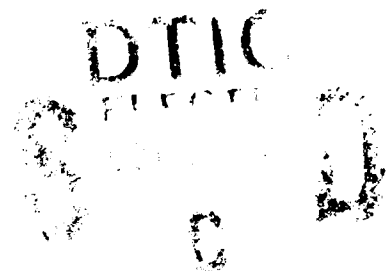


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NAVAL POSTGRADUATE SCHOOL

Monterey, California



THESIS

COMPUTER SIMULATION OF RANDOM AND
NON-RANDOM SECOND-PHASE
DISTRIBUTIONS IN TWO-PHASE MATERIALS

by

Michael E. Pas

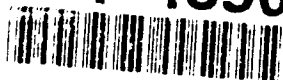
December 1990

Thesis Advisor
Co-Advisor

Terry R. McNelley
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91-13908



91 10 23 023

Unclassified

Security classification of this page

REPORT DOCUMENTATION PAGE

1a Report Security Classification Unclassified		1b Restrictive Markings	
2a Security Classification Authority		3 Distribution Availability of Report	
b Declassification Downgrading Schedule		Approved for public release; distribution is unlimited.	
4 Performing Organization Report Number(s)		5 Monitoring Organization Report Number(s)	
6a Name of Performing Organization Naval Postgraduate School	6b Office Symbol (if applicable) 33	7a Name of Monitoring Organization Naval Postgraduate School	
6c Address (city, state, and ZIP code) Monterey, CA 93943-5000		7b Address (city, state, and ZIP code) Monterey, CA 93943-5000	
8a Name of Funding Sponsoring Organization	8b Office Symbol (if applicable)	9 Procurement Instrument Identification Number	
6c Address (city, state, and ZIP code)		10 Source of Funding Numbers	
		Program Element No	Project No
		Task No	Work Unit Accession No

1 Title (Include security classification): **COMPUTER SIMULATION OF RANDOM AND NON-RANDOM SECOND-PHASE DISTRIBUTIONS IN TWO-PHASE MATERIALS**

2 Personal Author(s) **Michael E. Pas**

3a Type of Report Master's Thesis	13b Time Covered From To	14 Date of Report (year, month, day) December 1990	15 Page Count 50
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6 Supplementary Notation The views expressed in this thesis are those of the author and do not reflect the official policy or position of the Department of Defense or the U.S. Government.

7 Cosati Codes			18 Subject Terms (continue on reverse if necessary and identify by block number) particle distribution computer simulation.
Field	Group	Subgroup	

9 Abstract (continue on reverse if necessary and identify by block number)

The mechanical properties of any material with a discontinuous second phase dispersed in a matrix are recognized to be influenced by the distribution of the second-phase particles. Current models for the prediction of material properties from particle distributions are based on the assumption of a random particle distribution. Through computer simulation, nearest-neighbor particle spacings have been calculated for random and non-random distributions. For low fractions, random distributions approach the theoretical spacing predicted from consideration of random, infinitesimal points. For finite sized particles, increasing fraction results in larger spacings than predicted for infinitesimal points. For very high fractions, the spacing approaches that for regular (crystalline) arrays. Also, metal matrix composites initially possess clustered particle distributions. Upon processing, such distributions can be transformed into banded distributions with areas of both high and low density. With sufficient processing, random distributions can be attained. Non-random (banded) distributions were simulated. Sufficient banding results in reduced average particle spacing

16 Distribution Availability of Abstract ☒ unclassified unlimited ☐ same as report ☐ DTIC users		21 Abstract Security Classification Unclassified	
2a Name of Responsible Individual Ferry R. McNelley		22b Telephone (include Area code) (408) 646-2586	22c Office Symbol 69HY

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Unclassified

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Computer Simulation of Random and Non-Random Second-Phase
Distributions in Two-Phase Materials

by

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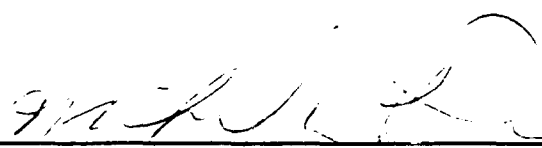
Submitted in partial fulfillment of the
requirements for the degree of

MASTER OF SCIENCE IN ENGINEERING SCIENCE

from the

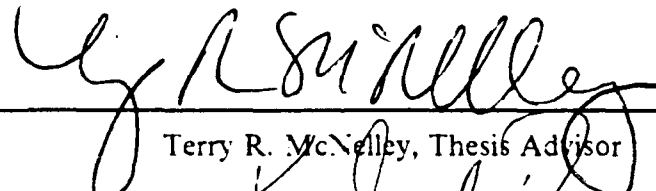
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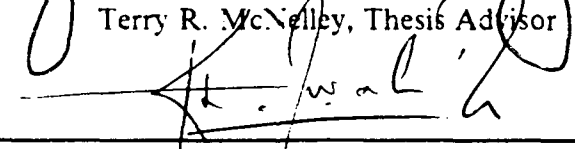


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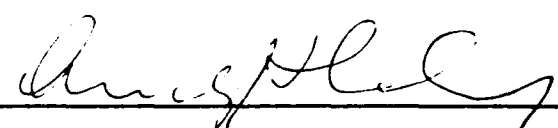
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ABSTRACT

The mechanical properties of any material with a discontinuous second phase dispersed in a matrix are recognized to be influenced by the distribution of the second-phase particles. Current models for the prediction of material properties from particle distributions are based on the assumption of a random particle distribution. Through computer simulation, nearest-neighbor particle spacings have been calculated for random and non-random distributions. For low fractions, random distributions approach the theoretical spacing predicted from consideration of random, infinitesimal points. For finite sized particles, increasing fraction results in larger spacings than predicted for infinitesimal points. For very high fractions, the spacing approaches that for regular (crystalline) arrays. Also, metal matrix composites initially possess clustered particle distributions. Upon processing, such distributions can be transformed into banded distributions with areas of both high and low density. With sufficient processing, random distributions can be attained. Non-random (banded) distributions were simulated. Sufficient banding results in reduced average particle spacing



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I. INTRODUCTION

In many two-phase materials, one phase is discontinuous and distributed in some manner in a matrix of the other phase. The mechanical properties of such two-phase materials may be altered according to how the second-phase particles are distributed throughout the material. Of course, the size and shape as well as distribution of these particles in the material may also influence the materials strength and ductility.

For example, the ability of dislocations to move in a material has a great effect on the materials strength and ductility. Blocking this dislocation movement through the presence of particles within the material represents a strengthening process. If these particles act as points which can pin the ends of dislocation segments and cause them to bow, the mechanism is termed precipitation hardening or dispersion strengthening. As the radius of curvature of the bowed dislocation is decreased the required stress increases. This leads to Orowan's equation [Ref. 1] for this mechanism

$$\tau = \frac{2Gb}{L} \quad (1.1)$$

where τ is the applied shear stress, G is the shear modulus, b is the dislocation Burger's vector and L the average distance between the two pinning particles and is a critical parameter in this equation. Different kinds of particles and their different types of distributions can have varying effects upon Orowan's equation. For instance, it is known that the strength of the particles themselves influences the overall strength of the material. Additionally, L , the characteristic distance, can be influenced by such parameters as the finite size of the particles, the volume fraction of the particles, and whether or not these particles are distributed in any particular pattern.

Alternatively, in an effort to produce stiff, strong, lightweight metallic materials considerable research has been done on the reinforcement of metallic materials with discontinuous fibers and particles. Much of the work done in this area has been concentrated on the reinforcement of materials using particles. Factors such as particle size and volume fraction have a known affect on the properties of materials [Ref. 2]. One such effect that has been demonstrated is the trade-off between strength and ductility in a metal matrix composite (MMC) material and this occurs as a result of increasing particle size [Ref. 3].

Processing techniques such as extrusion can also have an effect on the distribution of the particles within the matrix [Ref. 2]. Many MMC's particle distributions change according to the processing to which they are subjected. Clusters of reinforcement particles may be broken up by rolling which leads to a more random distribution. Rolling can also cause the distributions to become banded. An example of random and banded particle distributions found in an Al 6061 MMC material are shown in Figure 1 and Figure 2. The reinforcement is Al_2O_3 in this material. The banding shown here evolved as a result of the material's thickness being reduced approximately 66 percent by rolling at 350°C. [Ref. 4]

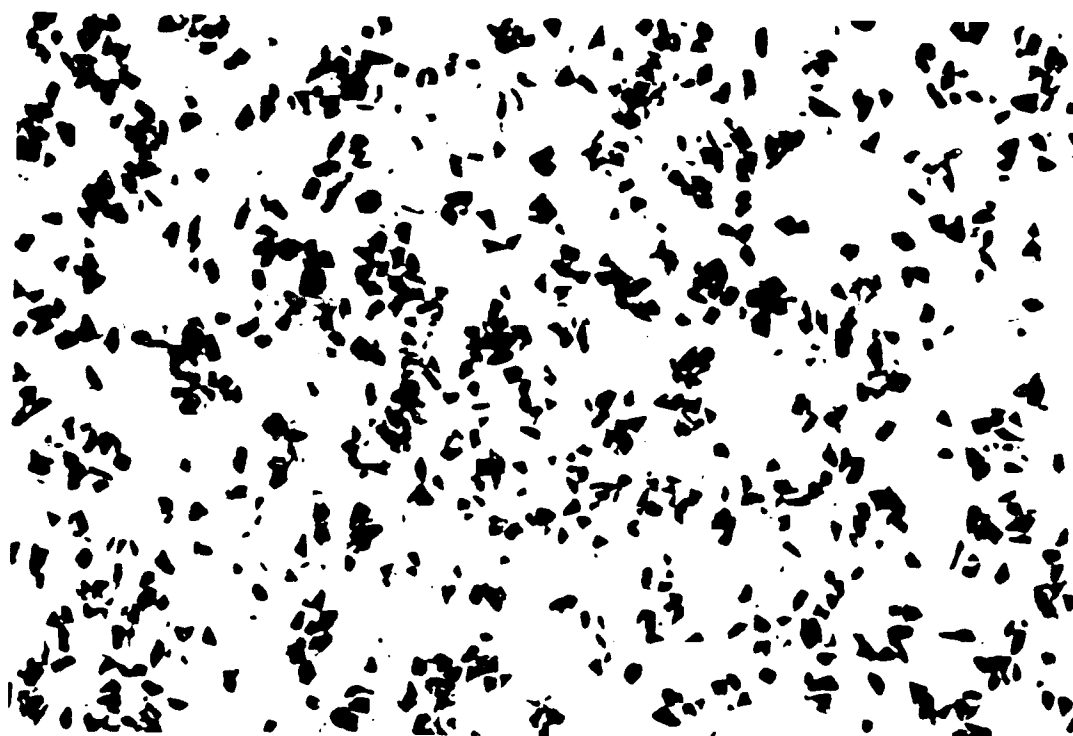


Figure 1. Random particle distribution in a fully processed Al 6061 alloy composite

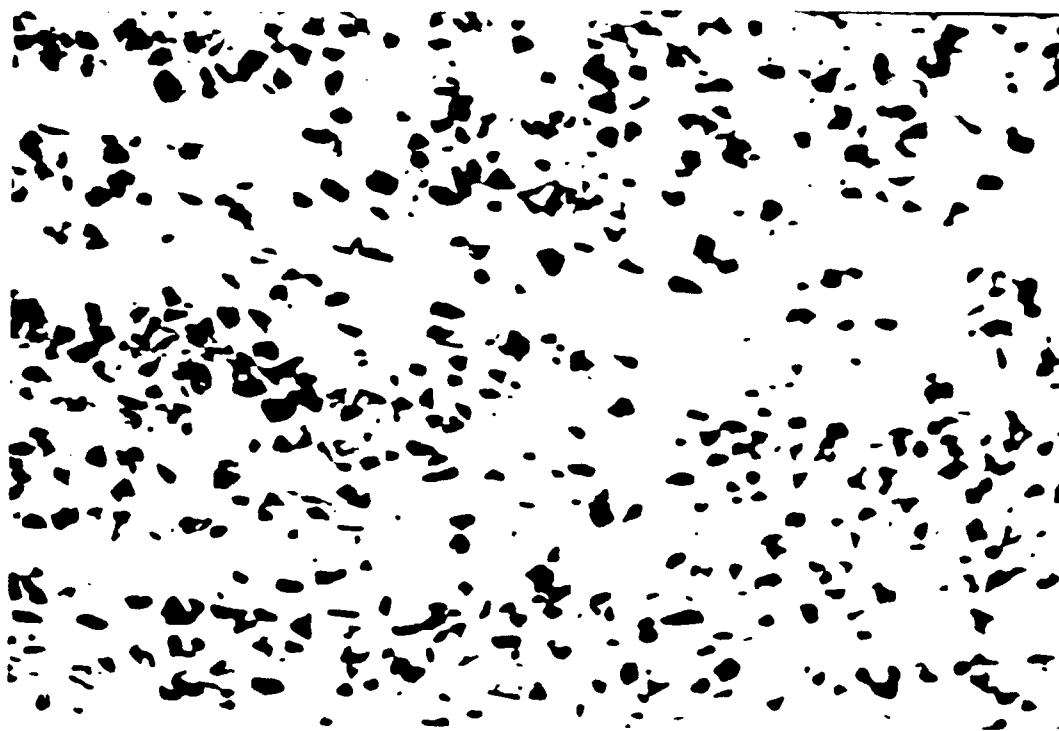


Figure 2. Banded particle distribution in a partially processed Al 6061 alloy composite

In order to accurately assess and compare these different types of microstructures it would be desirable to be able to quantitatively measure a characteristic parameter of these particle distributions such as average nearest neighbor particle spacing. Properties of materials containing particle distributions might then be inferred from this measurement. However, existing methods which attempt to do this can only be used on materials with random particle distributions. These models also assume that these particles are infinitesimal points, which is clearly not valid for real materials. There are models which can be used for finite sized particles, but these models require that the particles be distributed in a regular array, for instance in a manner analogous to a closed-packed arrangement in a crystal lattice.

This study was initiated to address the problem of random distributions of finite sized, non-overlapping particles using a computer simulation method. This simulation was then modified so that banding could be introduced into these finite sized, non-overlapping particle distributions. Calculations of the average nearest neighbor particle

spacing for different distributions were then made. For both mathematical and computational convenience it was decided to restrict the analysis to two dimensional representations as opposed to three dimensional models. The two dimensional approach makes graphics much easier, and reduces the computing time required. At the same time, the two dimensional results will be applicable to the three dimensional distribution through inference.

II. BACKGROUND

Existing approaches for calculating average nearest neighbor particle spacings on a two dimensional planar section assume that the particles are infinitesimal points and that they are distributed randomly. One common method for calculating average nearest neighbor particle spacing for random distributions of point particles is described by Underwood [Ref.5]. The approach begins with the above assumption that the particles are infinitesimally small, mathematical points. These points must then be distributed completely random throughout an area. Arbitrarily starting at any one of these points, he develops a function which describes the probability of finding another particle nearby. Starting at an arbitrary particle, the probability function is integrated over an expanding circle of radius r about the infinitesimal point as indicated in Figure 4.

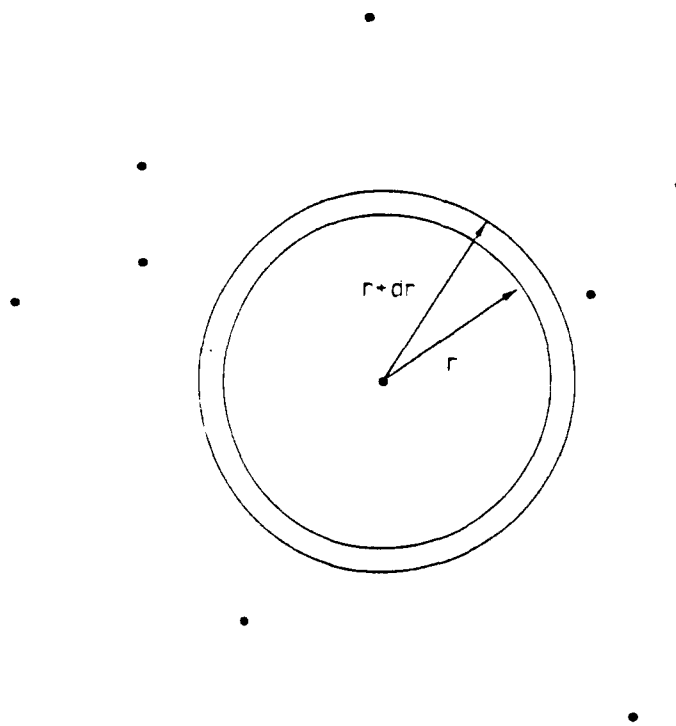


Figure 3. Integration about an infinitesimal point

The final result is

$$\delta = 0.5N^{-0.5} \quad (2.1)$$

where δ is the average value of the nearest neighbor particle spacing and N is the number of particles per unit area. The number of particles per unit area is usually calculated in practice by marking out an area on a micrograph of the material being studied and then counting the number of particles within that area, which provides then a value of N . In turn, δ is then calculated via equation (2.1).

At the opposite end of the spectrum from randomly distributed infinitesimal points is a perfectly regular distribution, such as hexagonal, of finite sized particles. A geometric analysis of a hexagonal distribution such as that shown in Figure 4

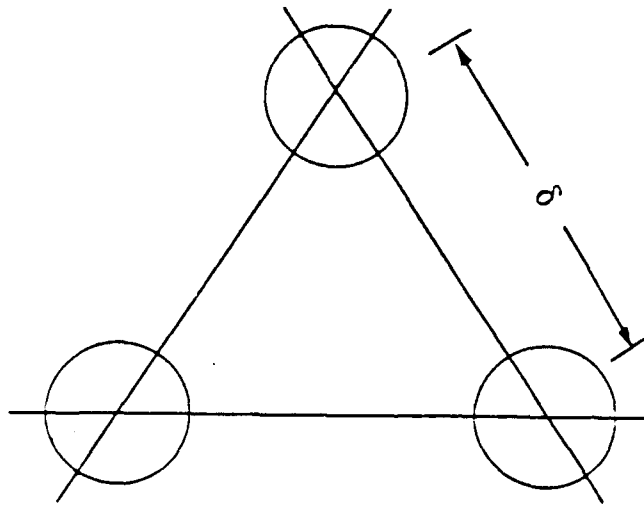


Figure 4. Hexagonal particle distribution

gives equation 2.2 as the result for average nearest neighbor particle spacing.

$$\delta = 1.075N^{-0.5} \quad (2.2)$$

Here again, δ is the average nearest neighbor particle spacing and N is the number of particles per unit area.

The above cases represents extremes in particle distributions. The first represents infinitesimally small points distributed randomly. However, real particles are not infinitesimal points, but instead, are of finite size and do not overlap. The fact that these particles are non-overlapping affects their distribution. Since these particles cannot overlap one another their distributions are not truly random because particles are prevented from occupying any position which would cause them to overlap with one another. This would affect the results of the integration process which resulted in equation (2.1) although this problem does not appear to have been addressed theoretically. The second case mentioned above applies only to distributions where the particle distributions are regular, which is also not an accurate description of real materials. Therefore, it can be said that real materials do not fit either of these models perfectly and that the accuracy of results obtained for such materials using the above methods is somewhat suspect.

In order to accurately apply Orowan's equation (2.1) it is necessary to know precisely what the characteristic parameter L is. For the above reasons a simple calculation for L in real materials is not possible. As a result of this it is often necessary to derive a value for L by actually counting the particles per unit area in a micrograph of the material. Even if it was possible to exactly calculate a value for L microstructurally, there is some question as to what L should really represent. Some doubt exists as to whether a dislocation actually bows between a particle and its nearest neighbor or between the particle and its second or third nearest neighbor [Ref. 6].

It is therefore necessary to develop a computer simulation which can handle both random and banded distributions of finite sized particles. Once these particle distributions are generated by the computer it is then possible through direct calculation to accurately compute the average nearest neighbor particle spacing for various particle distributions.

It is recognized that a computer simulation inherently contains many limitations. For ease of calculation this program generates two dimensional particle distributions versus real material three dimensional particle distributions. Additionally all of the particles are required to be of uniform size and shape. This simulation does not take into account how or why the particles become distributed as they are. It cannot account for particle-particle interactions that can also affect their distributions, or the effect of various processing techniques which can introduce these different distributions. Finally,

it is recognized that the statistics of such a model are complex. Varying such parameters as the size of the particles, the number of particles being positioned and changing the size of the area into which the particles are being positioned can introduce statistical variations into the results being obtained. Therefore several sets of data were generated in an attempt to minimize the statistical variations.

III. EXPERIMENTAL PROCEDURE

A. OVERVIEW

The construction of the particle distribution model and calculation of the spacing parameters was accomplished with a computer simulation. The programs needed to create these simulations were written in Turbo Pascal and run on an IBM personal computer. The programs were based upon a program written by A. Geltmacher [Ref. 7] which randomly positioned holes within a square array. A copy of these programs is provided in appendices A and B.

For this project it was necessary for the computer to place particles of finite size in both random and banded distribution patterns without the particles overlapping. In order to accomplish this, two separate but similar programs had to be written, one for the random distributions, and one for the banded distributions. From the random and banded particle distributions that were generated, nearest neighbor particle spacing calculations were made. The algorithm that these two programs followed is summarized in Figure 5.

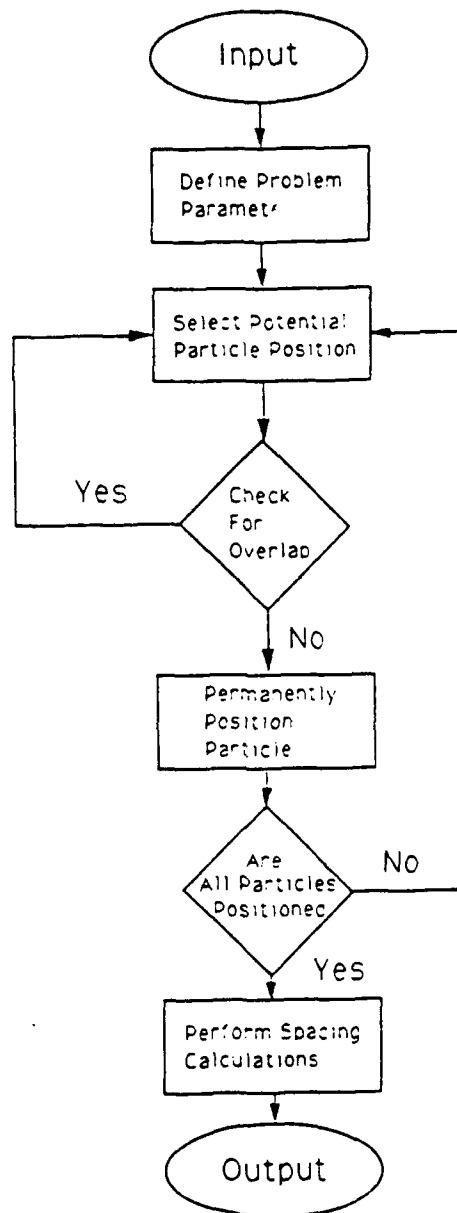


Figure 5. Program flow algorithm

B. RANDOM PARTICLE DISTRIBUTIONS

The input portion of this program requires the operator to input the size of the two dimensional area that is to be filled with particles. In addition, the size of the particles and the area fraction of the specified two dimensional area that is to be filled with particles, must also be input. The define parameters portion of the program then determines the number of particles that must be positioned to satisfy the area fraction requirements.

The next step of the program is to position the particles. Here, a random number generator is called that gives both an X and Y coordinate at which the particle can temporarily be positioned within the specified area. After this has been accomplished the computer checks to insure that the particle presently being positioned does not overlap any previously positioned particles. If, for example, the computer is attempting to position particle number five, it must calculate the center to center spacing from particle five to each of the four previously positioned particles. If any of these center to center spacing measurements is less than twice the radius of a particle, particle overlap has occurred and this potential position for particle five is rejected. The computer then cycles back to the random number generator, picks a new X and Y coordinate into which the particle is temporarily placed. The particle overlap check is again performed and if it is found that the new position does not overlap any previously positioned particle, then particle five is permanently positioned. This process is repeated until all of the particles that must be positioned to satisfy the area fraction requirements have been sited.

After the particle distributions have been generated the computer is ready to calculate the average nearest neighbor particle spacing. This is accomplished by calculating for each particle the center to center distance to every other particle. The smallest value obtained is the nearest neighbor particle spacing for that particular particle being considered. This calculation is made for every particle that has been positioned. The nearest neighbor particle spacing for each of these particles is then summed together and this sum is divided by the total number of particles. This result yields the average nearest neighbor particle spacing.

C. BANDED PARTICLE DISTRIBUTIONS

The program for generating these banded distributions is similar to the program for random distributions. However, in the input portion, in addition to having to input the

size of the area, the particle size, and area fraction, the operator must also provide input on how much banding is to be introduced into the distribution.

In order to cause banding to occur the original area into which particles are to be positioned is arbitrarily divided into five sub-regions of equal area, each containing 20 percent of the original area. Additionally, three of these sub-regions were designated as high particle density zones and the remaining two sub-regions as low particle density zones, as shown in Figure 6.

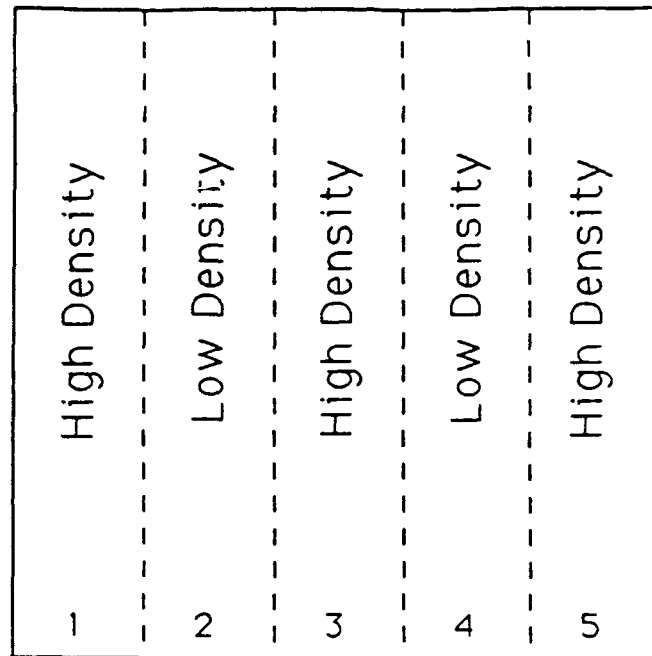


Figure 6. High and low particle region designations

The decisions to make five sub-regions of equal area and to designate three of them as high density zones and two as low density zones were made arbitrarily and numerous other arrangements can be envisioned.

In the define parameters portion of the program based upon the input from the operator the computer determines how many of the particles are to be allocated to each of the five sub-regions. If for example, the operator determines 80 percent of the particles will be placed in the high density zones, the computer will place 80 percent of the

total number of particles to be positioned in the three high density zones which comprise 60 percent of the total area. The remaining 20 percent of the particles will then be placed in the two low density zones or the remaining 40 percent of the area. By changing the percentage of particles which the operator wishes to place in the high density zones the severity of the banding can then be changed.

Particle overlap checks and the average nearest neighbor particle spacing calculation are performed in exactly the same manner as those described for the random distribution program.

IV. RESULTS AND DISCUSSION

A. OVERVIEW

To begin this study, plots were generated for random particle distributions of varying area fractions. From these distributions, the average nearest neighbor particle spacings were then calculated. After all of the data for the random distributions was collected, plots were then generated where banding was introduced into the distribution. Again values for the average nearest neighbor particle spacing were calculated for the banded particle distributions.

B. BANDED PARTICLE DISTRIBUTIONS

In order to generate the data that was required for this study the computer program had to be run several times. Each time the program is run it generates one particle distribution scheme and calculates the average nearest neighbor particle spacing for that particular distribution. It was therefore necessary to run the program several times for each set of the input parameters so that a statistical average could be obtained. As the area fraction that is to be covered with particles is decreased the number of particles to be positioned consequently is decreased and this can be expected to have an adverse effect on the statistics. In order to address this problem it was necessary to increase the number of particles being positioned at low area fractions by either reducing the radius of the particles or by increasing the size of the array into which they are being positioned. A minimum of 50 particles positioned appeared to be sufficient to offset the adverse effects of smaller total number of particles on the statistics. Shown below in Figures 7 through 10 are examples of random particle distributions of varying particle size and area fraction.

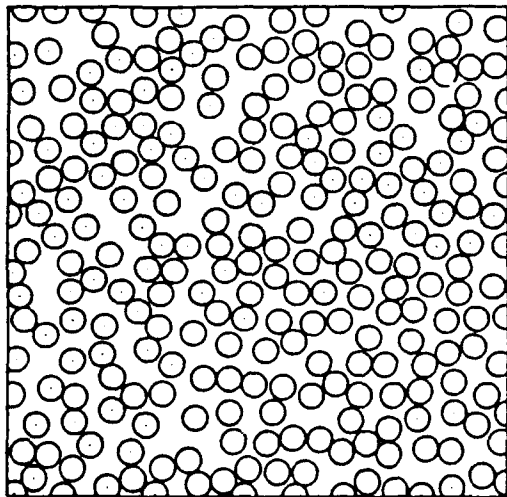


Figure 7. Random distribution with an area fraction of 0.50

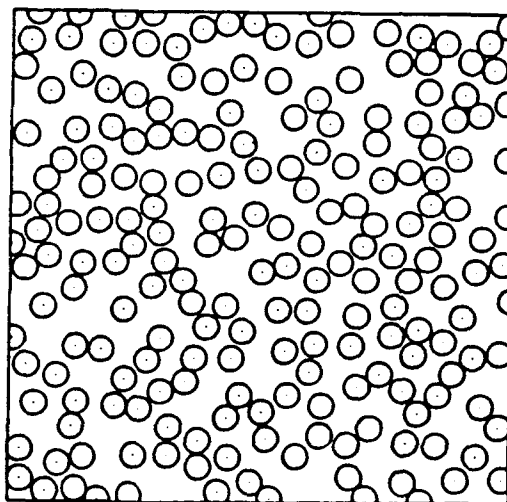


Figure 8. Random distribution with an area fraction of 0.40

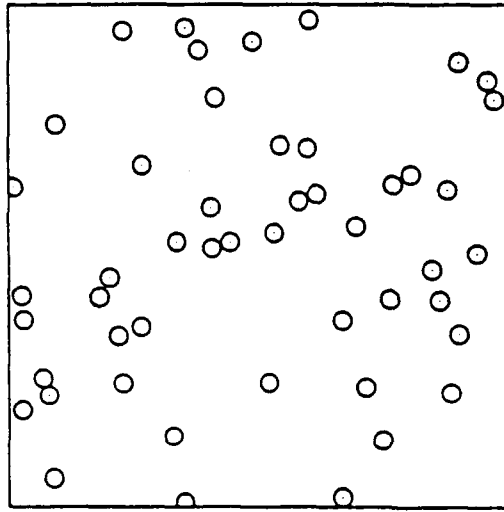


Figure 9. Random distribution with an area fraction of 0.05

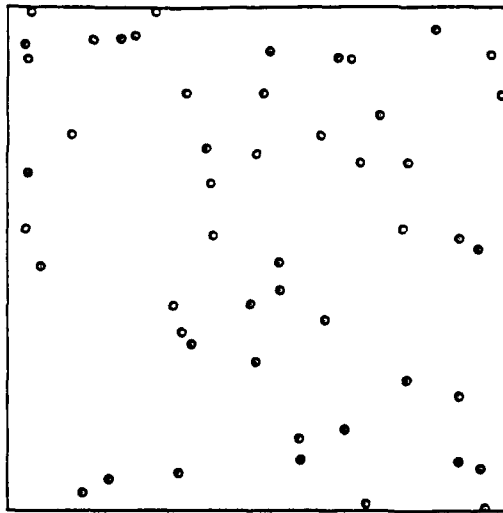


Figure 10. Random distribution with an area fraction of 0.01

Additionally in this study average nearest neighbor particle spacing data was generated for random distributions of particles of three different sizes, namely, 0.10, 0.25, and 0.50 units. For these three different sizes of particles, parameters such as area fraction, and array size were varied. The data collected is presented below in Tables 1 through 3 along

with the number of particles per unit area and how many times the program was run for each condition.

Table 1. DATA FOR PARTICLES OF RADIUS 0.10 UNITS

Area Fraction	Array size	Number of runs	δ	N
0.01	20×20	10	1.0495	0.3157
0.05	10×10	5	0.4507	1.5900
0.10	10×10	2	0.3400	3.1800
0.15	10×10	1	0.2956	4.7700
0.20	10×10	1	0.2688	6.3600
0.30	10×10	1	0.2458	9.5400
0.40	10×10	1	0.2295	12.7100

Table 2. DATA FOR PARTICLES OF RADIUS 0.25 UNITS

Area Fraction	Array size	Number of Runs	δ	N
0.01	30×30	10	2.3705	0.0511
0.05	30×30	10	1.1389	0.2544
0.10	10×10	10	0.8859	0.5600
0.15	10×10	10	0.7839	0.7600
0.20	10×10	10	0.6736	1.0200
0.30	10×10	2	0.6186	1.5300
0.40	10×10	2	0.5785	2.0300

Table 3. DATA FOR PARTICLES OF RADIUS 0.50 UNITS

Area Fraction	Array Size	Number of Runs	δ	N
0.01	60×60	5	4.9205	0.0127
0.05	60×60	2	2.7874	0.0636
0.10	30×30	2	1.9761	0.1273
0.15	30×30	2	1.6041	0.1909
0.20	30×30	2	1.4969	0.2546
0.30	30×30	2	1.2741	0.3819
0.40	10×10	5	1.1877	0.5100

Typical standard deviations as result of the data that was generated for random distributions of area fractions of 0.10, 0.15, and 0.20 are 0.0479, 0.0271, and 0.0283 units respectively. The total number of particles positioned in the 10×10 area were 51, 76 and 102 respectively.

In Figure 11, the computer generated spacing data are plotted versus number of particles per unit area for each of the three particle sizes employed. Three resultant curves were obtained. The theoretical variation of δ with N is shown for both random distributions of points and regular (hexagonal) arrays. Equation (2.1) and (2.2) will plot as straight lines of slope equal to $-\frac{1}{2}$ on double logarithmic axes. The computer simulations tend to a limit for δ which is the random point distribution for small values of N. Conversely, as the area fraction increases, the spacing decreases but less rapidly than suggested by the $N^{-0.5}$ dependence. It appears that the simulation data can be extrapolated to the solution predicted for a hexagonal array in each case. The area fraction in each such case is 0.91 and the particles are then in contact. Conversely, the random point solution predicts particles in contact at an area fraction of 0.2 for finite, uniform sized particles.

These results have important implications. Estimates of particle spacing based on particle counts in conjunction with equation (2.1) are inherently in error. The finite size of the particles preclude placement of particles such that overlap would occur and this results in non-randomness in the distribution. The effect of this can be seen in the upward shift in spacing (relative to the $N^{-0.5}$ dependence) as area fraction is increased. Indeed, as area fraction increases, simulation run time increased disproportionately to the

increase in numbers of particles as overlap resulted in increasing rejection of possible sites.

Finally, these results suggest that a normalized plot of $\frac{\delta}{r_p}$ (r_p equals particle radius) versus N will result in a single curve. This in turn suggest a functional relationship among these parameters although determination of this relationship is beyond the scope of this work.

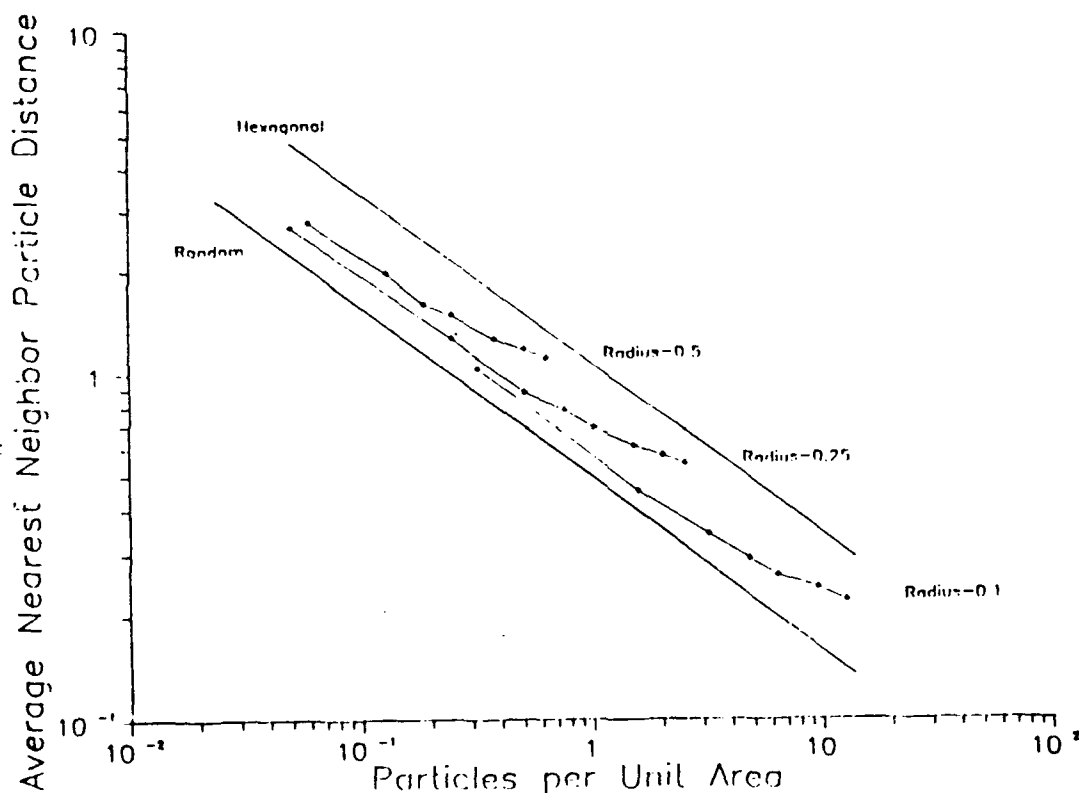


Figure 11. Random distributions of particles

C. EFFECT OF BANDING

This portion of the study examined banded particle distributions similar to those shown in Figure 2. It is known thermomechanical processing can result in distributions in which particles are present in bands of high concentration. It should also be noted

that the microstructure of wrought materials can also exhibit this banding of their microstructural constituents.

The computer generated distributions are an attempt to simulate distributions which are similar to those described above. These distributions had area fractions of 0.10, 0.15, and 0.20 which are typical values of many MMC's. For this portion of the study the size of the array was held constant at 10×10 units and a uniform particle size of 0.25 units was used. Different degrees of banding were produced by varying the percentage of particles placed in the three high density zones. Sample plots of random particle distributions and the associated banded distributions, which were created by placing 90 percent of the particles in the three high density zones, are shown in Figures 12 through 17. for the area fractions being considered here. Additional plots that were generated for this portion of the study are shown in Figures 19 through 30 in Appendix C. In calculating δ for each of these different situations the same approach was used. The results for each of these calculations are also shown below in Tables 4 through 9.

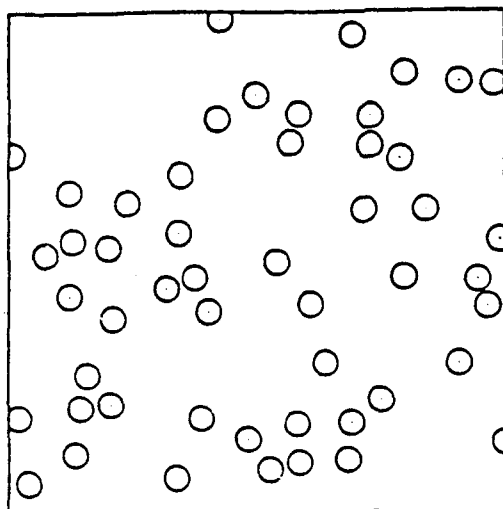


Figure 12. 0.10 Area fraction with a random distribution

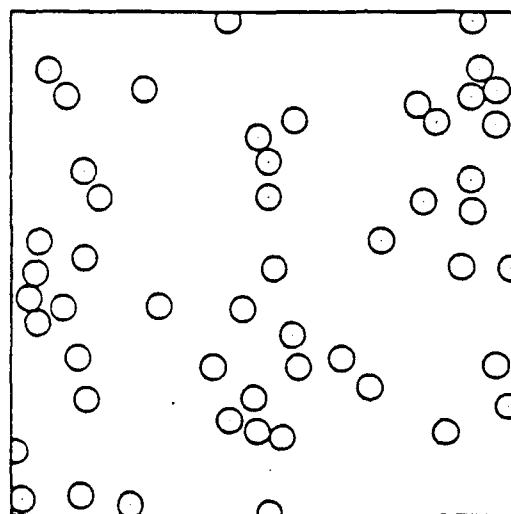


Figure 13. 0.10 Area fraction with 90% of particles in high density zones

Table 4. NEAREST NEIGHBOR SPACINGS FOR 0.10 AREA FRACTION

Percentage of Particles Placed in High Concentration Bands	60%(random)	70%	75%	80%
Particle Spacing	0.8304	0.8692	0.8162	0.9039
	0.8106	0.9417	0.9599	0.8700
	0.9266	0.9702	0.9489	0.7755
	0.9154	0.9472	0.8539	0.8542
	0.8722	0.8171	0.8992	0.9091
	0.9883	0.8318	0.9020	0.9233
	0.8324	0.9330	0.9273	0.8883
	0.8803	0.9141	0.8471	0.8908
	0.9216	0.9057	0.8727	0.9216
	0.8904	0.8655	0.8234	0.8700
Average Particle Spacing	0.8859	0.8933	0.8851	0.8807

Table 5. NEAREST NEIGHBOR SPACINGS FOR 0.10 AREA FRACTION

Percentage Placed in High Concentration Bands	85%	90%	100%
Particle Spacing	0.8212	0.8622	0.7978
	0.8468	0.7582	0.8008
	0.7825	0.8978	0.7158
	0.8596	0.8717	0.8198
	0.8978	0.8189	0.7901
	0.8333	0.8686	0.7945
	0.7984	0.9220	0.8268
	0.8729	0.8368	0.7443
	0.8791	0.9593	0.8363
	0.8297	0.7915	0.7809
Average Particle Spacing	0.8421	0.8587	0.7907

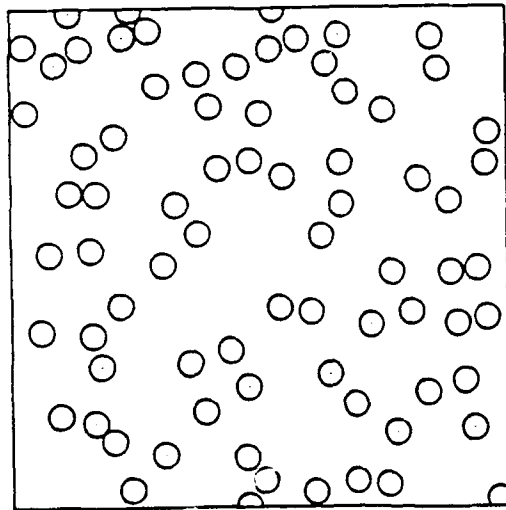


Figure 14. 0.15 Area fraction with a random distribution

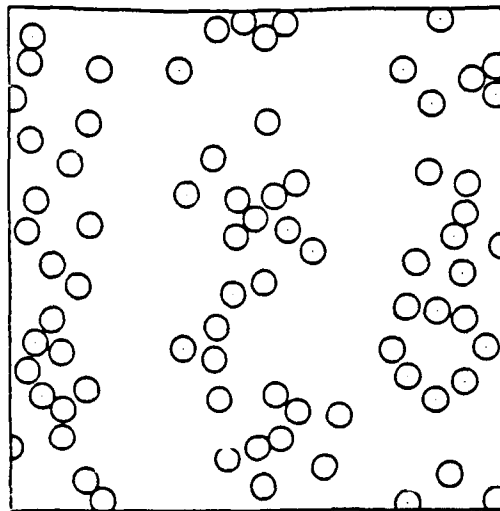


Figure 15. 0.15 Area fraction with 90% of particles in high density zones

Table 6. NEAREST NEIGHBOR SPACINGS FOR 0.15 AREA FRACTION

Percentage of Particle Placed in High Concentration Bands	60%(random)	70%	75%	80%
Particle Spacing	0.8370	0.7559	0.7504	0.7629
	0.8084	0.7676	0.7753	0.7573
	0.7475	0.7701	0.7782	0.7798
	0.7766	0.7824	0.7729	0.7706
	0.7580	0.7576	0.7615	0.7582
	0.7512	0.7365	0.7921	0.8107
	0.7669	0.7411	0.7903	0.7754
	0.8098	0.7939	0.8011	0.7058
	0.7877	0.7544	0.7607	0.7608
	0.7963	0.7629	0.7908	0.7486
Average Particle Spacing	0.7839	0.7622	0.7773	0.7631

Table 7. NEAREST NEIGHBOR SPACINGS FOR 0.15 AREA FRACTION

Percentage of particles place in high concentration bands.	85%	90%	100%
Particle Spacing	0.7075	0.7281	0.7024
	0.7578	0.7275	0.6620
	0.7426	0.7077	0.6725
	0.7495	0.7756	0.7233
	0.7337	0.7488	0.6603
	0.7616	0.7587	0.7064
	0.6883	0.7166	0.6611
	0.7339	0.7698	0.7008
	0.7369	0.7394	0.6978
	0.7462	0.7017	0.6714
Average Particle Spacing	0.7357	0.7374	0.6858

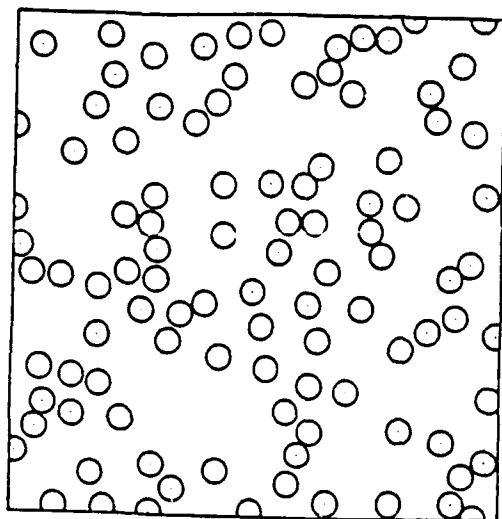


Figure 16. 0.20 Area fraction with a random distribution

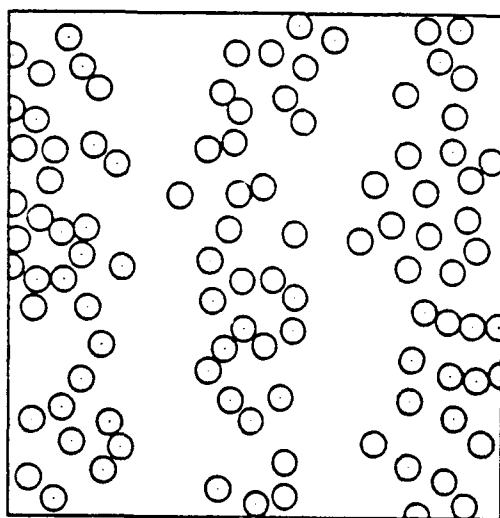


Figure 17. 0.20 Area fraction with 90% of particles in high density zones

Table 8. NEAREST NEIGHBOR SPACINGS FOR 0.20 AREA FRACTION

Percentage of Particles Placed in High Concentration Bands	60%(random)	70%	75%	80%
Particle Spacing	0.6712	0.7215	0.6728	0.6950
	0.6975	0.6897	0.6979	0.6631
	0.6922	0.6941	0.6913	0.6639
	0.7007	0.7004	0.6935	0.7144
	0.6948	0.6841	0.6724	0.7217
	0.7013	0.6827	0.6861	0.6819
	0.6668	0.6941	0.6794	0.6883
	0.7162	0.6774	0.6714	0.6824
	0.6803	0.7087	0.6717	0.6828
	0.6791	0.6887	0.6916	0.7073
Average Particle Spacing	0.6900	0.6941	0.6828	0.6901

Table 9. NEAREST NEIGHBOR SPACINGS FOR 0.20 AREA FRACTION

Percentage of Particles Placed in High Concentration	85%	90%	100%
Particle Spacing	0.6826	0.6577	0.6220
	0.6842	0.6371	0.6367
	0.6757	0.6703	0.6362
	0.6927	0.6754	0.6380
	0.6589	0.6676	0.6205
	0.6852	0.6513	0.6416
	0.6423	0.6559	0.6113
	0.6533	0.6729	0.6109
	0.6732	0.6522	0.6347
	0.6875	0.6824	0.6279
Average Particle Spacing	0.6736	0.6623	0.6280

The influence of banding can best be summarized by plotting the average nearest neighbor particle spacing versus the percentage of particles that are placed in the high density zones from the data presented above and this is shown in Figure 18.

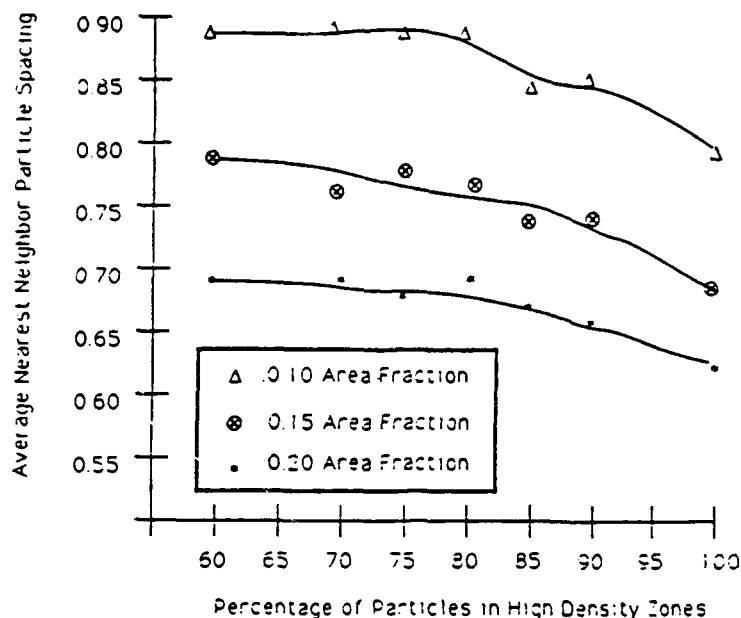


Figure 18. Effect of banding on average nearest neighbor particle spacing

Figure 18 clearly demonstrates that as the severity of the banding of the distribution is increased, that the average nearest neighbor particle spacing decreases. This result also has important implications in the quantitative assessment of microstructures. The presence of non-uniform distributions of particles or other microstructural constituents will result again in spacings which differ from those predicted by equation (2.1) and obtained by experimental determination of the parameter. It is recognized that the banding introduced here was devised in an arbitrary manner and that other forms of non-uniformity could yield a different result. It is likely, however, that decreased particle spacing will result in any circumstance of non-uniform particle distribution and this, in turn, will influence theoretical assessment of the role of particles in processes such as yielding and fracture. For example, experimental determination of δ through evaluation of N by quantitative metallographic methods will result in errors due to banding as well as errors due to the finite-size problem described in Section B.

D. CONCLUSIONS AND RECOMMENDATIONS

When dealing with random distributions of finite sized particles care must be taken if the models for infinitesimal random points is to be used since the average nearest neighbor calculations that this approach yields can be in error by as much of a factor of two. It appears that the infinitesimal random point method and the method for regular hexagonal arrays of finite sized particles represent a lower and upper bound, respectively, for actual distributions of uniform particles.

In addition, it appears that there is a functional relationship among particle size, average nearest neighbor particle spacing and the number of particles per unit area. However, this study did not determine this relationship. Finally, if the average nearest neighbor particle is a characteristic parameter chosen to describe materials with particle distributions, then sufficient banding alone can alter (i.e. decrease) this parameter.

Future research using this approach should address distributions of points and consider the statistics (i.e., standard deviations) in more detail. Subsequent studies should then include particles of varying size through introduction of a size distribution. Finally, the problem of non-random distributions should include varying kinds of non-randomness and particle size distributions as well.

APPENDIX A. PROGRAM RANDOMPOINT

```

Program Randompoint;
{Assign variable types and variables}
type
  largearray=array[1..1000] of real;
  label 51,52,53,54,55;

var
  tothigh,highsect,totlow,lowsect,num,
  ran1,ran2,dx1,dx2,dist,d1,totarea,parea,dsum,cumavg,avg,mindis,
  totmindis,avgmindis,harea,radius,space,y,x,af:real;

  elsect,e2sect,e3sect,e4sect,e5sect,i,k,m:integer;

  minavg,avgsum,posx,posy:largearray;

  da30r:text;

  (*****
begin (program randompoint)

  {Open the data file}
  assign(da30r,'da30r.txt');
  rewrite(da30r);

  (*****
  {Enter initial conditions}
  writeln('What is the total area fraction of particles?');
  readln(af);
  writeln('What is the length of the X-scale?');
  readln(x);
  writeln('What is the length of the Y-scale?');
  readln(y);
  writeln('What is the minimum spacing between particles?');
  readln(space);
  writeln('What is the radius of each particle?');

  readln(radius);

  (*****
  {Calculate the total area of the matrix}
  totarea:=x*y;

  {Calculate the total area of the matrix covered by particles}
  af:=(af/100)*totarea;

  {Calculate the area covered by each particle}
  parea:=3.1459*radius*radius;

  {Calculate the total number of particles}

  num:=af/parea;

  {Determine the number of particles found in both the high and
  low concentration areas}

  writeln('What percentage of the particles do you want in the');
  writeln('high concentration areas?');
  readln(harea);
  tothigh:=harea/100*num;
  
```

```

highsect:=tothigh/3;
totlow:=num-tothigh;
lowsect:=totlow/2;

(Determine the total number of particles up to the end of each section)
elsect:=round(highsect);
e2sect:=round(highsect+lowsect);
e3sect:=round(2*highsect+lowsect);
e4sect:=round(2*highsect+2*lowsect);
e5sect:=round(3*highsect+2*lowsect);

(*****)
(Position the particles in the first high concentration section)
randomize;
for i:=1 to elsect do
  begin
    51:ran1:=random;
    if (ran1>0.2) then
      goto 51;
    ran2:=random;
    posx[i]:=ran1*x;
    posy[i]:=ran2*y;

    (check for overlap)
    for k:=1 to (i-1) do
      begin
        dx1:=posx[i]-posx[k];
        dx2:=posy[i]-posy[k];
        d1:=sqrt(dx1*dx1+dx2*dx2);
        dist:=(2*radius+space);
        if (d1<dist) then
          goto 51;
      end;
    writeln('The position of particle ',i,' is');
    writeln(posx[i]);
    writeln(posy[i]);
  end;

(*****)
(Position the particles in the low first concentration section)
for i:=(elsect+1) to e2sect do
  begin
    52:ran1:=random;
    if (ran1<0.2) or (ran1>0.4) then
      goto 52;
    ran2:=random;
    posx[i]:=ran1*x;
    posy[i]:=ran2*y;

    (check for overlap)
    for k:=1 to (i-1) do
      begin
        dx1:=posx[i]-posx[k];
        dx2:=posy[i]-posy[k];
        d1:=sqrt(dx1*dx1+dx2*dx2);
        dist:=(2*radius+space);
        if (d1<dist) then
          goto 52;
      end;
    writeln('The position of particle ',i,' is');
  end;

```

```

        writeln(posx[i]);
        writeln(posy[i]);
    end;

    (*****
    {Position the particles in the second high concentration section}
    for i:=(e2sect+1) to e3sect do
        begin
            53:ran1:=random;
            if (ran1<0.4) or (ran1>0.6) then
                goto 53;
            ran2:=random;
            posx[i]:=ran1*x;
            posy[i]:=ran2*y;

            {check for overlap}
            for k:=1 to (i-1) do
                begin
                    dx1:=posx[i]-posx[k];
                    dx2:=posy[i]-posy[k];
                    d1:=sqrt(dx1*dx1+dx2*dx2);
                    dist:=(2*radius+space);
                    if (d1<dist) then
                        goto 53;
                end;
            writeln('The position of particle ',i,' is');
            writeln(posx[i]);
            writeln(posy[i]);
        end;

    (*****
    {Position the particles in the second low concentration zone}
    for i:=(e3sect+1) to e4sect do
        begin
            54:ran1:=random;
            if (ran1<0.6) or (ran1>0.8) then
                goto 54;
            ran2:=random;
            posx[i]:=ran1*x;
            posy[i]:=ran2*y;

            {Check for overlap}
            for k:=1 to (i-1) do
                begin
                    dx1:=posx[i]-posx[k];
                    dx2:=posy[i]-posy[k];
                    d1:=sqrt(dx1*dx1+dx2*dx2);
                    dist:=(2*radius+space);
                    if (d1<dist) then
                        goto 54;
                end;
            writeln('The position of particle ',i,' is');
            writeln(posx[i]);
            writeln(posy[i]);
        end;

    (*****
    {Position the particles in the third high concentration zone}
    for i:=(e4sect+1) to e5sect do
        begin

```

```

55:ran1:=random;
  if (ran1<0.8) then
    goto 55;
  ran2:=random;
  posx[i]:=ran1*x;
  posy[i]:=ran2*y;

  {Check for overlap}
  for K:=1 to (i-1) do
    begin
      dx1:=posx[i]-posx[k];
      dx2:=posy[i]-posy[k];
      d1:=sqrt(dx1*dx1+dx2*dx2);
      dist:=(2*radius+space);
      if (d1<dist) then
        goto 55;
    end;
  writeln('The position for particle ',i,' is');
  writeln(posx[i]);
  writeln(posy[i]);
end;

{*****}
{Compute the average distance between particles}
writeln;
writeln('Please wait, computing the average distance between particles. ');
for i:=1 to e5sect do
  begin
    dsum:=0;
    for k:=1 to (i-1) do
      begin
        dx1:=posx[i]-posx[k];
        dx2:=posy[i]-posy[k];
        d1:=sqrt(dx1*dx1+dx2*dx2);
        dsum:=dsum+d1;
      end;
    if (i-1<>0) then
      avgsum[i-1]:=dsum/(i-1);
  end;
cumavg:=0;
for m:=1 to (e5sect-1) do
  begin
    cumavg:=cumavg+avgsum[m];
  end;
avg:=cumavg/(e5sect-1);
writeln('The average distance between particles is ',avg);
writeln;
writeln('Please wait, computing the average minimum particle distance');

{*****}
{Compute the average distance to the closest particles}
for i:=1 to e5sect do
  begin
    {Compute maximum possible separation between any two particles}
    mindis:=sqrt(x*x+y*y);
    for k:=1 to (e5sect) do
      begin
        dx1:=posx[i]-posx[k];
        dx2:=posy[i]-posy[k];
        d1:=sqrt(dx1*dx1+dx2*dx2);

```

```

for i:=1 to num do
begin
mindis:=sqrt(x*x+y*y);
for k:=1 to (num) do
begin
dx1:=posx[i]-posx[k];
dx2:=posy[i]-posy[k];
d1:=sqrt(dx1*dx1+dx2*dx2);
if (d1<mindis) and (d1<>0.0) then
mindis:=d1;
end;
minavg[i]:=mindis;
end;

totmindis:=0;
for m:=1 to (num) do
begin
totmindis:=totmindis+minavg[m];
end;
avgmindis:=totmindis/(num);
writeln('The average minimum particle distance is ',avgmindis);
end.

```


APPENDIX B. PROGRAM ONLYRAN

```

Program Onlyran;
type
  largearray=array[1..1700] of real;
  label 51;

var
  dx1,dx2,dist,d1,mindis,totmindis,avgmindis,
  ran1,ran2,af,parea,x,y,totarea,space,radius:real;

  num,i,k,m:integer;
  minavg,avgsum,posx,posy:largearray;

  {*****}
begin
  writeln('What is the area fraction of particles?');
  readln(af);
  writeln('What is the length of the X-scale?');
  readln(x);
  writeln('What is the length of the Y-scale?');
  readln(y);
  writeln('What is the minimum spacing between particles?');
  readln(space);
  writeln('What is the radius of each particle?');
  readln(radius);

  {*****}
  totarea:=x*y;
  af:=(af/100)*totarea;
  parea:=3.1459*radius*radius;
  num:=round(af/parea);

  {*****}
  randomize;
  for i:=1 to num do
    begin
      51:ran1:=random;
      ran2:=random;
      posx[i]:=ran1*x;
      posy[i]:=ran2*y;

      {check for overlap}
      for k:=1 to (i-1) do
        begin
          dx1:=posx[i]-posx[k];
          dx2:=posy[i]-posy[k];
          d1:=sqrt(dx1*dx1+dx2*dx2);
          dist:=(2*radius+space);
          if (d1<dist) then
            goto 51;
        end;
      writeln('The position of particle ',i,' is');
      writeln(posx[i]);
      writeln(posy[i]);
    end;
  writeln('Please wait, computing the average nearest particle spacing');

  {*****}
  {compute the average distance to the nearest neighbor}

```

```

        if (d1<mindis) and (d1<>0.0) then
            mindis:=d1;
        end;
        minavg[i]:=mindis;
    end;
    {Compute the average of the closest particle spacings}
    totmindis:=0;
    for m:=1 to (e5sect) do
        begin
            totmindis:=totmindis+minavg[m];
        end;
    avgmindis:=totmindis/(e5sect);
    writeln('The average minimum particle distance is ',avgmindis);
    writeln;
    writeln;

    {*****}
    {Write positions to a data file}
    for m:=1 to e5sect do
        begin
            writeln(da30r,posx[m]);
            writeln(da30r,posy[m]);
        end;
    close(da30r);
    end.

```

APPENDIX C. PARTICLE DISTRIBUTION PLOTS

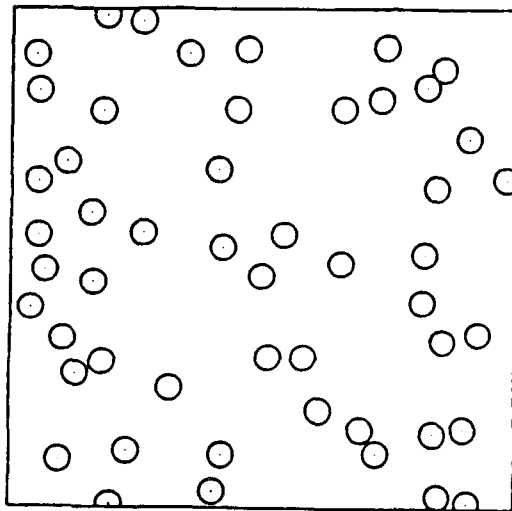


Figure 19. 0.10 Area fraction with 70% of particles in high density zone

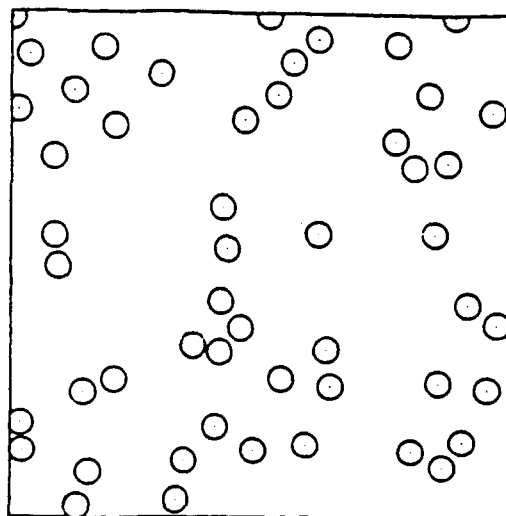


Figure 20. 0.10 Area fraction with 75% of particles in high density zone

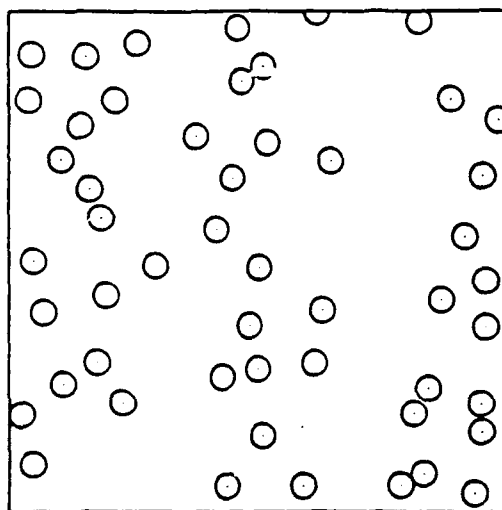


Figure 21. 0.10 Area fraction with 80% of particles in high density zone

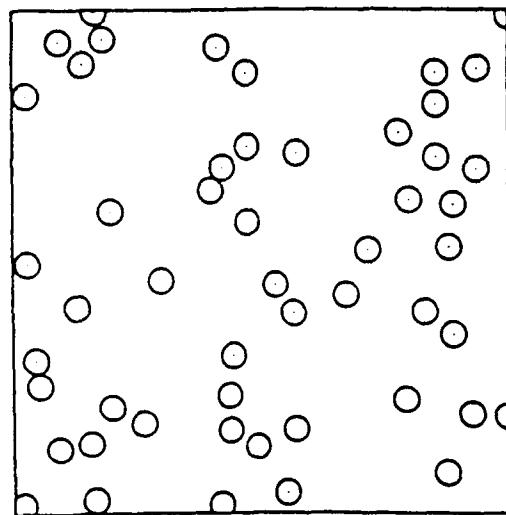


Figure 22. 0.10 Area fraction with 85% of particles in high density zone

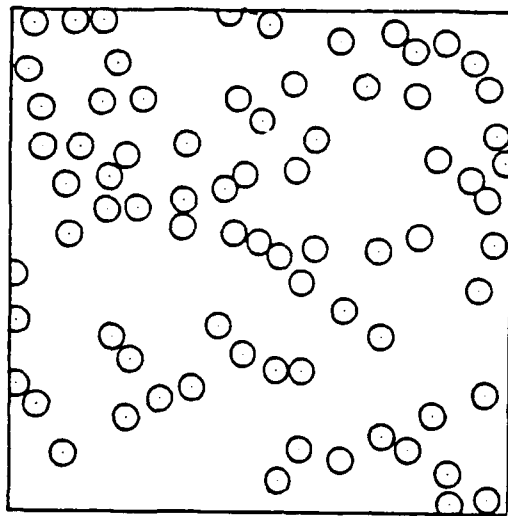


Figure 23. 0.15 Area fraction with 70% of particles in high density zone

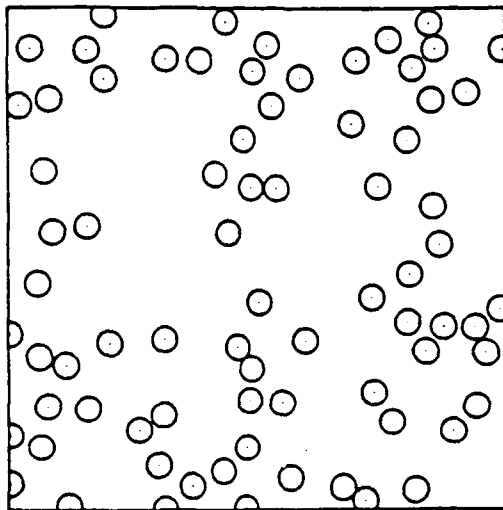


Figure 24. 0.15 Area fraction with 75% of particles in high density zone

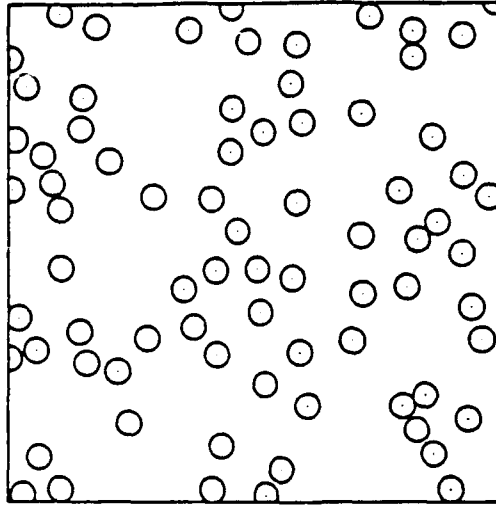


Figure 25. 0.15 Area fraction with 80% of particles in high density zone

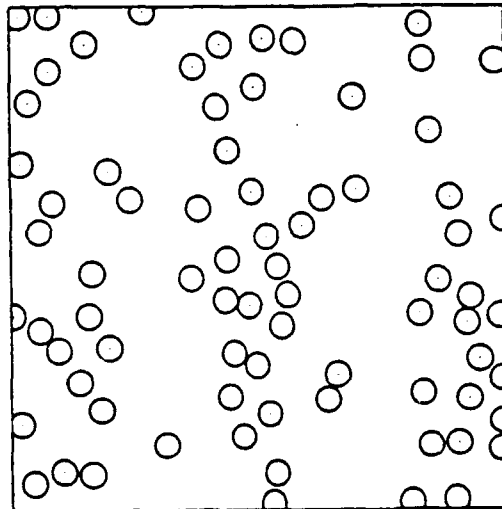


Figure 26. 0.15 Area fraction with 85% of particles in high density zone

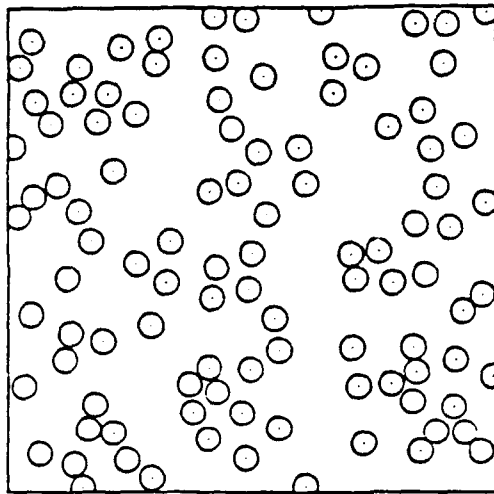


Figure 27. 0.20 Area fraction with 70% of particles in high density zone

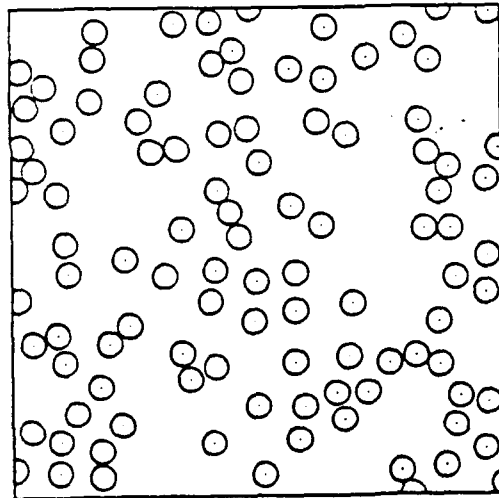


Figure 28. 0.20 Area fraction with 75% of particles in high density zone

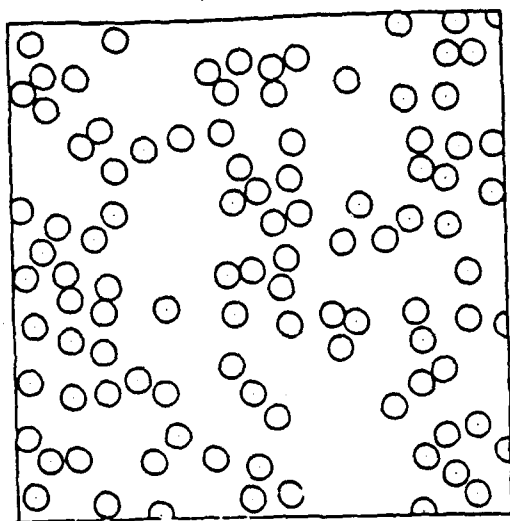


Figure 29. 0.20 Area fraction with 80% of particles in high density zone

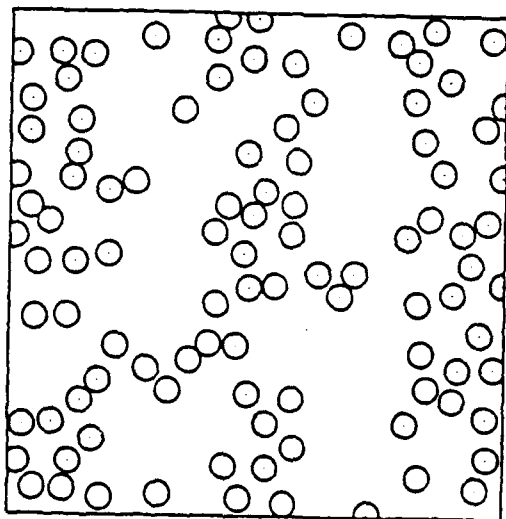


Figure 30. 0.20 Area fraction with 85% of particles in high density zone

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