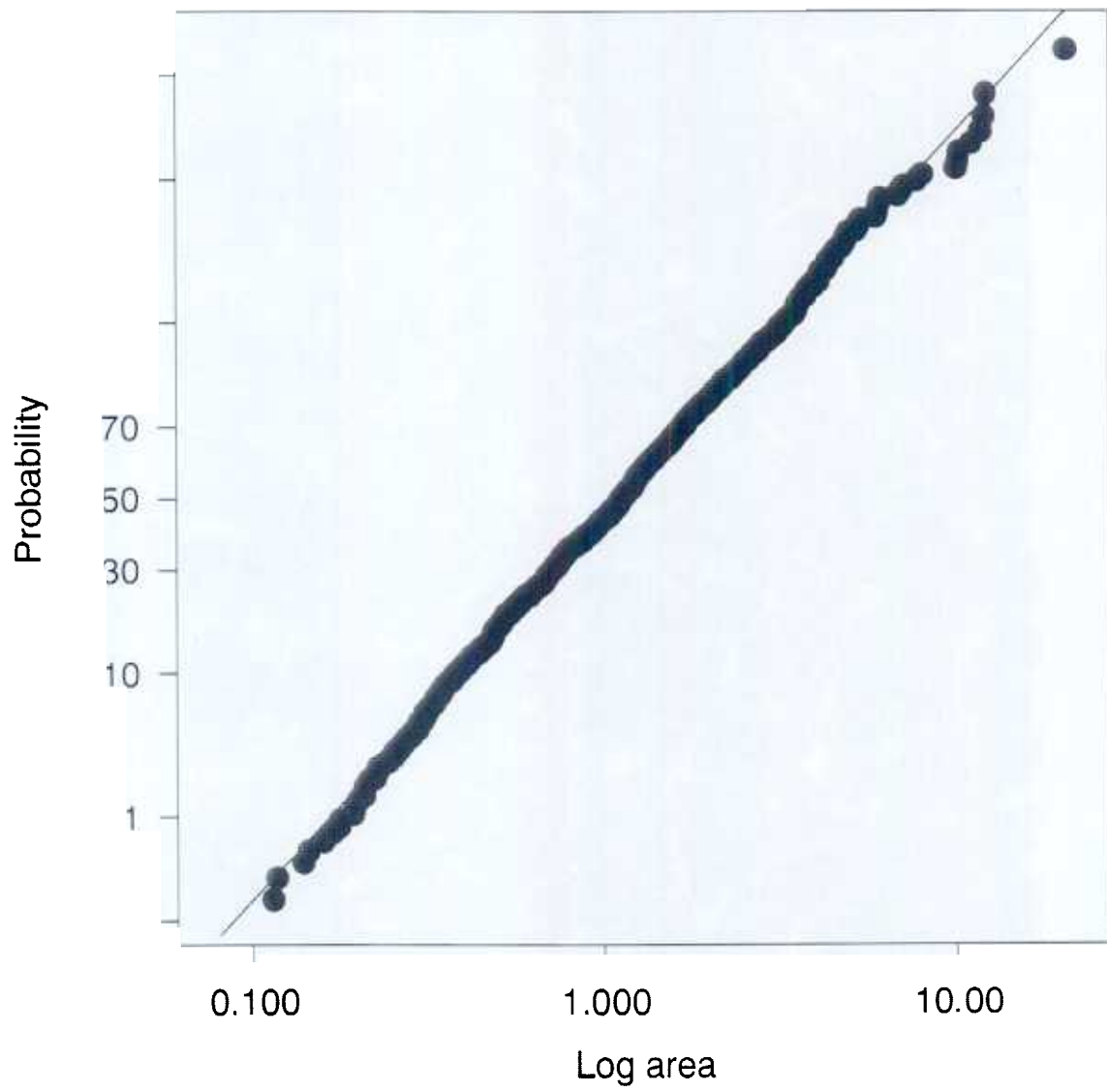


Figure 8

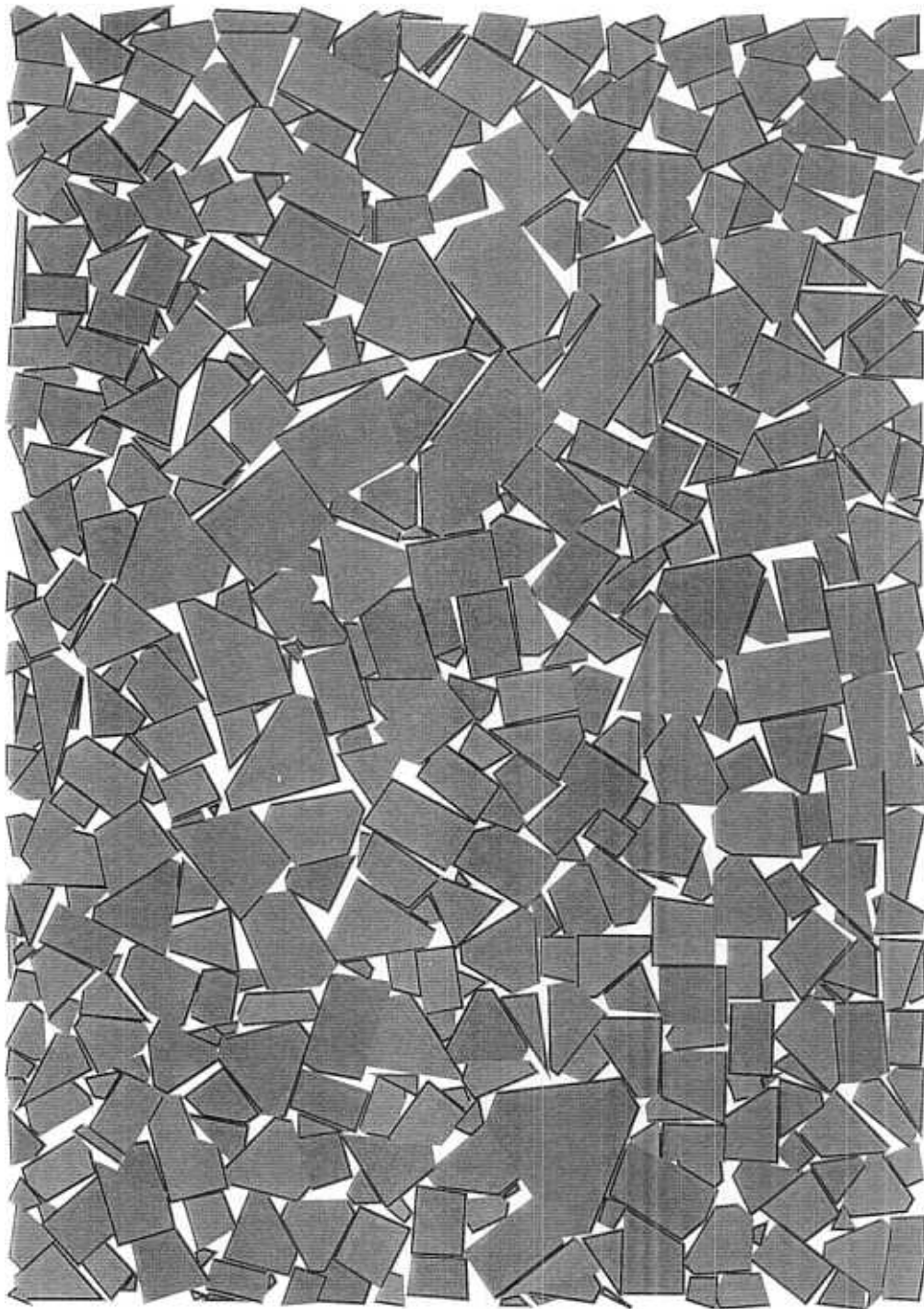


Figure 9

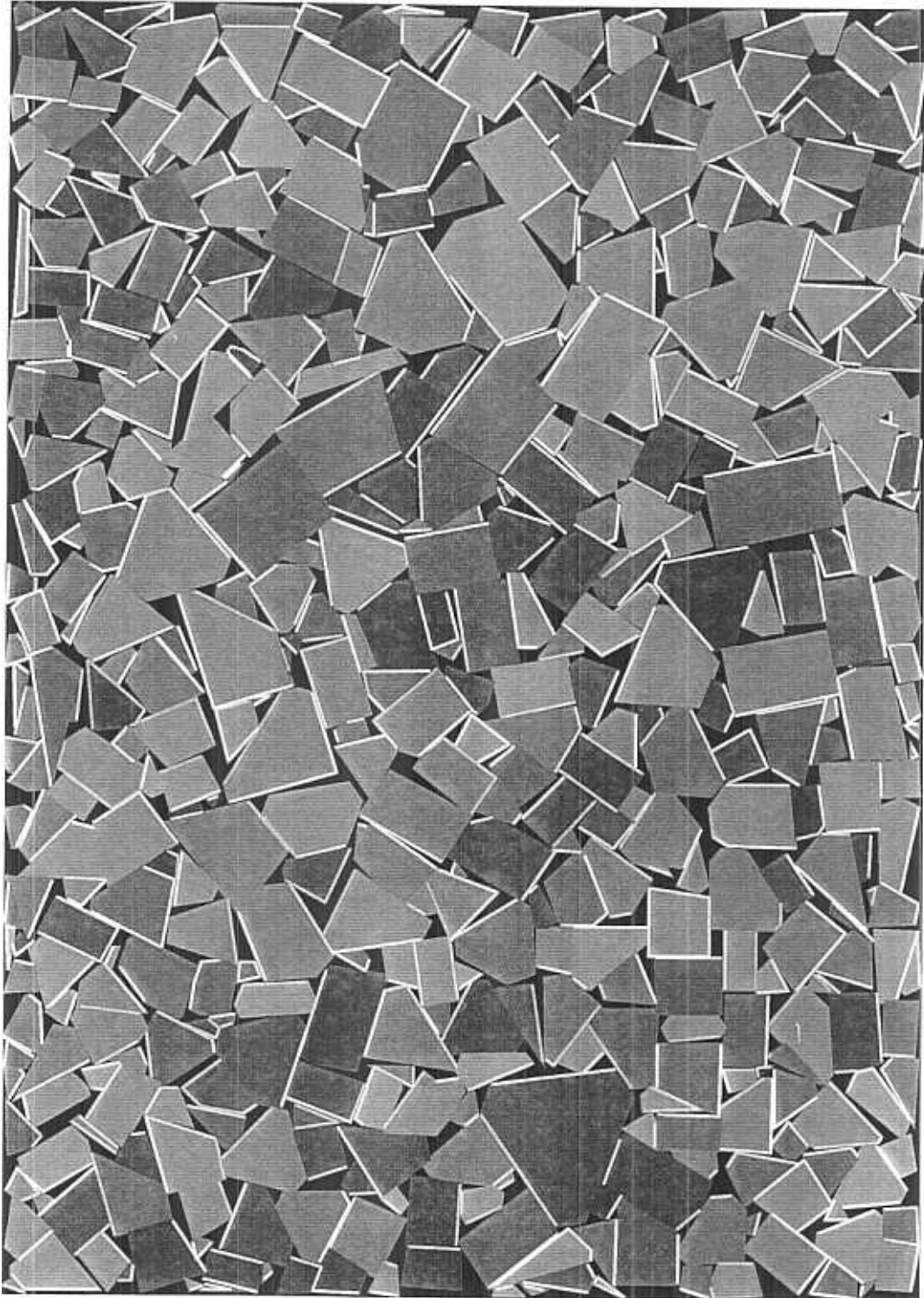


Figure 10

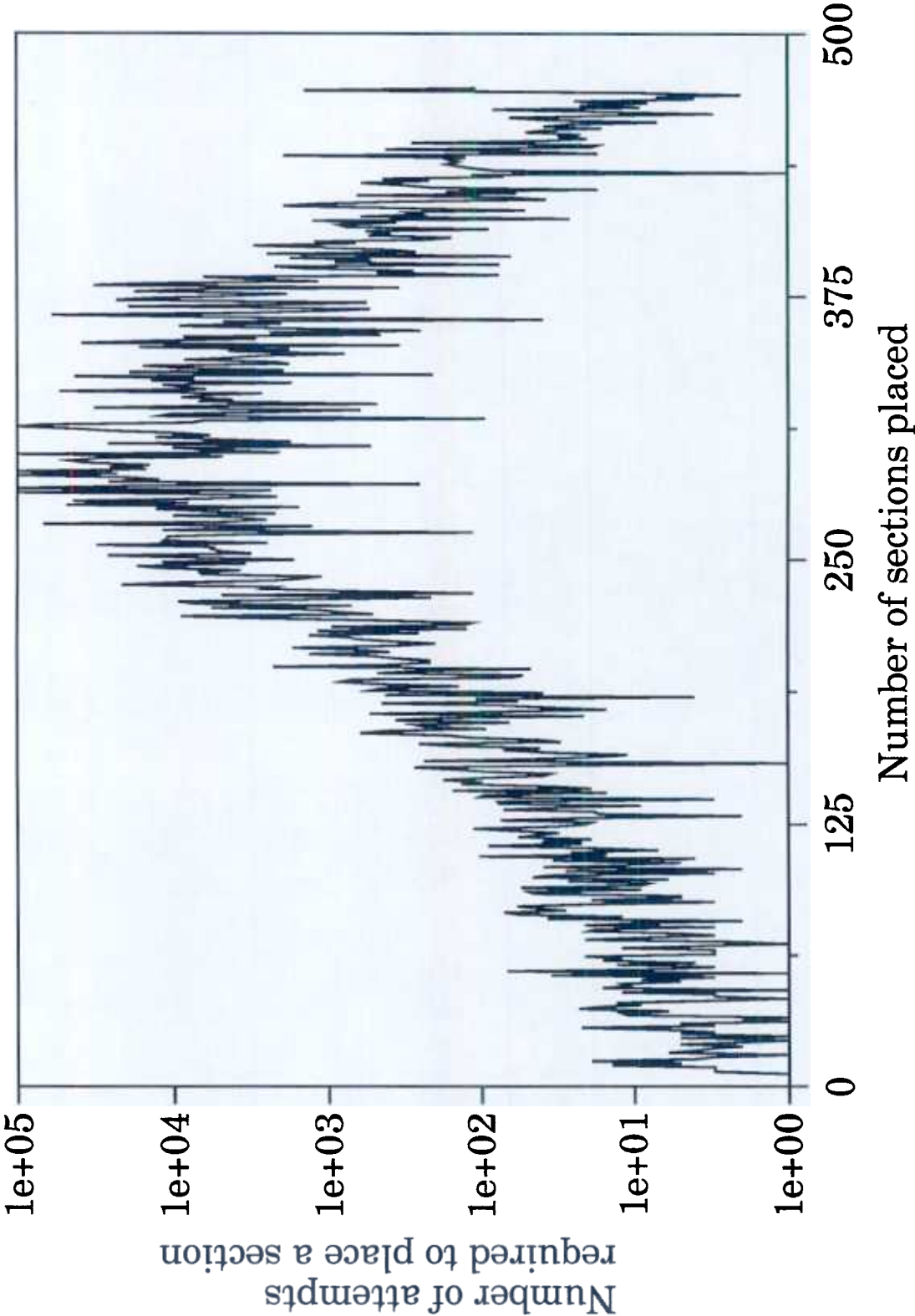


Figure 11

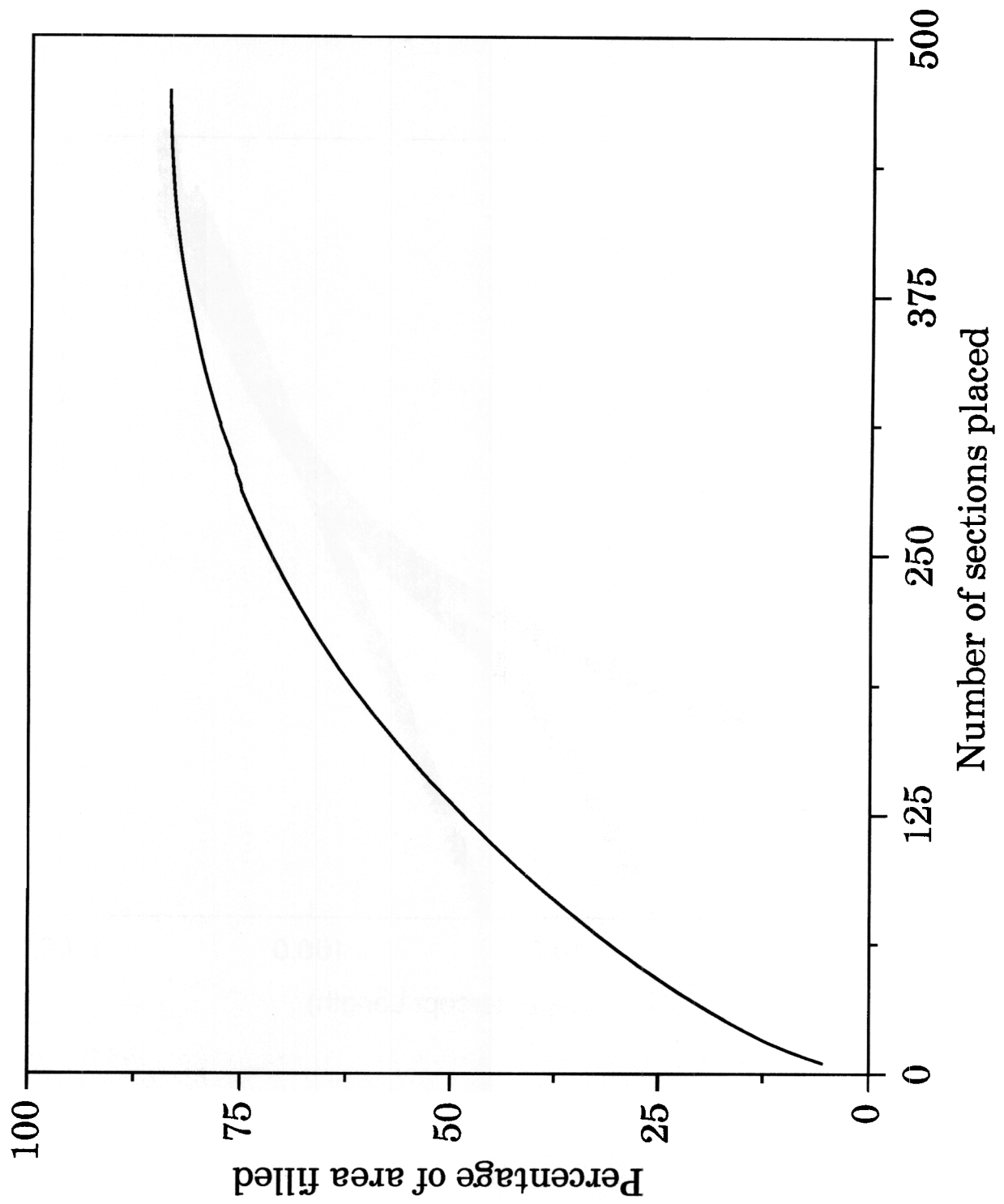


Figure 12

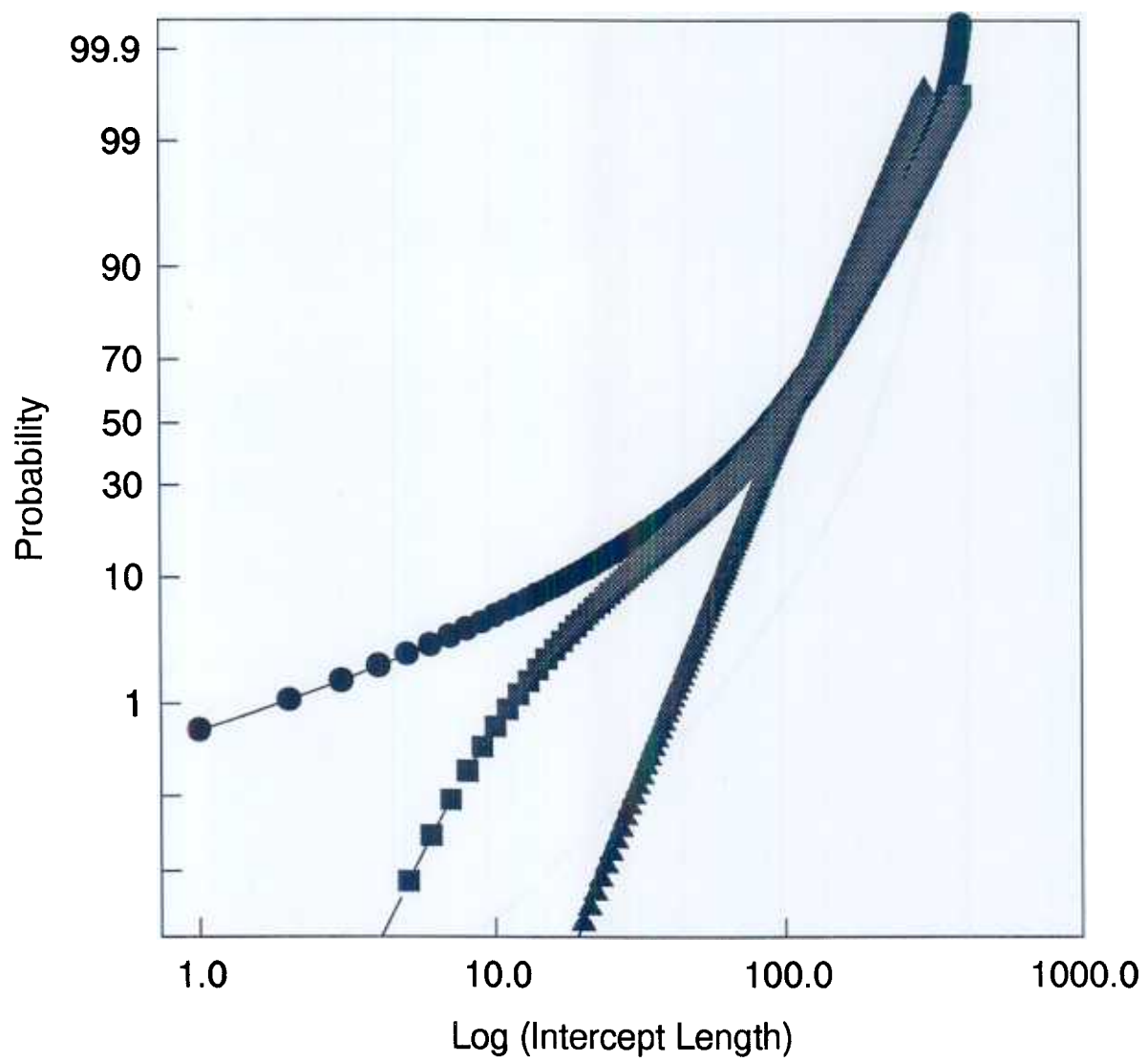
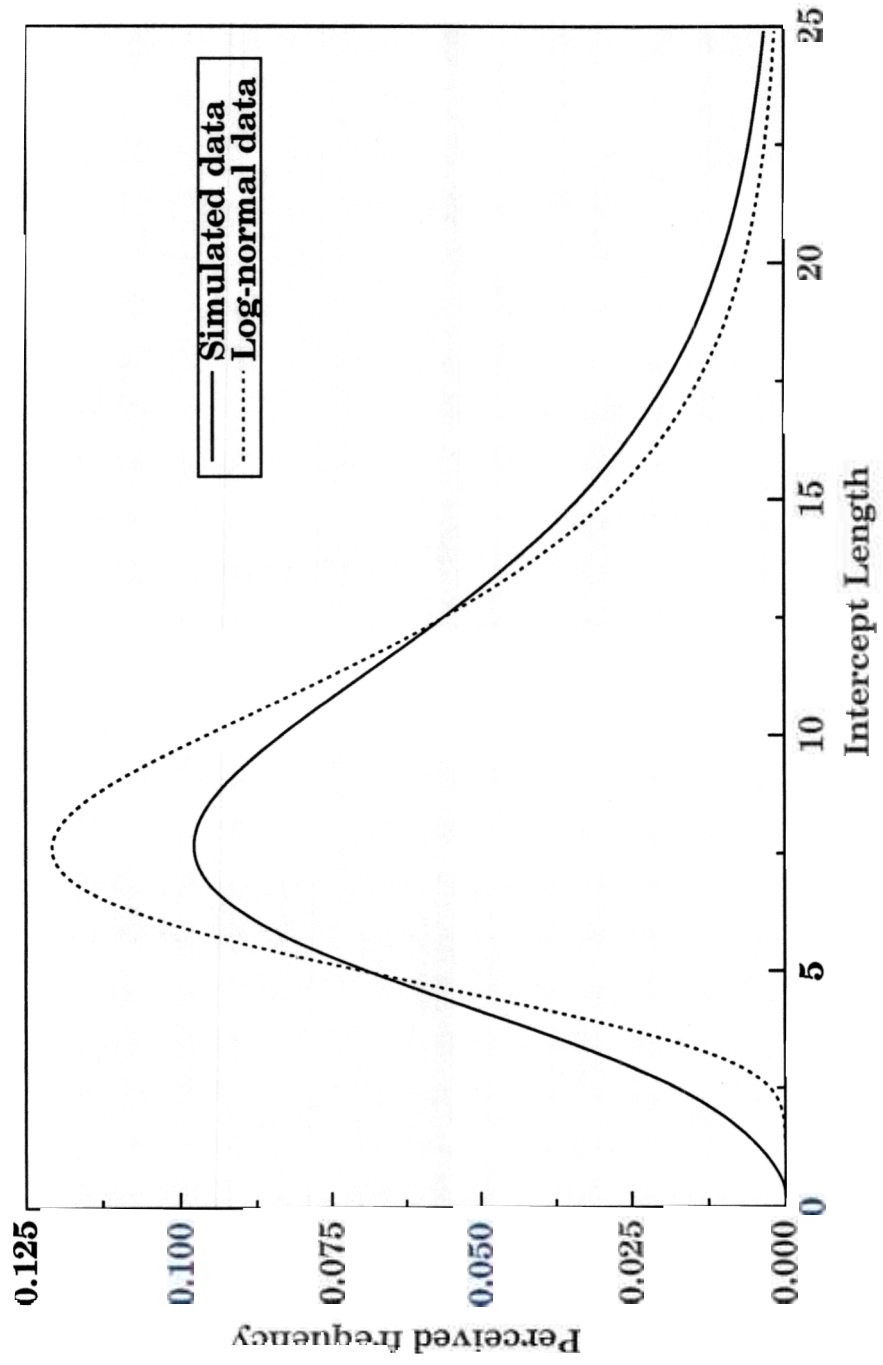


Figure 13



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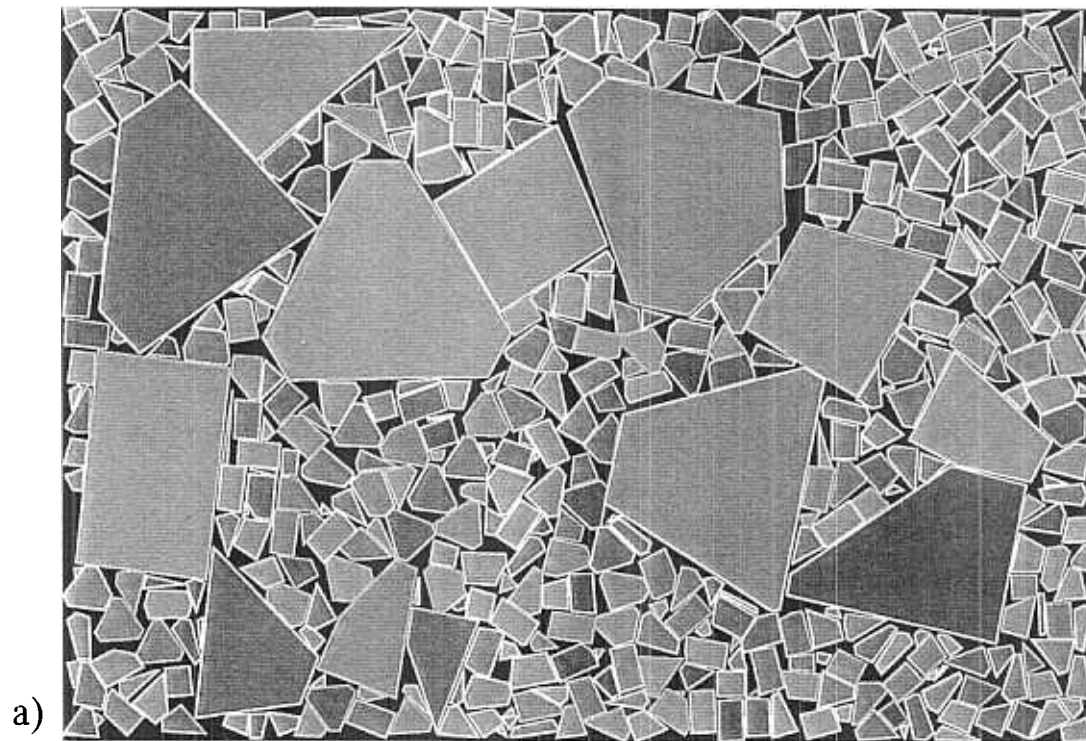


Figure 15 (a)

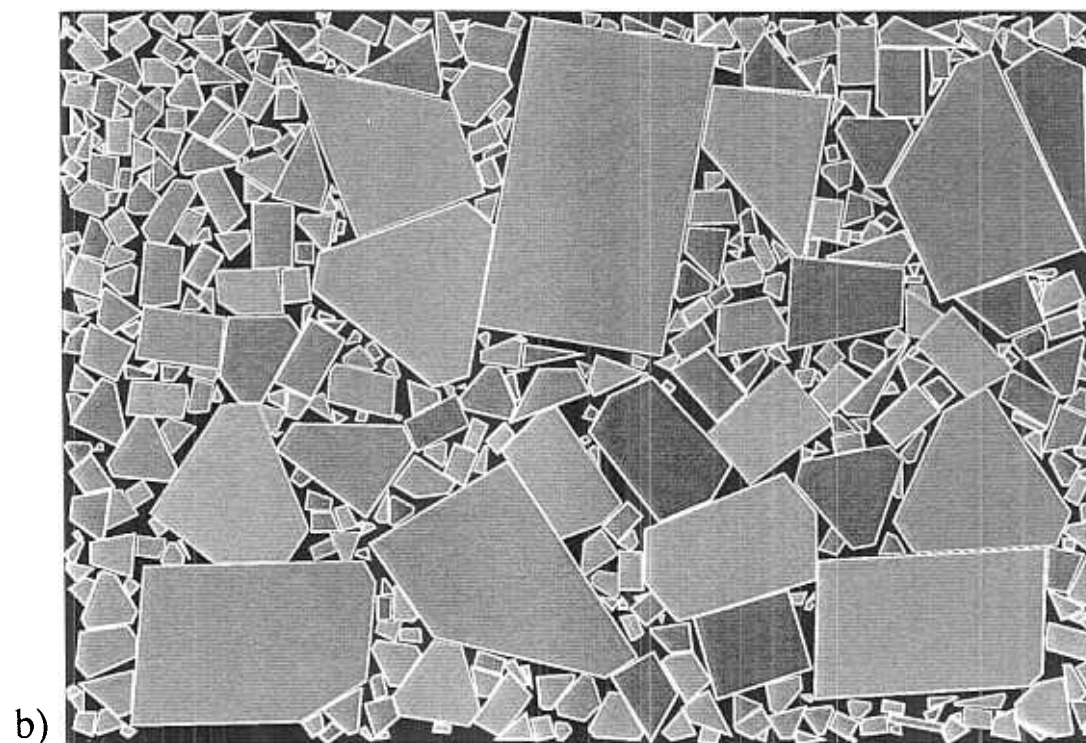


Figure 15 (b)

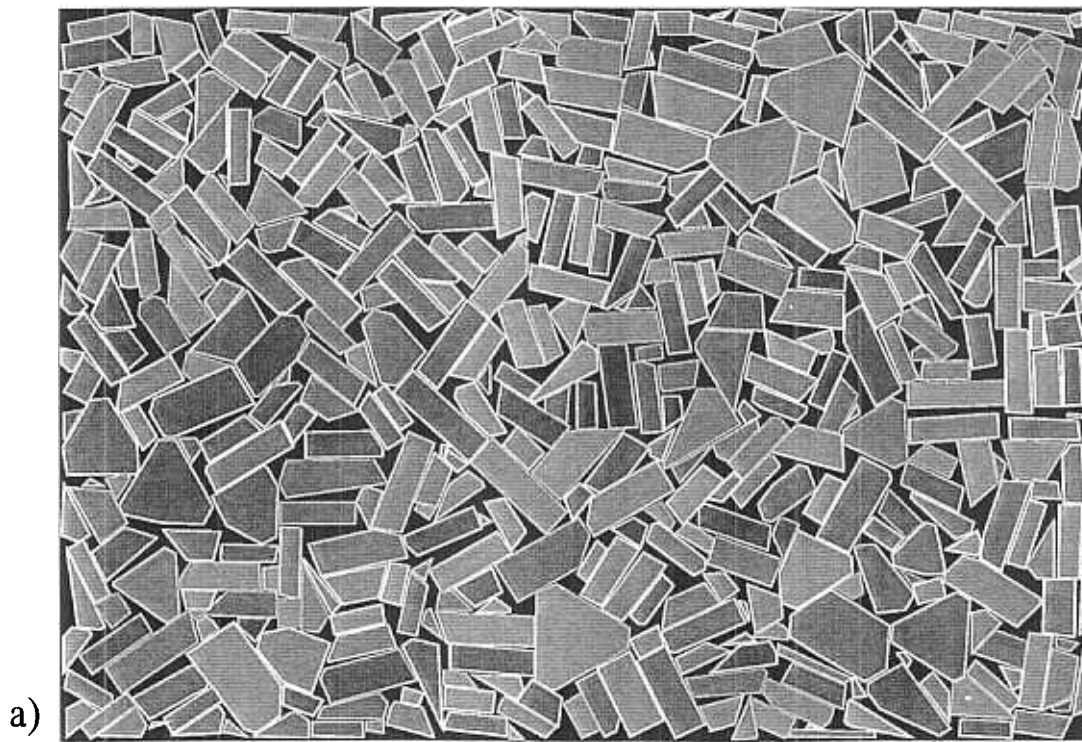


Figure 16 (a)

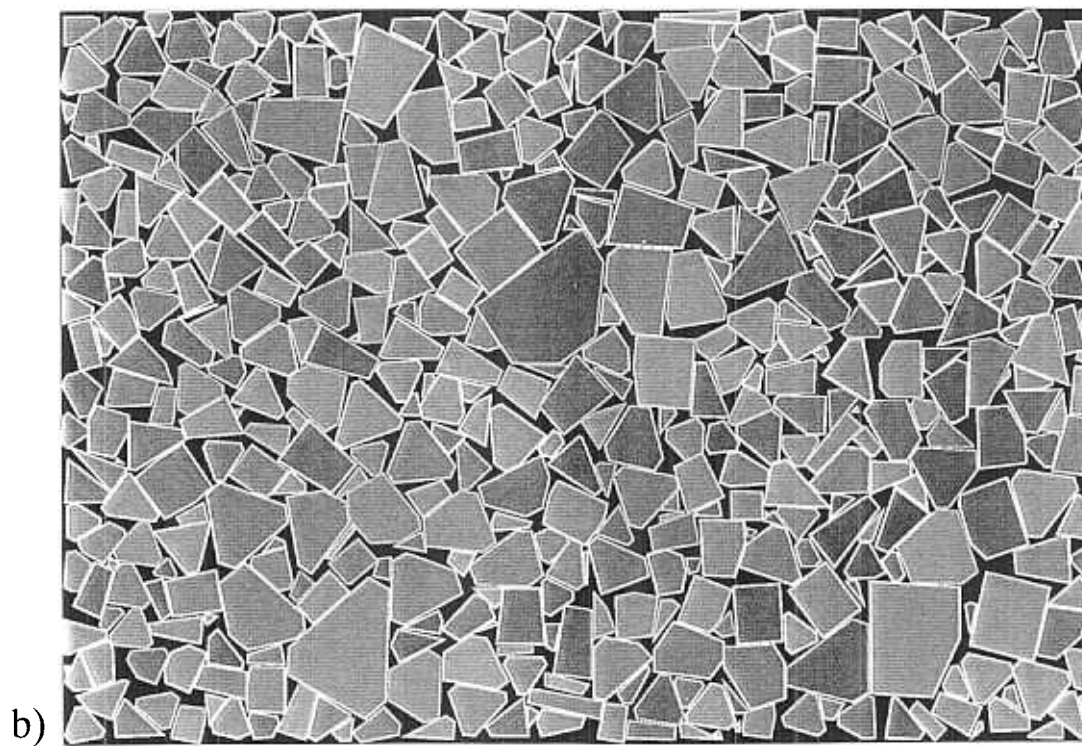


Figure 16 (b)