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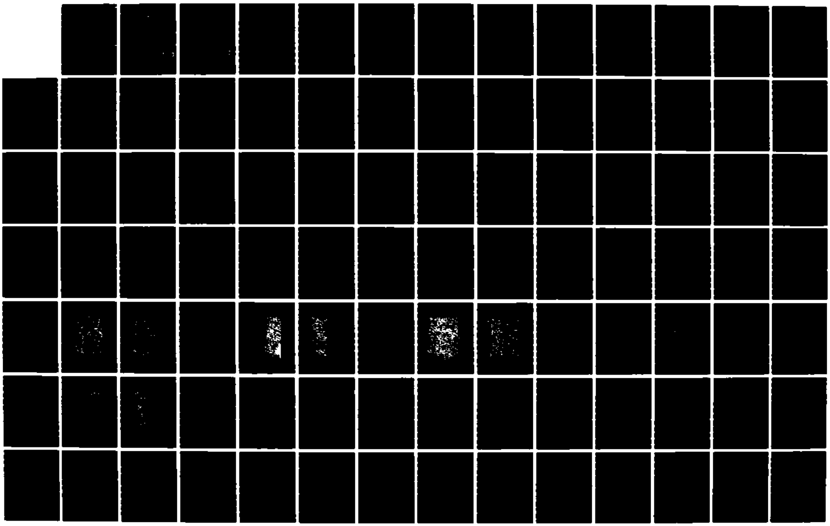

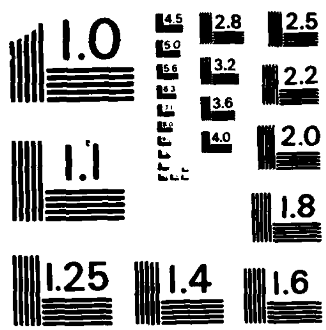

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AN IMPROVED MODEL OF

THIN FILM GROWTH

THESIS

David J. Doryland
Second Lieutenant, USAF

AFIT/GEP/ENP/85D-2

DEPARTMENT OF THE AIR FORCE

AIR UNIVERSITY

AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

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AN IMPROVED MODEL OF THIN FILM GROWTH

THESIS

Presented to the Faculty of the School of Engineering

of the Air Force Institute of Technology

Air University

In Partial Fulfillment of the

Requirements for the Degree of

Master of Science (Engineering Physics)

David J. Doryland, B.S.

Second Lieutenant, USAF

December 1985

Preface

The purpose of this study was to develop a computer program that could model thin film growth by vapor deposition. Although other computer programs have been written to do the same, this one is unique in that it incorporates several deposition parameters both new and old. Some of these include the variation of the angle of incidence about some main angle, the mobility of molecules, the doping of impurities into the microstructure, the creation of multilayered films and the ability to vary the substrate. Like many other models this is a two-dimensional simulation.

The program is written in FORTRAN 77 and was designed to be used on a VAX computer under a VMS operating system.

Throughout the program development, a process which took over five months, it was neccessary to rewrite sections of the program in order to get rid of bugs and/or make improvements. Although the resulting program is fairly sophisticated in nature, it is by no means the ultimate in the modeling of vapor deposition. More programs should be written in the future to provide a better understanding of thin films and the effect vapor deposition has on their growth.

While producing the computer model and writing this thesis I was very fortunate to be surrounded by several kind and dedicated individuals. I am deeply indebted to my faculty advisor, Major John Wharton, for having faith in me and for his assistance in times of need. I also wish to thank Dr. David Lee of the math department for his assistance in the early stages of program development. A word of thanks is also owed to the system manager Frank Bakos for his help in answering my many questions concerning the computer. Finally, I wish to thank my wife Litza for her understanding on the nights I was away at the computer room.

David J. Doryland

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Abstract

A VAX-11/785 computer was used to simulate the two-dimensional growth of thin films produced by vapor deposition. In this model molecules and impurities were represented by three different sized disks. In order to simulate varying deposition conditions and evaporants, several variable parameters were introduced. Among these parameters were the variation of the deposition angle about some main angle, the mobility of the disks upon collision, the ability to introduce impurities into the microstructure, the simulation of multilayered coatings and the ability to introduce imperfections into the substrate.

The results obtained by this model show that disks can be used to simulate some of the main features exhibited by vapor deposited films. Among these features are the formation of columns and their compliance with the "tangent rule", and the disappearance of this structure in the case of large disk mobility. Another feature found to be exhibited in the modeled films is that under certian conditions, impurities and substrate imperfections can produce large voids and/or nodules. Other characteristics found in the simulated films include pores which could allow water absorption, and increased packing density for films produced with angle variations along with a moderate amount of disk mobility.

AN IMPROVED MODEL OF THIN FILM GROWTH

I. Introduction

Thin films are widely used for various scientific and industrial applications, most notably in microelectronics and optics. In microelectronics, their use is predominately in the manufacturing of integrated circuits as in the isolation of circuit elements. In optics, however, thin films have been used for a variety of purposes such as antireflection coatings, mirrors, sun protection coatings as well as band-pass filters. The fabrication technique used in producing thin films varies but the most commonly used technique in optics is vapor deposition.

Since the advent of using vacuum chambers for the vapor deposition of thin films, the process by which the mircostructure is formed has not been completely understood. The amorphous and sometimes crystalline thin films produced by this type of deposition are usually characterized by voids, pores and other vacancies. However, the most dominant feature of these films is their columnar shape. More specifically, the microstructure consist of an array of somewhat parallel columnar regions of high density material surrounded by a network of material of lower density. It is also a characteristic of this microstructure that the diameters of the individual columns are approximately uniform. This structure has been observed by microfractography (13,18-21,29,40,41), by transmission electron microscopy (6,29,36-38,43,48), as well as by both small angle electron (29,38,46), and x-ray scattering (4,34,45). Experiments have shown that this columnar structure can also change some of the properties of the material when compared to those of the bulk material. Some of the changes that have been noted include magnetic (19-21, 29,33,40,41,43), optical (7,8), electrical (8,22,42) and mechanical (41) properties.

In an effort to try to understand the growth patterns of the columnar structure and how this might affect the properties of the film, the deposition process was first simulated by use of nucleation models (1,2, 9,25,42). Since then researchers have used computer models to simulate the vertical structure of thin films (3,5,10,11,15,16,24,26,28,30,31,46, 47,49). The results of these latest models confirm the fact that shadowing plays a major role in the growth of films deposited at oblique incidence. However, the columns comprising the mircrostructure produced by the models are approximately one to two orders of magnitude too small in diameter. Other characteristics that past models fail to properly simulate include the tendency of the models to produce films with low packing densities, and a failure to produce films with a crystalline structure.

Objective

The objective of this research was to improve upon a previous two-dimensional computer model (47) of thin film vapor deposition; and in doing so, incorporating into the new model parameters which could be changed at will by the user of the program. This allows the user to then examine the simulated film and make observations concerning the effect a particular parameter has made. The first parameter to be introduced into the model was the variation of the angle of deposition about some main angle. Other parameters introduced into the new model include allowing a certain percentage of molecules to undergo more than normal mobility, the ability to simulate the doping of impurities into the microstructure as well as being able to modify the substrate to model imperfections. The final parameter to be put into the program was the ability to deposit two different sized molecules and in doing so simulate multilayered coatings.

General Approach

The approach used to accomplish the objective was to divide the problem into three parts. First, after the problem had been defined and goals set, a comprehensive literature search was made from available material. In particular, any papers found containing computer simulations of vapor deposition were especially scrutinized. The second step in solving the problem consisted of developing the computer program used to model the film growth. This included making any simplifying assumptions, developing the mathematics and the model, as well as testing the program. The last step consisted of running the program and then analyzing the resulting films. Throughout this last step the previously mentioned parameters were varied and any significant changes to the film noted.

Sequence of Presentation

The results of this study will be presented in the five remaining chapters and three appendices. In chapter two, some of the current knowledge pertaining to the new model on thin films will be reviewed. In chapter three, the basic requirements needed to produce a computer model and how these are incorporated into the new model will be discussed. Chapter four will present the new model and how it was derived including its organization and implementation. The fifth chapter will show some of the resulting films produced by the computer simulation as well as the analysis of these films. A summary of conclusions and recommendations will be presented in the sixth chapter.

The final section of this thesis contains three appendices which are provided for follow on studies. Appendix A contains several mathematical derivations used in the development of the program, while Appendix B contains the actual Fortran code. The last appendix, which is extremely important for follow on studies, contains the documentation of the computer program, a brief explanation of how the program is organized, and a list of the variables used along with a description of their purpose.

II. Summary of Knowledge

Although there are several ways of depositing thin films onto a substrate, the most commonly used technique for producing optical components is by physical vapor deposition. The reason for using this technique is that it tends to produce a more uniform coating of the substrates. In most cases this process is accomplished inside a vacuum chamber where the bulk material is either heated resistively or by an electron beam which is directed into the material (23). Upon heating, the vapor thus produced coats the substrates placed inside the chamber by condensation.

Columnar Structure

As mentioned previously in chapter one, the most dominant feature exhibited by vapor deposited films is their columnar structure. It is important to realize, however, that not all vapor deposited films exhibit this columnar structure due to the mobility of the molecules. This process will be discussed in a future section.

Tangent Rule. Of all the parameters which affect the columnar structure exhibited by some films, the most influential is the angle of deposition (36,37,39,44). In 1966 Nieuwenhuizen and Haanstra (39) introduced an empirically derived expression which has become known as the "tangent rule." This expression relates the angle of growth of the film to the angle of deposition in the following manner:

$$2 \tan B = \tan A \qquad (1)$$

where B is the angle of growth of the film as measured from the substrate normal, and A is the angle of deposition also measured relative to the substrate normal. Figure 1 shows a graph of the tangent rule for deposition angles from 0 to 90 degrees (49). It is true that not all films exhibiting columnar structure follow the rule exactly, but for the most part the tangent rule is still obeyed.

Shadowing. One of the main reasons that vapor deposited films produce a columnar structure and that most films follow the tangent rule is due to a phenomenon called "shadowing." Put simply, shadowing is an effect which limits the eventual placement of the incident molecules in the microstructure due to previously deposited molecules blocking their path. Under actual deposition conditions, a molecule's trajectory is a straight line due to the fact that the process takes place in a vacuum. In other words, the molecule's mean free path is very large implying that the molecules first collision will be with the substrate or previously deposited film. If one allows disks to represent molecules, the idea of shadowing can be understood in figure 2. If disk X represents a previously deposited molecule, it can be thought of as a barrier which other molecules may encounter. For instance, if disk Y had a trajectory to the left of disk X at an angle A, the closest that it could impact the substrate would be some distance away. In other words, previously deposited molecules or even imperfections in the substrate shield or shadow unoccupied sites, thus creating voids. If the mobility of the molecules after condensation do not fill up the voids, the void structure is maintained and grows with subsequent deposition of molecules. As implied in figure 2, the larger the angle of deposition the larger the resulting voids.

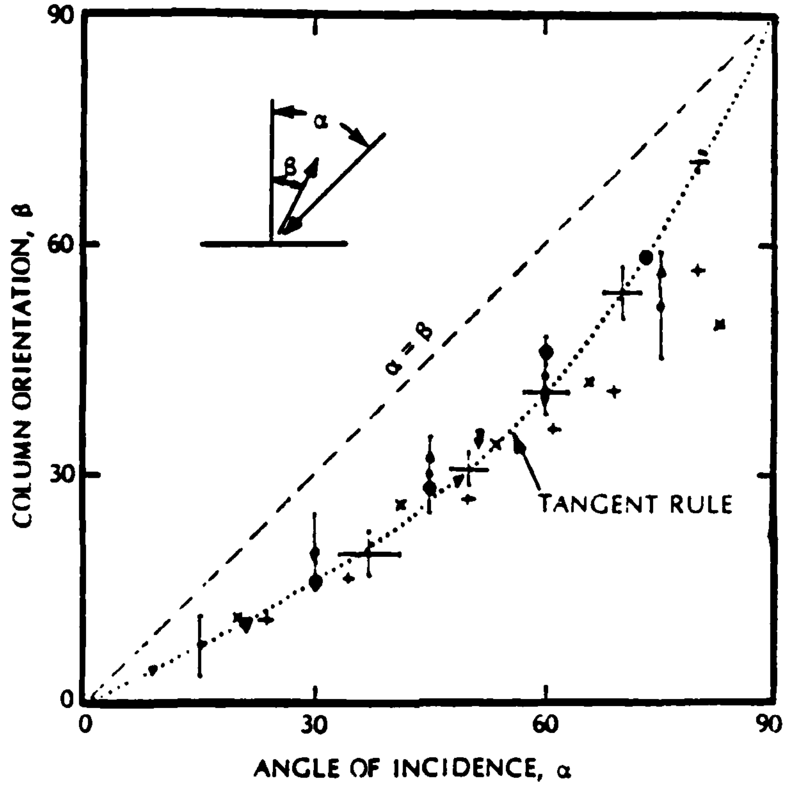


Figure 1. Tangent Rule

(Taken from Reference 49)

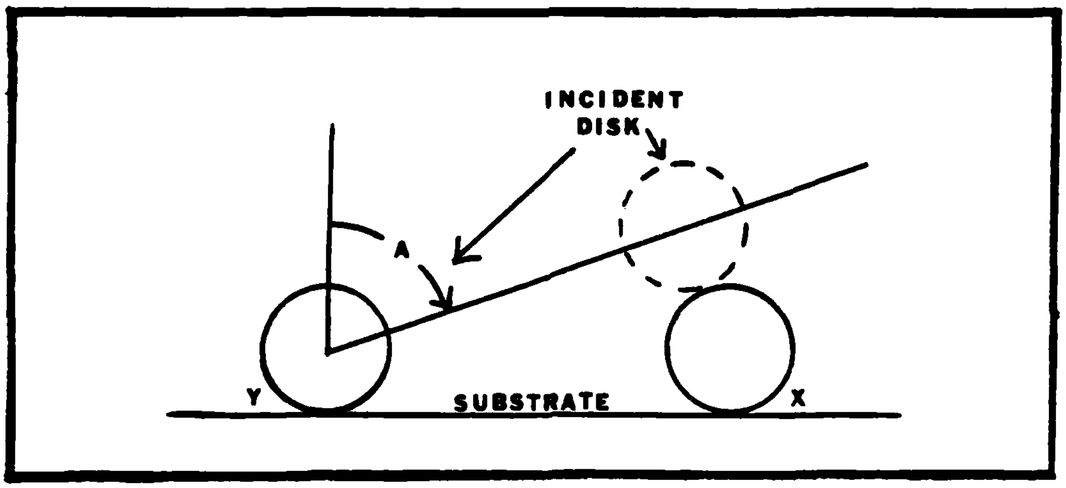


Figure 2. Shadowing

Shape of the Columnar Structure. The angle of deposition also has an effect on the shape of the individual columns. For normal deposition the cross sections of the columns tend to be circular. However, films deposited at oblique incidence yield columns with cross sections that are elliptical in shape. Contrary to what one might think, the axis of elongation occurs in a plane perpendicular to the plane of incidence (30), and is a direct result of shadowing. A figure exhibiting this elongation can be seen in figure 3. As the angle of deposition increases this columnar shape becomes more elliptical, and the void regions between the columns become thinner along a direction parallel to the incident plane.

Another characteristic of columnar shape that is gaining more support is that the individual columns are made up of even smaller columns, usually referred to as dendrites (10,31). These dendrites, which may only be a few molecules in diameter, are thought to come together in the early stages of growth and intertwine, thus forming the relatively large columns seen by transmission electron microscopy.

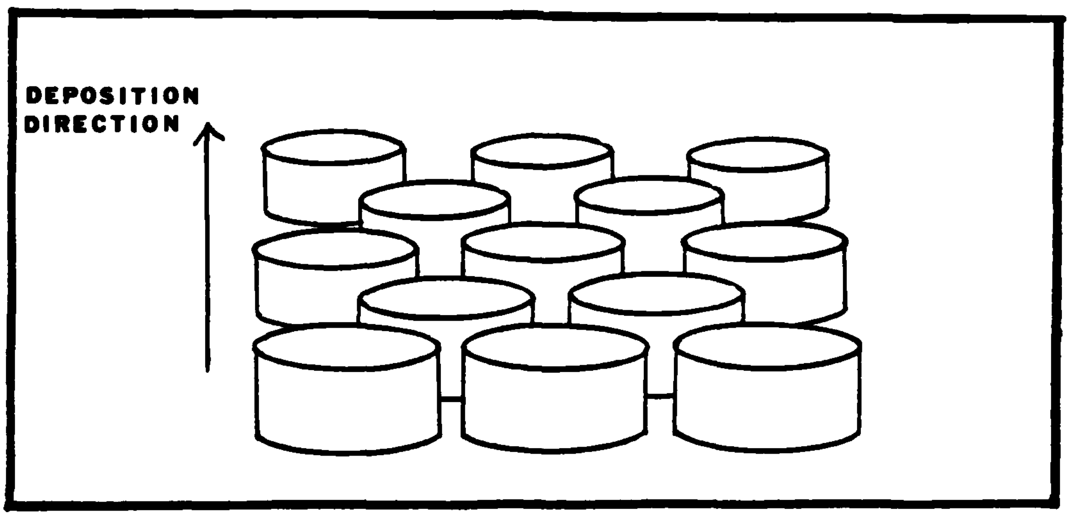


Figure 3. Columnar Elongation

__Density__. Because the amount of voids is related to the angle of incidence, the resulting density of the film is also affected. As expected, the density of the films decreases with an increasing angle of deposition. The density of a film can be defined in several ways, but the most commonly referred to density is the packing density. Packing density is usually defined as follows:

$$p = \frac{\text{Volume of the solid part of the film}}{\text{Total volume of the film (solid + voids)}} \tag{2}$$

where p is the packing density.

__Angle Variation__. One of the many ways that people have gone about affecting the packing density and producing more uniform coatings is by rotating the substrates. By rotating the substrates the angle of deposition is varied over time, thereby smoothing out the film and making it more uniform. This also tends to increase the overall density of the film. As to date, there have been few if any studies looking at the amount of variation as well as the speed of rotation, and how this affects the structure of the film.

__Mobility__

In order to further affect the density of the films, that is trying to produce more dense films, many people have tried to increase the mobility of the molecules as they are being deposited. There are basically two reasons why one would want to affect the mobility of the incident molecules as they are being deposited. One, as just mentioned, would be to try to produce a film with a higher packing density. The reason this is desirable is that if the density of the film can approach that of the bulk material, the properties of the film will tend to be more stable, especially the optical ones. The second reason for wanting to affect the mobility of the molecules is to help cut down on the amount of water absorption. As more water is absorbed into the mircro-structure the properties of the film change, and in the case of optical properties wavelength shifts can occur (31).

Substrate Temperature. It is well known that when the ratio of the substrate temperature to that of the bulk material (the material being deposited as a film) is extremely high, the resulting mircrostructure is without columnar structure (16). This is due to the fact that the mobility of the molecules is large and most, if not all, of the voids are filled. The high substrate temperature also has the effect that it increases the density of the film. The problem with using substrate temperature to increase the density of films is that most films are composed of several layers and the high temperature would destroy the layered structure.

Ion Bombardment. The use of ions to increase the mobility of the molecules making up the film has two primary purposes. First, ion bombardment has been used to help anneal the film to the substrate. Second, the use of bombarding ions has been used to help increase the overall packing density of the film. In both cases, authors (32) have experimented with varying current densities in hopes of producing films with greater substrate adhesion and packing densities.

Ultra-Violet Radiation. Another technique used to increase the mobility of the molecules under deposition has been the use of UV radiation (14,49). Although this technique has not had as much success as ion bombardment, the packing density of films have been increased somewhat.

Nodular Defects

Although there have been attempts to try to improve the microstructure of thin films by such processes as ion bombardment and UV irradiation, defects within the film still arise due to growth asperities (11-13,17,27,31). In thin film circles these defects are usually referred to as nodules. Put simply, a nodule is a structure protruding from the thin film surface in a domelike manner. A cross section of a nodule shows that their shape is like that of an inverted cone, either parabolic or linear, increasing their diameter above the tip of the cone. See figure 4 for an example of the general shape of a nodule. Micrographs of multilayer stacks (11,13,17) show that the individual layering sequence is maintained within the stack even though a nodule may be present. This evidence has led some to believe that nodules are growth defects and not massive spatter particles or empty bubbles. Therefore a

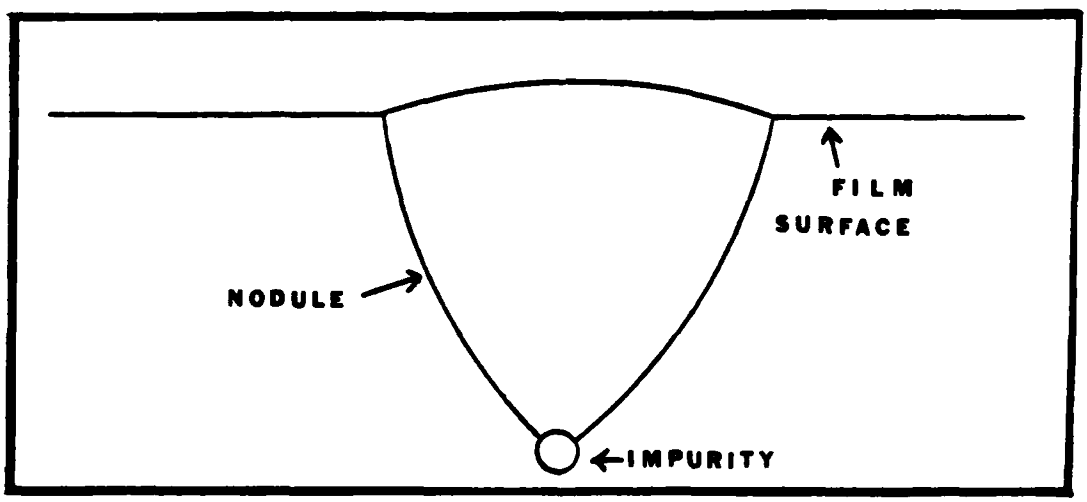


Figure 4. Shape of Nodule

nodule can be thought of as a reproduction of an individual minute particulate. The problem with nodules occurring in films is basically twofold. First, the non-uniform structure that these nodules present affect the properties of the film. Second, nodules have a tendancy to separate from the film, leaving behind a hole which can also cause problems with some of the film properties.

Substrate. One cause of nodules is surface asperities. Even though most substrates are thought to be "flat", there usually exists some defects with the substrate. These may arise due to surface roughness caused by insufficient polishing, or may even be caused by small polishing grains left over due to the polishing process (10). Whatever may be the cause of these small defects, there is much evidence leading to the belief that surface asperities can and do cause the formation of nodules.

Impurities. Another cause of nodular defects within films is due to impurities which get trapped within the microstructure during deposition. These impurities may vary from hydrogen molecules from oil diffusion pumps as well as nitrogen, oxygen or water vapor which may still reside in the vacuum chamber (10). Another cause of impurities may even be large spatterings of the material being used to produce the film coating. The effect that these impurities have within the microstructure is to provide the deposition material an asperity to grow on.

Intentional doping of impurities into films have shown a reduction in the tensile strength. This is due to the fact that the doped impurities form grain boundaries which affect the surface energy. This in turn influences the internal mechanical stress of the thin films (11).

Multilayers

The use of multilayers in thin film optics is primarily due to the interference effects caused by layers which are a quarter of a wavelength in thickness. Although most of the properties caused by this phenomenon are known, the growth patterns and the microstructure making up these layers is still not completely understood.

By the use of electron mircrographs, the layered structured within multilayered films has been seen along with a columnar microstructure making up the individual layers (10,13,17). However, these same mircrographs have shown that there are obvious discontinuities at the interfaces between these layers. This effect has caused some researchers to investigate the water absorption problems caused by these discontinuities at the boundaries (31).

III. Modeling

The purpose of this study was to improve upon a previous computer model of thin film growth by vapor deposition. In order to accomplish this task several concepts as to how the model would work had to be thought out. Some of these included how the molecules would be represented, the movement of the molecules after collision and the final placement of the molecules within the film. In an effort to gain an insight on how these questions could be answered, past models in the literature were reviewed.

Past Models

Although thin films by vapor deposition have been around for many years, the process by which films grow is not clearly understood. Therefore, since computers have been used increasingly in the scientific community, people have used computers to model thin film growth (1-3,5,9-11,15,16,24-26,28,30,31,42,46,47,49). These models fall into two main categories, with the first being nucleation models and the second belonging to a group hereafter referred to as the columnar category. Although nucleation theory may be a relevant concept, this report deals with the columnar nature of thin film growth, and therefore nucleation models will not be discussed.

Of all the columnar growth models of interest, the most notable is the one produced by Dirks and Leamy (5). In this model, a two-dimensional simulation, both the aspects of shadowing and atomic relaxation are discussed along with some aspects of three dimensional models.

Mobility. Whatever is used to model the actual molecules making up the film (disks are usually used in two dimensions and spheres in three dimensions), the amount of mobility given to the "molecules" is the most important aspect in the development of the simulation. Dirks and Leamy showed that in order to approach the proper modeling of vapor deposited films, the molecules (i.e. disks or spheres) must possess some sort of limited mobility. This can be explained by looking at the two possible extremes. In the case of no mobility, the simulated "film" produced by Dirks and Leamy was extremely porous and showed no columnar structure, but was rather composed of a chain-like structure. The other extreme would be when the molecules possessed infinite mobility, meaning that the molecules would continue to move until they found the point in the film which possessed the lowest potential energy. This of course would produce a very dense film, hexagonal closed packed in two dimensions, and was not even considered by Dirks and Leamy. Therefore they assumed a "limited mobility" which is somewhere in between the two extremes. More specifically, in the case of two dimensions the incident disks making up the evaporant were allowed to relax into the nearest "saddle" or "pocket" made by two disks. In the case of three dimensions this pocket was composed of three spheres. The films produced by this limited mobility were composed of columns three to five disks in diameter. Since then other models have used this same limited mobility in their simulations (10,11,16,24,26,28,31,46,47,49).

Defects. Other than trying to produce columnar structures within simulated films, computer models have been used to understand how nodules are formed within the mircrostructure and how this affects the growth of the film. The most well known works concerning the modeling of defects have been by Karl Guenther (11,15). His models have been able to produce nodular growths in films by both substrate imperfections and the doping of impurities within the microstructure. As far as substrate imperfections are concerned, this has been accomplished by modifying the substrates in such a way as to produce bumps and other surface asperities. When it comes to simulating the doping of impurities into the film, large spatterings of approximately three times the size of the simulated molecules have been used.

Form Birefringence. In addition to simulating columnar structure, three dimensional models have been used to study form birefringence (26). Put simply, films deposited at oblique incidence produce variations in the index of refraction due to the density of the films being different in various directions, a phenomenon caused by the columnar structure.

Assumptions

After a study of the past models had been reviewed, it was then necessary to make some simplifying assumptions in order to produce the new model. These are provided below along with any reasons as to why the assumptions were made:

1. The deposition of thin films can be represented by a two-dimensional computer model. Although a three-dimensional model may be more applicable or realistic, it is still possible to learn new things from a two-dimensional model.
2. The incident particles (atoms or molecules) making up the evaporant were assumed to be disks of a particular diameter. Of the three different size disks in the model, the smaller two were used to simulate the

evaporant. The largest disk, being approximately eight times the size of the smallest, was used to simulate an impurity being trapped in the mircrostructure. Although the size of the molecules may differ from one to the next in reality, the order of magnitudes are approximately correct for use in the model.

3. Each disk, independent of size, was assumed to travel on a straight line at an angle A relative to the substrate normal. It continued on this trajectory until coming into contact with one of the already deposited disk or the substrate. This is in good agreement with what actually happens in vapor deposition. The reason being that the deposition takes place in a vacuum plant, and there are few if any molecules removed from their trajectory.

4. Each individual disk was assumed to be deposited serially. Although the actual deposition rate of the molecules may be such that parallel activities take place (i.e. two molecules arriving at the substrate at the same time), the probability of these two events being close enough to affect one another is rare.

5. It was assumed that after an incident disk came into contact with an already deposited disk, it still had a limited mobility. This mobility allowed the disks to come to rest in one of two ways. First, the incident disk remained in contact with the first disk and then relaxed into the nearest "pocket" until it made contact with another previously deposited disk. Second, a set percentage of the incident particles were given an extra mobility allowing them to move to a pocket farther away but still maintaining contact with the first disk. The reason these types of mobility were introduced into the model was to find the amount

of limited mobility needed to produce realistic films, as discussed in the previous chapter.

Further discussion of why some of these assumptions were made and how they were used in the model can be found in the following sections.

Disk Size and Shape

After reviewing the literature it became evident that the most common shape used to represent molecules was a sphere for three-dimensional models and circles/disks for two dimensions. Even though these are relatively simple shapes compared to molecules actually used in vapor deposition, they are relatively easy to represent mathematically. It is for this reason, and the fact that the old model used disks, that this model also used disks to represent the molecules.

The size of the disk used to represent the molecules in the film was determined by looking at the two-dimensional arrays used to hold the disks. More specifically, three arrays (each 300 wide and 200 in height), were used to represent the film, accounting for 60000 unit cells. The first array was used to store occupancy data of the x-y field (i.e. whether or not a unit cell was occupied). The second and third arrays were used to store the x coordinates and y coordinates of the disks respectively. In order to avoid the problem of two or more disks occupying a single cell, the diameter of the smallest disk was equal to the square root of two (see figure 5). Since the model was to simulate multilayered coatings, a second disk of diameter equal to two times the square root of two was used to simulate a larger molecule or one with a greater interaction distance. Finally, in order to simulate

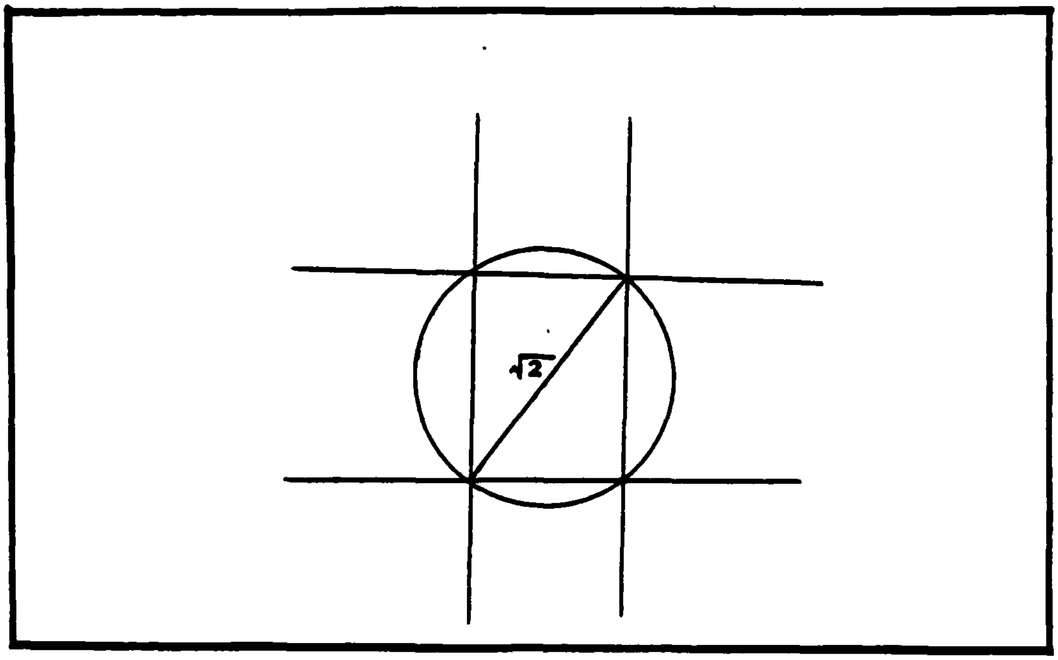


Figure 5. Size of Smallest Disk

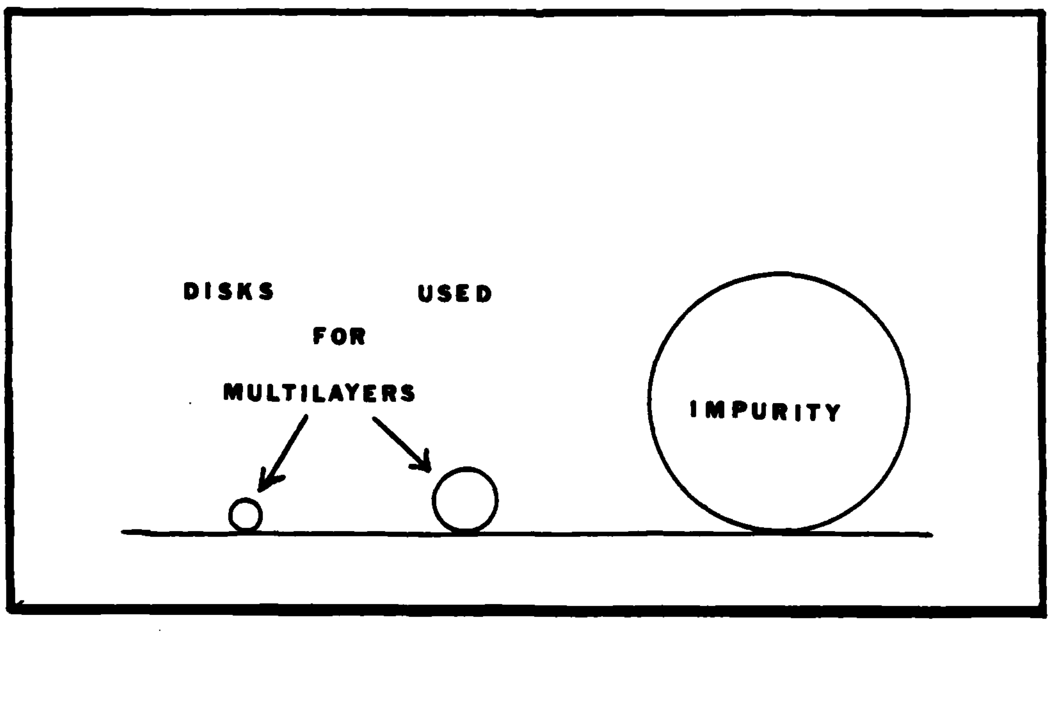


Figure 6. Comparitive Sizes of Disks

impurities a third disk was chosen to be eight times the square root of two in diameter or eight times the size of the smaller disk. See figure 6 for a comparative sketch of the three different disk sizes.

Disks are represented in the computer by the radius of the individual disks and its center coordinates. Once the address of a cell has been determined by truncating its coordinates, the information is stored in the arrays. In the occupation array a zero represents that the cell is unoccupied; while a one, two or eight specify the size of disk with its center located inside the particular cell.

Contact Circles

As an incident disk approaches those that have been previously deposited the position of the incident disk when it first collides, as well as its final resting position, needs to be determined. In order to accomplish this task the idea of contact circles from the old model was invoked. Put simply, the contact circle of an individual disk is a circle about the disk, whose radius is such that the edge of the circle passes through the center of the neighboring disk when they are in contact. An example of two contact circles can be seen in figure 7 where the smaller disk is in incident on the larger one. Implied is the fact that it is possible for one disk to have more than one size contact circle when it is surrounded by different size disks.

The idea of contact circles is first used in the model in determing the position of an incident disk after collision. As an incident disk approaches an already deposited disk or the substrate, which is composed of disks (a matter discussed in chapter 4), the position of the disk immediately upon collision can be determined mathematically. More

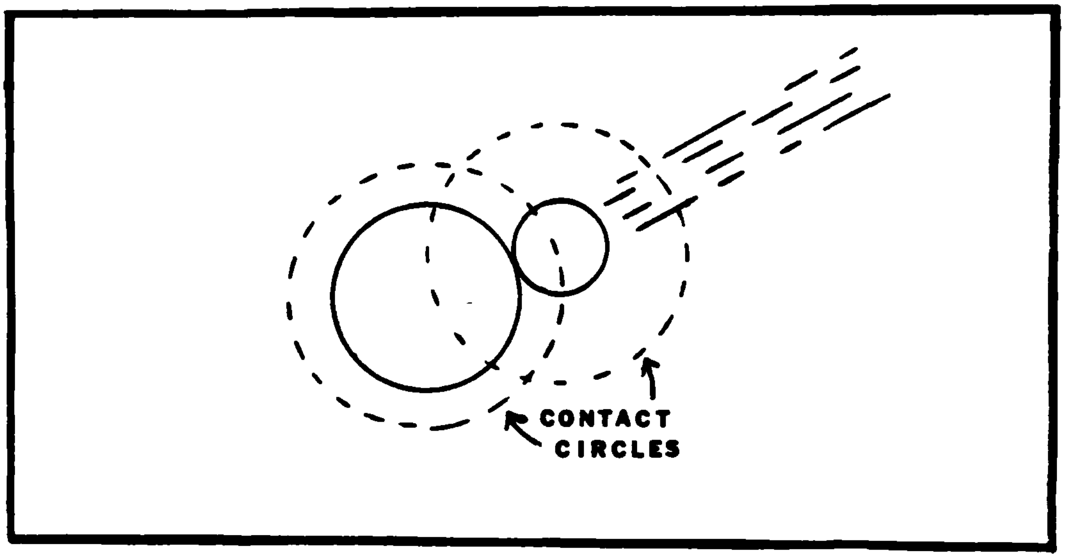


Figure 7. Contact Circles

specifically, the x and y values can be determined by finding the intercept of the contact circle of the collision disk and the line simulating the trajectory of the center of the incident disk (see figure 8). The

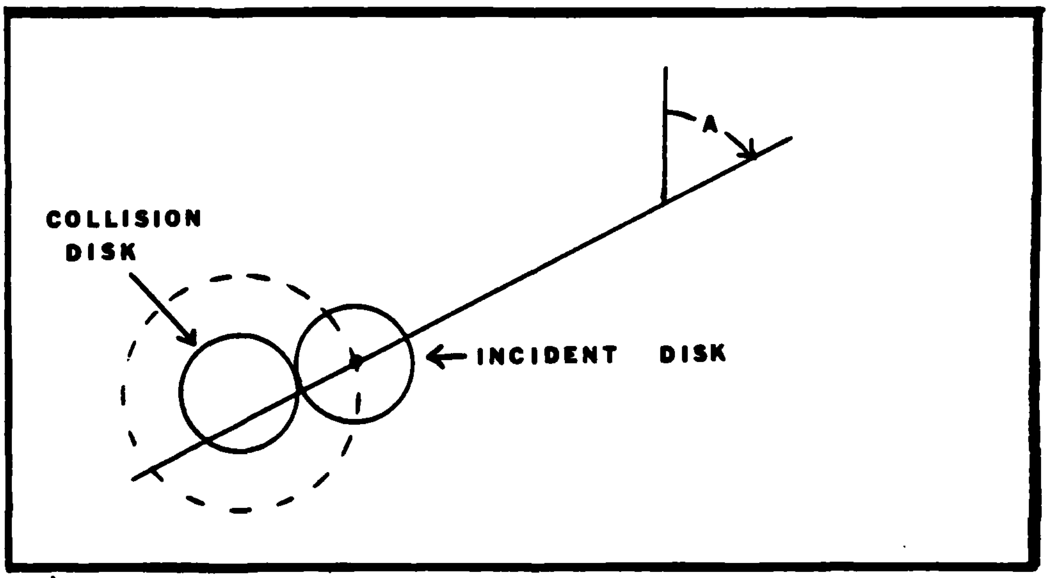


Figure 8. Collision Point Contact Circle

equations used to find the x and y intercepts are

$$Y = \frac{-\{[(a-h)/m] - k\} + \{r^2*[(1/m^2) + 1] - [(a-h) + (k/m)]^2\}^{1/2}}{[(1/m^2) + 1]} \tag{3}$$

$$X = Y/m + a \tag{4}$$

where the significance of the variables as well as the derivation of the equations can be found in appendix A.

The second place where the idea of contact circles comes into play is determining the final resting point of the incident disk. As stated above, the incident disk will come to rest in a "pocket" formed by the disk in which it first makes contact, known as the collision disk, and a neighboring or rest disk. In order to calculate the position of the center of the disk after it comes to rest, the contact circles of the collision and rest disk (whose radii are determined by the radius of the incident disk and their own respectively) are used as in figure 9. By

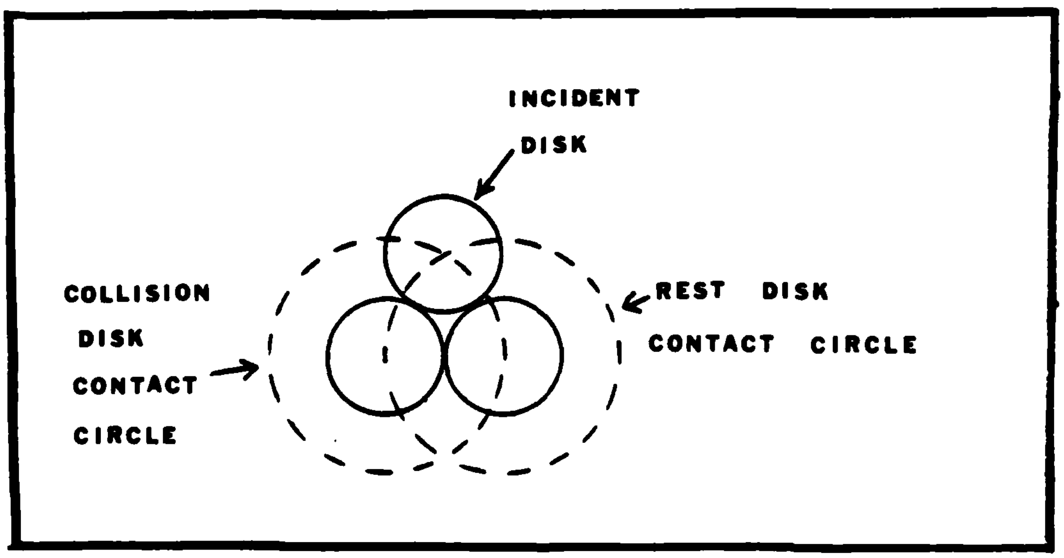


Figure 9. Rest Point Contact Circles

finding the intersection of the two contact circles the rest point can be determined. The mathematical formulas used to calculate the rest coordinate are

$$Y = [-a*k +/- (a^2*k^2 - c*b)]/c \quad (5)$$

$$X = [-a*h +/- (a^2*h^2 - c*b)]/c \quad (6)$$

where the significance of the variables and the derivations of the equations can be found in appendix A. Because these formulas actually specify two distinct points, the point which allows the disk to move the least is chosen as the rest point, except in the case of added mobility; a point which will be discussed in the next section.

Mobility

As stated earlier in the section concerning past models, the mobility of the disks after initial collision should be limited. In an effort to try to understand how much mobility the molecules should have after collision, the new model allows the user to look at three different mobilities. The first type of mobility that the disks can undergo is no mobility at all. When disks undergo no mobility, the resting point of the disk is determined by the collision point coordinates previously mentioned. Therefore, whenever the disk first comes into contact with another disk, the deposition process for that disk is complete. As shown in figure 10 the resulting film is very loosely packed. The second type of mobility possible is what will be referred to as normal mobility. Under normal mobility, the final resting point of the incident disk is determined by the disk coming to rest in the nearest pocket. As shown in figure 11, normal mobility implies that

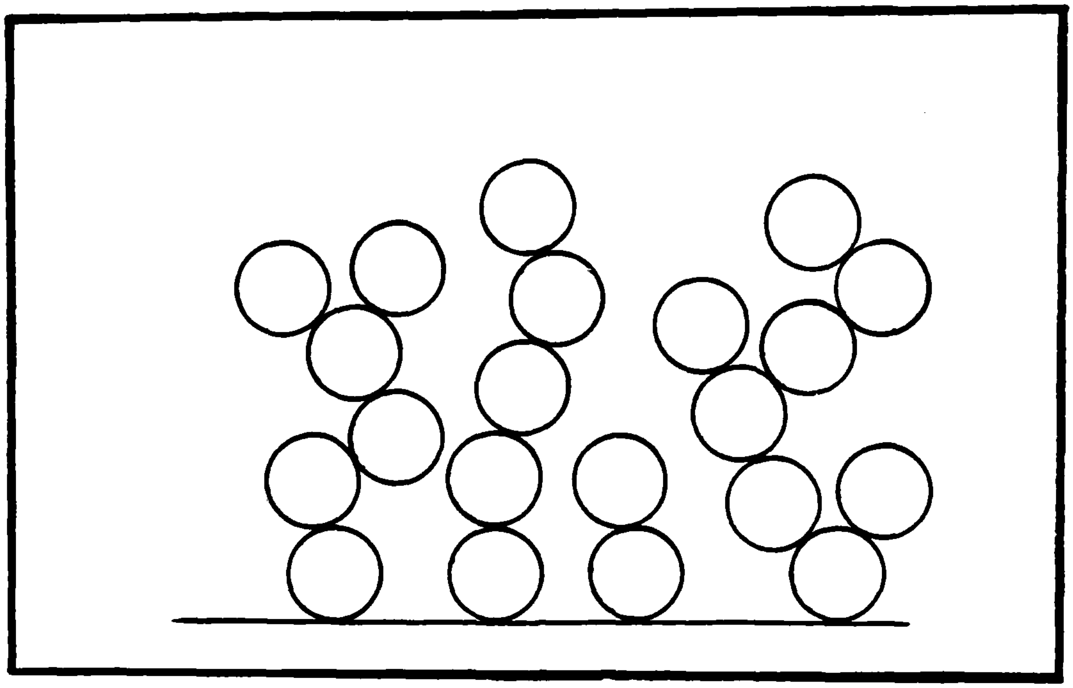


Figure 10. No Disk Mobility

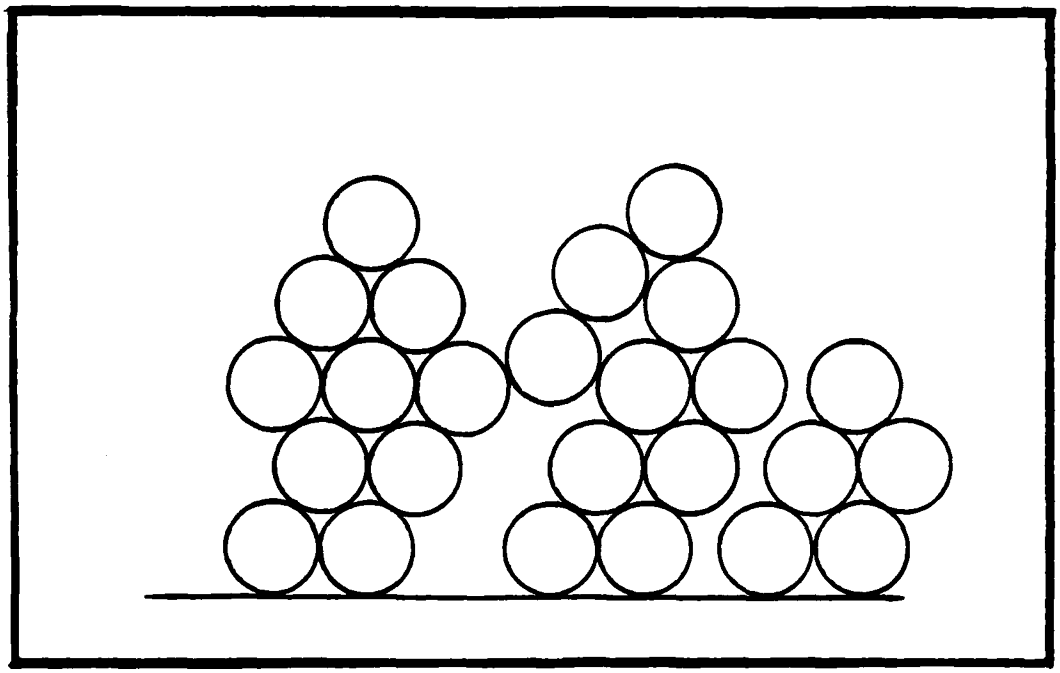


Figure 11. Normal Disk Mobility

each individual disk is in contact with at least two other disks.

The third type of mobility, which will be referred to as added or extra mobility, was introduced as one of the parameters in the new model. The reason for introducing this parameter is to try to produce films with greater packing densities and larger individual columns. Under extra mobility, the incident disk comes to rest in the pocket which allows the disks greater movement before coming to rest. As shown in figure 12, normally the incident disk will come to rest at point A. However, when extra mobility is introduced the incident disk will come to rest at point B making the column wider than before. More specifically, under extra mobility the incident disk still remains in contact with the collision disk but just rolls to the next available pocket produced by surrounding disks.

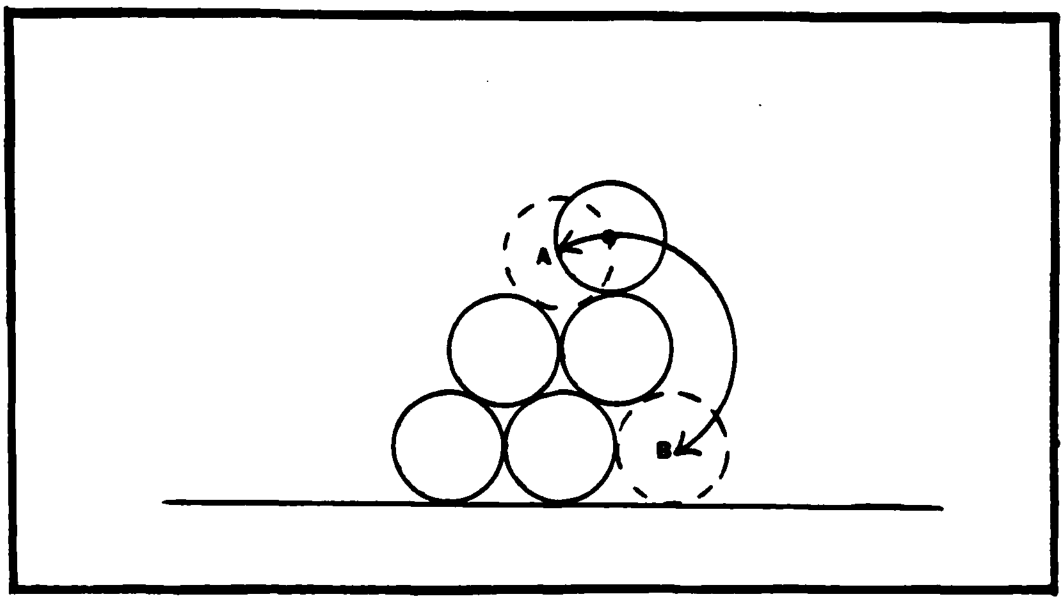


Figure 12. Extra Disk Mobility

IV. Program Implementation

In order to simulate the vapor deposition of thin films by use of a computer, it was first necessary to decide what the program was to model. That is, what specific tasks was the program going to be asked to do. In order to model the deposition process properly, the following major tasks needed to be incorporated into the program. One, the program had to be able to produce a substrate, and to simulate an actual substrate it was essential that it be able to produce imperfections. Two, the program needed to deposit a film onto the substrate, and in doing so the deposition process needed to contain parameters that could be changed to simulate different deposition conditions. Three, in order to analyze the results, the program needed to have an analysis section for calculating such variables as packing density and angle of growth by the film. And lastly, the results of the deposition needed to be plotted, so a fourth task of the program was to make possible the plotting of the deposited film and substrate.

The program listed in appendix B is able to take care of the four tasks by means of four subroutines. Each subroutine is connected to the other by a main interface loop. The names of the four subroutines in the program are simply the substrate, deposition, analysis and moving subroutines.

Substrate Subroutine

The substrate subroutine is divided into five areas allowing for the initialization, creation, storing, recalling and transferring of substrates. The movement between these sections is controlled by an interface loop at the beginning of the subroutine.

In an effort to keep the user from destroying valuable information, the subroutine uses a set of buffer arrays for manufacturing the substrate. These arrays (namely xc, yc and subbuf), each of which is 300 in width and 10 in height, are used to create the substrate before being transferred to the main arrays. More specifically, the information contained in these arrays hold information concerning the x coordinate, y coordinate and occupation (i.e. whether or not a cell is occupied) of the 3000 cells used to produce the substrate.

As in the previous model the substrate is composed of disks, each of which is the square root of two in diameter. In order to produce the substrate these disks are laid down either one on top of the other or side by side so that each disk just comes into contact with its neighbor. See figure 13 for an example of how these disks can be stacked.

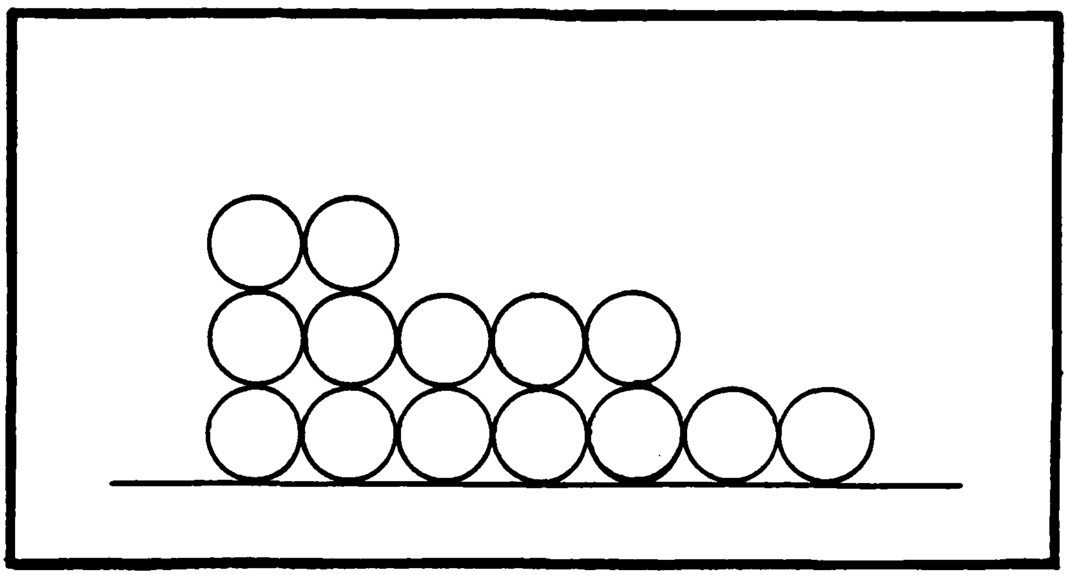


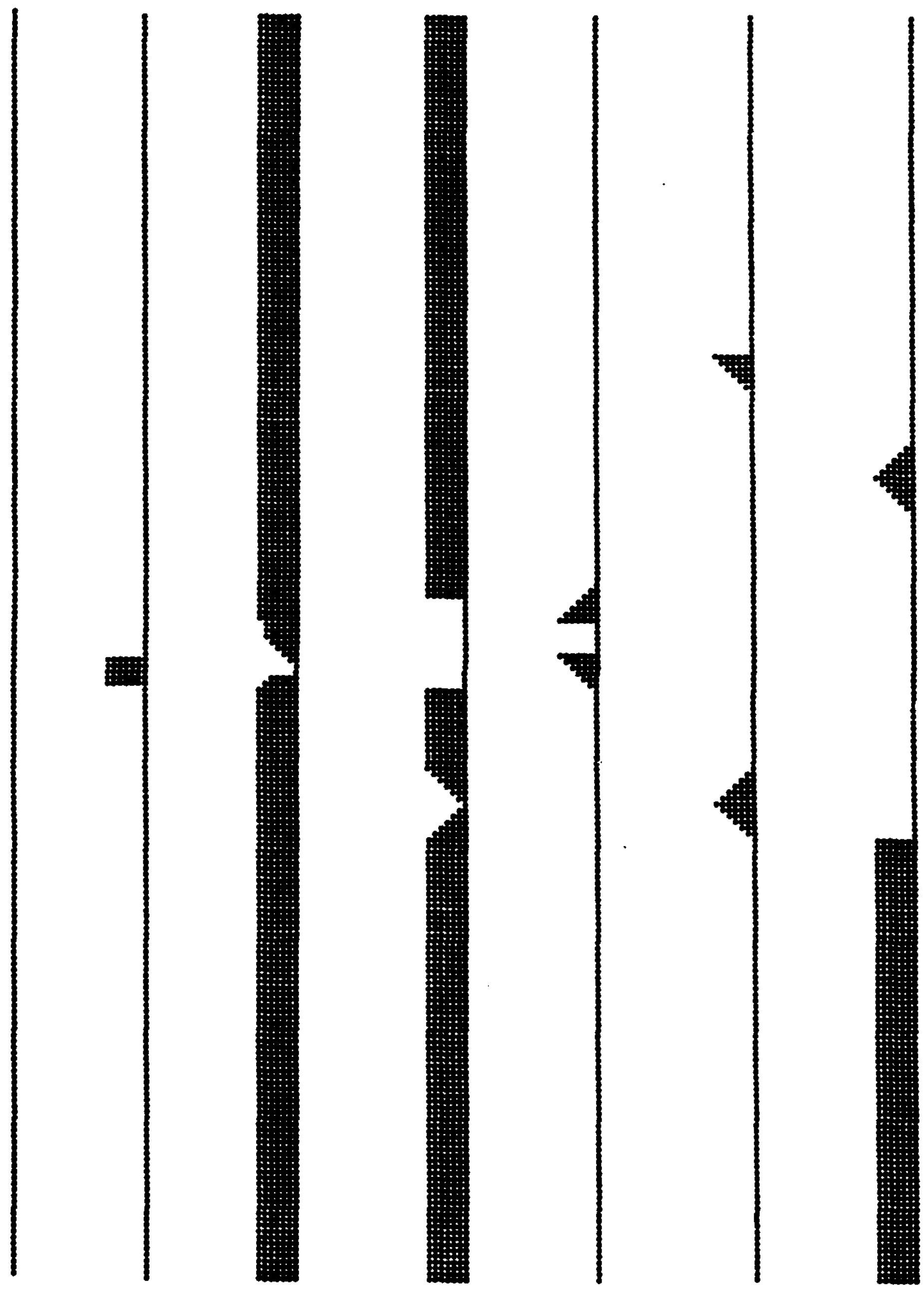
Figure 13. Substrate Stacking of Disks

Because the arrays are 300 wide and the diameter of each disk is the square root of two, a total of 213 disks can be laid across the bottom of the array thus producing a "flat" substrate. See figure 14 for an example. Although this may not appear to be flat due to the shape of the disks, it must be remembered that some optical substrates are nothing more than cleaved NaCl which is not "flat" on an atomic scale.

In order to produce a more complicated substrate, that is one which contains imperfections, the remaining parts of the buffers are used. Since the arrays are 10 high, the number of disks that can be stacked one upon another comes to 7, implying that 1491 disks can be used to create the substrate. The fact that there are 213 disks across the bottom of the arrays is used to envision 213 columns within the substrate, with each column having a maximum possible height of 7 disks. By specifying the height in each column it is then possible to produce substrates, as seen in figures 15 through 20.

Since the program was intended to be user friendly, it is not required that the user enter the height in each column to produce a substrate. In fact, after initializing the buffers and entering into the creation part of the subroutine, a flat substrate like the one in figure 14 is automatically produced. Furthermore, if the user desires a more complicated substrate and this substrate contains a section where the height remains constant over several columns, the user is spared the trouble of entering the same height over and over.

After entering the height in a particular column, the program asks whether or not the height is to be continued and if so to what column this should occur. An example of how the creation of a substrate may



Figures 14 through 20. Different Substrates take place is given below with the prompts and appropriate answers.

Do you wish to create more than just a horizontal line for the substrate?

If yes - Enter 1
Otherwise - Hit Return

1

There are 213 columns columns across the bottom of the substrate. Each one of these must have a height specified to it. The following steps will help in that process.

You are in column 1
Enter height (must be 7 or less)

1

Do you wish this height (1) to continue?

If yes - Enter 1
Otherwise - Hit Return

1

To what column should this continue?
(must be 213 or less)

100

You are in column 101
Enter height (must be 7 or less)

7

Do you wish this height (5) to continue?

If yes - Enter 1
Otherwise - Hit Return

1

To what column should this continue?
(must be 213 or less)

105

You are in column 106
Enter height (must be 7 or less)

1

```
Do you wish this height (1) to continue?

 If yes - Enter 1
 Otherwise - Hit Return

1

To what column should this continue?
      (must be 213 or less)

213

The substrate is now complete!!
Ready for transfer to film matrices.
```

A sample of the substrate just created by the above commands can be seen in figure 15.

Once the substrate has been produced, whether it is just flat or some imperfection has been introduced, the user may wish to store the values of the substrate for future use. This is accomplished by the third section of the subroutine. The fourth section is the counterpart of the previous section and allows the user to recall substrates so that they do not have to be reproduced. The final section of the subroutine takes care of transferring the values of the buffer arrays into the main arrays used in the deposition of the film. Once this has occurred the user may enter the deposition subroutine and prepare to deposit the film onto the substrate.

Deposition Subroutine

The deposition subroutine is divided into three sections, allowing for the initialization of the main arrays, the setting of the deposition variables and lastly the deposition of the film onto the substrate. As in the substrate subroutine, movement between these sections is controlled by an interface loop located at the beginning of the subroutine.

After the initialization of the main arrays takes place, the user of the program is then able to set the deposition variables which con- control the deposition process. The first parameter specified by the user is the number of disks to be deposited. In order to look at changes in the overall packing density of the film, the user should enter more disks than desired. The reason for this is that deposition of the film continues until either all the disks have been used or until the arrays become full. Therefore, by specifying more disks than the arrays can hold, the effect that other parameters have on the packing density can be measured.

The second parameter that the user has control of is the main angle of deposition. The angle entered by the user is the angle as measured from the substrate normal. Therefore if zero degrees were entered, deposition would occur at normal incidence. In order to simulate the rotation of substrates, the user also has the ability to vary the angle of incidence as well as the speed at which the variation takes place. This is accomplished by the user entering the angle which corresponds to the total amount of variation as in figure 21. If the main angle of

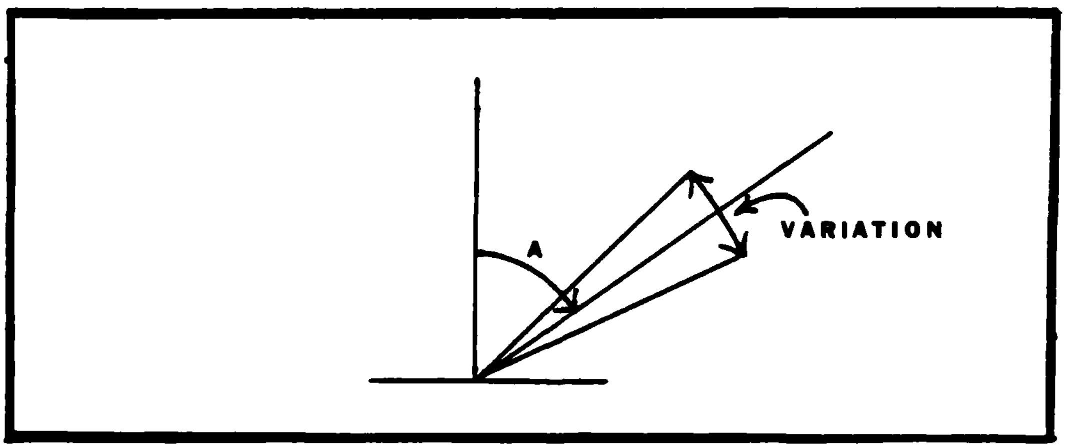


Figure 21. Full Angle Variation

incidence is at 35 degrees and the amount of variation is specified to be 10 degrees, then deposition will occur between 30 and 40 degrees. The speed at which the angle changes is determined by the size of the angle increment, implying that the smaller the angle increment the slower the angle changes over time. An example of how these variables are entered occurs below with the prompts and possible answers given.

```
At what angle do you wish the film to be deposited?
Please enter angle in degrees - Enter in real format.

27.0

Do you wish to vary the angle of incidence?

 If yes - Enter 1
 Otherwise - Hit Return

1

How many degrees (full angle) do you wish to vary the angle?
Enter degrees in real format.

6.0

What size angle do you wish to increment the angle of incidence?
Enter degrees in real format.

.01
```

With the above answers given to the prompts, the main angle of deposition will occur at 27 degrees and will vary between 24 and 30 degrees with the angle being changed 0.01 degrees after every disk.

The next set of parameters that the user is able to specify concerns the amount of mobility the disks have after making initial contact with a previously deposited disk or the substrate. The user has the choice of three different disk mobilities. First, the user may option to let the disk have no mobility. This of course would produce a film with a very low packing density like that of Dirks and Leamy (5), and does not simulate real films. Second, normal mobility may be chosen in which the disks come to rest in a "pocket" produced by two other disks. The final option the user may choose is allowing a predetermined percentage of disks to undergo an extra mobility as discussed in chapter three. The percentage is determined by the user entering the number of disks to be deposited before an extra mobility iteration occurs. Therefore if the user wishes 20 percent of the disks to undergo an extra mobility, the number 5 is entered.

The fourth parameter the user enters determines whether or not a single impurity, the size of which was discussed in chapter three, is to be deposited within the mircrostructure. If the user does decide to implant an impurity, the placement of the impurity is determined randomly by the computer.

The last set of parameters the user has control over is the size of the disk to be deposited. The user may decide to deposit only one size disk, either small or large, or he may decide to create a multilayered film. If the user decides upon creating a multilayered film, the program then prompts the user which size disk is to be deposited first and then the depth of the layers in terms of the film arrays.

After the deposition variables are set, the deposition of the film onto the designed substrate may be invoked. It should be noted that the five major parameters, number of disks, the angle of deposition, mobility of the disks, deposition of impurities and the size of disks, are all independent of one another. Therefore, any combination of these parameters may take place.

Deposition of film. The deposition of the film onto the substrate is the heart of the entire program. It is this section of the program that all other sections were designed around. The section itself is divided into three areas which are responsible for calculating collision partners and coordinates, rest point coordinates and, when needed, the rest point coordinates for disks which undergo an extra mobility.

Collision Coordinates. When an incident disk approaches a previously deposited disk or the substrate, it is necessary to know with what disk it makes contact and the position of the incident disk when this occurs. The reason for wanting to know the position of the incident disk upon collision comes about when finding the proper rest disk. In order to accomplish this task the collision corridor method used in the previous thesis (47) was utilized with some modifications since multiple sized disks were used in the new model.

Put simply, the collision corridor method uses parallel streamers to search the area around an incident disk trajectory for possible collision partners. Each individual streamer scans until reaching a cell not previously encountered by another streamer. Once an occupied cell is found the y coordinate of the incident disk is calculated by the algorithm in chapter three. Once each streamer has preformed its scan, the collision partner which yields the largest incident disk y coordinate is chosen as the collision disk. The x coordinate of the incident disk is then found by using the y value just obtained.

The number of streamers necessary to define the collision corridor is dependent upon two parameters. First, the spacing between the individual streamers needs to be such that no matter what the angle of deposition, no unit cell can be placed between them. Second, the width of the corridor has to be large enough that all unit cells capable of containing collisional partners are checked. This second parameter is therefore dependent on the size of the incident disk, as well as the size of the previously deposited disks. As an example, the case which calls for the least number of streamers occurs when only the smallest disks are being deposited. In this case for a collision to occur the center of the incident disk needs to be one disk diameter away from the center of another disk; namely, one square root of two. The minimum number of streamers necessary to check around the incident disk in this particular example is four (as shown in figure 22). When larger disks are deposited the number of streamers increases, as in the case when 16 streamers are used when an impurity is incident on large disks.

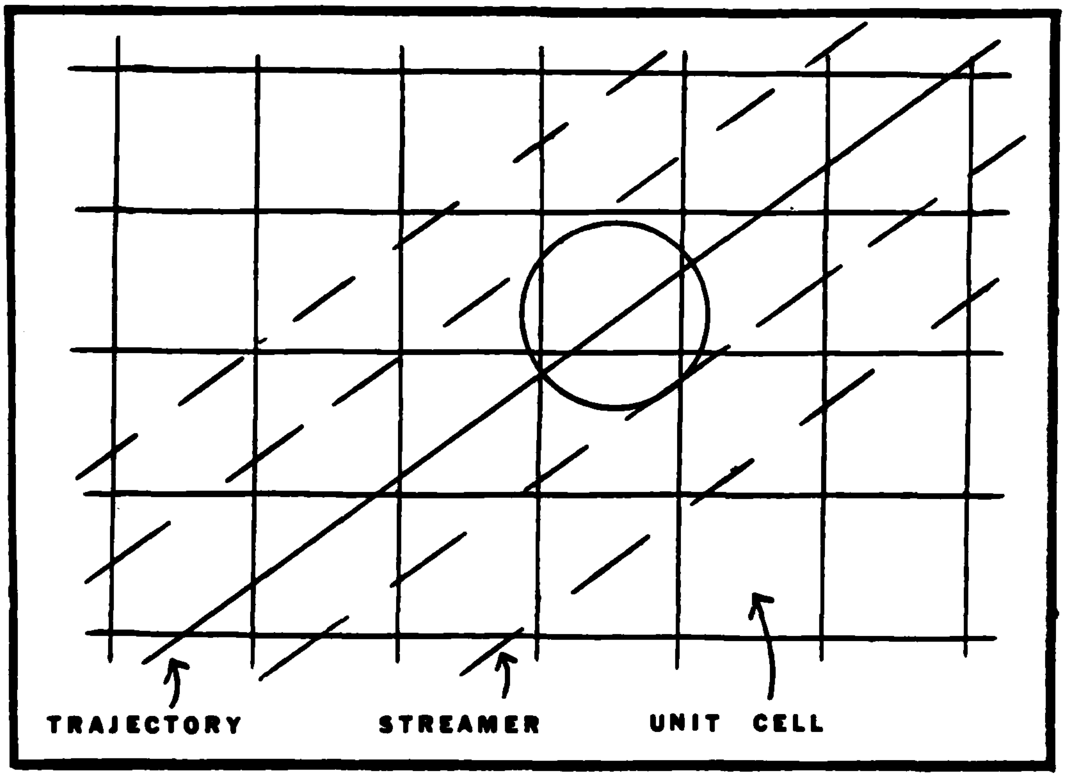


Figure 22. Example of Streamers

Rest Point Coordinates. Once a collision disk is determined and the position of the incident disk upon collision known, the final resting place of the disk can be determined. As mentioned previously, the user of the program has three options as far as the mobility of the disks are concerned. With no relaxation of the disks, it is implied that the collision coordinates of the incident disk become the rest point coordinates. For the case of extra mobility, this subject will be presented in the next area.

When normal relaxation of disks occurs, the final resting place is determined by the mathematical derivation explained in chapter three. That is, find a third disk or rest disk with which the incident disk rolls into contact with, while still maintaining contact with the collision disk. The program algorithm used to accomplish this task involves using an array search around the collision disk. The rest disk is then found by determining which disk allows the incident disk to move the shortest distance before coming to rest. If no further relaxation is to occur the rest position of the incident disk is then recorded in the main arrays by truncating the final position coordinates.

Extra Mobility Coordinates. In order to simulate some disks undergoing more than "normal mobility", the third area in the deposition section calculates the rest point coordinates of these disks. In essence, this part of the section finds the rest coordinates for the incident disks, which allows it to move to the "next" shortage distance in comparision to that of normal mobility. Like normal mobility, the incident disk is allowed to remain in contact with the collision disk.

Although the algorithm for normal mobility may be simple, the task of finding an alternate rest place is more difficult. Since the incident disk is to maintain contact with the collision disk and the resting place for normal mobility is to be ignored, there exists only one other possible resting position. Due to the way the algorithm was derived, the second resting place may or may not correspond to the position which allows the incident disk to move the next shortest distance. As shown in figure 23 (a condition immediately after contact has been made), position 1 is where the incident disk would come to rest under the condition of normal mobility. Although positions 2 through 5 correspond to places where the algorithm would designate as possible rest points, these are either occupied or physically impossible due to surrounding disks. Position 6 on the other hand is the second of the two possible resting points. In order to arrive at this decision using a computer, the extra mobility routine uses a set of seven stored posi-

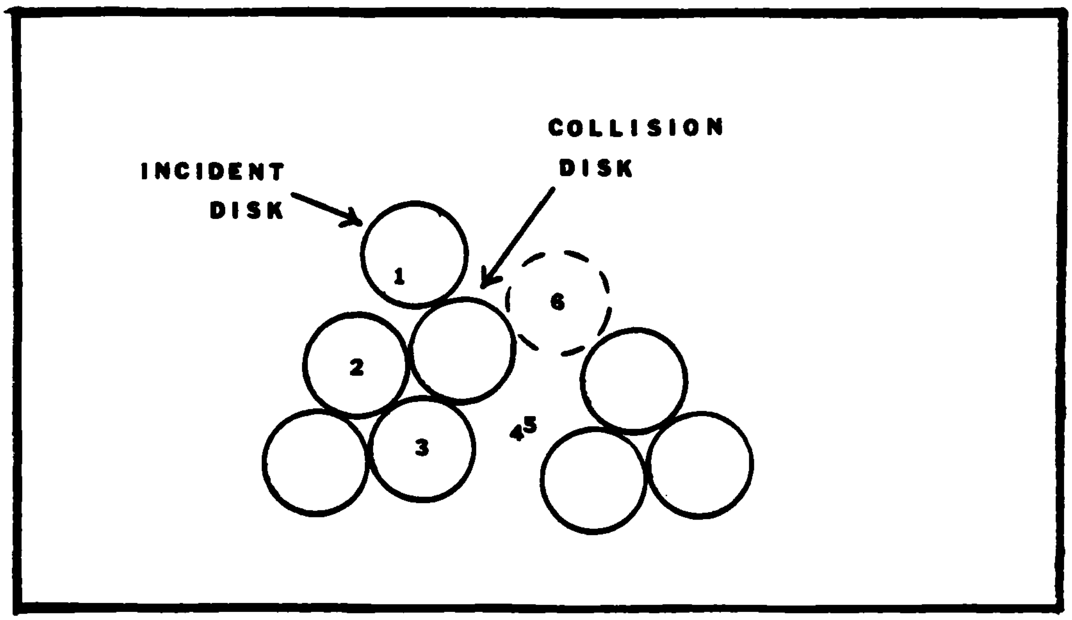


Figure 23. Extra Mobility Placement

tions and then tests whether each is occupied or physically plausible. Immediately after the testing of the seven different positions, another test looks at the y coordinate of the extra mobility position in comparison with the y coordinate determined for normal relaxation. If the extra mobility position is significantly higher than that for normal relaxation the position is considered invalid. The reason for doing this is to ensure that the resulting film becomes more dense rather than less dense. In the case where none of the seven positions are found to be suitable and/or the height position test fails, the final position of the disk is decided by default to be the position determined by normal relaxation. The next disk, in order to make up for the failure of the test, is then given extra mobility. This continues until a suitable disk is found.

Periodic Boundaries. In order to save on space within the memory of the computer, periodic boundaries were incorporated into the model. More specifically, this condition allowed incident disks which would normally disappear off the left side to reappear on the right and visa versa. The result of introducing periodic boundaries can be seen in in the next chapter where the figures give the impression that one section of the film is being viewed.

Analysis Subroutine

After a film has been produced it is necessary to characterize its properties. In this subroutine two properties of the simulated film are analyzed by two separate sections, namely the packing density and angle of growth of the film. The movement between these sections is controlled by an interface loop as in the first two subroutines.

Packing Density Analysis. As mentioned in chapter one when the density of the film increases, the properties of the film approach those of the bulk material. This is desirable because the optical properties of the film become more stable. An example would be the reduction of water absorption due to increased packing density, which in turn reduces the amount of wavelength shift. In order to monitor the density of the film, the first section of this subroutine is dedicated to that purpose.

Reviewing from chapter two, the packing density of the film is simply:

$$p = \frac{\text{volume of the solid part of the film}}{\text{total volume of the film (solid + voids)}} \tag{2}$$

where p is the packing density. This implies that the value of 1.00 is the largest value the packing density can achieve. In order to make the program more user friendly the value of p is multiplied by 100 making it a percentage.

In order to calculate the packing density of the film, where only one size disk has been deposited, the number of cells which are occupied are counted and then divided by the total number of cells. This number is then multiplied by the area of a disk relative to a cell, and then multiplied by 100. However, in the case where different sized disks are used, separate counters are needed for each size disk. After calculating the individual percentages for each size disk, the percentages are then added to obtain the total packing density. With the three different sized disks used in the program the individual packing densities were calculated as follows:

psmall = (number of cells with small disk/60000)*1.570796*100 (7)

plarge = (number of cells with large disk/60000)*6.283185*100 (8)

pimpur = (number of cells with impurities/60000)*100.5309*100 (9)

where psmall, plarge and pimpur are the respective packing densities of the three different disks.

Because films produced by vapor deposition tend to be amorphous in nature, this implies that the packing density throughout the film may not be uniform. In an effort to look for spatial variations within the simulated films the density algorithm was modified. Not only is it possible to find the total packing density of the film, but spatial variations in both the horizontal and vertical directions are possible. Therefore, the user of the program may look at individual areas within the film. This was accomplished by simply specifying the upper and lower heights for vertical variations, and left and right boundaries for horizontal variations. The values entered correspond to the addresses of the unit cells of the arrays.

Angle of Growth. The angle of columnar growth by the film is responsible for many characteristics as noted in chapter one, and is dependent on the deposition angle via the tangent rule in many films. In order to calculate the angle of growth the algorithm used in the previous model (47) was invoked.

This algorithm calculates the angle of growth by looking at variations in the density of the film at varying angles. In doing so, the angle of growth can be found at different heights within the film, amounting to vertical variations within the film.

Moving Subroutine

The moving subroutine was developed in order to store the values of the main arrays making up the film for future analysis and/or plotting. This is accomplished by dividing the subroutine into four sections. Again, as in the previous subroutines, the movement between the sections is controlled by an interface loop.

The first two sections of the subroutine provide a somewhat inefficient way of storing and retrieving values in that all values of the main arrays, both zero and non-zero, are moved around. Although this is not memory efficient it may prove to be useful for certain types of graphing devices.

The third section of the subroutine, like the first, stores the values of the main arrays into files; however, in this case only the non-zero values are stored. More specifically, this section produces two files for storing values for plotting. The first is a master file containing data on all the disks independent of size, and holds information concerning the occupancy of the unit cells as well as the x and y coordinates of the individual disks. The second file, on the other hand, con-contains similar data regarding only the larger sized disks.

The fourth section of the subroutine, somewhat like the second, reads back into the program the values stored in a file by section three. What makes this section different from the second is that only the data concerning the occupancy of the unit cells is read back. This in turn allows for only an analysis of the film, namely density calculations and determination of the angle of growth.

V. Results and Analysis

As with any program, it is necessary to analyze the results and then make conclusions based on the analysis. The purpose of this chapter is to look at the resulting films and then try to analyze the films based on the parameters under which the films were deposited. Throughout the last stages of program development and finally during the running of the program to obtain results, approximately 35 films were printed out and the results examined. However, to conserve on space only 13 of the most interesting films will be discussed in this chapter.

In order to provide a control upon which the films could be compared, 5 films were deposited at various angles. With these films, none of the deposition parameters were varied, therefore allowing future films to be compared against them. Three of these films can be seen in figures 24 through 26. The other films provided in this report (figures 27 through 36), all have at least one parameter that was introduced. In order to refresh the reader these parameters are the temporal variation of the angle of deposition, the mobility of the disks upon collision, the doping of impurities into the microstructure, the ability to introduce imperfections into the substrate and the simulation of multilayered coatings.

Controls

By viewing the three control films (figures 24 - 26), some of the main characteristics exhibited by other columnar models can be seen. In figure 24, a film deposited under normal incidence, columns 3 to 5 disks

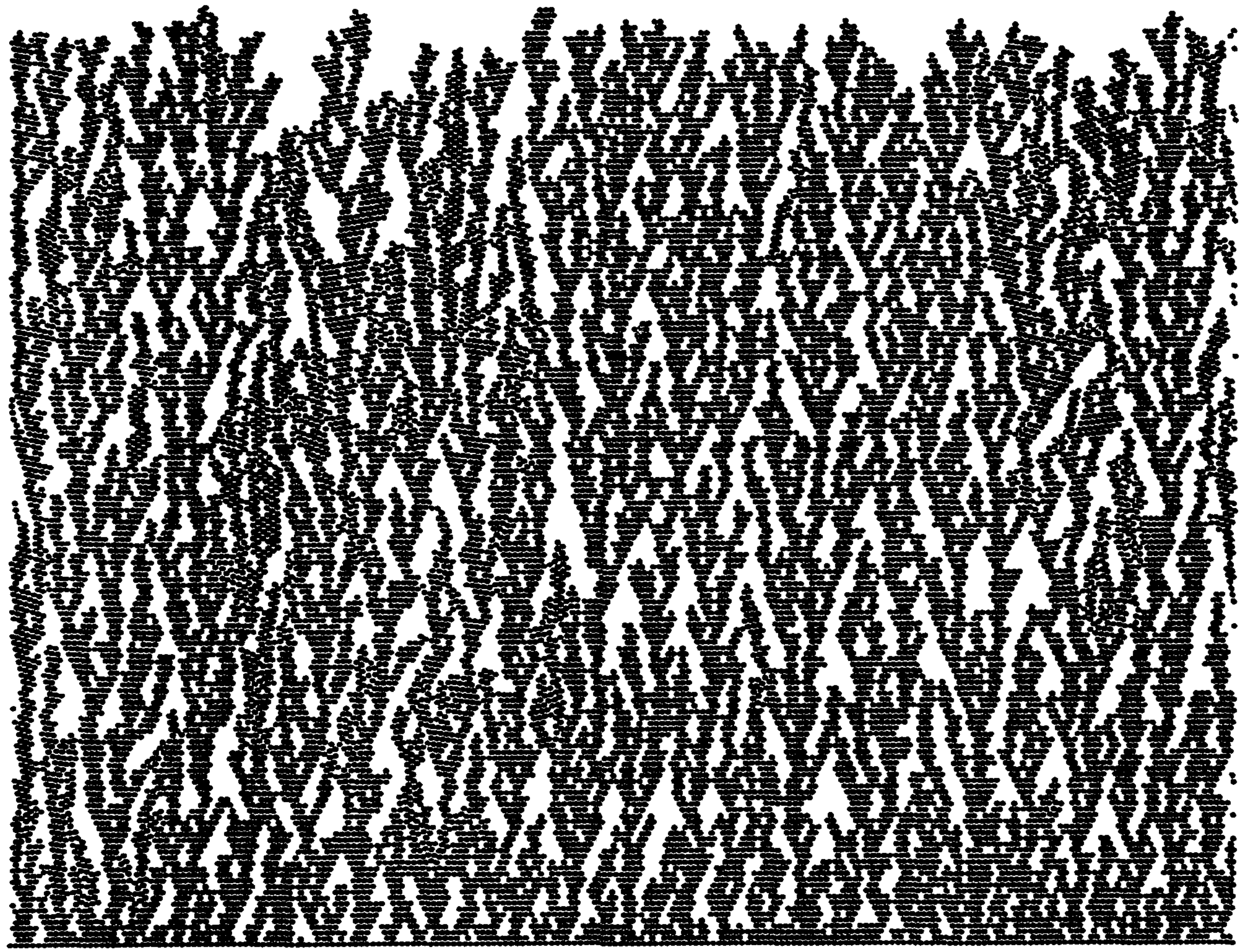


Figure 24. Control Film at Normal Incidence

thick can be seen branching in both the left and right directions due to the normal incidence. When the angle of deposition is increased to 25 degrees as in figure 25, little if any branching takes place that is headed toward the left. In figure 26, the film is definitely leaning towards the right due to the angle of incidence being 50 degrees. It can also be seen that the overall density of the film is less than that for normal incidence, and that the spacing between the columns is significantly larger than that for either normal incidence or at 25 degrees. Comparisons of the overall densities of the films show that the largest density occurs for the film deposited at normal incidence, and that this density decreases for increasing angles of deposition. The amount of decrease from normal incidence to 50 degrees is approximately 10 percent. The angle of growth by the control films is in very good agreement with what the tangent rule predicts. For example, at 50 degrees the angle of growth by the film was found to be approximately 29 degrees, where the tangent rule predicts 30.7 degrees.

All of the above results correspond very well to results that other models have produced. Therefore, it can be assumed that the new model is not predicting anything radical and that other results presented in this chapter should be considered as reliable.

Angle Variations

Films produced with angle variations showed no consistently reproducible results. However, there were some characteristics that could be gleaned from the resulting films. First of all, films produced with angle variations were able to produce columns that were on the average a little wider than those with no variations, but the spacing between the

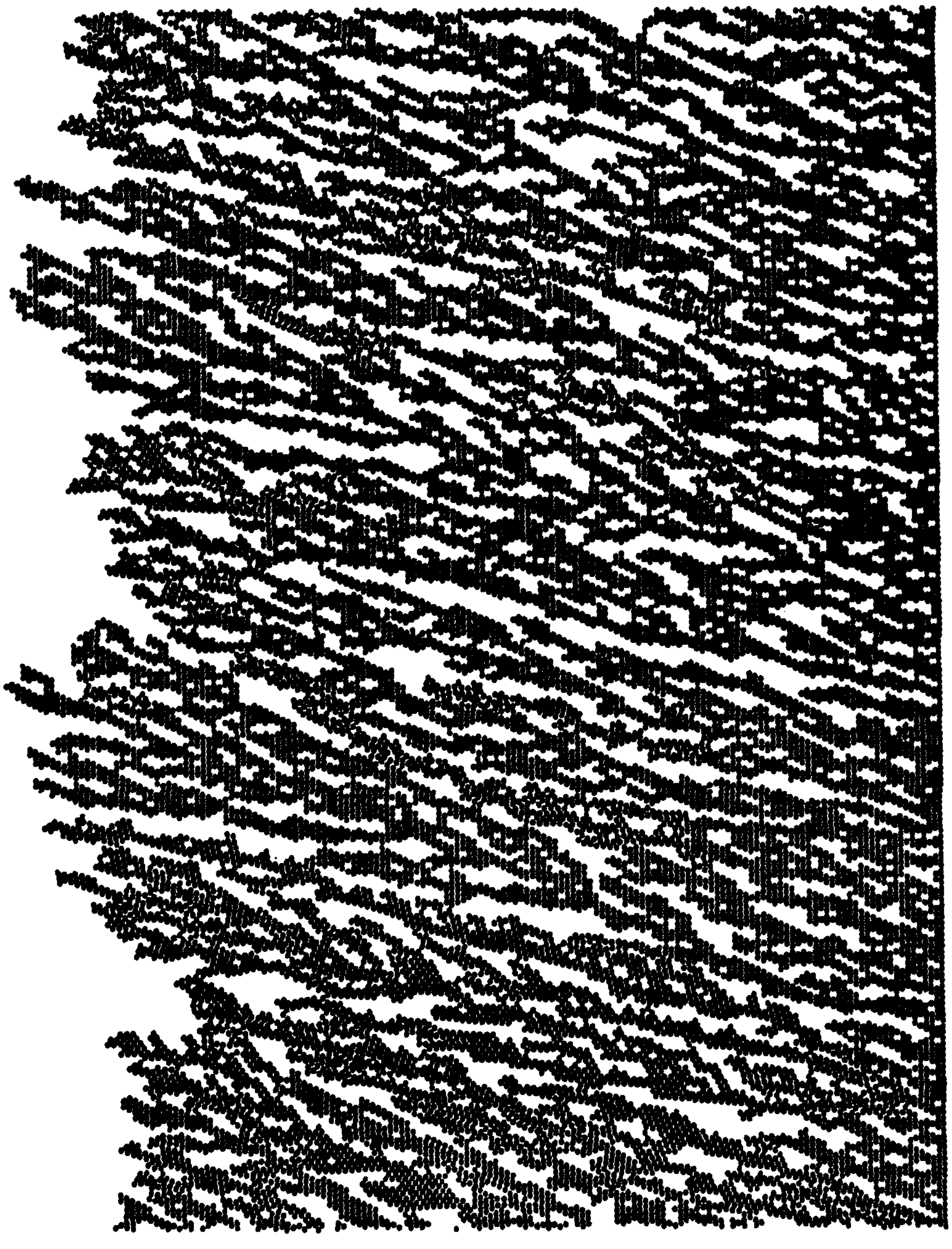


Figure 25. Control Film at 25 Degrees

Figure 26. Control Film at 50 Degrees

columns increased, which resulted in decreased density. The most interesting results came when angle variations were carried out with a reasonable amount of extra mobility on the part of the disks. As shown in figure 27, a multilayered film with disk mobility occurring on 5 percent of the disks, the dendrites formed are wider than normal but the columnar structure is fairly random. When this mobility is brought together with angle variation as in figure 28, large columns are formed from smaller dendrites which begins to model actual films. In this figure, 9 percent of the disks have undergone mobility and are deposited with 5 degrees of angle variation.

Mobility

One interesting result obtained during this research occurred when extra mobility was given to a percentage of the incident disks (figures 27,28,29,30,31). As noted above, larger columns were formed when the extra mobility of disks were introduced with angle variations. However, this alone was not the only significant result.

As the percentage of disks undergoing extra mobility was increased, three distinct phenomenon were found to exist. First, the packing density of the films was increased (figure 29). Although this comes as no surprise, the amount of increase for films deposited at oblique incidence was fairly substantial when compared to films deposited at normal incidence. In figure 30, a film deposited at 40 degrees with 20.1 percent mobility, the total density was found to be 68.1 percent. When this is compared to the control at 50 degrees (figure 25) with a packing density of 56.3 percent this corresponds to a 11.8 percent increase. The film in figure 31 (deposited at normal incidence), with a mobility

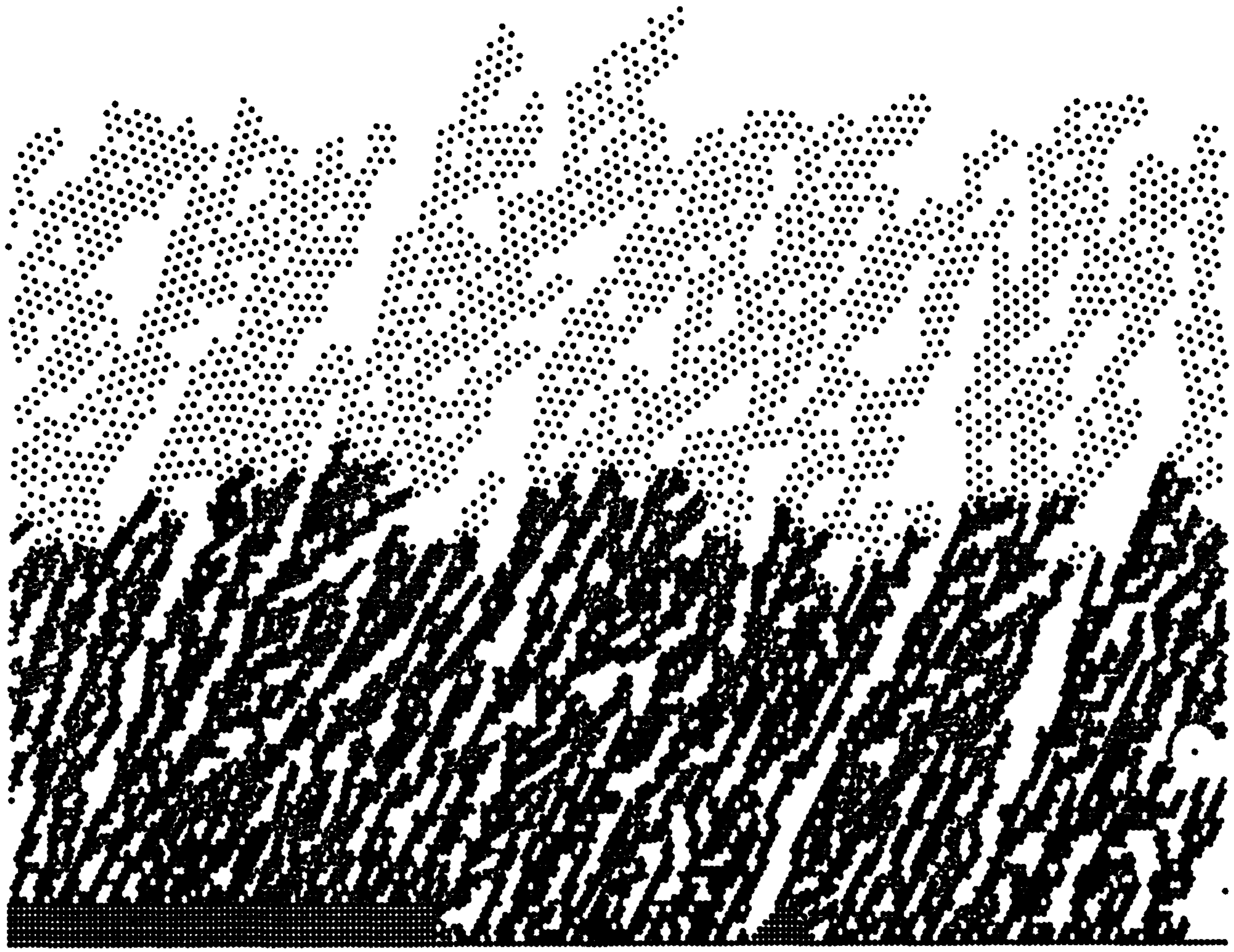


Figure 27. Multilayered Film at 40 Degrees with 4.5% mobility and an Impurity in the Lower Right Hand Corner

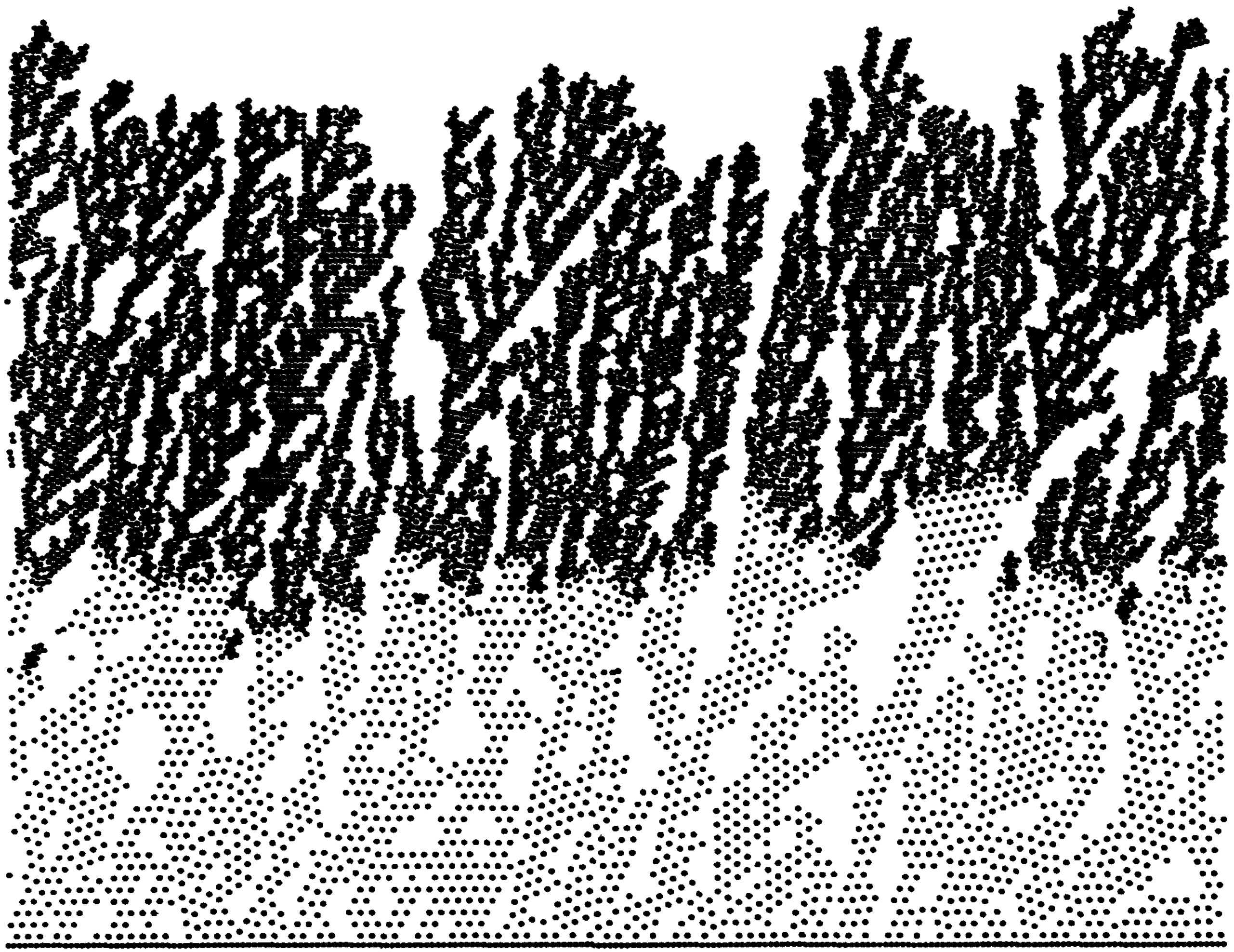


Figure 28. Multilayered Film at 25 Degrees with 9.3% mobility
and an Impurity in the Lower Left Hand Corner

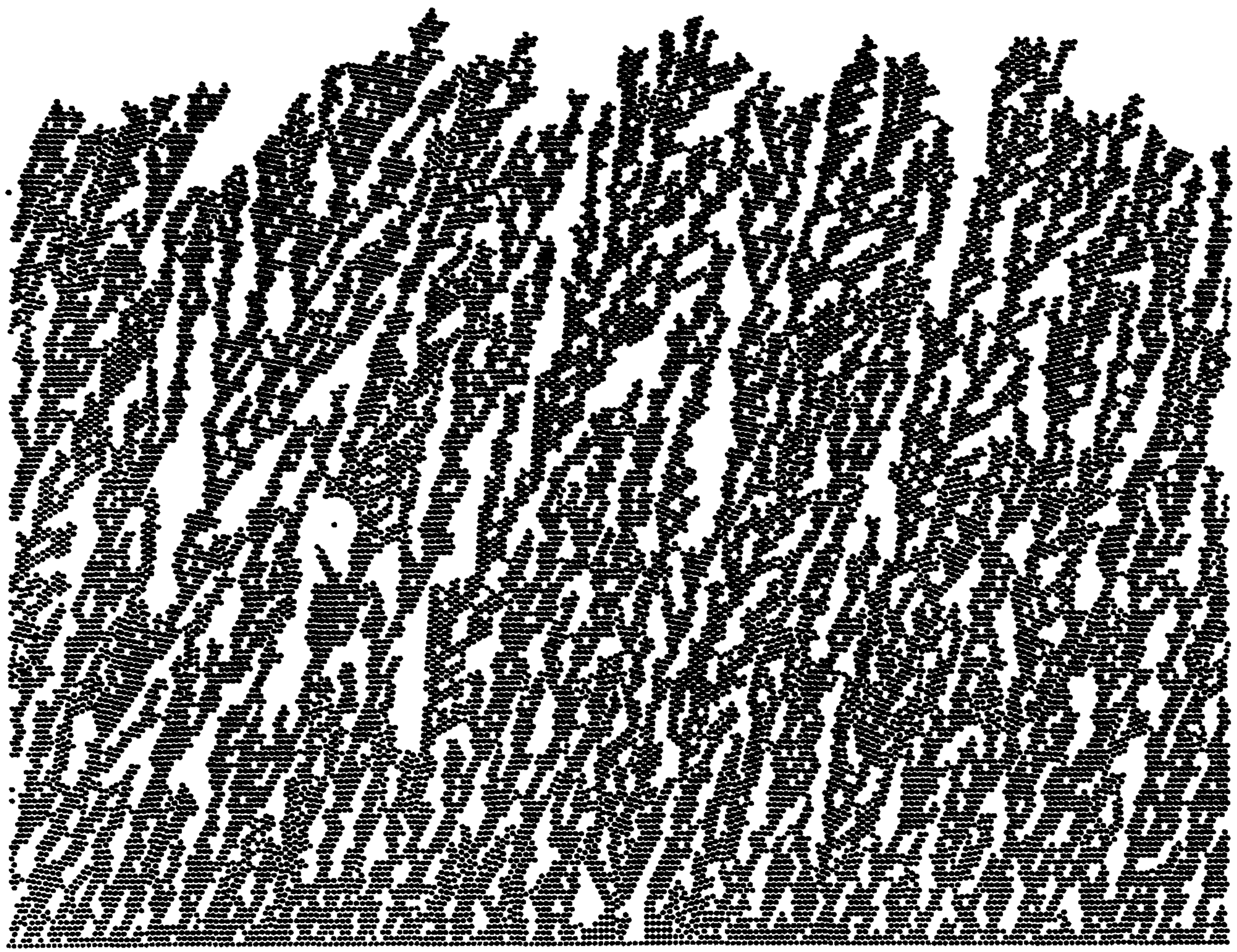


Figure 29. Small Disks Film at 27.1 Degrees with 4.5% mobility and an Impurity in the Lower Left Hand Corner

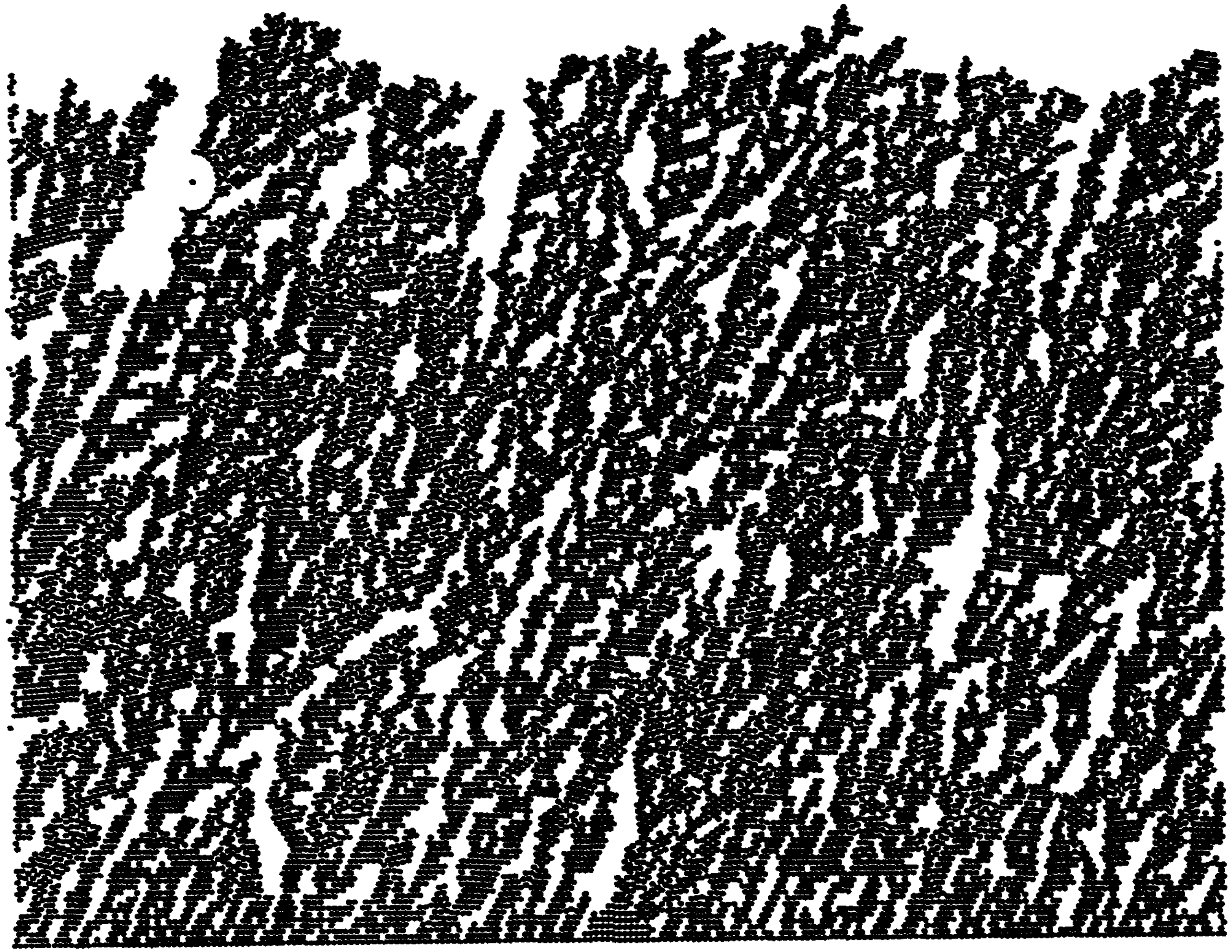


Figure 30. Small Disks Film at 40 Degrees with 20.1% Mobility and an Impurity in the Upper Left Hand Corner

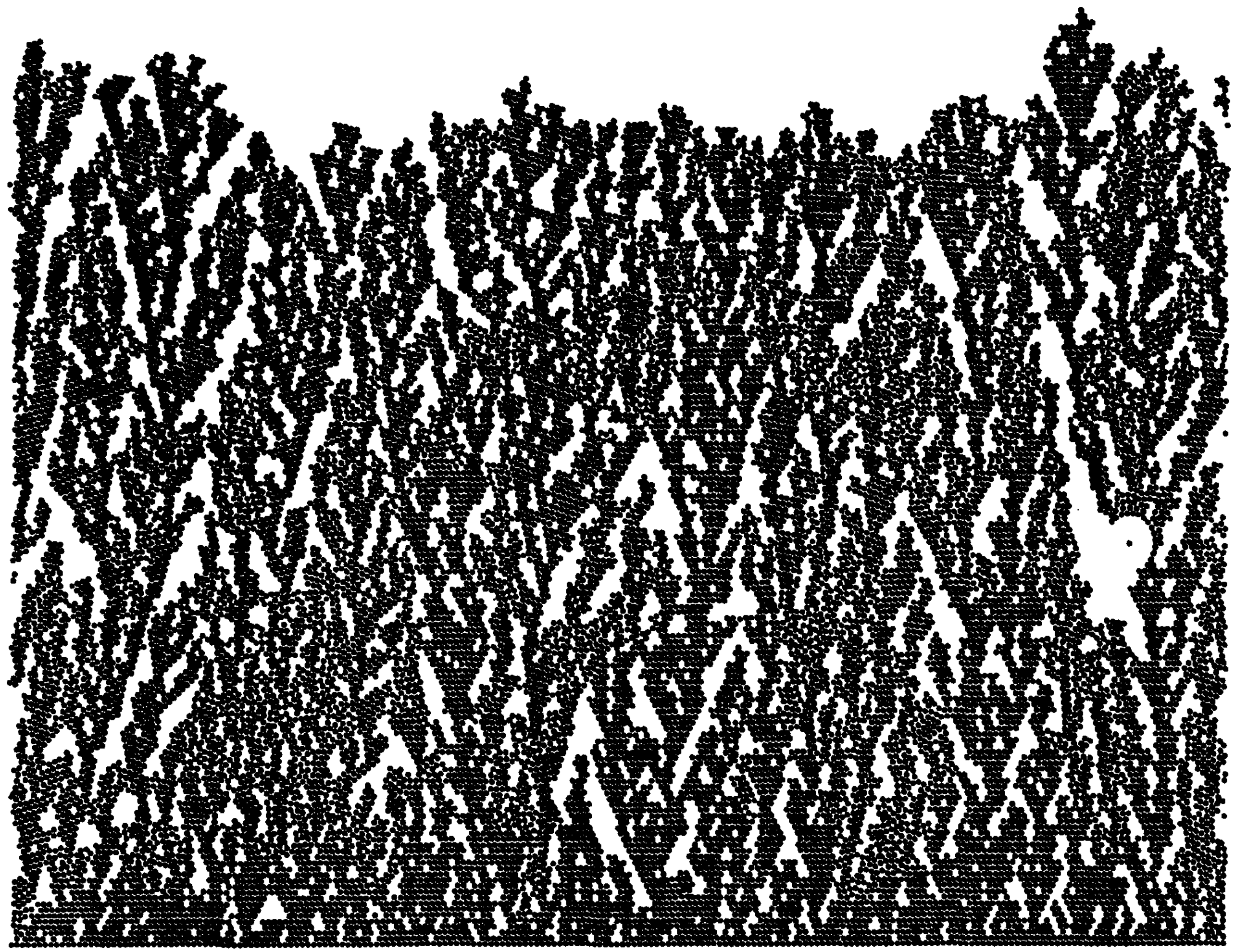


Figure 31. Small Disks Film at Normal Incidence with 21.6% Mobility and an Impurity in the Lower Right Hand Corner

of 21.6 percent, only showed a 0.8 percent increase in the packing den-density, compared to the control deposited at the same angle of deposition. This would seem to imply that mobility has little, if any, effect for films deposited at normal incidence, as far as increasing packing density is concerned.

The second phenomenon that occurred as a result of disk mobility was the disappearance of a visible columnar structure. In figures 27,28 and 29 where the mobility of disks was kept between 5 and 10 percent, a visible columnar structure is still maintained. However, when the mobility of the disks is increased to around 20 percent and greater as in figures 30 and 31, the columnar structure starts to break down and eventually goes away. This disappearance is in agreement with what Nakahara had found for films with large structural relaxation, such as in copper and permalloy films (35).

The third phenomenon found in films deposited with mobility was that the films possessed a more uniform packing density throughout the thickness of the film. A density analysis of the control film at normal incidence showed that the density of the film tends to decrease the farther away one gets from the substrate. When the same analysis was done on the film in figure 31, the packing density did not exhibit a consistent drop and the density near the top of the film was significantly greater than that for no mobility. This was found to be true for all films deposited with extra mobility. Although no major study has been made concerning the uniformity of density throughout the thickness of a film, the results would confirm or deny that shadowing plays a role in density variations of a film, if they exist.

Nodular Defects

As stated earlier in chapter three, there are basically two different ways that people have tried to produce nodular defects in the film; namely, through the use of substrate imperfections and the doping of impurities into the microstructure. Throughout the course of this research both of these methods were tried, the results of which varied.

Substrate Imperfections. As can be seen back in figures 15-20, the substrate subroutine had the ability to produce almost any number of substrates. Some of these were used in the deposition of films, namely those in figures 27,29,30,32 and 33. Although no nodules were formed as a result of the imperfections, some were able to produce an amorphous clump of disks in the immediate vicinity around the imperfection. This can be seen in figures 29,30 and 33. The reason for the amorphous nature of the film around the substrate imperfections can only be attributed to the irregularity of the imperfections themselves. As to why the substrates were not able to produce nodules, it seems to be due to the fact that the imperfections tend to be too small in comparison to the size of the disks used.

Impurities. The use of impurities to produce nodules was by far more effective than using substrate imperfections. As can be seen in figures 30 and 31 (especially in figure 30), distinct nodules can be seen within the mircostructure. Other attempts to produce nodules by the use of impurities can be seen in figures 27,28,29,32,33 and 34. Although these did not produce nodules, they did produce an amorphous structure immediately in their vicinity, which can be attributed to the irregularity of the structure, just as in the case of the substrate im-

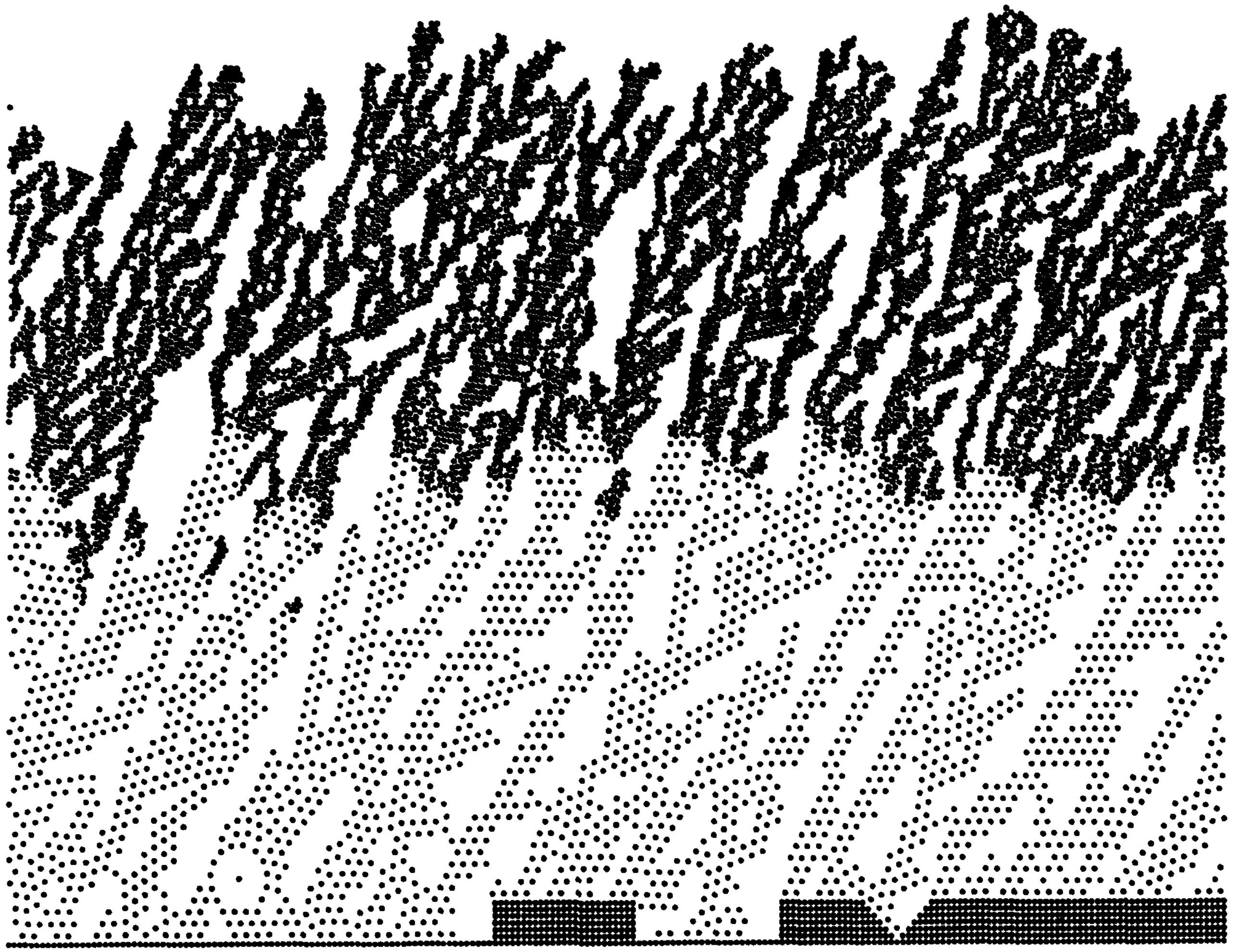


Figure 32. Multilayered Film at 40 Degrees with an Impurity in the Lower Left Hand Corner

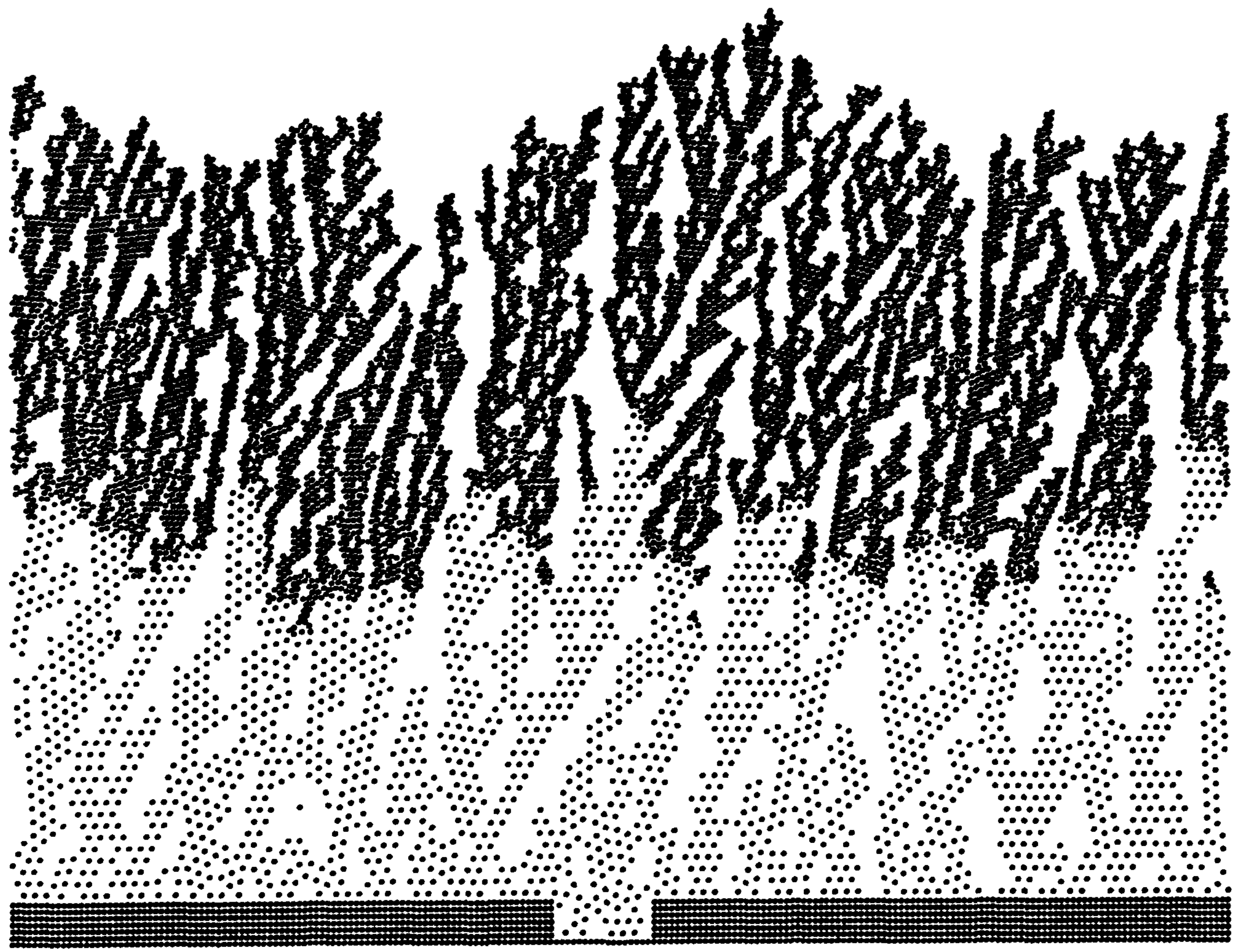


Figure 33. Multilayered Film at Normal Incidence with an Impurity in the Lower Left Hand Corner

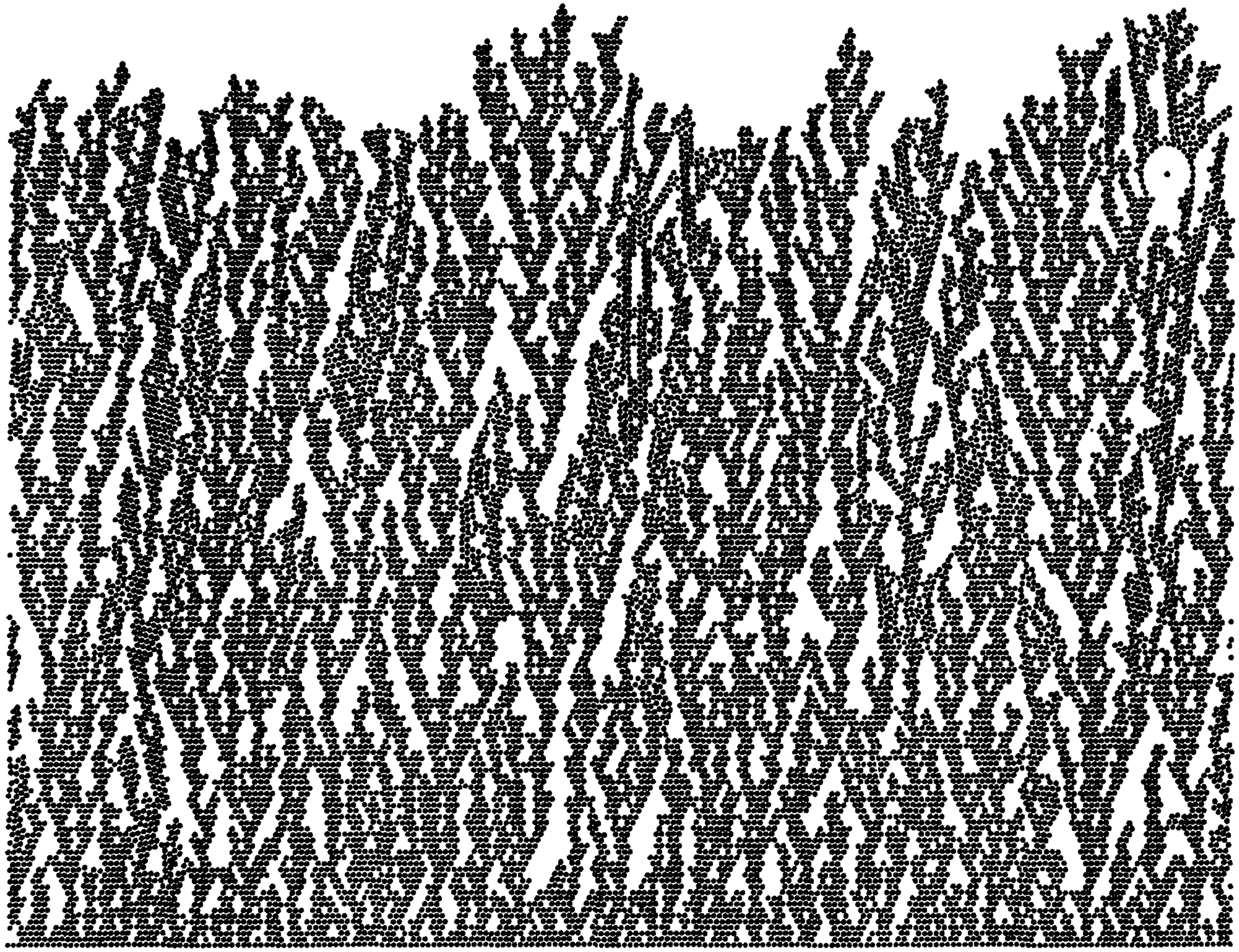


Figure 34. Small Disks Film at Normal Incidence with an Impurity in the Upper Right Hand Corner

perfections. Another characteristic common to the film growth around the impurities is the fact that the nodule or amorphous structure grows in a direction parallel with the angle of deposition. For example, in figure 30 the nodule at the top of the film grew at an angle of 40 degrees, which happens to be the angle of deposition for that film. One last characteristic which is common among some of the doped films is that the growth of the film immediately above the impurity extends above the top of the film. This can be seen in figures 30,31 and 34.

It would appear then that impurities can be used to create nodules and nodular effects such as the production of an amorphous structure. It is also implied that one reason for the creation of nodules in films is due to shadowing, since no physical parameters such as electrostatic charge are dealt with in the model.

Multilayers

Perhaps the most interesting results obtained during this research occurred when two different size disks were used to simulate multilayered films (figures 27,28,32,33,35,36). In the films produced when the smaller disks were deposited first, as in figures 27 and 35, there did not appear to be any outstanding features to note. The reason for this is that the boundaries between the layers appeared to be continuous in nature. However, when the larger disks were deposited first, two distinct features were noticed. First, some of the smaller disks from the top layer were able to penetrate through openings in the top of the lower layer, which made for a discontinuous boundary. This is especially evident in figures 32 and 36. Even though one would expect this to occur, one reason for choosing different sized disks was not neces-

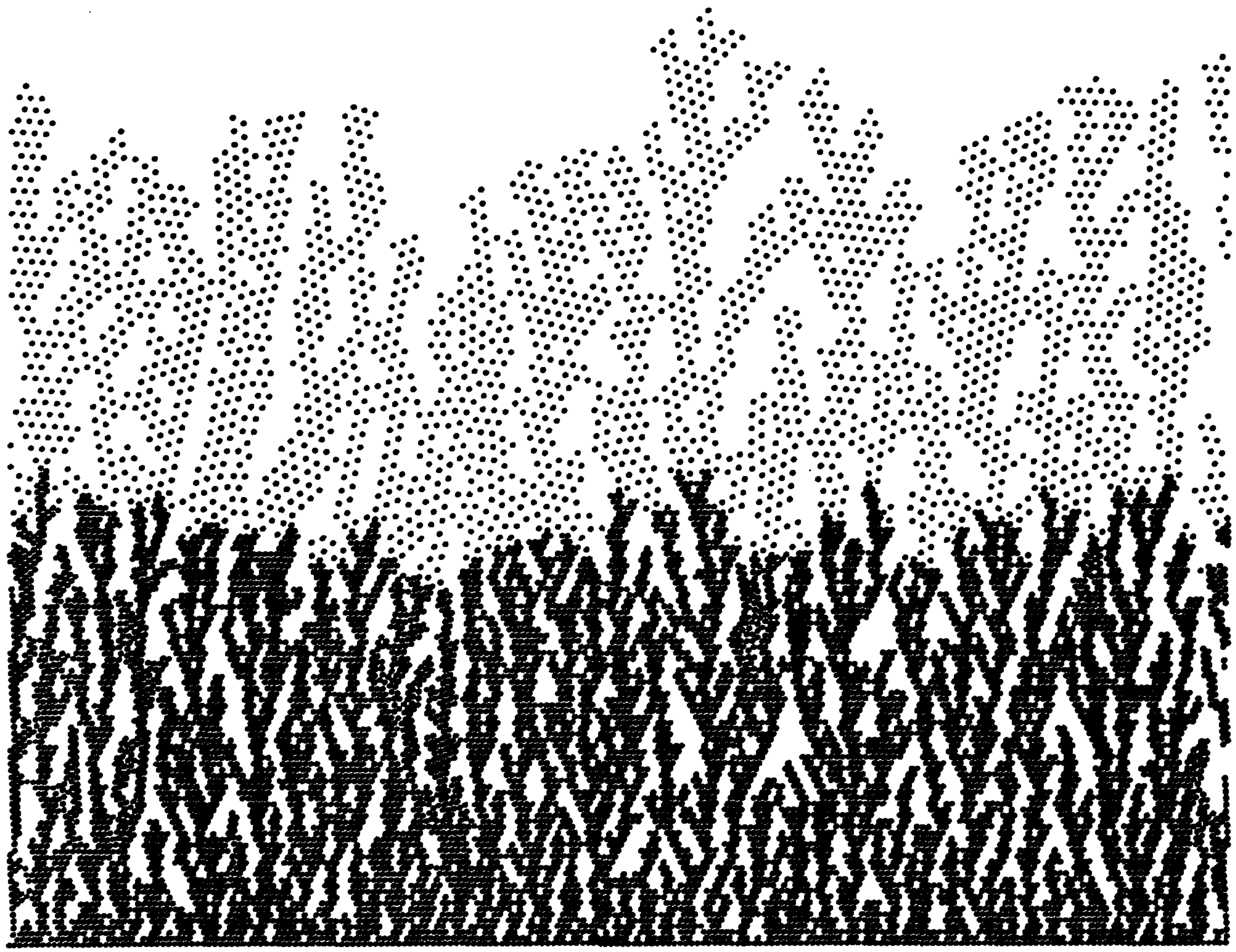


Figure 35. Multilayered Film at Normal Incidence with the Small Disks Deposited First

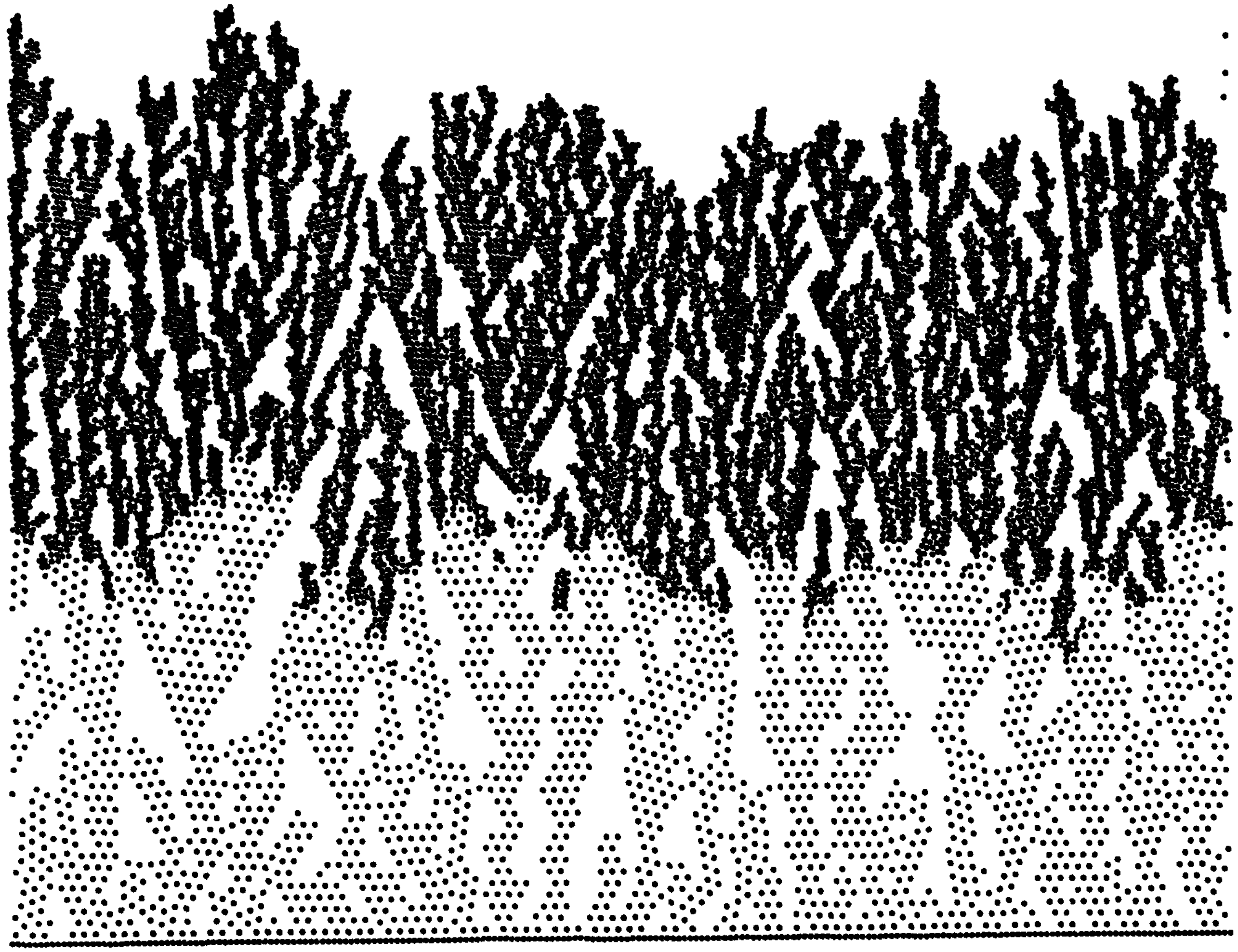


Figure 36. Multilayered Film at Normal Incidence with the Large Disks Deposited First

sarily to simulate molecules of different size, but to simulate molecules which possessed different interaction distances. The second feature exhibited by the films when the larger disks were deposited first, was that this tended to produce pores in the microstructure which could allow for water absorption (see figures 27,28,32). As stated in chapter two, one of the problems with vapor deposited films is that they are subject to water absorption. Therefore, these films would tend to imply that the mechanical properties of film growth, like shadowing, are one reason why water absorption occurs.

Other Characteristics

One result obtained from the research, that was not expected, was the fact that the density of the modeled film immediately above the substrate was significantly greater than the average density of the film. More specifically, the packing density of the area three to four unit cells above the substrate was found to be 25 to 30 percent greater than any other region in the film. The main reason that the density of the film near the substrate is so much greater, is most likely due to the fact that the shadowing effect of the film is negligible during the early stages of growth. Then as the columns in the film become larger, shadowing starts to play a more important role in the growth of the film, until the time when the film is high enough above the substrate that the density begins to approach that of the average.

VI. Conclusion and Recommendations

Conclusion

Based on the results obtained in chapter five, it is evident that the objectives of the research were met. That is, the ability to produce a computer simulation of thin film growth with variable parameters was accomplished.

Deposition Angle. It was shown during this thesis that the angle of deposition plays an important role in the growth of a film. Not only do the width of the individual columns making up the mircostructure decrease with increasing angle, but the packing density of the film decreases as well. The variation of the angle of incidence also played a role in determining the resulting structure. For relatively small angle variations (less than 10 degrees) the density of the film went up, but for larger angle variations the density went down producing a rather amorphous microstructure.

Mobility. By varying the percentage of disks undergoing extra mobilities, three results were obtained. First, the larger the percentage of disks undergoing extra mobility, the greater the packing density of the film. Second, for films with a relatively large amount of disk mobility, the columnar structure all but disappeared; a result which is in agreement with experimental work. Third, films deposited with disks undergoing extra mobility possessed a more uniform packing density.

Impurities. Although there were very few nodules formed by the doping of impurities, there were two interesting results. First, the film deposited immediately around the impurity was extremely more amorphous than other sections of the film which contained no impurities. Second, the angle of the nodule and/or amorphous growth was parallel with the angle of deposition.

Substrates. Out of the many substrates produced by the model none of them produced nodules of any great size, if at all. One reason for this may be due to the fact that the highest imperfection able to be created was only seven disks high. However, the imperfections in the substrate did create an unusually amorphous structure about them, somewhat like the impurities, which could have resulted in nodules had the film thickness not been so great.

Multilayers. The multilayered films produced by this computer simulation were the most interesting of all the films produced. It is apparent by looking at the films that the boundary layer between the different sized disks appeared to be discontinuous in nature, an outcome which is in complete agreement with experimental results. This was especially true of the cases in which the large disks were deposited first, for this allowed the smaller disks to slip through holes left by the larger ones. Other things of interest found in the multilayered films were large cracks or pores which could account for water absorption, and some nodule growth due to the discontinuity of the boundary layer.

Other Characteristics. It was found that the density of the film within a few unit cells of the substrate was significantly higher than the average packing density (25 to 30 percent). This is thought to occur as a result of shadowing playing a minor role in the early stages of growth.

Ending Remarks. Although more two-dimensional computer models using disk mechanics may be developed in the future, the results obtained should not be significantly different from those presented in this thesis. Three-dimensional models, on the other hand, may provide information about form birefringence and other properties that cannot be studied in two dimensions. However, for the most part computer simulated growth using disk mechanics can only give so much information. Not until the time when physical properties such as electrical charge and chemical bounding are routinely used to construct the model, will computer simulations tell people more about thin film growth.

Recommendations

In order to improve upon this new model of thin film growth there are several things which can be done. First, if computer space will allow, a simulation in three dimensions using disk mechanics is probably the next logical step. Upon the completion of modeling a three dimensional film, the introduction of physical parameters into the model will ultimately make the model more useful and realistic. Some of the parameters which could be introduced are the use of chemical bonds in order to produce films with a crystalline structure, the variation of the sub-temperature to allow for different molecule energies, as well as using electrical charge on individual molecules to determine the microstructure.

Appendix A

Mathematical Derivations used to Construct Program

This appendix is divided into two sections. Its purpose is to show the mathematical derivations used to develop the code in appendix B. The first section gives the mathematical derivations needed to find the incident disk coordinates after a collision has occurred. The equations for the final position of the incident disk are derived in the second section.

Incident Disk Coordinates After Collision

The equation of the trajectory taken by the center of the incident disk is a line. Rewriting the slope intercept form of a line by solving for x has the form:

$$X = (1/m)*Y + a \qquad (10)$$

where

m = slope of the line
a = X intercept

The equation of a contact circle discussed in chapter two can be writen in the form:

$$r^2 = (X - h)^2 + (Y - k)^2 \qquad (11)$$

where

h = X coordinate of the center of the contact circle
k = Y coordinate of the center of the contact circle
r = radius of the contact circle

In order to solve for the value of y, the value of x in the first equation is substituted for x in the second equation giving the following:

$$r^2 = [(Y/m) + a - h]^2 + [Y - k]^2 \qquad (12)$$

Expanding the squares and putting the equation into quadratic form gives:

$$[(1/m^2) + 1]*Y^2 + 2*[(a - h)/(m - k)]*Y + (a - h)^2 + k^2 - r^2 = 0 \qquad (13)$$

Solving the above equation for y gives:

$$Y = \frac{-\{[(a - h)/m] - k\} + \{r^2*[(1/m^2) + 1] - [(a - h) + (k/m)]^2\}^{1/2}}{[(1/m^2) + 1]} \qquad (3)$$

The square root is added, and not subtracted since the collision occurs at the larger y value. In order to solve for the value of x, the value of y is simply put back into the equation of the trajectory. Because the angle of incidence is measured from the substrate normal the value of $[(1/m^2) + 1]$ is actually the secant squared of the incident angle, and is represented by sc2ang in the program. The value of $[(a-h) + (k/m)]^2$ is represented by g and the value of $[(a-h)/m - k]$ by f.

Incident Disk Rest Point Coordinates

Given the equations of the collision and rest disk contact circles respectively as

$$r1^2 = X^2 + Y^2 \qquad (14)$$

$$r2^2 = (X - h)^2 + (Y - k)^2 \qquad (15)$$

r1 is the radius of the collision disk contact circle, r2 the radius of the rest disk contact circle, h the x seperation between the two disks and k the y seperation betweenthe two disks.

It is important to note that the equations above are written for circles which have been translated to the origin. Solving for x in equation 14 gives:

$$X = +/- (r1^2 - Y^2)^{1/2} \qquad (16)$$

Substituting this value for x into equation 15 gives:

$$r2^2 = [(r1^2 - Y^2)^{1/2} - h]^2 + (Y - k)^2 \qquad (17)$$

After expanding the squares and cancelling values, the equation looks like the following:

$$r2^2 = r1^2 + h^2 - 2h(r1^2 - Y^2)^{1/2} + k^2 - 2ky \qquad (18)$$

Through algerbraic manipulation this can be transformed into the the following quadratic equation:

$$(k^2 + h^2)*Y^2 + 2aky + (a^2 - h^2*r1^2) = 0 \qquad (19)$$

where $a = (r2^2 - r1^2 - h^2 - k^2)/2$. Solving this quadratic equation yields the two possible values of y namely

$$Y = [-a*k +/- (a^2*k^2 - c*b)]/c \qquad (5)$$

where $b = (a^2 - h^2*r1^2)$ and $c = (k^2 + h^2)$. The two values of x can be solved for in a likewise manner yielding the following equation:

$$X = [-a*h +/- (a^2*h^2 - c*b)]/c \qquad (6)$$

Appendix B

Fortran Program Code

The following pages of this appendix contain the Fortran code used to model thin film growth by vapor deposition. More specifically the program code is composed of Fortran 77 and contains a fortran statement using IMSL (International Mathematical and Statistical Libraries), a library of subroutines used for statistical purposes. In this program the IMSL statement (ggubfs) is used as a random number generator for evenly distributing the simulated evaporate over the substrate.

Questions concerning the use of particular variables within the program can be addressed by referring to appendix C, which contains a list of the variables along with a brief discription of their purpose.

```
C
C
C                'THIN FILM GROWTH SIMULATOR - AN IMPROVED MODEL'
C                                  VERSION - 2
C                         WRITTEN BY DAVID J. DORYLAND
C                                   30 SEP 85
C
C
C       LIKE ITS PREDECESSOR, THE PURPOSE OF THIS PROGRAM IS TO SIMULATE
C       THE VAPOR DEPOSITION OF THIN FILMS.  THE PROGRAM ITSELF IS DI-
C       VIDED INTO 4 MAJOR AREAS WITH EACH CONTAINING A BRIEF DESCRIP-
C       TION OF ITS FUNCTION.  THE REASON BEHIND THIS IS THAT IT PROVIDES
C       NOT ONLY AN EASIER WAY TO DEBUG THE PROGRAM BUT IT ALSO HELPS OR-
C       GANIZE IT.  THIS PROGRAM IS WRITTEN IN FORTRAN 77 AND REQUIRES A
C       WORKING KNOWLEDGE OF IMSL AND S (FOR FUTURE PLOTTING).  IT WAS DE-
C       SIGNED TO RUN ON A VAX/VMS COMPUTER.
C
C
C                   ****************************************
C                   *                                      *
C                   *          MAIN PROGRAM START-UP       *
C                   *           AND INTERFACE LOOP         *
C                   *                                      *
C                   ****************************************
C
C
C       THE PURPOSE OF THIS SECTION IS TO DECLARE AND INITIALIZE THE MAIN
C       VARIABLES USED THROUGHOUT THE PROGRAM.  IT ALSO INCLUDES A SIGN
C       ON MESSAGE, A HELP MESSAGE, THE READING OF THE DATE AND THE MAIN
C       INTERFACE LOOP.
C
C
C                   ********** VARIABLE DECLARATION **********
C
      REAL DATE, XCOORD(300,200), YCOORD(300,200)
      INTEGER FILM(300,200), IVAR
C
C
C                        ********** SIGN ON **********
C
      WRITE (6,0010)
 0010 FORMAT (10(2X/),15X,'THIN FILM GROWTH SIMULATOR - AN IMPROVED MODE
     CL'/,32X,'VERSION - 2'/,33X,'=========='/,25X,'WRITTEN BY DAVID J.
     CDORYLAND'/,33X,'30 SEP 85'/,2(2X/),19X,'THIN FILM RESEARCH - A GRE
     CAT WAY OF LIFE'/,7(2X/))
C
C
C                   ********** READING OF THE DATE **********
C
      WRITE (6,0015)
 0015 FORMAT (1X,'ENTER DATE AND TIME (MMDDHHMM)')
      READ (5,0016) DATE
 0016 FORMAT (F8.0)
C
C
C                     ********** HELP MESSAGE **********
C
      WRITE (6,0017)
 0017 FORMAT (10(1X/),10X,'TO OPERATE THIS PROGRAM, ANSWER THE QUESTIONS
     C ASKED BY USING'/,10X,'THE KEYPAD LOCATED ON THE RIGHT SIDE OF THI
```

```
     CS TERMINAL.  AT THE'/,10X,'CONCLUSION OF EACH NUMBERED SECTION, PR
     CESS THE CARRIAGE RETURN'/,10X,'KEY TO CONTINUE WITH THE PROGRAM.
     CIN ORDER TC EXIT THE PROGRAM'/,10X,'AT ANY TIME, PRESS CONTROL C (
     CCTRL/C).  TO ENTER THE PROGRAM,'/,10X,'PRESS THE CARRIAGE RETURN.'
     C,7(1X/))
      READ (5,0021)
C
C
C               ********** MAIN INTERFACE LOOP **********
C
 0019 WRITE (6,0020)
 0020 FORMAT (15(2X/),29X,'MAIN INTERFACE LOOP'///,20X,'ENTER APPROPRIAT
     CE NUMBER TO CONTINUE'/,2(2X/),26X,'1 - SUBSTRATE SUBROUTINE'/,26X,
     C'2 - DEPOSITION SUBROUTINE'/,26X,'3 - ANALYSIS SUBROUTINE'/,26X,'4
     C - MOVING SUBROUTINE'/,26X,'CTRL/C - EXIT TO OPERATING SYSTEM'/,6(
     C2X/))
C
 0031 READ (5,0021) IVAR
 0021 FORMAT (I1)
C
      IF (IVAR .EQ. 1) THEN
           CALL SUB(FILM,XCOORD,YCOORD,HEIGHT)
           GOTO 0019
      ELSE IF (IVAR .EQ. 2) THEN
           CALL DEPO(FILM,XCOORD,YCOORD,HEIGHT,DATE)
           GOTO 0019
      ELSE IF (IVAR .EQ. 3) THEN
           CALL ANAL(FILM,XCOORD,YCOORD)
           GOTO 0019
      ELSE IF (IVAR .EQ. 4) THEN
           CALL MOVE(FILM,XCOORD,YCOORD)
           GOTO 0019
      ENDIF
      WRITE (6,0030)
 0030 FORMAT (20X,'INCORRECT RESPONSE DUMMY!! - TRY AGAIN'///)
      GOTO 0031
C
      END
C
C
C                    ******************************
C                    *                            *
C                    *     SUBSTRATE SUBROUTINE   *
C                    *                            *
C                    ******************************
C
C     THIS SUBROUTINE CONSIST OF 5 AREAS: THAT IS THE INITIALIZING, PRO-
C     DUCING, STORING, TRANSFERING AND RECALLING OF SUBSTRATES. EACH
C     SECTION CONTAINS A BRIEF DESCRIPTION OF ITS PURPOSE AND/OR ITS AP-
C     PROACH.
C
      SUBROUTINE SUB (FILM,XCOORD,YCOORD,HEIGHT)
C
C     LOCAL VARIABLES
C
      REAL XCOLD, HGT, XPOS, YCOLD, HEIGHT, YC(300,10), XC(300,10)
      REAL XCOORD(300,200), YCOORD(300,200)
      INTEGER SUBBUF(300,10), COL, XCOL, ANS, IVAR, FILM(300,200), YHGT
C
C
```

```
C              ********** SUBSTRATE INTERFACE LOOP **********
C
 0040 WRITE (6,0041)
 0041 FORMAT (15(2X/),25X,'SUBSTRATE INTERFACE LOOP'///,20X,'ENTER APPRO
     CPRIATE NUMBER TO CONTINUE'/,2(2X/),26X,'1 - INITIALIZE SUBSTRATE'/
     C,26X,'2 - CREATE SUBSTRATE'/,26X,'3 - STORE SUBSTRATE'/,26X,'4 - R
     CECALL SUBSTRATE'/,26X,'5 - MOVE SUBSTRATE (TO FILM MATRIX)'/,26X,'
     C9 - EXIT TO MAIN INTERFACE LOOP'/,26X,'CTRL/C - EXIT TO OPERATING
     CSYSTEM'/,5(2X/))
C
 0049 READ (5,0050) IVAR
 0050 FORMAT (I1)
C
      IF (IVAR .EQ. 1) THEN
          GOTO 0060
      ELSE IF (IVAR .EQ. 2) THEN
          GOTO 0070
      ELSE IF (IVAR .EQ. 3) THEN
          GOTO 0080
      ELSE IF (IVAR .EQ. 4) THEN
          GOTO 0090
      ELSE IF (IVAR .EQ. 5) THEN
          GOTO 0100
      ELSE IF (IVAR .EQ. 9) THEN
          RETURN
      ENDIF
      WRITE (6,0051)
 0051 FORMAT (21X,'YOU BLEW IT BLOCKHEAD!! - TRY AGAIN'///)
      GOTO 0049
C
C
C             ********** SUBSTRATE INITIALIZATION **********
C
C THIS PART OF THE SUBROUTINE INITIALIZES SUBBUF, XC, YC TO ZERO SO THAT
C A NEW SUBSTRATE CAN BE CREATED.  UPON ENTERING THIS SECTION THE INTIAL-
C IZATION DOES NOT AFFECT THE FILM MATRICES (FILM,XCOORD,YCOORD).
C
 0060 WRITE (6,0064)
 0064 FORMAT (10X,'UPON ENTERING YOU MAY LOSE THE CONTENTS OF THE SUBROU
     CTINE BUFFER!'/,10X,'DO YOU WISH TO SAVE THE OLD CONTENTS?'//,11X,'
     CIF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0080
      ENDIF
C
      DO 0061 X = 1,300,1
         DO 0062 Y = 1,10,1
            SUBBUF(X,Y) = 0
            XC(X,Y) = 0.0
            YC(X,Y) = 0.0
 0062    CONTINUE
 0061 CONTINUE
C
      WRITE (6,0063)
 0063 FORMAT(10X,'ALL VALUES OF THE SUBROUTINE BUFFER HAVE BEEN SET TO Z
     CERO'//)
      PRINT *,'                                              HIT RETURN'
      READ (5,0050)
```

```
      GOTO 0040
C
C
C                ********** SUBSTRATE CREATION **********
C
C THIS PART OF THE SUBROUTINE ALLOWS THE PROGRAMMER TO CREATE A SUBSTRATE.
C THE FIRST STEP IS TO LAY DOWN A SINGLE LAYER OF DISK.  AFTER THE SINGLE
C LAYER HAS BEEN LAYED DOWN, THEN THIS PART OF THE SUBROUTINE HELPS IN CREAT-
C ING THE REMAINDER OF THE SUBSTRATE.  THIS IS DONE BY NOTING THAT EACH
C DISK IS THE SQUARE ROOT OF TWO IN DIAMETER AND THAT THESE CAN BE STACKED
C ONE UPON ANOTHER.
C
 0070 WRITE (6,0072)
 0072 FORMAT (10X,'JUST A REMINDER.  UPON ENTERING INTO THIS PART OF THE
     C'/,10X,'SUBROUTINE YOU MAY BE DESTROYING A PREVIOUS SUBSTRATE.'/,1
     C0X,'DO YOU WISH TO SAVE THE OLD SUBSTRATE?'//,11X,'IF YES -  ENTER
     C 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0080
      ENDIF
C
C CREATES A HORIZONTAL SUBSTRATE WITH NO DEFECTS
C
      XC(1,1) = 1.0
      YC(1,1) = 1.0
      SUBBUF(1,1) = 1
      XCOLD = 1.0
 0071 IF (XCOLD .LT. 300) THEN
          XCOLD = XCOLD + 1.4142136
          X = AINT(XCOLD)
          XC(X,1) = XCOLD
          YC(X,1) = 1.0
          SUBBUF(X,1) = 1
          GOTO 0071
      ENDIF
      HEIGHT = 1.0
C
      WRITE (6,0073)
 0073 FORMAT (5X,'DO YOU WISH TO CREATE MORE THAN JUST A HORIZONTAL LINE
     C FOR THE SUBSTRATE?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HI
     CT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0074
      ELSE
          GOTO 0040
      ENDIF
C
 0074 WRITE (6,1073)
 1073 FORMAT (10X,'THERE ARE 213 COLUMNS ACROSS THE BOTTOM OF THE SUBSTR
     CATE.'/,10X,'EACH ONE OF THESE MUST HAVE A HEIGHT SPECIFIED TO IT.'
     C/,10X,'THE FOLLOWING STEPS WILL HELP IN THAT PROCESS.'//)
C
      COL = 0
      HEIGHT = 0
 1074 IF (COL .EQ. 213) THEN
          GOTO 0079
```

```
      ELSE
          COL = COL + 1
          WRITE (6,0075) COL
 0075     FORMAT (10X,'YOU ARE IN COLUMN',I4/,10X,'ENTER HEIGHT (MUST BE
     + 7 OR LESS)'//)
C
 1080     READ (5,0050) YHGT
          IF (YHGT .EQ. 1) THEN
              GOTO 0076
          ELSE IF (YHGT .GT. 7) THEN
              WRITE (6,1075)
 1075         FORMAT (10X,'HEIGHT TOO HIGH - TRY AGAIN!'//)
              GOTO 1080
          ELSE
C
C CREATES THE HEIGHT SPECIFIED FOR AN INDIVIDUAL COLUMN
C
              YCOLD = 1.0
              XPOS = 1.0 + (COL - 1)*1.4142136
              X = AINT(XPOS)
              HGT = YHGT - 1
              DO 0077 I = 1,HGT,1
                  YCOLD = YCOLD + 1.4142136
                  IF (YCOLD .GT. HEIGHT) THEN
                      HEIGHT = YCOLD
                  ENDIF
                  Y = AINT(YCOLD)
                  XC(X,Y) = XPOS
                  YC(X,Y) = YCOLD
                  SUBBUF(X,Y) = 1
 0077         CONTINUE
C
 0076         WRITE (6,0078) YHGT
 0078         FORMAT (10X,'DO YOU WISH THIS HEIGHT (',I1,') TO CONTINUE?
     C'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
              READ (5,0050) ANS
              IF (ANS .EQ. 1) THEN
                  WRITE (6,1070)
 1070             FORMAT (10X,'TOO WHAT COLUMN SHOULD THIS CONTINUE?'/,1
     C8X,'(MUST BE 213 OR LESS)'//)
 1077             READ (5,1050) XCOL
 1050             FORMAT (I3)
                  IF (XCOL .GT. 213) THEN
                    WRITE (6,1078)
 1078               FORMAT (10X,'COLUMN NUMBER TOO LARGE - TRY AGAIN'//)
                    GOTO 1077
                  ENDIF
C
C FILLS IN THE SUBSTRATE MATRICES TO THE COLUMN SPECIFIED WITH THE LAST
C ENTERED HEIGHT.
C
                  COL = COL + 1
                  IF (YHGT .EQ. 1) GOTO 1079
                  DO 1071 I = COL,XCOL,1
                      XPOS = 1.0 + (I - 1)*1.4142136
                      X = AINT(XPOS)
                      YCOLD = 1.0
                      DO 1072 J = 1,HGT,1
                          YCOLD = YCOLD + 1.4142136
```

```
                          Y = AINT(YCOLD)
                          XC(X,Y) = XPOS
                          YC(X,Y) = YCOLD
                          SUBBUF(X,Y) = 1
1072                   CONTINUE
1071                CONTINUE
1079                COL = XCOL
                    GOTO 1074
               ELSE
                    GOTO 1074
               ENDIF
           ENDIF
       ENDIF
C
 0079 WRITE (6,1076)
 1076 FORMAT (10X,'THE SUBSTRATE IS NOW COMPLETE!!'/,10X,'READY FOR TRAN
     CSFER TO FILM MATRICES.'///)
      PRINT *,'                                                HIT RETURN'
      READ (5,0050)
      GOTO 0040
C
C
C                   ********** SUBSTRATE STORAGE **********
C
C THIS PART OF THE SUBROUTINE ALLOWS ONE TO TEMPORARILY STORE THE CONTENTS
C OF SUBBUF, XC AND YC IN THE FILE CALLED FOR011.DAT.  IT DOES NOT DESTROY
C CONTENTS OF THESE MATRICES, BUT MERELY COPIES THEM FOR FUTURE REFERENCE.
C
 0080 WRITE (6,0081)
 0081 FORMAT (10X,'UPON ENTERING THIS PART OF THE SUBROUTINE, THE SUBROU
     CTINE'/,10X,'BUFFER WILL BE STORED IN A FILE CALLED FOR011.DAT.'/,1
     C0X,'IS THIS YOUR DESIRE?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE
     C - HIT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          PRINT *,' '
          PRINT *,'WORKING'
          GOTO 0088
      ELSE
          GOTO 0040
      ENDIF
C
 0088 OPEN (UNIT = 11,FILE = 'FOR011.DAT',STATUS = 'NEW')
C
      DO 0082 X = 1,300,1
         DO 0083 Y = 1,10,1
               WRITE (11,0084) SUBBUF(X,Y), XC(X,Y), YC(X,Y)
 0084          FORMAT (1X,I2,3X,F8.4,3X,F8.4)
 0083    CONTINUE
 0082 CONTINUE
C
      CLOSE (UNIT = 10)
C
      WRITE (6,0086)
 0086 FORMAT (10X,'THE VALUES OF THE SUBROUTINE BUFFER HAVE NOW BEEN'/,1
     C0X,'COPIED INTO THE FILE FOR011.DAT'//)
      PRINT *,'                                                HIT RETURN'
      READ (5,0050)
      GOTO 0040
```

```
C
C                 ********** SUBSTRATE RECALLING **********
C
C THIS PART OF THE SUBROUTINE ALLOWS ONE TO ACCESS AND RECALL THE CON-
C TENTS OF A FILE CALLED TAKE.DAT.  IN DOING SO, THE VALUES OF A PRE-
C VIOUSLY DEVELOPED SUBSTRATE WILL BE ENTERED INTO THE MATRICES SUBBUF,
C XC AND YC.
C
 0090 WRITE (6,0091)
 0091 FORMAT (10X,'JUST A REMINDER.  UPON ENTERING THIS PART OF THE SUBR
     COUTINE'/,10X,'THE CURRENT VALUES OF THE SUBROUTINE BUFFER MAY BE L
     COST.'/,10X,'THE REASON FOR THIS IS THAT NEW VALUES FROM TAKE.DAT W
     CILL BE READ IN.'/,10X,'DO YOU WISH TO SAVE THE CURRENT VALUES OF T
     CHE BUFFER?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE TO CONTINUE -
     C HIT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0080
      ENDIF
      PRINT *,'WORKING'
C
      OPEN (UNIT = 11,FILE = 'TAKE.DAT',STATUS = 'OLD')
      REWIND (UNIT = 11)
C
      DO 0095 X = 1,300,1
         DO 0096 Y = 1,10,1
             READ (11,0097) SUBBUF(X,Y), XC(X,Y), YC(X,Y)
 0097        FORMAT (1X,I2,3X,F8.4,3X,F8.4)
 0096    CONTINUE
 0095 CONTINUE
C
      CLOSE (UNIT = 11)
C
      HEIGHT = 10
C
      WRITE (6,0098)
 0098 FORMAT (10X,'THE NEW VALUES OF THE SUBROUTINE BUFFER HAVE NOW BEEN
     C'/,10X,'READ IN FROM THE FILE TAKE.DAT'//)
      PRINT *,'                                                HIT RETURN'
      READ (5,0050)
      GOTO 0040
C
C
C                 ********** SUBSTRATE MOVING **********
C
C THIS PART OF THE SUBROUTINE COPIES THE CURRENT VALUES OF SUBBUF, XC AND
C YC INTO THE MATRICES FILM, XCOORD AND YCOORD RESPECTIVELY.  THE REASON
C FOR THIS, IS SO THAT THE DEPOSITION PROCESS CAN BE INVOKED WITH A SUB-
C STRATE IN PLACE.
C
 0100 WRITE (6,0101)
 0101 FORMAT (10X,'UPON ENTERING THIS PART OF THE SUBROUTINE THE CURRENT
     C VALUES'/,10X,'OF THE SUBROUTINE BUFFER WILL BE COPIED INTO THE FI
     CLM MATRICES.'/,10X,'IS THIS YOUR DESIRE?'//,11X,'IF YES -  ENTER 1
     C'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0103
```

```
      ELSE
          GOTO 0040
      ENDIF
C
 0103 DO 0104 X = 1,300,1
          DO 0105 Y = 1,10,1
              XCOORD(X,Y) = XC(X,Y)
              YCOORD(X,Y) = YC(X,Y)
              FILM(X,Y) = SUBBUF(X,Y)
 0105     CONTINUE
 0104 CONTINUE
C
      WRITE (6,0106)
 0106 FORMAT (10X,'THE SUBROUTINE VALUES HAVE BEEN TRANSFERED'//)
      WRITE (6,0107)
 0107 FORMAT (10X,'DO YOU WISH TO RETURN TO THE MAIN INTERFACE LOOP?'//,
     C11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0050) IVAR
      IF (IVAR .EQ. 1) THEN
          RETURN
      ELSE
          GOTO 0040
      ENDIF
      END
C
C
C
C                    ********************************
C                    *                              *
C                    *     DEPOSITION SUBROUTINE    *
C                    *                              *
C                    ********************************
C
C     THIS SUBROUTINE CONSIST OF 3 AREAS: THAT IS THE INITIALIZING OF
C     THE FILM MATRICES, THE SETTING OF THE DEPOSITION VARIABLES AND
C     THE DEPOSITION OF THE FILM ON A SUBSTRATE.  EACH SECTION CONTAINS
C     A BRIEF DESCRIPTION OF ITS PURPOSE AND/OR ITS APPROACH.
C
      SUBROUTINE DEPO(FILM,XCOORD,YCOORD,HEIGHT,DATE)
C
C     LOCAL VARIABLES
C
      REAL DATE
      REAL ANG,ANGVAR,RANG,OLDANG,ANGINC,HEIGHT,RANNUM,YTEST,YBNC(6)
      REAL XCOORD(300,200),YCOORD(300,200),H,K,A,B,C,RBNC(6),XBNC(6)
      DOUBLE PRECISION DSEED,RESTY,RESTX,R1,R2,DRESTX
      DOUBLE PRECISION TEST1,TEST2,TEST3,TEST4,TESTY,DRESTY
      INTEGER FILM(300,200),IVAR,NODSK,BNCVAR,HGTLAY,LAYER,SIZE,BNCCTR
      INTEGER YSUB,YFILM,NDEP,DEPCTR,XCOLL,YCOLL,HCTR,IMPX,BCTR
C
C
C            ********** DEPOSITION INTERFACE LOOP **********
C
 0110 WRITE (6,0111)
 0111 FORMAT (15(2X/),26X,'DEPOSITION INTERFACE LOOP'///,20X,'ENTER APPR
     COPRIATE NUMBER TO CONTINUE'/,2(2X/),25X,'1 - INITIALIZE FILM MATRI
     CX'/,25X,'2 - SET DEPOSITION VARIABLES'/,25X,'3 - DEPOSITION OF FIL
     CM'/,25X,'9 - EXIT TO MAIN INTERFACE LOOP'/,25X,'CTRL/C - EXIT TO O
     COPERATING SYSTEM'/,6(2X/))
```

```
C
 0114 READ (5,0115) IVAR
 0115 FORMAT (I1)
C
      IF (IVAR .EQ. 1) THEN
          GOTO 0120
      ELSE IF (IVAR .EQ. 2) THEN
          GOTO 0130
      ELSE IF (IVAR .EQ. 3) THEN
          GOTO 0160
      ELSE IF (IVAR .EQ. 9) THEN
          RETURN
      ENDIF
      WRITE (6,0116)
 0116 FORMAT (23X,'WRONG SCREWBALL!! - TRY AGAIN'///)
      GOTO 0114
C
C
C            ********** DEPOSITION INITIALIZATION **********
C
C THIS PART OF THE SUBROUTINE INITIALIZES ALL THE VALUES OF FILM, XCOORD
C AND YCOORD - FROM Y = 11 TO Y = 200 - TO ZERO.  THIS IS DONE TO ENSURE
C THAT ANY PREVIOUS DEPOSITION TRIALS ARE CLEARED OUT.
C
 0120 WRITE (6,0121)
 0121 FORMAT (10X,'UPON ENTERING THIS SECTION, ALL VALUES OF THE FILM MA
     CTRICES'/,10X,'WILL BE DESTROYED.  IN ORDER TO SAVE THESE VALUES YO
     CU MUST'/,10X,'EXIT THIS SUBROUTINE.'/,10X,'DO YOU WISH TO SAVE THE
     CSE VALUES?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'
     C//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
          RETURN
      ENDIF
      PRINT *,'WORKING'
C
      DO 0125 X = 1,300,1
         DO 0126 Y = 11,200,1
             FILM(X,Y) = 0
             XCOORD(X,Y) = 0.0
             YCOORD(X,Y) = 0.0
 0126    CONTINUE
 0125 CONTINUE
C
      WRITE (6,0127)
 0127 FORMAT(2(1X/),10X,'THE VALUES OF THE FILM MATRICES HAVE BEEN SET T
     CO ZERO.'/,10X,'DEPOSITION VARIABLES ARE READY TO BE SET!'//)
      PRINT *,'                                                HIT RETURN'
      READ (5,0115)
      GOTO 0110
C
C
C          ********** READING OF DEPOSITION VARIABLES **********
C
C THIS PART OF THE SUBROUTINE READS IN SUCH VARIABLE AS:  THE NUMBER OF
C DISKS TO BE DEPOSITED, THE ANGLE OF INCIDENCE, ANY VARIATION IN THE
C ANGLE OF INCIDENCE, WHETHER OR NOT BOUNCING WILL OCCUR, WHETHER AN IM-
C PURITY IS TO BE DEPOSITED AND THE SIZE OF THE DISKS TO BE USED IN CON-
C JUNCTION WITH THE DEPTH OF THE LAYERS.  THIS IS ACCOMPLISHED BY ASKING
```

```
C A NUMBER OF QUESTIONS.
C
 0130 WRITE (6,0131)
 0131 FORMAT (10X,'BEFORE GOING FARTHER, IT IS ASSUMED THAT A SUBSTRATE
     CHAS'/,10X,'BEEN PRODUCED OR RECALLED AND THEN TRANSFERED TO THE FI
     CLM'/,10X,'MATRICES.  IT IS ALSO ASSUMED THAT THE TOP PORTION OF TH
     CE'/,10X,'FILM MATRICES HAVE BEEN INITIALIZED.'/,10X,'IS THIS CORRE
     CCT?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0132
      ELSE
          RETURN
      ENDIF
C
C INITIALIZATION OF QUESTION VARIABLES
C
 0132 NODSK = 0
      OLCANG = 0.0
      ANGVAR = 0.0
      ANGINC = 0
      BNCVAR = 0
      NOMOB = 0
      IMPUR = 0
      LAYER = 0
      HGTLAY = 0
      SIZE = 1
C
C QUESTION PERTAINING TO THE NUMBER OF DISK
C
 0133 WRITE (6,0134)
 0134 FORMAT(10X,'HOW MANY DISKS DO YOU WISH DEPOSITED?'/,10X,'ENTER VAL
     CUE IN INTEGER FORMAT.'//)
      READ *,NODSK
      WRITE (6,0135) NODSK
 0135 FORMAT (2(1X/),10X,I5,' DISK WILL BE DEPOSITED, UNLESS FILM MATRIC
     CES BECOME FULL'//)
C
C QUESTIONS PERTAINING TO THE ANGLE OF DEPOSITION
C
      WRITE (6,0136)
 0136 FORMAT (10X,'AT WHAT ANGLE DO YOU WISH THE FILM TO BE DEPOSITED?'/
     C,10X,'PLEASE ENTER ANGLE IN DEGREES - ENTER IN REAL FORMAT.'//)
      READ *,OLCANG
C
      WRITE (6,0137)
 0137 FORMAT (10X,'DO YOU WISH TO VARY THE ANGLE OF INCIDENCE?'//,11X,'I
     CF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0138
      ELSE
          GOTO 0141
      ENDIF
C
 0138 WRITE (6,0139)
 0139 FORMAT (10X,'HOW MANY DEGREES (FULL ANGLE) DO YOU WISH TO VARY THE
     C ANGLE?'/,10X,'ENTER DEGREES IN REAL FORMAT.'//)
```

```
      READ *, ANGVAR
      WRITE (6,0140)
 0140 FORMAT (2(1X/),10X,'WHAT SIZE ANGLE DO YOU WISH TO INCREMENT THE A
     CNGLE OF INCIDENCE?'/,10X,'ENTER IN REAL FORMAT.'//)
      READ *,ANGINC
C
C QUESTIONS PERTAINING TO THE MOBILITY OF THE DISKS
C
 0141 WRITE (6,0142)
 0142 FORMAT (2(1X/),10X,'DO YOU WISH ANYTHING OTHER THAN NORMAL MOBILIT
     CY?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
           GOTO 1143
      ELSE
           GOTO 0155
      ENDIF
C
 1143 WRITE (6,1144)
 1144 FORMAT (10X,'IF YOU WISH NO MOBILITY - ENTER 1'/,10X,'IF YOU WISH
     CEXTRA MOBILITY - ENTER 2'//)
C
 1145 READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
         NOMOB = 1
         GOTO 0155
      ELSE IF (IVAR .EQ. 2) THEN
         GOTO 0143
      ELSE
         PRINT*,'TRY AGAIN'
         GOTO 1145
      ENDIF
C
 0143 WRITE (6,0144)
 0144 FORMAT (10X,'ENTER THE NUMBER OF DISKS TO BE DEPOSITED BEFORE AN E
     CXTRA'/,10X,'MOBILITY ITERATION TAKES PLACE - ENTER IN INTEGER FORM
     CAT.'//)
      READ *,BNCVAR
C
C QUESTION PERTAINING TO WHETHER OR NOT AN IMPURITY SHOULD BE DEPOSITED.
C
 0155 WRITE (6,0156)
 0156 FORMAT (2(1X/),10X,'DO YOU WISH AN IMPURITY TO BE DEPOSITED?'//,11
     CX,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
         IMPUR = 1
      ELSE
         GOTO 0146
      ENDIF
C
C QUESTIONS PERTAINING TO THE SIZE OF DISK DEPOSITED
C
 0146 WRITE (6,0147)
 0147 FORMAT (2(1X/),10X,'DO YOU WISH TO USE TWO DIFFERENT SIZE DISK?'//
     C,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
```

```
      IF (IVAR .EQ. 1) THEN
           LAYER = 1
           GOTO 0148
      ELSE
           GOTO 1150
      ENDIF
C
 0148 WRITE (6,1149)
 1149 FORMAT (10X,'DO YOU WISH THE LARGE DISK TO BE DEPOSITED FIRST?'//,
     C11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
         SIZE = 2
      ENDIF
C
      WRITE (6,0149)
 0149 FORMAT (10X,'HOW MANY ROWS HIGH (IN TERMS OF FILM MATRIX) DO YOU W
     CISH'/,10X,'THE LAYERS TO BE? - ENTER IN INTEGER FORMAT.'//)
      READ *,HGTLAY
C
C PRINTING OUT QUESTION VARIABLES
C
 1150 WRITE (6,0150)
 0150 FORMAT (12(2X/))
      PRINT *,'THE NUMBER OF DISK TO BE DEPOSITED =',NODSK
      PRINT *,'THE ANGLE OF DEPOSITION WILL BE =',OLDANG,'DEGREES'
C
      IF (ANGVAR .EQ. 0.0) THEN
          PRINT *,'NO ANGLE VARIATION WILL TAKE PLACE.'
      ELSE
          PRINT *,'THE AMOUNT OF ANGLE VARIATION =',ANGVAR,'DEGREES.'
          PRINT *,'THE ANGLE INCREMENT =',ANGINC,'DEGREES.'
      ENDIF
C
      IF (NOMOB .EQ. 1) THEN
         PRINT*,'DEPOSITION WILL OCCUR WITH NO RELAXATION.'
      ELSE
         IF (BNCVAR .EQ. 0) THEN
            PRINT *,'DEPOSITION WILL OCCUR WITH NORMAL RELAXATION.'
         ELSE
            PRINT *,'AN EXTRA MOBILITY WILL BE GIVEN AFTER EVERY',BNCVAR
     C,' ITERATIONS.'
         ENDIF
      ENDIF
C
      IF (IMPUR .EQ. 0) THEN
          PRINT *,'NO IMPURITY WILL BE DEPOSITED.'
      ELSE
          PRINT *,'ONE IMPURITY WILL BE DEPOSITED RANDOMLY.'
      ENDIF
C
      IF (LAYER .EQ. 0) THEN
          PRINT *,'ONLY ONE SIZE DISK WILL BE DEPOSITED.'
      ELSE
          IF (SIZE .EQ. 1) THEN
              PRINT *,'TWO DIFFERENT SIZE DISK WILL BE DEPOSITED - THE FI
     CRST BEING SMALL'
          ELSE
              PRINT *,'TWO DIFFERENT SIZE DISK WILL BE DEPOSITED - THE FI
     CRST BEING LARGE'
```

```
            ENDIF
            PRINT *,'THE DEPTH OF EACH LAYER WILL BE ',HGTLAY
         ENDIF
C
C LAST CHECK BEFORE DEPOSITION
C
      WRITE (6,0151)
 0151 FORMAT (2(1X/),10X,'DO YOU WISH TO CHANGE ANY OF THE ABOVE VARIABL
     CES?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0132
      ENDIF
C
      WRITE (6,0153)
 0153 FORMAT (10X,'DEPOSITION VARIABLES HAVE NOW BEEN SET.'/,10X,'DEPOSI
     CTION IS READY TO OCCUR!!'//)
      PRINT *,'                                                   HIT RETURN'
      READ (5,0115)
      GOTO 0110
C
C
C               ********** DEPOSITION OF FILM **********
C
C THIS PART OF THE SUBROUTINE IS THE HEART OF THE ENTIRE PROGRAM.  ITS
C PURPOSE IS TO DEPOSIT THE "FILM" ONTO THE FABRICATED "SUBSTRATE".
C ALL NECCESSARY VARIABLES TO RUN THIS SECTION, SHOULD HAVE BEEN READ IN
C BY EARLIER SUBROUTINES OR SECTIONS.  FOR MORE INFORMATION ON HOW THIS
C PART OF THE SUBROUTINE WORKS CONSULT THE THESIS - AN IMPROVED MODEL OF
C THIN FILM GROWTH (AFIT - SCHOOL OF ENGINEERING).
C
 0160 WRITE (6,0161)
 0161 FORMAT (10X,'HAVE ALL THE DEPOSITION VARIABLES BEEN READ IN AND'/,
     C10X,'THE FILM MATRICES INITIALIZED?'//,11X,'IF YES - ENTER 1'/,11X
     C,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0115) IVAR
      IF (IVAR .EQ. 1) THEN
          GOTO 0162
      ELSE
          GOTO 0110
      ENDIF
C
C BEGINNING OF DEPOSITION
C
 0162 WRITE (6,0163)
 0163 FORMAT (22X,'DEPOSITION PROCESS HAS NOW BEGUN!!'///)
C
C SETTING OF THE SEED FOR RANDOM NUMBER GENERATION.
C
      DSEED = 123457.D0
      DSEED = (DSEED*(DATE/1000.0))
C
C INITIALIZATION OF DEPOSITION VARIABLES
C
      BNCCTR = 0
      BCTR = 0
      IMPSET = 0
      HGTIMP = 0
```

```
      SET = 0
      HOSIZE = SIZE
      YCK = 0
      IMPHGT = 0
      IMPX = 0
      YHGT = AINT(HEIGHT) + 3
      YFILM = AINT(HEIGHT)
      ANGMAX = OLDANG + ANGVAR/2
      ANGMIN = OLDANG - ANGVAR/2
      ANG = OLDANG
      NO = 0
      P = 1
      HCTR = 0
C
C DETERMINATION OF WHEN IMPURITY WILL BE DEPOSITED
C
      IF (IMPUR .EQ. 1) THEN
         RANNUM = GGUBFS(DSEED)
         RANDY = (RANNUM * 179) + YHGT
         HGTIMP = AINT(RANDY)
C         HGTIMP = 10
      ENDIF
C
C
C     *****COLLISION POINT DETERMINATION*****
C
C RANDOM X DETERMINATION
C
      DO 0170 DEPCTR = 1,NODSK,1
           IF (YHGT .GT. 199) GOTO 0201
           RANNUM = GGUBFS(DSEED)
           RANDX = (RANNUM * 300) + 1
C
C ANGLE DIRECTION CHANGE SECTION
C
           IF (ANGVAR .EQ. 0.0) THEN
                GOTO 0175
           ELSE
                ANG = ANG + P*ANGINC
                IF (ANG .GT. ANGMAX) THEN
                     P = -1
                     ANG = ANGMAX - ANGINC
                ELSE IF (ANG .LT. ANGMIN) THEN
                     P = 1
                     ANG = ANGMIN + ANGINC
                ENDIF
           ENDIF
 0175      RANG = ANG/57.2957751
           COSANG = COS(RANG)
           TANANG = TAN(RANG)
           SC2ANG = TANANG**2 + 1
C
C SIZE AND COUNTER MODIFICATION FOR IMPURITIES
C
           IF (IMPUR .EQ. 1) THEN
               IF (SET .EQ. 1) THEN
                  SIZE = HOSIZE
                  GOTO 0177
               ENDIF
               IF (YCK .EQ. 0) THEN
```

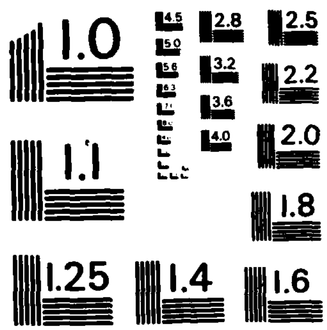
```
                    IF (YHGT .GE. HGTIMP) THEN
                       YCK = 1
                       IMPSET = 1
                       SET = 1
                       HDSIZE = SIZE
                       SIZE = 8
                       CTR = 15
                       GOTO 0180
                    ENDIF
                 ENDIF
              ENDIF
C
C DETERMINATION OF SCAN COUNTER
C
 0177         IF (IMPSET .EQ. 0) THEN
                 IF (LAYER .EQ. 0) THEN
                    CTR = 3
                    GOTO 0180
                 ELSE
                    CTR = 6
                    GOTO 0179
                 ENDIF
              ELSE
                 IF (LAYER .EQ. 0) THEN
                    CTR = 14
                    GOTO 0180
                 ELSE
                    CTR = 15
                    GOTO 0179
                 ENDIF
              ENDIF
C
C SIZE CHANGING SECTION FOR DIFFERENT SIZE DISK
C
 0179         IF (((YHGT-1) - YFILM) .GE. HGTLAY) THEN
                 YFILM = YHGT
                 IF (SIZE .EQ. 1) THEN
                    SIZE = 2
                 ELSE IF (SIZE .EQ. 2) THEN
                    SIZE = 1
                 ENDIF
                 HDSIZE = SIZE
              ENDIF
C
 0180         Y2 = 0
              X2 = 0
              DYINT = 0
              DYINT = 0
              XCOLL = 0
              YCOLL = 0
              A2 = 0.0
           DO 0181 STRCTR = 0,CTR,1
C
C DETERMINATION OF X INTERCEPT
C
              IF (IMPSET .EQ. 1) THEN
                 IF (SIZE .EQ. 1) THEN
                    XINCT = RANDX + (6.363961/COSANG)
                 ELSE
                    XINCT = RANDX + (7.0710678/COSANG)
```

```
            ENDIF
          ELSE
            XINCT = RANDX + (SIZE * 1.4142136)/COSANG
          ENDIF
C
C DETERMINATION OF STREAMER INTERCEPT
C
          SINCT = RANDX + .942809416 * (STRCTR/COSANG)
C
          XPOS = YHGT * TANANG + SINCT - 1
          OXPOS = XPOS
          COLL = 0
C
C BEGINNING OF STREAMER SEARCH
C
          DO 0190 Y = YHGT,1,-1
               XPOS = Y * TANANG + (SINCT - 1)
               ISHFT = ((AINT(XPOS/301)) * 300)
               NEWX = AINT(XPOS - ISHFT)
               OLDX = AINT(OXPOS - ISHFT)
               DO 0195 X = OLDX,1,-1
                    IF (FILM(X,Y) .NE. 0) THEN
                       IF ((X .EQ. OXINT).AND.(Y .EQ. OYINT)) GOTO 0194
                       NXINCT = XINCT - ISHFT
                       G = (NXINCT-XCOORD(X,Y))+(TANANG * YCOORD(X,Y))
C
C COLLISION CIRCLE RADIUS DETERMINATION
C
                       IF (FILM(X,Y) .EQ. 1) THEN
                          IF (SIZE .EQ. 1) THEN
                             RAD2 = 2
                          ELSE IF (SIZE .EQ. 2) THEN
                             RAD2 = 4.5
                          ELSE IF (SIZE .EQ. 8) THEN
                             RAD2 = 40.5
                          ENDIF
                       ELSE IF (FILM(X,Y) .EQ. 2) THEN
                          IF (SIZE .EQ. 1) THEN
                             RAD2 = 4.5
                          ELSE IF (SIZE .EQ. 2) THEN
                             RAD2 = 8
                          ELSE IF (SIZE .EQ. 8) THEN
                             RAD2 = 50
                          ENDIF
                       ELSE IF (FILM(X,Y) .EQ. 8) THEN
                          IF (SIZE .EQ. 1) THEN
                             RAD2 = 40.5
                          ELSE IF (SIZE .EQ. 2) THEN
                             RAD2 = 50
                          ENDIF
                       ENDIF
C
C TESTING FOR POSSIBLE COLLISION PARTNER
C
                       TEST1 = (RAD2 * SC2ANG - G**2)
                       IF (TEST1 .LT. 0.0) THEN
                          GOTO 0194
                       ELSE
                          F = YCOORD(X,Y) - TANANG*(NXINCT-XCOORD(X,Y))
                          YI = (F + SQRT(TEST1))/SC2ANG
```

```
                              QXINT = X
                              QYINT = Y
                              IF (YI .GT. Y2) THEN
                                  Y2 = YI
                                  A2 = NXINCT
                                  XCCLL = X
                                  YCCLL = Y
                              ENDIF
                              COLL = 1
                           ENDIF
                        ENDIF
0194                    IF (X .EQ. NEWX) GOTO 0196
0195               CONTINUE
0196               CXPOS = XPOS
                   IF (COLL .EQ. 1) GOTO 0181
0190          CONTINUE
0181       CONTINUE
C
C DETERMINATION OF X COLLSION POSITION
C
           X2 = Y2 * TANANG + A2
C
C TEST FOR NO MOBILITY
C
           IF (NOMOB .EQ. 1) THEN
              RESTX = X2
              RESTY = Y2
              GOTO 0221
           ENDIF
C
C     *****REST POINT DETERMINATION*****
C
C
 0205      SHORT = 10000
           MIN = 0
           MAX = 0
C
C INTIALIZATION FOR MOBILITY ROUTINE
C
           IF (BNCVAR .NE. 0) THEN
              DO 0207 B = 1,6,1
                 RBNC(B) = 10000
                 XBNC(B) = 0.0
                 YBNC(B) = 0.0
 0207         CONTINUE
           ENDIF
C
C DETERMINATION OF THE SIZE OF THE ARRAY SEARCH
C
           IF (IMPSET .EQ. 0) THEN
              IF (LAYER .EQ. 0) THEN
                 MIN = -3
                 MAX = 3
                 GOTO 0210
              ELSE
                 WIDTH = FILM(XCOLL,YCOLL) + SIZE
                 IF (WIDTH .EQ. 2) THEN
                    MIN = -4
                    MAX = 4
                 ELSE IF (WIDTH .EQ. 3) THEN
```

AD-A167 147 AN IMPROVED MODEL OF THIN FILM GROWTH(U) AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH SCHOOL OF ENGINEERING D J DORYLAND DEC 85 AFIT/GEP/ENP/85D-2 2/2

UNCLASSIFIED F/G 7/4 NL



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

```
                  MIN = -5
                  MAX = 5
               ELSE IF (WIDTH .EQ. 4) THEN
                  MIN = -6
                  MAX = 6
               ENDIF
            ENDIF
         ELSE
            IF (LAYER .EQ. 0) THEN
               MIN = -8
               MAX = 8
               GOTO 0210
            ELSE
               WIDTH = FILM(XCOLL,YCOLL) + SIZE
               IF (WIDTH .EQ. 2) THEN
                  MIN = -8
                  MAX = 8
               ELSE IF (WIDTH .EQ. 3) THEN
                  MIN = -10
                  MAX = 10
               ELSE IF (WIDTH .EQ. 4) THEN
                  MIN = -10
                  MAX = 10
               ELSE IF (WIDTH .EQ. 9) THEN
                  MIN = -9
                  MAX = 9
               ELSE IF (WIDTH .EQ. 10) THEN
                  MIN = -10
                  MAX = 10
               ENDIF
            ENDIF
         ENDIF
C
C BEGINNING OF SEARCH AROUND COLLISION PARTNER
C
 0210    DO 0220 J = MIN,MAX,1
            Y = 0
            Y = J + YCOLL
            IF ((Y .LT. 1) .OR. (Y .GT. YHGT)) GOTO 0220
            DO 0230 I = MIN,MAX,1
               X = 0
               X = I + XCOLL
               SHFT = 0
               IF (X .LT. 1) THEN
                  X = X + 300
                  SHFT = 1
               ELSE IF (X .GT. 300) THEN
                  X = X - 300
                  SHFT = 300
               ENDIF
C
C INITIALIZATION OF REST POINT VARIABLES
C
               IF (FILM(X,Y) .NE. 0) THEN
                  A = 0.0
                  B = 0.0
                  C = 0.0
                  D = 0.0
                  R1 = 0.0
                  R2 = 0.0
```

```
                    H = 0.0
                    K = 0.0
                    TEST2 = 0.0
                    RINC = 0.0
C
C SETTING OF REST CIRCLE RADII
C
                    IF (SIZE .EQ. 1) THEN
                       RINC = .707106781
                    ELSE IF (SIZE .EQ. 2) THEN
                       RINC = 1.414213562
                    ELSE IF (SIZE .EQ. 8) THEN
                       RINC = 5.6568542
                    ENDIF
C
C DETERMINATION OF REST POINT VARIABLES
C
                    R1 = (FILM(XCOLL,YCOLL) * .707106781) + RINC
                    R2 = (FILM(X,Y) * .707106781) + RINC
C
                    IF (SHFT .EQ. 0) THEN
                       H = XCOORD(X,Y) - XCOORD(XCOLL,YCOLL)
                    ELSE IF (SHFT .EQ. 1) THEN
                       H = XCOORD(X,Y) - 300.0 - XCOORD(XCOLL,YCOLL)
                    ELSE IF (SHFT .EQ. 300) THEN
                       H = XCOORD(X,Y) + 300.0 - XCOORD(XCOLL,YCOLL)
                    ENDIF
C
                    K = YCOORD(X,Y) - YCOORD(XCOLL,YCOLL)
                    A = (R2*R2 - R1*R1 - H*H - K*K)/2
                    B = A*A - (H*H)*(R1*R1)
                    C = (K*K + H*H)
                    IF (C .EQ. 0.0) GOTO 0230
                    TEST2 = (A*A*K*K - (C*B))
C
C TESTING FOR POSSIBLE REST PARTNERS
C
                    IF (TEST2 .LT. 0.0) THEN
                       GOTO 0230
C
C DETERMINATION OF POSSIBLE REST POINTS
C
                    ELSE
                       DO 0250 L = -1,1,2
                          Y1 = (-(A*K) + L*SQRT(TEST2))/C
                          DO 0260 M = -1,1,2
                             D = A*A - (K*K)*(R1*R1)
                             TEST3 = (H*H*A*A - (C*D))
                             IF (TEST3 .LT. 0.0) GOTO 0250
                             X1 = (-(H*A) + M*SQRT(TEST3))/C
                             TEST4 = ((X1 - H)**2 + (Y1 - K)**2)
                             TCL = ABS(TEST4 - R2*R2)
                             IF (TCL .LT. .005) THEN
                                XDIST = X1 + XCOORD(XCOLL,YCOLL) - X2
                                YDIST = Y1 + YCOORD(XCOLL,YCOLL) - Y2
                                R = (XDIST**2 + YDIST**2)
C
C STORING OF VALUES FOR MOBILITY ROUTINE
C
                                IF (BNCVAR .NE. 0) THEN
```

```
                         DO 0255 BNC = 1,6,1
                           IF (R .LT. RBNC(BNC)) THEN
                               IF (BNC .EQ. 6) GOTO 0257
                               BNC1 = BNC + 1
                               DO 0256 B1 = 5,BNC1,-1
                                 RBNC(B1) = RBNC(B1-1)
                                 XBNC(B1) = XBNC(B1-1)
                                 YBNC(B1) = YBNC(B1-1)
 0256                          CONTINUE
 0257                          RBNC(BNC) = R
                               XBNC(BNC) = X1+XCOORD(XCOLL,YCOLL)
                               YBNC(BNC) = Y1+YCOORD(XCOLL,YCOLL)
                               GOTO 0258
                           ELSE
                               GOTO 0255
                           ENDIF
 0255                    CONTINUE
                       ENDIF
C
C TEMPORARY STORAGE OF REST POINT VALUES
C
 0258                  IF (R .LT. SHORT) THEN
                          TSHORT = SHORT
                          SHORT = R
                          TRESTX = 0.0
                          TRESTY = 0.0
                          TRESTX = RESTX
                          TRESTY = RESTY
                          RESTX = 0.0
                          RESTY = 0.0
                          TESTY = 0.0
                          TESTY = Y1 + YCOORD(XCOLL,YCOLL)
                          IF (TESTY .LT. 2.0) GOTO 0260
                          RESTY = Y1 + YCOORD(XCOLL,YCOLL)
                          RESTX = X1 + XCOORD(XCOLL,YCOLL)
C
C MOVEMENT OF DISK IF NOT WITHIN BOUNDARIES
C
                          IF (RESTX .GE. 301.0) THEN
                             RESTX = RESTX - 300.0
                          ELSE IF (RESTX .LT. 1.0) THEN
                             RESTX = RESTX + 300.0
                          ENDIF
C
C TESTING OF POSITION FOR OCCUPATION
C
                          TPX3 = DINT(RESTX)
                          TPY3 = DINT(RESTY)
                          IF (FILM(TPX3,TPY3) .NE. 0) THEN
                             IF (TRESTX .NE. 0.0) THEN
                                SHORT = TSHORT
                                RESTX = TRESTX
                                RESTY = TRESTY
                             ENDIF
                          ENDIF
                          ORESTX = RESTX
                          ORESTY = RESTY
C
                       ENDIF
                     ELSE
```

```
                                     GOTO 0260
                                  ENDIF
 0260                          CONTINUE
 0250                       CONTINUE
                         ENDIF
                      ENDIF
 0230              CONTINUE
 0220           CONTINUE
C
C ******************************************************************
C
C                   EXTRA MOBILITY ROUTINE
C
C          PRINT*,' '
C          PRINT*,'RX RY',RESTX,RESTY
          IF (BNCVAR .EQ. 0) THEN
             GOTO 0221
          ELSE
C
C TEST TO MAKE SURE THE FILM IS HIGH ENOUGH
C
             Y3 = DINT(RESTY)
             IF (SIZE .EQ. 1) THEN
                IF (Y3 .LE. (1+HEIGHT)) GOTO 0221
             ELSE IF (SIZE .EQ. 2) THEN
                IF (Y3 .LE. (2+HEIGHT)) GOTO 0221
             ELSE IF (SIZE .EQ. 8) THEN
                IF (Y3 .LE. (4+HEIGHT)) GOTO 0221
             ENDIF
C
             BNCCTR = BNCCTR + 1
C             PRINT*,BNCCTR
             IF (BNCCTR .GE. BNCVAR) THEN
               DO 0235 B = 1,6,1
C
                 IF (XBNC(B) .GT. 300.0) THEN
                    XBNC(B) = XBNC(B) - 300.0
                 ELSE IF (XBNC(B) .LT. 1.0) THEN
                    XBNC(B) = XBNC(B) + 300.0
                 ENDIF
C
C INTIAL CHECK FOR REDUNDANCY
C
                 IF ((XBNC(B).NE.ORESTX).AND.(YBNC(B).NE.ORESTY)) THEN
                   IF ((XBNC(B).NE.0.0).AND.(YBNC(B).NE.0.0)) THEN
                      TXBNC = AINT(XBNC(B))
                      TYBNC = AINT(YBNC(B))
                      IF (FILM(TXBNC,TYBNC) .EQ. 0) THEN
C
C BEGINNING OF DISTANCE AREA CHECK
C
                        DO 0236 JJ = MIN,MAX,1
                           YBCK = JJ + TYBNC
                           DO 0237 II = MIN,MAX,1
                              XBCK = II + TXBNC
                              BSHFT = 0
C
                              IF (XBCK .GT. 300) THEN
                                 XBCK = XBCK - 300
                                 BSHFT = 300
```

```
                          ELSE IF (XBCK .LT. 1) THEN
                            XBCK = XBCK + 300
                            BSHFT = 1
                          ENDIF
C
                          IF (FILM(XBCK,YBCK) .NE. 0) THEN
                            YBDIST = YCOORD(XBCK,YBCK) - YBNC(B)
                            IF (BSHFT .EQ. 0) THEN
                              XBDIST = XCOORD(XBCK,YBCK) - XBNC(B)
                            ELSE IF (BSHFT .EQ. 300) THEN
                              XBDIST = XCOORD(XBCK,YBCK)+300-XBNC(B)
                            ELSE IF (BSHFT .EQ. 1) THEN
                              XBDIST = XCOORD(XBCK,YBCK)-300-XBNC(B)
                            ENDIF
                            TESTS = (XBDIST**2 + YBDIST**2)
C
C DETERMINING THE TOLERANCE DISTANCE
C
                            IF (FILM(XBCK,YBCK) .EQ. 1) THEN
                              IF (SIZE .EQ. 1) THEN
                                BTOL = 1.98
                              ELSE IF (SIZE .EQ. 2) THEN
                                BTOL = 4.45
                              ELSE IF (SIZE .EQ. 8) THEN
                                BTOL = 40.4
                              ENDIF
                            ELSE IF (FILM(XBCK,YBCK) .EQ. 2) THEN
                              IF (SIZE .EQ. 1) THEN
                                BTOL = 4.45
                              ELSE IF (SIZE .EQ. 2) THEN
                                BTOL = 7.9
                              ELSE IF (SIZE .EQ. 8) THEN
                                BTOL = 49.0
                              ENDIF
                            ELSE IF (FILM(XBCK,YBCK) .EQ. 8) THEN
                              IF (SIZE .EQ. 1) THEN
                                BTOL = 40.4
                              ELSE IF (SIZE .EQ. 2) THEN
                                BTOL = 49.0
                              ENDIF
                            ENDIF
C
C TESTING FOR DISTANCE TOLERANCE
C
                            IF (TESTS .LT. BTOL) GOTO 0235
                          ENDIF
 0237                   CONTINUE
 0236                 CONTINUE
                      RESTX = XBNC(B)
                      RESTY = YBNC(B)
                      YTEST = ORESTY + .3
                      IF (RESTY .GT. YTEST) GOTO 0235
                      BNCCTR = 0
                      BCTR = BCTR + 1
                      GOTO 0219
                    ENDIF
                  ENDIF
                ENDIF
 0235         CONTINUE
              GOTO 0219
```

```
            ENDIF
          ENDIF
C
C LAST CHECK AND DEFAULT STRUCTURE
C
 0218     IF (RESTY .LT. 1.0) THEN
             BCTR = BCTR - 1
 0219        RESTX = DRESTX
             RESTY = DRESTY
             BNCCTR = (BNCVAR - 1)
          ENDIF
C          PRINT*,'RX RY',RESTX,RESTY
C
C ****************************************************************
C
 0221     X3 = DINT(RESTX)
          Y3 = DINT(RESTY)
C
C TESTING FOR OVERWRITES
C
          IF (FILM(X3,Y3) .NE. 0) THEN
              HCTR = HCTR + 1
          ENDIF
C
C FIXING OF DISK POSITION
C
          XCOORD(X3,Y3) = RESTX
          YCOORD(X3,Y3) = RESTY
          FILM(X3,Y3) = SIZE
C
C SETTING OF THE STARTING HEIGHT FOR NEXT DISK
C
          IF (YCK .EQ. 1) THEN
             YCK = 0
             TYHGT = YHGT - (Y3 + 6)
             IF (TYHGT .GT. 0) THEN
                YHGT = YHGT
             ELSE
                YHGT = Y3 + 9
             ENDIF
          ELSE
             IF (Y3 .GE. YHGT) THEN
                YHGT = Y3 + 3
             ENDIF
          ENDIF
C
C INCREMENTING THE DISK COUNTER
C
          ND = ND + 1
          IF (ND .EQ. 500) THEN
             WRITE (6,0200) DEPCTR
 0200        FORMAT (28X,I5,' DISKS DEPOSITED')
             ND = 0
          ENDIF
C
C RESETTING OF PARAMETERS IN THE CASE OF IMPURITIES
C
          IF (IMPSET .EQ. 1) THEN
             IF (YHGT .GT. (HGTIMP+50)) THEN
                IMPSET = 0
```

```
               ENDIF
            ENDIF
C
C FINDING THE POSITION OF IMPURITY
C
         IF (SIZE .EQ. 8) THEN
             IMPHGT = Y3
             IMPX = X3
         ENDIF
C
C MESSAGE CENTER FOR END OF DEPOSITION
C
 0170 CONTINUE
 0201 WRITE (6,0202) (DEPCTR - 1)
 0202 FORMAT (2(1X/),15X,'DEPOSITION COMPLETED WITH ',I5,' DISKS DEPOSIT
     CED!'///)
C
      WRITE (6,0225) HCTR
 0225 FORMAT (23X,'THERE WERE ',I2,' OVERLAPPING DISKS'//)
C
      IF (BNCVAR .NE. 0) THEN
         WRITE (6,0229) BCTR
 0229    FORMAT (18X,I5,' DISKS WERE GIVEN AN EXTRA MOBILITY'//)
      ENDIF
C
      IF (IMPHGT .EQ. 0) THEN
         GOTO 0226
      ELSE
         WRITE (6,0227) IMPHGT
 0227    FORMAT (22X,'THE Y HEIGHT OF THE IMPURITY IS ',I3)
         WRITE (6,0228) IMPX
 0228    FORMAT (21X,'THE X POSITION OF THE IMPURITY IS ',I3//)
      ENDIF
C
 0226 WRITE (6,0222)
 0222 FORMAT(9X,'DEPOSITION VARIABLES ARE READY TO BE ANALYZED AND/OR ST
     CORED.'//)
      PRINT *,'                                                 HIT RETURN'
      READ (5,0115)
      RETURN
C
      END
C
C
C
C                       ********************************
C                       *                              *
C                       *      ANALYSIS SUBROUTINE     *
C                       *                              *
C                       ********************************
C
C     THIS SUBROUTINE CONSIST OF 2 AREAS: THAT IS THE CALCULATING OF THE
C     DENSITY OF THE FILM MATRICES AND THE DETERMINATION OF THE ANGLE OF
C     THE DEPOSITED FILM.  EACH SECTION CONTAINS A BRIEF DESCRIPTION OF
C     ITS PURPOSE AND/OR ITS APPROACH.
C
      SUBROUTINE ANAL(FILM,XCOORD,YCOORD)
C
C     LOCAL VARIABLES
C
```

```
      REAL XCOORD(300,200),YCOORD(300,200),RSMLDN,RLRGDN,TOTDEN,CORR(90)
      REAL LOCDEN,LLRGDN,LSMLDN,SLNDEN,LLNDEN,CORFAC,ISHFT,XPOS,OXPOS
      REAL ANG,RANG,TANANG,TLNDEN,LARGE1,LARGE2,LARGE3,AVGANG
      INTEGER FILM(300,200),IVAR,SMLCTR,LRGCTR,TOTCTR,SDNCTR,LDNCTR
      INTEGER LOCCTR,BOTHGT,TOPHGT,SUB,CELCTR,LDKCTR,SDKCTR,MAXCNT,A
      INTEGER TEST,ANGLE1,ANGLE2,ANGLE3,DENCK,LEFT,RIGHT
C
C
C                ********** ANALYSIS INTERFACE LOOP **********
C
 0400 WRITE (6,0401)
 0401 FORMAT (19(2X/),27X,'ANALYSIS INTERFACE LOOP'///,20X,'ENTER APPROP
     CRIATED NUMBER TO CONTINUE'/,2(2X/),25X,'1 - CALCULATION OF DENSITY
     C'/,25X,'2 - CALCULATION OF ANGLE'/,25X,'9 - EXIT TO MAIN INTERFACE
     C LOOP'/,25X,'CTRL/C - EXIT TO OPERATING SYSTEM'/,6(2X/))
C
 0405 READ (5,0406) IVAR
 0406 FORMAT (I1)
C
      IF (IVAR .EQ. 1) THEN
         GOTO 0410
      ELSE IF (IVAR .EQ. 2) THEN
         GOTO 0430
      ELSE IF (IVAR .EQ. 9) THEN
         RETURN
      ENDIF
      WRITE (6,0407)
 0407 FORMAT(25X,'SORRY CHARLIE!! - TRY AGAIN'///)
      GOTO 0405
C
C
C                ********** CALCULATION OF DENSITY **********
C
C THIS PART OF THE SUBROUTINE IS USED TO CALCULATE THE DENSITY OF THE DE-
C POSITED FILM. THIS IS ACCOMPLISHED BY SCANNING THE ENTIRE FILM MATRIX
C AND CHECKING FOR OCCUPATION BY EITHER SMALL,LARGE OR IMPURITY DISKS.
C AFTER COUNTING THE NUMBER OF DISK THE AREA TAKEN UP BY THE DISK IS COM-
C PARED TO THE TOTAL POSSIBLE AREA THUS CREATING THE PACKING DENSITY.  A
C LOCAL DENSITY IS ALSO CALCULATED TO STUDY THE AFFECTS OF CHANGING CER-
C TIAN PARAMETERS.
C
 0410 WRITE (6,0411)
 0411 FORMAT (10X,'IT IS ASSUMED UPON ENTERING THIS SECTION OF THE SUBRO
     CUTINE THAT'/,10X,'YOU WISH TO FIND THE DENSITY OF THE CURRENT FILM
     C MATRICES.'/,10X,'IS THIS CORRECT?'//,11X,'IF YES - ENTER 1'/,11X,
     C'OTHERWISE - HIT RETURN'//)
C
      READ (5,0406) IVAR
      IF (IVAR .EQ. 1) THEN
         ANGCK = 0
         GOTO 0412
      ELSE
         GOTO 0400
      ENDIF
C
 0412 WRITE (6,0413)
 0413 FORMAT (10X,'IF YOU WISH TO LOOK AT VARIATIONS IN Y - ENTER 1'/,10
     CX,'IF YOU WISH TO LOOK AT VARIATIONS IN X - ENTER 2'/,10X,'IF YOU
     CWISH TO LOOK AT VARIATIONS IN BOTH X AND Y - ENTER 3'//)
C
```

```
      READ (5,0490) DENCK
 0490 FORMAT (I1)
C
      IF (DENCK .EQ. 1) THEN
         GOTO 0415
      ELSE IF (DENCK .EQ. 2) THEN
         GOTO 0480
      ELSE IF (DENCK .EQ. 3) THEN
         GOTO 0415
      ELSE
         PRINT*,'TRY AGAIN'
         GOTO 0412
      ENDIF
C
 0415 WRITE (6,0416)
 0416 FORMAT (10X,'IN ORDER TO CHECK FOR VERTICAL VARIATIONS IN DENSITY
     CTWO HEIGHTS'/,10X,'NEED TO BE SPECIFIED.  PLEASE ENTER THE Y VALUE
     CS IN INTEGER FORMAT.'//)
C
 0434 PRINT*,'ENTER BOTTOM HEIGHT'
 0418 READ (5,0417) BOTHGT
 0417 FORMAT (I3)
      IF (BOTHGT .LT. 1) THEN
         PRINT*,'           BOTTOM HEIGHT TOO LOW - TRY AGAIN'
         GOTO 0418
      ENDIF
      PRINT*,'ENTER TOP HEIGHT'
 0419 READ (5,0417) TOPHGT
      IF (TOPHGT .GT. 200) THEN
         PRINT*,'           TOP HEIGHT TOO HIGH - TRY AGAIN'
         GOTO 0419
      ENDIF
      PRINT*,' '
C
      IF ((ANGCK .EQ. 1).OR.(DENCK .EQ. 1)) THEN
         LEFT = 1
         RIGHT = 300
         PRINT*,'WORKING'
         GOTO 0433
      ENDIF
C
 0480 WRITE (6,0481)
 0481 FORMAT(10X,'IN ORDER TO CHECK FOR HORIZONTAL VARIATIONS IN DENSITY
     C TWO WIDTHS'/,10X,'NEED TO BE SPECIFIED.  PLEASE ENTER THE X VALUE
     CS IN INTEGER FORMAT.'//)
C
      PRINT*,'ENTER LEFT BOUNDARY'
 0482 READ (5,0417) LEFT
      IF (LEFT .LT. 1) THEN
         PRINT*,'        LEFT BOUNDARY TOO FAR LEFT - TRY AGAIN'
         GOTO 0482
      ENDIF
      PRINT*,'ENTER RIGHT BOUNDARY'
 0483 READ (5,0417) RIGHT
      IF (RIGHT .GT. 300) THEN
         PRINT*,'        RIGHT BOUNDARY TOO FAR RIGHT - TRY AGAIN'
         GOTO 0483
      ENDIF
C
      IF (DENCK .EQ. 2) THEN
```

```
          TOPHGT = 200
          BOTHGT = 1
       ENDIF
C
       PRINT*,' '
       PRINT*,'WORKING'
C
C INTIALIZATION OF DENSITY VARIABLES
C
 0433  TOTCTR = 0
       LRGCTR = 0
       SMLCTR = 0
       IMPCTR = 0
       IDNCTR = 0
       SDNCTR = 0
       LDNCTR = 0
       LOCCTR = 0
C
C COUNTING OF DISK FOR DENSITY CALCULATIONS
C
       DO 0420 Y = 1,200,1
          DO 0421 X = 1,300,1
             IF (FILM(X,Y) .EQ. 1) THEN
                  SMLCTR = SMLCTR + 1
             ELSE IF (FILM(X,Y) .EQ. 2) THEN
                  LRGCTR = LRGCTR + 1
             ELSE IF (FILM(X,Y) .EQ. 8) THEN
                  IMPCTR = IMPCTR + 1
             ENDIF
             IF ((Y .GE. BOTHGT).AND.(Y .LE. TOPHGT)) THEN
                  IF ((X .GE. LEFT).AND.(X .LE. RIGHT)) THEN
                       IF (FILM(X,Y) .EQ. 1) THEN
                          SDNCTR = SDNCTR + 1
                       ELSE IF (FILM(X,Y) .EQ. 2) THEN
                          LDNCTR = LDNCTR + 1
                       ELSE IF (FILM(X,Y) .EQ. 8) THEN
                          IDNCTR = IDNCTR + 1
                       ENDIF
                       LOCCTR = LOCCTR + 1
                  ENDIF
             ENDIF
 0421     CONTINUE
 0420  CONTINUE
C
C FINDING THE TOTAL NUMBER OF DISK
C
       TOTCTR = SMLCTR + LRGCTR + IMPCTR
       IF (ANGCK .EQ. 1) GOTO 0429
C
C OUTPUT FOR THE NUMBER OF DISK
C
       WRITE (6,0422) SMLCTR
 0422  FORMAT (10X,'THE NUMBER OF SMALL DISKS DEPOSITED = ',I5)
       WRITE (6,0423) LRGCTR
 0423  FORMAT (10X,'THE NUMBER OF LARGE DISKS DEPOSITED = ',I5)
       WRITE (6,1423) IMPCTR
 1423  FORMAT (10X,'THE NUMBER OF IMPURITIES = ',I1)
       WRITE (6,0424) TOTCTR
 0424  FORMAT (10X,'THE TOTAL NUMBER OF DISK DEPOSITED = ',I5)
C
```

```
C CALCULATIONS OF THE DENSITIES
C
 0429 RSMLDN = (SMLCTR*1.5707963*100)/60000
      RLRGDN = (LRGCTR*6.2831853*100)/60000
      RIMPDN = (IMPCTR*100.53096*100)/60000
      TOTDEN = RSMLDN + RLRGDN + RIMPDN
      LSMLDN = (SDNCTR*1.732050808*100)/LOCCTR
      LLRGDN = (LDNCTR*6.2831853*100)/LOCCTR
      LIMPDN = (IDNCTR*100.53096*100)/LOCCTR
      LOCDEN = LSMLDN + LLRGDN + LIMPDN
C
      IF (ANGCK .EQ. 1) GOTO 0435
C
      PRINT*,' '
C
C OUTPUT OF THE DENSITIES
C
      WRITE (6,0425) RSMLDN
 0425 FORMAT (10X,'SPACE OCCUPIED BY SMALL DISK = ',F5.2,'%')
      WRITE (6,0426) RLRGDN
 0426 FORMAT (10X,'SPACE OCCUPIED BY LARGE DISK = ',F5.2,'%')
      WRITE (6,1426) RIMPDN
 1426 FORMAT (10X,'SPACE OCCUPIED BY IMPURITIES = ',F5.2,'%')
      WRITE (6,0427) TOTDEN
 0427 FORMAT (10X,'THE TOTAL PACKING DENSITY = ',F5.2,'%')
      PRINT*,' '
      WRITE (6,0428) LOCDEN
 0428 FORMAT (10X,'THE LOCAL PACKING DENSITY = ',F6.2,'%'//)
      WRITE (6,0404)
 0404 FORMAT (10X,'DENSITY CALCULATIONS ARE COMPLETE'//)
      PRINT*,'                                                    HIT RETURN'
      READ (5,0406)
      GOTO 0400
C
C
C                    ********** CALCULATION OF ANGLE **********
C
C THIS PART OF THE SUBROUTINE IS USED TO CALCULATE THE ANGLE OF THE FILM
C GROWTH.  THIS IS ACCOMPLISHED BY SCANNING THE DEPOSITED FILM AT ANGLES
C RANGING FROM 1 TO 80 DEGREES.  AFTER THIS THE LARGEST "CORRELATION" FAC-
C TOR IS CHOSEN AS THE ANGLE OF FILM GROWTH.  THE IDEA HERE IS THAT A
C LARGE "CORRELATION" WILL OCCURR WHEN THE VARYING ANGLE EQUALS THE ANGLE
C OF FILM GROWTH.  IT HAS BEEN FOUND OUT THROUGH TRIAL AND ERROR THAT THE
C BEST RESULTS ARE OBTAINED WHEN THE SEPERATION BETWEEN THE TWO HEIGHT LE-
C VELS ARE BETWEEN 10 AND 20.
C
 0430 WRITE (6,0431)
 0431 FORMAT (10X,'IN THIS PART OF THE SUBROUTINE THE ANGLE OF THE FILM
     CGROWTH'/,10X,'WILL BE CALCULATED USING A SCANNING TECHNIQUE.'/,10X
     C,'IS THIS YOUR DESIRE?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE -
     C HIT RETURN'//)
C
      READ (5,0406) IVAR
      IF (IVAR .EQ. 1) THEN
         ANGCK = 1
         GOTO 0459
      ELSE
         GOTO 0400
      ENDIF
C
```

```
 0459 WRITE (6,0460)
 0460 FORMAT (10X,'IN ORDER TO SPEED UP THE ANGLE CALCULATIONS TWO HEIGH
     CT LEVELS NEED'/,10X,'TO BE SPECIFIED.  PLEASE ENTER THE Y VALUES I
     CN INTEGER FORMAT.'//)
C
      GOTO 0434
C
C BEGINNING OF ANGLE ANALYSIS
C
 0435 MAXCNT = 299+TOPHGT-BOTHGT
      DO 0437 C = 0,89,1
         CORR(C) = 0.0
 0437 CONTINUE
C
C BEGINNING OF INDIVIDUAL ANGLE CHECKS
C
      DO 0438 A = 1,80,1
         ANG = FLOAT(A)
         WRITE (6,0455) A
 0455    FORMAT (23X,'ANALYZING FILM ANGLE AT ',I2,' DEGREES')
         RANG = ANG/(57.2957751)
         TANANG = TAN(RANG)
         CRSTRM = 0.0
         DO 0439 SUB = 1,300,1
C
C INTIALIZATION OF ANGLE ANALYSIS VARIABLES
C
            SDKCTR = 0
            LDKCTR = 0
            IDKCTR = 0
            CELCTR = 0
            SLNDEN = 0.0
            LLNDEN = 0.0
            ILNDEN = 0.0
            TLNDEN = 0.0
            XPOS = (TANANG * TOPHGT) + SUB
            OXPOS = XPOS
C
C START OF THE ARRAY SEARCH
C
            DO 0440 Y = TOPHGT,1,-1
               XPOS = (TANANG * Y) + SUB
               ISHFT = ((AINT(XPOS/301)) * 300)
               NEWX = AINT(XPOS - ISHFT)
               OLDX = AINT(OXPOS - ISHFT)
               DO 0441 X = OLDX,1,-1
C
C COUNTING OF THE DISKS
C
                  IF (FILM(X,Y) .NE. 0) THEN
                     IF (FILM(X,Y) .EQ. 1) THEN
                        SDKCTR = SDKCTR + 1
                     ELSE IF (FILM(X,Y) .EQ. 2) THEN
                        LDKCTR = LDKCTR + 1
                     ELSE IF (FILM(X,Y) .EQ. 8) THEN
                        IDKCTR = IDKCTR + 1
                     ENDIF
                  ENDIF
C
                  X2 = X + 1
```

```
                    IF (X2 .GT. 300) THEN
                       X2 = X2 - 300
                    ENDIF
C
                    IF (FILM(X2,Y) .NE. 0) THEN
                       IF (FILM(X2,Y) .EQ. 1) THEN
                          SDKCTR = SDKCTR + 1
                       ELSE IF (FILM(X2,Y) .EQ. 2) THEN
                         LDKCTR = LDKCTR + 1
                       ELSE IF (FILM(X2,Y) .EQ. 8) THEN
                          IDKCTR = IDKCTR + 1
                       ENDIF
                    ENDIF
                    CELCTR = CELCTR + 2
C
                    IF (CELCTR .GE. MAXCNT) GOTO 0442
                    IF (X .EQ. NEWX) GOTO 0443
 0441             CONTINUE
 0443             OXPOS = XPOS
                  IF (Y .LE. 30THGT) GOTO 0442
 0440           CONTINUE
C
C CALCULATION OF THE LINE DENSITIES
C
 0442           SLNDEN = ((SDKCTR*1.5707963)/CELCTR)
                LLNDEN = ((LDKCTR*6.2831853)/CELCTR)
                ILNDEN = ((IDKCTR*100.53096)/CELCTR)
                TLNDEN = SLNDEN + LLNDEN + ILNDEN
C
                IF (TLNDEN .LE. (LOCDEN/100)) THEN
                   CORFAC = (((LOCDEN/100) - TLNDEN)/(LOCDEN/100))**2
                ELSE
                   CORFAC = ((TLNDEN - (LOCDEN/100))/(1-(LOCDEN/100)))**2
                ENDIF
C
                CRSTRM = CRSTRM + CORFAC
 0439     CONTINUE
C
C DETERMINING THE CORRELATION NUMBER
C
          CORR(A) = CRSTRM/300
 0438 CONTINUE
C
C FINDING THE THREE LARGEST CORRELATION NUMBERS
C
        ANGLE1 = 0
        ANGLE2 = 0
        ANGLE3 = 0
        LARGE1 = 0.0
        LARGE2 = 0.0
        LARGE3 = 0.0
        DO 0470 TEST = 1,30,1
           IF (CORR(TEST) .GT. LARGE1) THEN
              ANGLE3 = ANGLE2
              ANGLE2 = ANGLE1
              ANGLE1 = TEST
              LARGE3 = LARGE2
              LARGE2 = LARGE1
              LARGE1 = CORR(TEST)
           ELSE IF (CORR(TEST) .GT. LARGE2) THEN
```

```
            ANGLE3 = ANGLE2
            ANGLE2 = TEST
            LARGE3 = LARGE2
            LARGE2 = CORR(TEST)
            GOTO 0470
         ELSE IF (CORR(TEST) .GT. LARGE3) THEN
            ANGLE3 = TEST
            LARGE3 = CORR(TEST)
         ENDIF
 0470 CONTINUE
C
C CALCULATION OF THE AVERAGE OF THE TOP THREE VALUES
C
      AVGANG = FLOAT((ANGLE1 + ANGLE2 + ANGLE3)/3)
C
C OUTPUT OF THE ANGLE ANALYSIS
C
      PRINT*,' '
      PRINT*,' '
      WRITE (6,0451) ANGLE1,ANGLE2,ANGLE3
 0451 FORMAT (13X,'THE TOP THREE CORRELATED ANGLES IN DECENDING ORDER AR
     CE'/,T30,I2,8X,I2,8X,I2/)
      WRITE (6,0453) AVGANG
 0453 FORMAT (18X,'THE AVERAGE CORRELATED ANGLE IS ',F4.1,' DEGREES'//)
      WRITE (6,0452)
 0452 FORMAT (20X,'THE FILM ANGLE CALCULATIONS ARE COMPLETE'//)
      PRINT*,'                                                 HIT RETURN'
      READ (5,0406)
      GOTO 0400
      END
C
C
C
C                      *********************************
C                      *                               *
C                      *       MOVING SUBROUTINE       *
C                      *                               *
C                      *********************************
C
C      THIS SUBROUTINE IS DIVIDED INTO 3 SECTIONS.  THE FIRST 2 SECTIONS
C      MOVE THE DEPOSITED FILM TO A FILE FOR STORAGE AND BACK AGAIN.  THE
C      LAST SECTION HELPS IN PREPARING THE DEPOSITED FILM FOR PLOTTING.
C      EACH SECTION CONTAINS A BRIEF DESCRIPTION OF ITS PURPOSE AND/OR
C      ITS APPROACH.
C
      SUBROUTINE MOVE (FILM,XCOORD,YCOORD)
C
C      LOCAL VARIABLES
C
      REAL XCOORD(300,200),YCOORD(300,200),XCOOR,YCOOR
      INTEGER FILM(300,200),IVAR,FIL,CTR,RECCTR
C
C
C                ********** MOVING INTERFACE LOOP **********
C
 0300 WRITE (6,0301)
 0301 FORMAT (18(2X/),27X,'MOVING INTERFACE LOOP'///,20X,'ENTER APPROPRI
     CATE NUMBER TO CONTINUE'/,2(2X/),25X,'1 - STORE FILM MATRICES'/,25X
     C,'2 - RECALL FILM MATRICES'/,25X,'3 - STORE FILM FOR PLOTTING'/,25
     CX,'4 - RECALL PLOTTING VALUES'/,25X,'9 - EXIT TO MAIN INTERFACE LO
```

```
     COP'/,25X,'CTRL/C - EXIT TO OPERATING SYSTEM'/,5(2X/))
C
 0305 READ (5,0306) IVAR
 0306 FORMAT (I1)
C
      IF (IVAR .EQ. 1) THEN
         GOTO 0310
      ELSE IF (IVAR .EQ. 2) THEN
         GOTO 0330
      ELSE IF (IVAR .EQ. 3) THEN
         GOTO 0350
      ELSE IF (IVAR .EQ. 4) THEN
         GOTO 0380
      ELSE IF (IVAR .EQ. 9) THEN
         RETURN
      ENDIF
      WRITE (6,0308)
 0308 FORMAT(21X,'YOU MESSED UP!! - TRY AGAIN'///)
      GOTO 0305
C
C
C              ********** STORING OF FILM MATRICES **********
C
C THIS PART OF THE SUBROUTINE STORES THE VALUE OF FILM, XCOORD, YCOORD
C INTO THE DATA FILE FOR012.DAT.  THIS IS DONE SO THAT FINISHED FILMS
C CAN BE STORED FOR FUTURE REFERENCE AND RECALLED FOR ANALYZING IF DE-
C SIRED.  THIS METHOD OF STORAGE IS SOMEWHAT INEFFICIENT IN THAT UN-
C OCCUPIED STORAGE CELLS ARE ALSO READ INTO THE FILE. THIS METHOD OF
C STORAGE SHOULD ONLY BE USED WHEN THE OPERATOR HAS ALOT OF SPACE IN
C HIS DIRECTORY.
C
 0310 WRITE (6,0311)
 0311 FORMAT (10X,'IN THIS PART OF THE SUBROUTINE THE CURRENT VALUES OF
     CTHE FILM'/,10X,'MATRICES WILL BE STORED IN A FILE CALLED FOR012.DA
     CT FOR FUTURE'/,10X,'REFERENCE.'/,10X,'IS THIS YOU DESIRE?'//,11X,'
     CIF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0306) IVAR
      IF (IVAR .EQ. 1) THEN
         PRINT*,' '
         PRINT*,'WORKING'
         GOTO 0315
      ELSE
         GOTO 0300
      ENDIF
C
 0315 OPEN (UNIT = 12, FILE = 'FOR012.DAT', STATUS = 'NEW')
C
      DO 0320 Y = 1,200,1
         DO 0325 X = 1,300,1
            WRITE (12,0326) FILM(X,Y),XCOORD(X,Y),YCOORD(X,Y)
 0326       FORMAT (1X,I2,3X,F8.4,3X,F8.4)
 0325    CONTINUE
 0320 CONTINUE
C
      CLOSE (UNIT = 12)
C
      WRITE (6,0327)
 0327 FORMAT(10X,'THE VALUES OF THE FILM MATRICES HAVE NOW BEEN COPIED'/
     C,10X,'INTO THE FILE FOR012.DAT.'//)
```

```
      PRINT*,'                                                      HIT RETURN'
      READ (5,0306)
      GOTO 0300
C
C
C             ********** RECALLING OF FILM MATRICES **********
C
C
C THIS PART OF THE SUBROUTINE RECALLS THE VALUES OF THE FILE FOR013.DAT
C SO THAT THEY MAY BE ANALYZED AND/OR READIED FOR PLOTTING.  THE VALUES
C READ IN ARE PLACED IN THE MATRICS FILM, XCOORD, YCOORD.  IN DOING SO
C THE VALUES STORED BY THE PREVIOUS SECTION ARE READ IN, THEREFORE THE
C VALUES NEED TO OF BEEN COPIED INTO A FILE CALLED FOR013.DAT.
C
 0330 WRITE (6,0331)
 0331 FORMAT (10X,'JUST A REMINDER. UPON ENTERING INTO THIS PART OF THE
     CSUBROUTINE'/,10X,'THE CURRENT VALUES OF THE FILM MATRICES WILL BE
     CLOST.  THE REA-'/,10X,'SON FOR THIS IS THAT THE NEW VALUES FROM TH
     CE FILE FOR013.DAT'/,10X,'WILL BE READ IN.'/,10X,'DO YOU WISH TO SA
     CVE THE CURRENT VALLES OF THE FILM MATRICES?'//,11X,'IF YES - ENTER
     C 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0306) IVAR
      IF (IVAR .EQ. 1) THEN
         GOTO 0310
      ENDIF
      PRINT*,'WORKING'
C
      OPEN (UNIT = 13,FILE = 'FOR013.DAT',STATUS = 'OLD')
      REWIND (UNIT = 13)
C
      DO 0335 Y = 1,200,1
         DO 0336 X = 1,300,1
            READ (12,0337) FILM(X,Y),XCOORD(X,Y),YCOORD(X,Y)
 0337       FORMAT (1X,I2,3X,F8.4,3X,F8.4)
 0336    CONTINUE
 0335 CONTINUE
C
      CLOSE (UNIT = 13)
C
      WRITE (6,0340)
 0340 FORMAT (10X,'THE NEW VALUES OF THE FILM MATRICES HAVE NOW BEEN'/,1
     C0X,'READ IN FORM THE FILE FOR013.DAT.'//)
      PRINT*,'                                                      HIT RETURN'
      READ (5,0306)
      GOTO 0300
C
C
C             ********** STORING OF FILM FOR PLOTTING **********
C
C THIS PART OF THE SUBROUTINE STORES THE NON-ZERO VALUES OF THE MATRICES
C FILM, XCOORD, AND YCOORD INTO THE FILES FOR007.DAT AND FOR014.DAT FOR
C FUTURE PLOTTING.  THIS IS ACCOMPLISHED BY CHECKING EACH ADDRESS OF THE
C TWO DIMENSIONAL AREAS FOR OCCUPATION AND THEN TRANSFERING ONLY THOSE
C STORAGE CELLS THAT HAVE NONE ZERO INFORMATION.
C
 0350 WRITE (6,0351)
 0351 FORMAT(10X,'WARNING!  UPON ENTERING INTO THIS PART OF THE SUBROUTI
     CNE THE'/,10X,'CURRENT VALUES OF THE FILM MATRICES WILL BE COPIED I
     CNTO THE'/,10X,'FILES FOR007.DAT AND FOR014.DAT.  IN DOING SO, THE
     CADDRESS OF'/,10X,'THE INDIVIDUAL POINTS WILL BE LOST SO THAT NO AN
```

```
     CALYSIS CAN BE'/,10X,'EVALUATED DIRECTLY.'/,10X,'IS THIS YOUR DESIR
     CE?'//,11X,'IF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0306) IVAR
      IF (IVAR .EQ. 1) THEN
         PRINT*,'WORKING'
         GOTO 0355
      ELSE
         GOTO 0300
      ENDIF
C
 0355 OPEN (UNIT = 7,FILE = 'FOR007.DAT',STATUS = 'NEW')
      OPEN (UNIT = 14,FILE = 'FOR014.DAT',STATUS = 'NEW')
C
      DO 0357 Y = 1,200,1
         DO 0358 X = 1,300,1
            IF (FILM(X,Y) .NE. 0) THEN
               WRITE (7,0359) FILM(X,Y),XCOORD(X,Y),YCOORD(X,Y)
 0359          FORMAT (1X,I2,3X,F8.4,3X,F8.4)
               IF (FILM(X,Y) .EQ. 2) THEN
                  WRITE (14,0356) FILM(X,Y),XCOORD(X,Y),YCOORD(X,Y)
 0356             FORMAT (1X,I2,3X,F8.4,3X,F8.4)
               ENDIF
            ELSE
               GOTO 0358
            ENDIF
 0358    CONTINUE
 0357 CONTINUE
C
      CLOSE (UNIT = 14)
      CLOSE (UNIT = 7)
C
      WRITE (6,0360)
 0360 FORMAT (10X,'THE VALUES OF THE FILM MATRICES HAVE BEEN COPIED TO'/
     C,10X,'THE FILES CALLED FOR007.DAT AND FOR014.DAT.'//,10X,'PLOTTING
     C OF THE FILM MATRICES CAN NOW OCCUR!'//)
      PRINT*,'                                             HIT RETURN'
      READ (5,0306)
      GOTO 0300
C
C
C            ********** RECALLING OF FILM FOR ANALYZING **********
C
C THIS LAST PART OF THE SUBROUTINE TAKES THE VALUES FILM, XCOORD, YCOORD
C FROM THE FILE FOR008.DAT SO THAT THEY CAN BE ANALYZED.  THIS IS ACCOM-
C PLISHED BY LOOKING AT THE VALUES OF XCOORD AND YCOORD AND TRUNCATING THE
C VALUES.  AFTER TRUNCATION THE FILM MATRIX IS THEN GIVEN THE PROPER VALUES.
C THIS SECTION IS THE COUNTERPART OF THE PREVIOUS SECTION IMPLYING THAT THE
C VALUES MUST BE COPIED INTO A FILE FOR008.DAT BEFORE ATTEMPTING TO READ
C FROM THE FILE.
C
 0380 WRITE (6,0381)
 0381 FORMAT (10X,'CAUTION! UPON ENTERING INTO THIS SECTION OF THE SUBRO
     CUTINE, THE'/,10X,'CURRENT VALUES OF FOR008.DAT WILL BE READ INTO T
     CHE FILM MATRICES'/,10X,'DESTROYING THE OLD VALUES.'/,10X,'HAVE THE
     C FILM MATRICES BEEN INITIALIZED TO ZERO?'//,11X,'IF YES - ENTER 1'
     C/,11X,'OTHERWISE - HIT RETURN'//)
C
      READ (5,0306) IVAR
      IF (IVAR .EQ. 1) THEN
```

```
            GOTO 0382
         ELSE
            GOTO 0386
         ENDIF
C
 0386 WRITE (6,0389)
 0389 FORMAT (10X,'DO YOU WISH TO INITIALIZE THE FILM MATRICES?'//,11X,'
     CIF YES - ENTER 1'/,11X,'OTHERWISE - HIT RETURN'//)
C
         READ (5,0306) IVAR
         IF (IVAR .EQ. 1) THEN
            PRINT*,'WORKING'
            GOTO 0397
         ELSE
            PRINT*,' '
            GOTO 0382
         ENDIF
C
 0397 DO 0398 X = 1,300,1
            DO 0399 Y = 1,200,1
               FILM(X,Y) = 0
 0399       CONTINUE
 0398 CONTINUE
C
 0382 WRITE (6,0383)
 0383 FORMAT (10X,'IN ORDER TO COMPLETE THIS PART OF THE SUBROUTINE ONE
     CMUST KNOW'/,10X,'THE NUMBER OF RECCRDS IN THE FILE TO BE READ.  IF
     C YOU KNOW THE'/,10X,'CORRECT NUMBER ENTER THAT BELOW.  IF NOT, EXI
     CT THE PROGRAM AND'/,10X,'FIND OUT!! - USE CTRL/C'//)
C
         PRINT*,'ENTER THE NUMBER OF RECORDS'
         READ (5,0385) NUMREC
 0385 FORMAT (I5)
C
         PRINT*,' '
         PRINT*,'WORKING'
C
         OPEN (UNIT = 8,FILE = 'FOR008.CAT',STATUS = 'OLD')
         REWIND (UNIT = 8)
C
         RECCTR = 0
         DO 0390 CTR = 1,NUMREC,1
            READ (8,0391) FIL, XCOOR, YCOOR
 0391       FORMAT (1X,I2,3X,F8.4,3X,F8.4)
            X = AINT(XCOOR)
            Y = AINT(YCOOR)
            FILM(X,Y) = FIL
            RECCTR = RECCTR + 1
            IF (RECCTR .EQ. 1000) THEN
               WRITE (6,0388) CTR
 0388          FORMAT (28X,I5,' RECCROS READ IN')
               RECCTR = 0
            ENDIF
 0390 CONTINUE
C
         CLOSE (UNIT = 15)
C
         PRINT*,' '
         WRITE (6,0396) (CTR-1)
 0396 FORMAT (21X,'A TOTAL OF ',I5,' RECCRDS WERE READ IN'//)
```

```
      WRITE (6,0395)
 0395 FORMAT (10X,'THE NEW VALUES OF THE FILM MATRICES HAVE BEEN READ IN
     C FROM THE'/,10X,'FILE FOR008.DAT AND ARE READY TO BE ANALYZED.'//)
      PRINT*,'                                                HIT RETURN'
      READ (5,0306)
      RETURN
C
      END
```

Appendix C

Program Documentation

The purpose of this appendix is to provide some documentation of the program listed in appendix B. This is accomplished by listing the variables used in the program and giving a short description of their purpose.

Introduction

This program is the second in a series of programs written by students attending the Air Force Institute of Technology located at Wright Patterson AFB, Ohio. The purpose of this program, like its predecessor, is to simulate the vapor deposition of thin films. It is written in Fortran 77 and contains a statement using IMSL (International Mathematical and Statistical Libraries), a library of intrinsic functions used for statistical purposes. It was designed to run on a VAX/VMS computer system.

The program is organized into five main sections which includes the the main start-up and four subroutines. The main start-up consist of a help message in order to get the user aquainted with the program and an interface loop. The substrate subroutine allows the user to intialize, create, store, recall and move substrates. The deposition subroutine is used to initialize the main arrays, read in deposition parameters and deposit the film onto the substrate. The analysis subroutine, provides the user the ability to check the density of the film and the angle of growth without having to print out the film. The moving subroutine allows the user to store and recall films for plotting and analysis.

Variable Listing

The following is a listing of the variables used in the program listed in appendix B along with a short description of their purpose. A qualifier on the end of the description, tells in what subroutine of the program the variable was used. The listing is in alphabetical order.

A - A variable derived in appendix A used to find the rest point of the incident disk. - depo

ANDVAR - The number of degrees (full angle) that the angle of incidence should vary about the main angle of deposition. - depo

ANG - The main angle of deposition measured from the subsrate normal. - depo,anal

ANGCK - This variable is used to help in the angle analysis of the film, especially in the density check. - anal

ANGINC - The amount of angle to be incremented or decremented from the old angle of deposition. - depo

ANGLE1,2,3 - Three variables used to hold the angles corresponding to the largest correlation numbers. - anal

ANGMAX - A variable which contains the largest angle, the angle of incidence can have when angle variation takes place. - depo

ANGMIN - A variable which contains the smallest angle, the angle of incidence can have when angle variation takes place. - depo

AVGANG - The average of the angles with the three largest correlation factors used in finding the angle of growth by the film. - anal

A2 - The x intercept of the trajectory for the center of the incident disk. - depo

B - A variable derived in appendix A used to find the rest point of an incident disk. - depo

BNCCTR - A counting variable used to monitor if an extra mobility is to occur. - depo

BNCVAR - The number specifying (indirectly) the percentage of disks to undergo an extra mobility. - depo

BOTHGT - Specifies the bottom height to be checked in the density and angle analysis routines. - anal

BSHFT - This variable used in the mobility routine helps maintain the periodic nature of the film and is like the other shift variables.- depo

BTOL - This variable is just like TOL but is used in the mobility routine. - depo

C - A variable derived in appendix A used to find the rest point of an incident disk. - depo

CELCTR - Counts the number of cells during a streamer check in the the angle analysis routine. - anal

COLL - A variable used to keep track of whether or not a collision has occured during checking of the collision corridor by the streamers. - depo

CORFAC - The correlation number of an individual streamer used to find the angle of growth by the film. - anal

CORR - An array used to hold the correlation numbers for finding the angle of growth by the film. - anal

COSANG - The cosine of RANG. - depo

CRSTRM - The summation of CORFAC across the bottom of the substrate. - anal

CTR - The variable used to specify the number of streamers in the scanning routine. - depo

D - A variable defined from the variables A, K and R1. - depo

DATE - The date and time entered are used to modify the seed of the random number generator in the deposition subroutine. - depo

DENCK - Used to signal that the density algorithm is to be used. - anal

DEPCTR - The main deposition counter which keeps track of how many disks are deposited. - depo

DRESTX - This default variable stores the value of RESTX and is used in case a test is failed in the mobility routine. - depo

DRESTY - The counter part of DRESTX but stores the value of RESTY.- depo

DSEED - The seed numbers used to determine the random numbers in deposition. - depo

F - A variable used to find the y coordinate of the collision point and is derived in appendix A. - depo.

FIL - A counterpart to FILM used to read back in the film for analysis. - move

FILM - A 300 by 200 array used to keep track of whether a cell is occupied by a disk. If its value is zero the cell is unoccupied. - sub, depo,anal,move

G - A variable used to find the y coordinate of the collision point and is derived in appendix A. - depo

H - A variable defined in appendix A and is used to find the rest point of the incident disk. - depo

HCTR - This counting variable keeps track of how many overlapping disks occur during the deposition process. - depo

HDSIZE - This variable holds the last used value of SIZE when an impurity is deposited. - depo

HEIGHT - A variable used to store the largest height of the substrate. - sub,depo

HGT - A variable read in during the creation of the substrate. Its value gives the height or the number of disks to be placed in a column. - sub

HGTIMP - A number determined randomly. If the value of YHGT equals or is greater than this value an impurity is deposited if this is desired. - depo

HGTLAY - Its value specifies the height of each layer in terms of the spatial arrays. - depo

IDKCTR - Counts the number of impurities in a streamer search to find the angle of growth by the film. - anal

IDNCTR - Counts the number of impurities in the local density variation check. - anal

ILNDEN - The line density of streamer for impurities in checking for angle of growth by the film. - anal

IMPCTR - Counts the total number of impurities in the film. - anal

IMPHGT - This variable stores the truncated value of the y position of the impurity after it is deposited. - depo

IMPSET - If equal to one an impurity is about to be or has been deposited into the film. Its value may change to zero if the impurity is covered. - depo

IMPUR - If this has the value of one then an impurity will be deposited randomly into the mircrostructure. - depo

IMPX - This variable stores the truncated value of the x position of the impurity after it is deposited. - depo

ISHFT - The truncated value of XPOS used to help maintain periodic boundaries. - depo

IVAR - This interface variable used throughout the program is responsible for reading in answers to questions asked by the program. - sub,depo,anal,move

K - A variable defined in appendix A and is used to find the rest point of the incident disk. - depo

LARGE1,2,3 - Three values which store the largest correlation numbers for finding the angle of growth by the film. - anal

LAYER - If this has the value of one then a multiple layered film will be produced. - depo

LDNCTR - Counts the number of large disks in the local density variation check. - anal

LDKCTR - A counter of large disks in the streamer search for finding the angle of growth by the film. - anal

LEFT - The default boundary condition on the left side for vertical variations. - anal

LIMPDN - The impurity packing density in the local area check - anal

LLNDEN - The line density of the large disks during a streamer search to find the angle of growth by the film. - anal

LLRGDN - The large packing density in the local area check. - anal

LOCCTR - Counts the number of cells in the local density variation check. - anal

LOCDEN - The total local packing density. - anal

LRGCTR - Counts the total number of large disks in the film. - anal

LSMLDN - The small packing density in the local area check. - anal

MAX - The value of this variable determines how far to the right and up, the area search is to take place around the collision disk looking for possible rest disk. - depo

MIN - The value of this variable determines how far to the left and down, the area search is to take place around the collision disk looking for possible rest disk. - depo

ND - A counting variable used to keep track of the number of disks that have been deposited. - depo

NEWX - The truncated value of XPOS minus ISHFT and is used to determine to what address the search is to take place along an individual row during the scanning routine. - depo

NODSK - The number of disk to be deposited in the deposition of the film if the spatial arrays do not become full. - depo

NOMOB - A variable used in determining the mobility of the disk. If equal to one no mobility will occur. - depo

NUMREC - The number of records to be read back in for analysis. - move

NXINT - The value of XINT minus ISHFT and is used to account for the perodic nature of the film. - depo

OLDANG - The main angle of deposition measured from the substrate normal. - depo

OLDX - The truncated value of OXPOS minus ISHFT and is used to determine from what address the search began along an individual row during the scanning routine. - depo

OXINT - A variable used to minimize the calculations made. It contains the truncated x position of the last streamer intercept. - depo

OXPOS - This variable contains the last new value of XPOS for an individual row during the scanning by a streamer. - depo

OYINT - A variable used to minimize the calculations made. It contains the truncated y position of the last streamer intercept. - depo

P - This variable has the value of 1 or -1 and is used in incrementing or decrementing the angle of incidence. - depo

R - This variable gives the distance squared that a disk has to move before coming to rest. - depo

RAD2 - The radius of the collision disk contact circle squared and is used to find the y coordinate of the collision point. - depo

RANDX - The random number between 1 and 301 used to deposit the disks evenly across the substrate. Its value is the x intercept of the left most streamer. - depo

RANG - The angle of deposition in radians. - depo

RANDY - The random number between 1 and 180 produced in order to decide where the impurity is to be deposited in the mircrostructure. - depo

RANNUM - The randum number between 0 and 1 produced by the IMSL subroutine named ggubfs. - depo

RBNC - An array seven in length and is used like SHORT to keep track of how far a disk has to move before coming to rest. It is used in the mobility routine. - depo

RECCTR - A counting variable used to keep track of how many records are read back in for analysis. - move

RESTX - The x coordinate of the final position of an incident disk. - depo

RESTY - The y coordinate of the final position of an incident disk. - depo

RIGHT - The default boundary on the right side used for vertical variation checks. - anal

RIMPDN - The total packing density due to impurities. - anal

RINC - The incremental radius used to calculate the values of R1 and R2 and is determined by the size of the incident disk. - depo

RLRGDN - The total packing density due to large disks. - anal

RSMLDN - The total packing density due to small disks. - anal

R1 - The radius of the collision disk contact circle and is used in finding the rest point of the incident disk. - depo

R2 - The radius of a possible rest disk contact circle and is used in finding the rest point of the incident disk. - depo

SC2ANG - The secant squared of RANG. - depo

SDKCTR - Counts the number of small disks in the streamer search for finding the angle of growth by the film. - anal

SDNCTR - Counts the number of small disks in the local density variation check. - anal

SET - If equal to one an impurity is about to be or has been deposited. - depo

SHFT - A variable like ISHFT used to keep the film periodic but is used in the rest point determination. - depo

SHORT - A variable used to keep track of how far an incident disk has to move before coming to rest. The smaller the value the shorter the distance. - depo

SINCT - The x intercept of the current streamer. - depo

SIZE - This variable contains information pertaining to the diameter of the disk in question. If equal to one the diameter equals the square root of two, if equal to two the diameter is two times the square root of two, it equal to eight the diameter equals eight times the square root of two. - depo,anal,move

SLNDEN - The line density due to the small disks and is used in finding the angle of growth by the film. - anal

SMLCTR - Counts the total number of small disks in the film. - anal

STRCTR - A variable which contains the current value of incrementation of the number of streamers used to search the collision corridor. - depo

SUBBUF - A 300 by 10 array used to store the occupancy data of the substrate in its development before being transfered to FILM. - sub

TANANG - The tangent of RANG. - depo

TESTY - A variable used to make sure the disk is not below the film array. - depo

TEST1 - A variable used for a number of test. This is used to make sure a collision is possible between two disks. - depo

TEST2 - A variable like TEST1. This is used to make sure the two contact circles do indeed intercept one another. - depo

TEST3 - A variable almost exactly like TEST2 but this one uses the x values to check for intersection between the circles. - depo

TEST4 - A variable used in conjuction with TOL to make sure that the values of X1 and Y1 go together. - depo

TLNDEN - The total line density of the streamer used to find the angle of growth by the film. - anal

TOL - A variable used in conjunctin with TEST4 to make sure that the values of X1 and Y1 go together. - depo

TOPHGT - This is used to specify the top height in the density and angle analysis routines. - anal

TOTCTR - Counts the total number of disks in the film. - anal

TOTDEN - The total packing density of the film. - anal

TPX3 - The truncated value of RESTX, it is used to check for prior occupancy by another disk. - depo

TPY3 - The truncated value of RESTY, it is used to check for prior occupancy by another disk. - depo

TRESTX - A temporary storage place used to store the last value of RESTX. - depo

TRESTY - A temporary storage place used to store the last value of RESTY. - depo

TSHORT - A temporary storage place used to store the last value of SHORT. - depo

TXBNC - The truncated value of XBNC and is used to check for occupancy in the mobility routine. - depo

TYBNC - The truncated value of YBNC and is used to check for occupancy in the mobility routine. - depo

WIDTH - A variable used to determine the values of MIN and MAX. - depo

XBNC - An array seven in length and stores possible x values of rest points for the mobility routine. - depo

XBCK - This is used in the area search of the mobility routine. - depo

XC - A 300 by 10 array used to store the y coordinates of the disks in the development of the substrate before being transfered to YCOORD. - sub

XCOL - Its value gives the current column that the substrate subroutine is working on in the creation of a substrate. - sub

XCOLD - A variable used to store the old values of XC in the manufacturing of the substrate. - sub

XCOLL - The integer value which contains the x address of the collision disk. - depo

XCOOR - A counterpart of XCOORD used for reading back in films for analysis. - move

XCOORD - A 300 by 200 array used to store the x coordinates of the disks. - sub,depo,anal,move

XDIST - A variable used in conjunction with YDIST to find how far a disk has to move before coming to rest. - depo

XINCT - This variable contains the x intercept of the center of the incident disks trajectory. - depo

XPOS - The address of the cell used to start the search of the collision corridor. - depo

X1 - A variable used to calculate the two possible x values of the rest point. - depo

X2 - The x position of the incident disk immediately upon collision with the collision disk. - depo

YBCK - A variable used in the area search of the mobility routine. - depo

YBNC - An array seven in length and stores possible y values of rest points for the mobility rountine. - depo

YC - A 300 by 10 array used to store the y coordinates of the disks in the development of the substrate before being transferred to XCOORD. - sub

YCOLD - A variable used to store the old values of YC in the manufacturing of a substrate. - sub

YCK - A variable used to recalculate the variable YGHT when an impurity is deposited. - depo

YCOLL - The integer value which contains the y address of the collision disk. - depo

YCOOR - The counterpart of YCOORD used to read back in the film for analysis. - move

YCOORD - A 300 by 200 array used to store the y coordinates of the disks. - sub,depo,anal,move

YDIST - A variable used in conjunction with XDIST to find out how far a disk has to move before coming to rest. - depo

YFILM - A variable used to store the largest height of the substrate in conjuntion with determing the thickness of the multilayers. - depo

YHGT - This variable stores the y starting point for the scanning routine for depositing the film. - depo

YI - A variable used to calculate the new possible y coordinate of the collision point. - depo

YTEST - A variable used in the mobility routine to make sure that the film does not become less dense. - depo

Y1 - A variable used to calculate the two possible y values of the rest point. - depo

Y2 - The y position of the incident disk immediately upon collision with the collision disk.

Y3 - The truncated value of RESTY and is used to make sure that mobility is possible near the substrate. - depo

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A VAX-11/785 computer was used to simulate the two-dimensional growth of thin films produced by vapor deposition. In this model molecules and impurities were represented by three different sized disks. In order to simulate varying deposition conditions and evaporants, several variable parameters were introduced. Among these parameters were the variation of the deposition angle about some main angle, the mobility of the disks upon collision, the ability to introduce impurities into the mircrostructure, the simulation of multi-layered coatings and the ability to introduce imperfections into the substrate.

The results obtained by this model show that disks can be used to simulate some of the main features exhibited by vapor deposited films. Among these features are the formation of columns and their compliance with the "tangent rule", and the disappearance of this structure in the case of large disk mobility. Another feature found to be exhibited in the modeled films is that under certian conditions, impurities and substrate imperfections can produce large voids and/or nodules. Other characteristics found in the simulated films include pores which could allow water absorption, and increased packing density for films produced with angle variations along with a moderate amount of disk mobility.

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