The background of the cover is a micrograph showing a complex network of dark, branching, and elongated structures against a lighter, yellowish-brown background. These structures resemble a solidification pattern, such as dendrites or a network of grain boundaries, typical of a metal alloy. The overall color palette is warm, ranging from light tan to deep brown.

Alloy Solidification Modeling

Edited by G. Antipas

Alloy

Solidification Modeling

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Alloy

Solidification Modeling

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Preface

‘Alloy’ is a computer program which predicts the way a material solidifies. The present version considers two components although more than two components can be created by the underlying numerical code. The program is based on the extensive theoretical and experimental studies of solidification that have occurred over the last thirty years. Much of the theory that has been developed has been gathered into the present program. The program itself is designed to be a research tool and a teaching aid. At present, about fifty binary systems are included in the data base but any system can be added and thus treated.

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Oxford 1996

The 'Alloy' computer programme

The 'Alloy' computer programme

1. Introduction:

Alloy is a computer program which predicts the way a material solidifies. The present version considers two components although more than two components can be treated by the underlying numerical code. Other versions of the program treating more components will become available in due course.

The program 'Alloy' is based on the extensive theoretical and experimental studies of solidification that have occurred over the last thirty years. Much of the theory that has been developed has been gathered into the present program. The program is designed to be a research tool and a teaching aid. At present about fifty binary systems are included in the data base but any system can be added and thus treated.

The installation procedure is described in section 2. The program can be operated very simply from the first mouse driven screen; the essential operating details are presented in section 2.1 and 2.2. Section 3 is used to describe the more complex features of the program and as a reference for the operating procedure.

Sections 4-6 are used to provide background information on solidification theory and on the way the theory is implemented in the present program. Section 7 is used to show how various aspects of solidification theory can be illustrated by the program. The limitations of the program are discussed in section 8.

It is suggested that users should read sections 1 and 2, and then load and run the program. Users should then go on to read the other sections once they are familiar with the basic program. In most cases a run takes less than a minute and the results can be viewed as the reactions proceed but in addition high quality hard copies can be produced as a permanent record.

2. Installation procedure:

From the 'DOS' prompt go to the 'ALLOY' floppy disk by typing a: (or b:).

Type *INSTALL* this will make a directory

C:\ALLOY and copy all the files on floppy disk 'ALLOY' onto C:\ALLOY

If a directory other than C:\ALLOY is required the INSTALL.BAT file should be edited.

2.1 Using the program:

The object of these initial instructions is to allow the user to operate the program with the minimum of delay. The various more complex features will be introduced at a later stage. The program may be run from

i) the C:\ALLOY > dos prompt by typing *ALLOY*

ii) the C:\ALLOY> dos prompt in WINDOWS by typing *ALLOY* or

iii) from WINDOWS using the PROGRAM MANAGER to run 'C:\ALLOY\ALLOY.BAT'

The first screen, which should appear after the program starts, is shown in figure 1.

Figure 1. First screen - Main menu.

The screen will show the last run phase diagram. The alloy composition can be altered by dragging the composition line inside the phase diagram using the left mouse button.

The program is run by clicking the 'Run' instruction on the right hand side of the screen or by pressing the return key. The screen changes to the 'run screen' showing four diagrams and the calculations start. An example of the run screen is shown in figure 2.

On the run screen the top left hand diagram is the phase diagram showing the alloy composition line and the initial growth temperature. The top right hand diagram shows the progress of temperature plotted against time. At the end of the run this will give the cooling curve. The temperature axis uses the same scale as that on the phase diagram.

The lower left hand diagram shows a segregation map. In this the composition axis is plotted on the same scale as the phase diagram. A phase boundary appears as a step in composition. During a run the boundary compositions can be seen to follow the phase diagram.

The fourth diagram on the lower right hand side is a schematic representation of the microstructure. The diagram shows the growing solid as cells, rounded dendrites, sharp dendrites, faceted dendrites or faceted needles. The diagram shows the volume fraction of the phases which are present. The phases are either coloured according to the average composition or according to the phases present (controlled by 'struct' flag in section 3.2). Eutectics appear as lamellae and eutectoids as finer lamellae.

Figure 2 The run screen

Unless interrupted by the temperature or time flags (see section 3.2), the program will run until the temperature reaches the lowest phase diagram temperature. Control is returned to the main menu by pressing 'Esc'. If any key other than Esc or F1 is pressed during a run, the program pauses. Any key (other than F1 and Esc) then continues the run.

Pressing 'Esc' at any level eventually returns to the main menu. At the main menu 'Esc' exits the program. At the main menu, the alloy composition and growth condition can be changed and further runs carried out. The next section describes how these changes are made.

2.2 Changing alloy composition, the growth conditions and the phase diagram:

The input data can be changed from within 'Menu F1' (see later) but it is much easier to change data using the mouse at the main menu.

Alloy composition: As mentioned earlier, the alloy composition can be changed by dragging the composition line using the left mouse button at the main menu screen (figure 1). Added control can be achieved by using the left and right arrow keys. The jump for each press can be 0.01, 0.1 or 1% and this is controlled by the up and down arrow keys.

Growth conditions: On the right hand side of the main menu there are a number of growth options. Two of the three, growth rate, temperature gradient and cooling rate will be lit (only

two are independent). These can be increased or decreased by clicking the relevant arrows on the screen. As the growth conditions or alloy composition are changed the cell/dendrite primary spacing and tip undercooling as well as other dependent variables are automatically calculated and displayed on the main menu screen.

Moving the composition line across the screen will mean that different solid phases are formed when solidification first starts. The phase and structure formed is given above the phase diagram on the left hand side. Near the eutectic composition, eutectic will be formed. As will be discussed in section 4.3, the initial phase/structure is predicted by that which grows at the highest temperature. The phases/structures checked are listed above the line showing the predicted phase/structure. Other listed information includes the liquidus temperature and the diffusion coefficients in the solid and liquid phases.

Changing the phase diagram: A new phase diagram may be selected by clicking another diagram from the list displayed on the left. New pages of diagrams can be selected by clicking 'PREV' or 'NEXT'. When a new diagram is selected and changes have been made to the phase diagram data file, an option for saving the changes is given before a new diagram is displayed.

3. Reference section for the Main menu, Menu F1, Editor F2 and Printer F3: Detailed operating procedure:

The program consists of a number of connected programs. The features described in section 2 considers the main part of the program. Three other parts of the program provide more complex control, editing and printing functions. The functions may be called from the main menu by clicking 'Menu F1', 'Editor F2' or 'Printer F3' boxes (alternatively pressing the F1, F2 or F3 keys)

The 'Menu F1' allows a number of different run options to be selected and records data from a previous run. This part of the program also allows a series of instructions to be carried out from a batch file 'DA' during a run. For instance cooling might be required, followed by annealing and then further cooling.

The 'Editor F2' allows the phase diagram to be edited on line and allows the data associated with the single, two and three phases to be changed.

The 'Printer F3' allows stored hard copy data to be viewed and printed as required.

Most of the features on the main menu were presented in section 2. A number of features which are available at the main menu were not covered.

3.1 Additional Main menu features:

A hard copy of the phase diagram can be prepared by pressing Alt F3. This can be printed by going to the 'Printer F3' controller see below.

The scale of phase diagram and later diagrams on the run screen can be adjusted by dragging the corners of the phase diagram using the right mouse button. When the right mouse button

is pressed, the cursor is attached to the nearest corner of the phase diagram. Dragging the corner changes the maximum and minimum temperature, and maximum and minimum composition. The diagram is rescaled by clicking the 'Scaled' box. If a return to the starting scale is required the 'Redraw' box should be clicked. This feature is useful when only a limited range of compositions are needed such as occurs in a dilute alloy.

Temperature flags 'tmin' and 'tmax' can be used to interrupt a run (see section 3.2 variable 12 and 13). The flag temperatures are displayed on the right hand side of the main menu phase diagram (as a $\top$ or $\perp$). The values may be dragged by using the left mouse button.

3.2 Menu F1:

'Menu F1' can be called from the 'main menu', from the 'run screen' or implicitly by the program. A typical 'Menu F1' screen is shown below.

```

Page # 2   File SE   Active keys PgUp, PgDn and F1=help.
nrec = 0.3200E+2, c_mode= 0.2000E+1, c_r = 0.1000E+0, vel = 0.7943E-5
liq_gr= 0.1585E+4, d_dist=-0.1000E+1, und_c =-0.1000E+1, gst =-0.1000E+1
dt =-0.1000E+1, dt2 = 0.1250E+1, error = 0.1000E-9, tmin = 0.2000E+3
tmax = 0.1110E+4, addtim=*****, damp = 0.1000E+1, s_run= 0.0000E+0
pause = 0.0000E+0, centrl= 0.1000E+1, 3d/2d = 0.0000E+1, tot_b= 0.5000E+2
struct= 0.0000E+0, plot = 0.7000E+1, c_r_r = 0.1259E-1, vel_r= 0.7943E-5
.t_gra= 0.1585E+4, .d_dst= 0.4050E-3, .und = 0.3376E+1, .gst = 0.2403E-1
.d_t = 0.1589E+1, .error= 0.1000E-9, Pb = 0.5578E+2, = 0.0000E+0
run = 0.0000E+0
Menu F1 will be called when the temp during a run goes below tmin in C.
0.0000000E+00
Use arrow keys to highlight number to be changed or line in DA to be edited
The DA batch file is as below
'*c_r_r' 0.8 multiply the cooling rate by 0.8
'-tmin' 50. move tmin down 50 K
run 1 run into next page
loops 100 carry it out up to 100 times
end 0 return to manual control

```

Figure 3. The 'Menu F1' screen

The screen shows two types of data; in the upper half, data held in the 'SE' file is displayed and in the lower part the 'DA' batch file is shown; both files may be edited on line.

Data held in the 'SE' file:

The upper section is a list of variables or flags which can be set and also data returned by the program when the program was last interrupted. Thirty three variables are displayed. These are altered most easily by using the arrow keys to move the highlight region to the variable which needs changing. In the figure the highlight region is on 'tmin'. As the highlight region is moved a single line description of the variable is displayed. Here it is 'Menu F1 will be called when the temperature during a run goes below tmin in C'. Where necessary, the line indicates the dimensions of the variable. Below the single line description, the value of the variable is displayed in more detail (this is useful for example for the value of 'addtim')

which on figure 3 is too large for display in the list). The old value of a variable is deleted and the new value entered when a number is typed. A return terminates the entry another return takes the cursor to the 'run' box.

A more sophisticated method of data entry is also available. The user will not need this method unless the 'DA' batch is to be used. The variables may be changed by typing the variable name followed by the value. As an example typing
vel 0.1

replaces the previous value of 'vel' with 0.1

Simple arithmetic operations may also be carried out. Typing

**vel' 1.2*

multiplies the previous value of 'vel' by 1.2. Typing

/vel' 1.1

divides the previous value of 'vel' by 1.1. Similarly for + and -. Note that the single quotation marks should be typed.

Variables starting with a '.' eg '.vel' indicate data returned by the program. These variables are automatically put to zero when a program is run. The presence of a minus sign on some of the variables, such as the diffusion distance, is used to indicate that the value should be calculated by the program.

The variables are stored in the file 'SE'; many different pages can be stored and used. The page number is given at the top left hand corner of the 'Menu F1' screen. On figure 3 'Page # 2' is shown. Different pages may be viewed by using the PgUp or PgDn keys. Details concerning the use of pages are given below when the 'run' variable is discussed.

Each of the variables are listed below with their function. The single line description which appears when the relevant variable is lit is shown in italics and the variable is shown in quotation marks.

1) *Number of records do not change.* 'nrec' This signals the number of records in the 'SE' file the value and should not be changed.

2) *Cooling mode, this should 1 2 or 3 and can be altered on main screen.* 'c_mode' This is the cooling mode flag; only 1, 2 or 3 are valid options. The value can also be changed using the mouse on the main screen. A value of 1 gives steady state cooling, a value of 2 cools at a constant rate and a value of 3 gives a constant rate of heat extraction. The different cooling modes are discussed in section 5.2.

3) *Cooling rate K/s. This will be ignored unless either vel or liq_gr are negative.* 'c_r' This is the imposed cooling rate but will be ignored unless either the tip velocity or the liquid temperature gradient is negative. Only two of the three variables cooling rate, tip velocity and liquid gradient can be imposed; the third depends on the other two. A negative value for the tip velocity or liquid temperature gradient signals that it is the dependent variable. To set a particular cooling rate set 'c_r' and either 'vel' or 'liq_gr'. This variable can be changed (if lit) using the mouse on the main screen.

4) *Imposed growth rate m/s. This will be ignored (ie c_r and liq_gr used) if negative.* 'vel'.

This is the imposed growth rate in m/s. If negative the value of 'vel' will be calculated from 'c_r' and 'liq_gr'. This variable can be changed if lit using the mouse on the main screen.

5) *Initial liquid gradient at tip K/m, will be ignored(c_r and vel used) if negative. 'liq_gr'.* This is the temperature gradient in the liquid at the tip. The value will be ignored if negative and its value calculated using 'vel' and 'c_r'. This variable can be changed if lit on the main screen.

6) *Diffusion distance in m, value will be calculated from the primary spacing if -ve. 'd_dist'.* This is the diffusion distance in m. When negative, the diffusion distance is calculated by the program. A positive entry allows a measured value to be used and the variable can be changed using the mouse on the main screen.

7) *Tip undercooling in K, value will be calculated if negative. 'und'.* This is the tip undercooling. A positive entry allows a measured value to be used and the variable can be changed using the mouse on the main screen.

8) *Fraction solid at tip, value will be calculated if negative. 'gst'.* This is the fraction solid at the tip. When negative it is calculated by the program. A negative entry allows a measured value to be used.

9) *Initial time step in s, the value will be calculated if negative. 'dt'.* This is the initial time step used in the calculation. When negative the value is taken to be one hundredth of the estimated time taken to freeze the sample. The time step is continually adjusted by the program during a run.

10) *This is the increment in dt for a single phase, typically 1.25. 'dt2'.* This is the increment in time step per cycle but is only applied when just one phase is present. At other times the time step depends on the rate of motion of the most rapidly moving two phase boundary.

11) *Initial limiting error which must be reached by each equation, typically 0.1e-9. 'error'.* This is the initial limiting error which must be reached in the composition and temperature equations. During a run the limiting error is modified as described in section 5.2.

12) *Menu F1 will be called when the temperature during a run goes below tmin in C. 'tmin'.* This is the temperature below which 'Menu F1' is called by the program so that new data can be entered from the 'DA' batch file. When a new phase diagram is loaded 'tmin' is set to the minimum temperature on the phase diagram. 'tmin' can also be set by dragging the markers on the right of the phase diagram of the main screen.

13) *Menu F1 will be called when the temperature during a run goes above tmax in C. 'tmax'.* This is the temperature above which 'Menu F1' is called by the program so that new data can be entered from the 'DA' batch file. When a new phase diagram is loaded 'tmax' is set to the maximum temperature on the phase diagram. 'tmax' can also be set by dragging the markers on the right of the phase diagram of the main screen.

14) *Menu F1 will be called when time exceeds time+addtim in s. 'addtim'.* When added to

the present time, it gives the time when 'Menu F1' will be called by the program so that new data can be entered from the 'DA' batch file. To prevent the batch file being called unintentionally 'addtim' should be set to a very large number.

15) *Fraction of change used in the Newton Raphson should be 1.0. 'damp'.* During a Newton Raphson iteration 'damp' is the fraction of the estimated change which is used. This should be set to 1.0

16) *When 0 starts a new run, when 1 the interrupted run is continued. 'srun'.* This is a flag which determines whether a run continues or another run starts. When 0 a new run is started, when 1 the interrupted run is continued. This flag is automatically set when Menu F1 is called by using 'tmin', 'tmax', 'addtim' or when a run is interrupted when the run screen is displayed. The flag is automatically cleared (set to 0) when the program starts or restarts.

17) *Pause flag. 0 no action, 1 pauses each iteration. 'pause'.* This is the pause flag. When set to 1 the program pauses after each Newton Raphson iteration; any key except 'Esc' continues the run. The feature is useful for slowing the program down.

18) *Central difference flag, 0 uses upwind, 1 uses central difference. 'centrl'.* This is the central difference flag. When set to 0 the upwind approximation is used; when set to 1 the central difference approximation is used. The upwind approximation is generally not needed unless very low diffusion coefficients are being used.

19) *Axisymmetry flag, 1 gives axisymmetry, 0 planar growth. '3d/2d'.* This flag determines whether the program uses the axisymmetric or planar solver.

20) *This is the approximate total number of control volumes, 50-800 typically 50. 'tot_b'.* This is the approximate total number of control volumes (or boxes) used to obtain the diffusion solution.

21) *Microstructure flag, 1 colour depends on phase, 0 colour depends on composition. 'struct'.* This is a flag which controls the colours shown on the schematic microstructure. When set to 0 the colour depends on composition. When set to 1 a new colour is used for each phase this is useful when phases have small composition differences. The hard copy options use 1 but do not change the value of 'struct',

22) *Plot flag, (see manual section 3.1), 1 runsceen, 2 fract solid, 4 microseg, 8 temp. 'plot'.* This is the flag which controls the diagrams which can be sent to the printer. The flag operates by adding the values for the different figures together. A value of 1 saves two pages which are similar to the final run screen; the value 2 saves the fraction of the phases present as a function of temperature; the value 4 draws a segregation plot at a series of temperatures or at different times; the value 8 means that temperature rather than time is used for the previous plot. The value $1+2=3$ would mean that the two run screen plots and the volume fraction plots were prepared. The value $4+8=12$ would mean that a series of segregation plots were prepared for various temperatures.

23) *Running cooling rate can be changed if program interrupted K/s. 'c_c_r'* This is the

cooling rate in K/second which was present when the program was interrupted. The value may be changed to a new value to be used if the present run is continued. A change to zero is not valid in cooling mode 1.

24) *Running tip velocity can be changed if program interrupted in m/s. 'cvel'* This is the value of the tip velocity when the program was interrupted. The value may be changed to a new value to be used if the present run is continued. A change to zero is not valid for modes 2 and 3.

Variables 25 to 30 are returned by the program.

25) *Liquid gradient when program interrupted, program output in K/m. '.t_grd'*

26) *Actual diffusion distance used in program in m, program output. '.ddist'*

27) *Actual tip undercooling used by program in K, program output. '.und'*

28) *Actual fraction solid at tip, program output. '.gst'*

29) *Actual time step in seconds, program output. '.dt'*

30) *Limiting error when program interrupted, program output. '.error'*

31) *Composition of alloy in at%. 'Pb'* The symbol shown will be the element which is the solute for the phase diagram. The value may be set in Menu F1 but also may be set using the mouse in the main menu.

32) Not at present used.

33) *Runs program in page see F1 help. 'run'* A value may be entered in the usual way by typing a number. An additional 'return' will exit 'Menu F1'. Control will return to the calling routine. If a run has been interrupted when the run screen was showing by the use of 'tmin', 'tmax', 'addtim' or key F1, it will return to the run screen and continue running; if it was called from the 'Main menu' it will return to the 'Main menu'. The number in the run variable determines which 'SE' page is used. If the starting page is 2 and changes in the options are made; then if 'run 5' is used the changes will be put into page 5 and no permanent alterations will be made to page 2. Any output from the program will be similarly recorded in page 5. Since the first available page is page 2, 'run 0' and 'run 1' have a special meaning. 'run 0' means run in the present page. 'run 1' means run in next page. The use of the 'Esc' key is equivalent to a 'run 0'. Care should be taken not to leave gaps in the pages.

The lower part of the 'Menu F1' screen is the 'DA' batch file.

The 'DA' batch file:

The use of the batch file is a sophisticated use of the program and will be of interest to some but not all users. The 'DA' file is an ASCII file which is a list of instructions which are

carried out if the temperature becomes less than 'tmin' or greater than 'tmax' or the time exceeds start_time + add_time (see variables 12,13 and 14 above). The instructions are identical to those which could be entered from the keyboard if a run was interrupted by the user with the F1 key. The 'DA' file is shown on the 'Menu F1' screen and can be edited by using the arrow keys to move to the line to be edited. A return starts a new line and Ctl (back delete) deletes and removes a line. In the example of the 'Menu F1' screen shown above the 'DA' file consists of.

```
'*c_r_r' 0.8           multiplies existing cooling rate by 0.8
'-tmin' 50.            moves tmin down 50 K
run 1                  runs into next page
loops 100              carry this out 100 times
end 0                  return to manual control
```

To use this batch file the cooling 'mode' flag could be set to 2. The 'tmin' should be set to some temperature say 50 degrees below the liquidus shown on the 'Main menu' screen. When the program is run and when the temperature becomes less than 'tmin', the 'DA' file will be called. The cooling rate will be multiplied by 0.8, 'tmin' will be reduced by 50 K and the program will be run into the next 'SE' page. The instruction 'loop 100' will be carried out when the program returns to the Menu F1 because the temperature becomes lower than the new 'tmin'. The instruction 'loops 100' will return the pointer in 'DA' to the beginning so that the instruction will be repeated. The loop could go round 100 times. The 'end 0' instruction just returns to manual control.

If the 'DA' file was

```
end 0                  return to manual control
loops 100              do it 100 times if necessary
```

When the program runs and for instance the temperature becomes less than 'tmin', the program will pause for manual entries. One of these should be to move 'tmin' so that a return does not immediately occur when the program restarts.

A more complicated 'DA' file would be

```
'*c_r_r' -1.          changes cooling to heating
'+tmin' -100           get the 'tmin' condition out of the way
'+tmax' -100           set the 'tmax' condition
run 1                  run into next page
'*c_r_r' -1.
'+tmin' 100            reset 'tmin'
'+tmax' 100            get 'tmax' out of the way
run 1                  run into next page
loops 100              repeat up to 100 times
end 0                  return to manual control
```

Another possible use would be to reproduce a cooling curve from an experiment. This could be done with a series of cooling rates imposed at different temperatures. The first 'tmin' and cooling rate would be set in 'c_r'.

```
c_r_r 1.1
tmin 620
```

```

run 1
c_r_r 1.2
tmin 580
run 1
c_r_r 1.3
tmin 540
run 1
c_r_r 0.8
tmin 0
run 1
end 0

```

3.3 The Editor F2:

Menu F1 controls the way the program runs; the Editor F2 allows the data associated with each phase diagram to be modified. All the phase diagram data is held in a single ASCII file 'DATA0'. The format of 'DATA0' is given in appendix A; an understanding of the format would be necessary to load a new phase diagram or to modify the data of an existing diagram by using an external editor. No detailed knowledge is necessary to use of the internal editor.

Figure 4, Editor F2.

Changes to the 'DATA0' can be made easily on line by using the internal F2 editor. The F2 editor is entered from the main screen by pressing F2 or clicking on Editor F2. The new screen which appears will be similar to that shown in figure 4.

Any changes made will be present until a new phase diagram is loaded or when the 'ALLOY' program is exited. If changes have been made an option to make the changes permanent will be made before the changes are lost.

Various features may be used:

- 1) Some of the points which make up the phase diagram are shown. Those shown can be dragged by using the left mouse button. Only the compositions can be changed (not the temperature).
- 2) New two phase points may be added. The cursor should be moved into a two phase region at the correct temperature. When the 'Ins' key is pressed a new point is added on each boundary by interpolation.
- 3) Points may be deleted by moving the cursor into the two phase region to a temperature nearest that of the points to be deleted. Pressing the 'Del' key changes the colour of the points and an option of removing the points is given.
- 4) The position of the diagram can be changed using the arrow keys.
- 5) The magnification on the screen can be increased using Ctrl ↑ key and decreased using the Ctrl ↓ key. The change in magnification leaves the cursor position unchanged. First move the cursor to the position which needs to be magnified; then press Ctrl ↑ a number of times.
- 6) A return to the main screen is achieved by using the 'Return' key or the 'Esc' key.

A brief summary of the features are given at the top of the 'Editor F2' screen. The composition and temperature of the cursor is given on the right bottom of the screen.

Changes can also be made by editing the text characters which make up the data. Where possible the cursor should be moved into the one or two phase region to be edited. Pressing the right mouse button then automatically brings up the data for the one or two phase region which may be edited. The single phase data entry will be similar to that shown below.

Aluminium		Single phase dat
0.0 2.4e-4	!Landolt	x,y Do=xC+y m2/s
0.0 1.39e5	!Landolt	x,y q=xC+y J/mol
2e6		Specfc ht J/m3 K
0.1e8		Excess Heat J/m3
150._		Conductvty W/m K

Figure 5.

The left hand side is the data, the source of the data is given in the centre (they are listed in appendix C) and the right hand side is a brief description of the data. If the data has no source, it has been estimated.

Line 1 is the phase, here Aluminium, Al₂Li₃ would mean Al₂Li₃

Line 2, two numerical entries which give D_0 (see section 6.3) this with q is used to give the diffusion coefficient.

Line 3, two numerical entries which give q (see section 6.3).

Line 4, the specific heat in J/m³ K

Line 5, the excess heat H_o in J/m³. The heat content $H = H_o + C_p T$ (see section 6.3)

Line 6, the conductivity in W/m K.

Initially the last line will be lit; the arrow keys may be used to move to the line and characters to be edited. The 'Return' key or 'Esc' returns to the calling screen.

Pressing the right mouse button when the cursor is in a two phase region brings up the relevant two phase data such as that shown below.

Liquid-Aluminium	Two phase region data
1 9	Phases a and b
6	Number of points
660 100 100	Temp, comp a at%, b at%
642.91 91.84 99.36	Temp, comp a at%, b at%
614.70 82.09 98.05	Temp, comp a at%, b at%
587.43 75.04 96.50	Temp, comp a at%, b at%
566.74 70.49 95.20	Temp, comp a at%, b at%
548 67.0 94.3	Temp, comp a at%, b at%
1 13 1 30	Reactn,nphase,opphase,eute
0 0.900E-07 ! --- , Gunduz	Faceting, GibbThomsn coef

Figure 6.

The first line gives the two phases in words, the second the number representing the two phases. The number of a phase is the number of the single phases in the list of single phases. Liquid is the first phase and solid aluminium is the ninth. The third line gives the number of points in the two phase region, here 6. The next 6 lines have three numbers representing temperature, composition of the first and composition of the second phase. The compositions are in the same order as the phases in line 1 and 2.

The penultimate line has four numbers which indicate to the program details of the reaction which occurs after the lowest temperature.

'Reactn' means reaction type. Peritectic (& peritectoid) =2, eutectic (& eutectoid) =1 and end of diagram (no reaction)= 0. Here a eutectic follows after 548 C.

'nphase' means new phase. This is the phase number of the phase which will appear below the 548 C, here it would be CuAl₂ which has the number 13.

'opphase' this means old phase and is the phase which should disappear below the lowest temperature. This would be liquid (ie. phase 1) for a eutectic.

'eute' means eutectic coefficient. This is the constant E_u which appears in the eutectic undercooling equation $\Delta T_E = E_u \sqrt{V}$. At present the same value **must** be entered in both of the two phase regions which occur above the eutectic (E_u is really the only piece of three phase data).

The last line contains two numbers. The first 'Faceting' is a flag which indicates whether faceting occurs. Non faceting=0, faceting=1 and highly faceting (ie needles)=2. The second number is the Gibbs Thomson coefficient. This is needed to calculate dendrite spacing and undercooling.

The values may be edited as for single phase data. Some single phase regions are so narrow that it is difficult to put the cursor inside the single phase region. The phases at the edges may be selected by going outside the phase diagram. For internal phases the name of the phase should be obtained from a two phase region. The single phase data can then be selected at the Editor F2 screen by pressing the F2 key.

3.3. Printer F3:

This is a routine which displays, prints, renames and deletes printer files. Twelve printer files can be prepared during a session. These go from PLOT12 to PLOT23. During a run the plot files which are prepared depends on the plot flag in 'Menu F1' (see 4.2). After a run when control has returned to the Main menu, pressing F3 or clicking the PrntF3 box goes to a screen such as that shown in figure 7. The screen shows the last prepared figure.

Figure 7 Printer F3 screen.

On the left hand side there are a list of options which can be obtained using the keys listed or by clicking the relevant box.

- 1) '*Print file F3*' Sends the present file to the printer (modified by the printer toggle see below)
- 2) '*Print all Shift F3*' This sends all the files made in the present session to the printer (modified by the printer toggle see below).
- 3) '*Rename file Ctl F3*' This allows the displayed file to be renamed and thus made permanent. At the beginning of a session using 'ALLOY.BAT' will delete any file labelled PLOT??. During a session up to twelve files can be prepared if more than twelve are prepared the first are overwritten.
- 4) '*Delete file Del*' This allows the displayed file to be deleted. Deleting a file named PLOT?? is unnecessary since these will be automatically be deleted.
- 5) '*Next file PgDn*' This displays the next printer file.
- 6) '*Previous file PgUp*' This displays the previous printer file. Pressing PgUp a number of times will eventually bring up any printer files made permanent on the present directory. These files can be printed renamed and deleted in the usual manner.
- 7) '*Toggle printer F7*' As the default, the program prepares high quality output for an HPIII printer in a combination of HP3GL and standard HPIII code. This code is sent to the LPT1: device. The program can also prepare 'Word Perfect' graphics code which is stored as a PLOT??.WPG. The latter is of poorer quality. An additional option is to store the HPIII code in a file named PLOT?? which can be sent to a HPIII printer at a later time by for example sending

COPY /b PLOT12 LPT1: at the dos prompt sends PLOT12 to the device LPT1. The */b* ensures the file is sent in the correct way to the printer. The different options can be toggled one after the other; the option chosen is shown by the first line on the left hand side. In the example given above the file displayed is PLOT15 and the data is being sent to the LPT1: device.

The routine displaying the figures is a stripped down version of a full mouse driven plotter/drawing/printing program 'PL' which can be supplied on request. The program 'PL' was used to plot the figures in this manual. The data for the graphs are stored in files 'PLOT??.T'. The format can be supplied on request.

4. Solidification theory:

The purpose of this section is to introduce terminology and to give reference to original work and other work where more detailed information can be obtained.

4.1 The growth of the primary phase:

A phase diagram is shown in figure 8. If alloy marked (i) is cooled, for instance by pulling it out of a furnace, the solid grows directionally into the liquid. Materials typically grow with either a faceted or non faceted interface. The presence of faceting can be predicted using the Jackson α factor[1,2].

Most metals have low α factors and grow with a non faceted interface. For a non-faceted material the solid grows with a planar, cellular or dendritic front[2]. At low enough growth

Figure 8.

rates the solid grows as a planar front. As the growth rate is increased the interface becomes cellular or dendritic. The transition at low velocities is predicted well by the constitutional undercooling condition[2,3]. At very high velocities the planar interface becomes stable again and this occurs at the absolute stability limit. Both transitions were treated by Mullins and Sekerka [2,4]. With a faceting material very roughly the same behaviour occurs. Some materials such as Sb or Bi are only 'slightly' faceted and dendrite like structures are formed. Others with very high α factors grow as needles.

At steady state, when an interface grows with a planar front, the composition in the liquid at the interface builds up until solid is deposited at the same composition as the bulk liquid. The interface grows at the undercooling shown by ΔT_0 on figure 8. During cellular or dendritic growth the cell or dendrite tips grow at a higher temperature (smaller undercooling). The tip temperatures have been measured experimentally[5] and predicted theoretically[6]. The undercooling approaches the plane front undercooling when the velocity approaches the constitutional undercooling condition and the absolute stability condition.

Cells or dendrites often grow as an array, the spacing between tips is called the primary spacing. At low velocities and high temperature gradients, there is a relatively small variation (a factor of about 2) in the spacing of the dendrites on a specimen. The spacings are such that there is a strong interaction between adjacent dendrites. The mechanism for spacing selection is discussed in detail in [6,7]. The smallest spacing is determined by the overgrowth of one cell or dendrite by another[6] and is defined as the array stability limit. The maximum spacing is determined by tip splitting for cells and the growth of a tertiary arm for dendrites. Good agreement has been obtained between theory and experiment for recent models[6,7]

Under other conditions dendrites grow with a wide range of primary spacings. This occurs

at low temperature gradients and high velocities [6,7]. In the present model these dendrites are termed 'Irregular dendrites'. The minimum spacing in this case occurs when dendrites just become close enough to interact near the tip. The tip of all dendrites irrespective of spacing grow near the 'marginal stability condition' [8,9,10]. Originally it was felt that the condition was necessary to define the dendrite tip radius. Recent work indicates that although the condition fits experiment, theoretical steady state shapes are not possible at other values of the tip radius. The problem is discussed in [6].

When cells or dendrites grow solute builds up in the liquid between the cells or dendrites (for a distribution coefficient $k = C_S/C_L < 1$). If diffusion in the solid is small, the build up leads to a variation in solute composition in the first and last liquid to freeze. This variation in composition is known as microsegregation. Traditionally two extreme conditions for microsegregation have been considered. When diffusion is negligibly slow the variation in solid composition C_S , with fraction solid g_S is given by the Scheil equation [eg. 2].

$$C_S = k C_o (1 - g_S)^{(k-1)} \quad \text{where } C_o \text{ is the bulk alloy composition.}$$

The derivation of the Scheil equation assumes complete mixing in the liquid and none in the solid. The other extreme is when diffusion is rapid enough to give an almost uniform composition in the solid. Under these conditions the fraction solid during solidification is given by the 'lever rule'. In practice most materials lie somewhere between the two extremes. A major feature of the present computer model is the numerical treatment of the more general diffusion problem.

To summarise:

- i) Materials grow with a faceted or non-faceted interface determined by the Jackson α factor.
- ii) Planar growth occurs at low and very high growth velocities determined by constitutional undercooling or the absolute stability limit.
- iii) Cells or dendrites grow at some fraction of the planar interface undercooling.
- iv) For cells and regular dendrites the minimum spacing is determined by the array stability limit and the maximum spacing is determined by tip splitting or growth of a tertiary arm.
- v) Microsegregation occurs between the cells or dendrites and determined mainly by the extent of solid state diffusion.

4.2 The peritectic reaction $L + \alpha \rightarrow \beta$:

An alloy of composition (ii) in figure 8 would probably go through the peritectic reaction near T_p . Initially for alloy (ii) dendrites of α would form and as the temperature drops below the peritectic temperature β would form. This would probably nucleate on the α but even if it did not the β would grow towards the α phase. Strictly speaking the peritectic reaction $L + \alpha \rightarrow \beta$ only takes place rapidly at the junction of α , β and L . This means that a layer of β rapidly covers the α phase. Once the α is covered the transformation of α to β is determined by diffusion through the solid phase. A schematic figure showing the steady state growth of a peritectic is shown in figure 9. Traditionally it is assumed that diffusion through the solid is very slow so that very little transformation takes place. In practice the amount of diffusion is usually significant and depends on how rapidly the β phase region expands with decreasing temperature and how much diffusion is necessary (determined by the width

of the α β region). An important feature of the present model is that the diffusion through the β is fully treated.

Figure 9.

Another aspect of growth near the peritectic temperature is that it is not immediately obvious which phase α or β is formed first. The liquidus and solidus of the α and β phases can be imagined to be extrapolated above and below the peritectic temperature. If the phase growing at the higher temperature (lower undercooling) is the β phase no peritectic reaction will take place. In general, because typically β dendrites grow at smaller undercoolings (narrower liquid solid regions), under some conditions β will grow rather than α even when the stable liquidus temperature is above the peritectic temperature. The present model predicts which phase grows by considering competitive growth. That is, the phase chosen is that which grows at the maximum temperature (minimum undercooling).

To summarize:

- i) The amount of β formed from the α phase depends mainly on the amount of solid state diffusion.
- ii) The phase formed initially depends on the interface or tip temperatures for the two different solid phases.

4.3 The eutectic reaction $L \rightarrow \beta + \gamma$:

Figure 8 also shows a eutectic reaction at T_E . Eutectic growth is the cooperative growth of two phases and in this reaction the growth of one solid aids the growth of the other. Generally eutectic spacings are very much finer than cell or dendrite spacings. The average composition of the solid β and γ will be very similar to the liquid composition from which it is formed. Models exist for eutectic growth [2, 11-13] and these are successful for two non

faceted phases. In these systems regular lamellar or rod-like structures are produced. The models predict the eutectic growth temperature and the lamellar or rod spacing. When a faceting phase is present the eutectics are much less regular and grow at larger undercoolings[2,12,13].

The lamellar growth model [11] and experiment shows that the interface undercooling ΔT_E , depends on the root of the growth velocity V .

Alloy (iii) in figure 8 would probably grow as a eutectic without any primary phase since its composition is near the eutectic composition. On the other hand alloy (iv) would probably grow as β dendrites followed by the eutectic. The extent of the eutectic range has been found to be determined by the competitive growth principle mentioned earlier. That is dendrites are present when they grow at a higher temperature. The precise form of the eutectic range differs at high and low temperature gradients. 'Alloy' describes the range equally well for all gradients.

To summarize.

- i) Eutectics grow with fine eutectic structures and with undercoolings below the eutectic temperature of the form $\Delta T_E = E_u \sqrt{V}$.
- ii) Typically the average composition of the eutectic α and β is almost the same composition as the liquid from which it is formed.
- iii) The eutectic range is determined by competitive growth.

5. The numerical model:

5.1 The physical basis:

The basis of the present numerical model is the solution of the diffusion problem for any number of components for any number of phases in two simple geometries, planar or axis-symmetric. A slice through a dendrite or cell such as that shown in figure 9 is followed as a function of time. Earlier more detailed work showed that the slice could be considered in isolation, that is little transport occurs in the direction of dendritic growth.

As a slice cools, the composition in contact with the boundary between phases follows the phase diagram. The change in composition at the boundary leads to diffusion and the movement of the boundary. If solid and liquid is present as the slice cools solidification occurs. If solid state diffusion is negligibly small, the variation in solid composition reproduces the Scheil equation and if the solid diffusion coefficient is large almost complete mixing occurs in both the solid and liquid. Any intermediate amount of diffusion is automatically treated by the 'Alloy' program.

When a peritectic reaction occurs a new solid phase is introduced between the solid and liquid. The growth of the new phase is determined by the interface conditions and diffusion in the three phases α β and liquid.

When a eutectic is formed a new pseudo single phase is considered to have been produced. The phase is assumed to be single phase because only one length scale is treated in the present model. If the eutectic was being fully treated, diffusion and the effect of curvature

would be necessary on the scale of the eutectic. In the present model the pseudo single phase is deposited with the same composition as the liquid.

5.2 The solution to the diffusion problem:

As mentioned earlier the diffusion model can handle any number of phases and any number of components. An implicit control volume technique is used [14]. Each phase is divided up into a number of control volumes (or boxes). A careful account is then made of the fluxes of solute into a box to give the change in composition inside the box. The flux through a control volume wall is the diffusive flux and that due to the motion of the wall. The accumulation of solute within a control volume takes into account the fluxes and the change in volume. The numerical technique is implicit; that is the composition and position at all the control volume centres at the end of the time step are used to calculate fluxes which would change the starting composition to the final composition. The fluxes are calculated by either using the upwind approximation or the central difference approximation [14].

The boundary between phases is placed at a control volume centre. The control volumes within a phase expand or contract as a phase grows or shrinks. An accumulation of solute equation exists for each control volume. The calculated compositions must also be consistent at each phase boundary with the temperature and the phase diagram. This boundary condition between the phases provides an additional equation which allows the boundary motion to be calculated. Since the model is implicit any time step is mathematically stable and the only limitation on step is loss of physical accuracy. A Newton Raphson technique is used to solve the non linear simultaneous equations. Usually three iterations are needed to give errors limited by double precision accuracy (typically 10^{-12} in composition). Flexibility is built in by decreasing the limiting error if less than five cycles are used but increasing it if more than five cycles are required.

All control volumes within a phase have the same size. The control volume size will generally be different for each phase. The size is monitored at each time step and changed by altering the number of control volumes within that phase; when the size is greater than 1.45 times the average size, more boxes are created; when the size is less than 0.69 the average size, boxes are removed. The new compositions and position of the box centres are obtained by interpolation. The minimum number of boxes is taken to be two. The time step is adjusted during a run so that no wall moves more than two box spacings.

Two controls within the program allow the central difference or upwind approximation to be used and allow planar or axi-symmetry to be imposed. Three different growth modes (cooling or heating modes) can be imposed:

- 1) In the first steady state directional growth is assumed. This would apply when a specimen is pulled from a furnace or during the directional growth of a turbine blade. The temperature drop in a time interval is that necessary to account for latent heat evolution and any change in conductivity resulting from the change in fraction of the phases.
- 2) The second mode simply assumes the cooling rate is constant. Since the cooling rate can be changed at will during the run, this means that a cooling curve, for example from a DC casting, can be exactly reproduced.
- 3) The third mode assumes a constant rate of heat extraction. In this mode the temperature at the end of the time step is calculated by the model. This mode produces cooling curves

similar to those obtained during traditional thermal analysis or during differential thermal analysis.

As will be seen later very different cooling curves are produced in mode 1 and 3.

6. Implementation of solidification theory:

6.1 The relevant diffusion length:

Clearly a dendrite cannot really be described by planar or axi-symmetry. A complete treatment of a three dimensional dendrite is not possible. The trick used in the present program and in all approximate analytic descriptions of microsegregation is based on the assumption that reasonable results can be obtained if a suitable length scale and the correct solid state diffusion coefficient is used. The difficulty comes in deciding how to choose the length scale as a function of alloy composition and growth conditions.

Recently, the numerical models mentioned earlier[6,7] have been successfully used to predict cell and dendrite primary spacing as a function of the growth conditions. Analytic expressions have been obtained by fitting the numerical results[6]. Slightly different expressions are used in the present model to predict primary spacings and tip undercoolings. These expressions behave more reasonably when the distribution coefficient approaches zero and can be used for any part of the phase diagram. The expressions are given in appendix B. For the cellular structure it is reasonable that the diffusion length scale should be the primary cell spacing. For dendrites a suitable length scale is more difficult to justify. In the present work, fractions of the primary spacing are arbitrarily assumed to be valid. The fraction is chosen by considering the relative contribution due to the GD/V term and the V^n term (the a_1 and a_2 terms in appendix B) in the undercooling expression. Figure 10 shows a typical plot of tip undercooling against velocity. The minimum undercooling occurs when $a_1 \approx a_2$. Cells are assumed to occur for velocities up to the minimum undercooling and the diffusion distance is taken to be the cell spacing; rounded dendrites are assumed to occur from the minimum undercooling up to the velocity where $10 a_1 = a_2$ and the diffusion distance is taken to be half the primary spacing; sharp dendrites are assumed to occur for larger velocities and diffusion distance is taken to 0.25 times the primary spacing. These values are based on experience and are at least qualitatively correct.

With less justification faceted growth is treated like rounded dendrites and faceted needles like sharp dendrites. Although the previous theoretical model [6] separately predicts cell and dendrite spacing and tip undercooling, only the dendrite results are used in the present work. At this stage the added complexity did not seem to justify separate expressions for cells and dendrites.

6.2. Growth of dendrites, eutectic and peritectic:

On entry to the program data is read from the data base for the relevant phase and the composition is taken from the cursor line on the phase diagram. The primary spacing and tip undercooling is calculated and this then allows the diffusion distance to be calculated. The program automatically checks the constitutional undercooling condition and the absolute stability condition.

When the run starts solid is assumed to be formed at the cell/dendrite growth temperature. Practically when a dendrite grows, the fraction solid increases very rapidly near the tip (see diagram figure 9). To approximate this, solid is assumed to form such that the amounts of solid and liquid are given by the phase diagram at the dendrite growth temperature. This is shown schematically by the dotted line in figure 9. Justification for this approximation is given by the more detailed numerical work[6].

In a system which is terminated by a eutectic reaction, the eutectic growth temperature is compared with the dendrite tip temperature. When the eutectic growth temperature is larger, eutectic rather than primary is assumed to form first. By changing the alloy composition or growth conditions the eutectic region can easily be mapped out. When a primary phase is formed first, eutectic is assumed to occur when the temperature drops to the eutectic growth temperature. As discussed earlier solid eutectic is assumed to have the same composition as the liquid at that temperature.

In a system which has a peritectic reaction, the primary phase formed first is taken to be that which grows at the highest temperature. Both the stable and metastable systems are tested. The metastable system is obtained by extrapolating the last points from the phase diagram below the peritectic temperature. If the high temperature phase forms first the new solid phase is assumed to form when the temperature is such that the new phase does not disappear when placed at the boundary between the original phases.

Monotectics, peritectoids and eutectoids are treated in exactly the same way as the eutectic or peritectic reactions.

6.3. Data:

Details of the way the data can be edited was given in section 4.2 and 4.3. The actual data is discussed in this section. Three types of data are needed. Data associated with single phases, data associated with the two phase boundaries and data associated with the eutectic reaction.

Single phase data:

The heat conductivity K_i and specific heat C_{pi} , are assumed to be constant within a phase. The heat content H_i , is assumed to be given by a constant value H_{oi} and the specific heat term.

$$H_i = H_{oi} + C_{pi}T$$

Latent heats for a transformation appears as the difference in heat content on either side of a phase boundary. The average conductivity and heat content depends on the fraction of the different phases which are present.

Because of the importance of solid state diffusion, the diffusion coefficient is set up as a function of both temperature and composition. The temperature variation is included in the usual way

$$D_i = D_{oi} e^{q_i/RT}$$

The composition variation is included by assuming a linear variation of D_{oi} and q_i with composition.

Two phase data:

The most important two phase data is that obtained from the phase diagram. The phase diagram is stored as a set of two phase regions. Each two phase region has the composition of the two phases listed at a limited number of temperatures. Between any two temperatures the temperature can be linearly related to the composition of one phase and temperature and composition of the two extremes. Similarly the composition on one side of the boundary can be related to the other by a linear expression of the form, $C_1 = a + bC_2$ where a and b are constants which can be expressed as in terms of composition and temperature of the upper and lower points. The general equation allows a reaction at any point in the phase diagram to be treated. Curvature in the phase boundary lines is easily handled by increasing the number of points.

Other listed data for a two phase region includes the Gibbs-Thomson coefficient (needed to calculate spacings) and a flag which determines whether faceting occurs.

Three phase data:

The only three phase data listed at the moment is the eutectic constant E_u relating the eutectic undercooling to the growth velocity ($\Delta T_E = E_u \sqrt{V}$).

7. Examples illustrating aspects of solidification theory.

For these examples ensure that up and down arrows are present for the velocity and temperature gradient on the main menu (see figure 1). If they are not present, go to Menu F1 and make the variable 'vel' (tip velocity) and the variable 'liq_gr' (liquid temperature gradient) positive. Initially, start out with a moderate velocity ($\sim 100 \mu/s$) and moderate temperature gradient ($\sim 2 \text{ K/mm}$). Many of the examples are carried out at the Main menu before a run is carried out.

7.1 Planar interface breakdown:

Select a phase diagram and alloy composition such that the composition line goes through the liquidus and solidus (that is it is not interrupted by a horizontal eutectic or peritectic line. eg alloy (i) figure 8). By clicking on the velocity arrow keys, reduce the velocity until a planar front is predicted (shown just above the left hand corner of the phase diagram). This is the constitutional undercooling limit. Increase the velocity until cells then dendrites are formed. Eventually with increasing velocity the interface again becomes planar and this is the absolute stability limit. The critical constitutional undercooling velocity is given by

$$V_c = \frac{Gk}{DmC_o(k-1)} .$$

The equation applies for a system on the left hand side of a phase diagram with straight solidus and liquid lines. The temperature difference between liquidus and solidus at C_o is given by:

$$\Delta T_o = mC_o - \frac{mC_o}{k} = \frac{mC_o(k-1)}{k}.$$

The temperature difference ΔT_o is shown on figure 8. Using ΔT_o allows a more general expression (which applies anywhere on the phase diagram) to be written as:

$$V_c = \frac{G}{D\Delta T_o}$$

Remembering that ΔT_o is the temperature gap between the liquidus and solidus check that V_c varies in the correct manner with G and ΔT_o .

The absolute stability velocity can be written as [2,6]:

$$V_a = \frac{D\Delta T_o}{\Gamma k}$$

Check that V_a does not depend on G but does depend on ΔT_o (a more general expression for k is given in appendix B).

7.2 Dendrite undercooling and primary spacing:

Repeat the procedure described in the previous section and watch the dendrite tip temperature. This is indicated by the horizontal line on the phase diagram. Near the critical constitutional supercooling velocity and the absolute stability velocity the temperature line on the phase diagram will cross the composition line at the solidus. This is the largest tip undercooling. At an intermediate velocity the undercooling will become very small and almost cross at the liquidus. Very approximately the undercooling is given by

$$\Delta T = GD/V + \left(\frac{\Gamma k \Delta T_o V}{D} \right)^{0.5}$$

The first term is dominant at low velocities and the second term becomes important after the minimum in the undercooling. The more accurate expression used in 'Alloy' is described in appendix B. The term $k\Delta T_o$ is shown on figure 14 and is really the liquidus slope times the difference in the solid and liquid compositions at the liquidus temperature.

Repeat the procedure by watching the primary spacing in the top left box of the Main menu. Except for a very small region near the constitutional undercooling limit the spacing decreases with increasing velocity. At high velocities (low temperature gradients) the label changes from primary spacing to irregular structures. At low velocities (and high gradients) the dendrites interact very strongly and the range of spacing on a specimen is small. At high velocities (and low gradients) little interaction occurs and the minimum spacing occurs when an interaction first begins to occur between the dendrites [6] (see also appendix B). There will be a wide range of spacings on a specimen when irregular structures are indicated.

The average spacing is given approximately by (see appendix B)

$$\lambda = 3.75(\Gamma \Delta T_o k)^{0.23} \left(\frac{V}{D} \right)^{-0.3} G^{-0.47} \left(1 - \frac{GD}{\Delta T_o V} \right)^{0.5}$$

The term on the extreme right is effectively one except near the constitutional undercooling limit. As before $k\Delta T_o$ is the liquidus slope times the difference in the solid and liquid

compositions at the liquidus temperature.

7.3 Temperature time plots - cooling curves:

As an example select the BiPb system using the left mouse button at the Main menu screen. Select a composition somewhere near the peritectic composition (33 At %). Select growth mode 3 and run the program. When the run is complete the top right diagram should show the cooling curve. Cooling mode 3 has a constant rate of heat extraction. This means that when latent heat is evolved there is a smaller decrease in temperature. When eutectic forms all the heat is given out at one temperature so that there is a horizontal plateau. This is the result that might be expected if a thermocouple was placed at the centre of a small casting and heat was extracted from the outer walls at an approximately constant rate. Most textbooks would suggest this is what always happens.

Change the cooling mode to mode 1 and run again. When the run is complete the temperature time trace will be very different. For mode 1 the cooling rate is that which would occur if a thermocouple was placed at one point in a specimen and the specimen was pulled directionally out of the furnace. The heat flow is assumed to be in one direction. When latent heat is evolved, more heat must be conducted down the specimen so that the temperature gradient should be steeper. The steeper gradient would mean that the temperature drops more rapidly. In fact the change in slope can be in either direction because the conductivity in the solid is usually greater than that in the liquid. At high enough velocities the curve should become steeper when latent heat is evolved.

The cooling mode has an appreciable effect on the amount of time spent at a high temperature and thus on the amount of microsegregation.

7.4 Microsegregation:

As discussed in section 4.1 the solid first formed at the dendrite tip can have a very different composition to that formed at a lower temperature. If it is assumed that no diffusion occurs in the solid, the solid composition varies as in the Scheil equation (see section 4.1). Often the amount of segregation critically depends on the amount of solid state diffusion which in turn depends on the scale of the structure and on the solid state diffusion coefficient.

Choose an alloy where the solidus composition varies with temperature. An example would be Bi 20 At% Pb. Carry out a run in growth mode 1. During the run watch the composition versus fraction solid plot on the lower left hand side of the run screen. The composition of the first solid formed gradually changes because solid state diffusion is occurring. Note the amount of eutectic which is present at room temperature. The effect of the solid state diffusion coefficient can be examined by increasing or reducing the diffusion coefficient in order of magnitude steps. This is done by going to the F2 editor, using the right mouse button to select the phase then altering the constant part of the D_0 term (do not make the diffusion coefficient too small as this may cause numerical instability). It should be possible to reproduce a Scheil like dependence. For a low diffusion coefficient an appreciable quantity of eutectic is formed. For a high value of the diffusion coefficient solidification is almost complete as soon as the solidus is crossed and no eutectic is formed. The change in D_0 will not become permanent in the file 'DATA0' unless the save option is taken when exiting the

program or phase diagram.

The cooling mode has an appreciable effect on the amount of microsegregation because of the time spent at a higher temperature. Adjust the solid state diffusion coefficient so that a small but appreciable amount of segregation occurs in mode 1. Then change to mode 3 and run again; the segregation should be considerably reduced.

It is often implied in elementary texts books that the amount of microsegregation is decreased by slow enough cooling. This is generally not true for continuous cooling because the structure gets coarser. The amount of microsegregation can easily be examined as a function of cooling rate using the program.

The amount of microsegregation within a single phase also depends on how much the composition being deposited changes. Move to a system which has an almost vertical solidus followed by a eutectic. In this case the solid composition is constant and the amount of eutectic is always given by the lever rule.

7.5 The eutectic range:

Choose a system such as AlSi, AlCu or PbBi which has a eutectic. Move the composition line to the eutectic composition on the main menu. The first solid 'Eutectic' should be indicated just above the top left corner of the phase diagram. Change the velocity by clicking the arrows. As the velocity increases the eutectic growth temperature decreases because of the eutectic undercooling. The eutectic undercooling (below the eutectic temperature) is determined by the eutectic coefficient E_u which is entered in the phase diagram data base. The value can be altered by using the Editor F2. The eutectic coefficient could be calculated from eutectic theory [11] but is here entered as a single value. The eutectic undercooling is assumed to be given by

$$\Delta T = E_u \sqrt{V}$$

Eutectic is formed without dendrites if the eutectic temperature is above the dendrite tip temperature. This is reasonable because dendrites cannot form if the material is completely solid [2,15]. The dendrite tip temperature was examined above in section 7.2. The dendrite undercooling is measured below the liquidus temperature for the alloy under consideration. This will mean that dendrites will be formed far enough away from the eutectic composition. Examine the transition using the arrow keys to alter the composition. The step for each key press can be 1.0, 0.1 or 0.01 % and can be adjusted using the up and down arrow keys. The structures examined at each composition are shown above the 'first solid' entry. Run the program for an alloy which should be eutectic and another when dendrites should be formed. Note that as soon as dendrites are formed a relatively large amount of primary phase is formed.

It is possible for the structure to be eutectic at low velocities when the GD/V term in the dendrite undercooling is dominant; then as the velocity is increased dendrites form and at higher velocities eutectic is formed once again because the second term in the dendrite undercooling becomes large. This can be demonstrated by moving away from the eutectic composition then clicking the velocity arrows.

Using the eutectic undercooling expression the eutectic growth temperature is given by

$$T_{IE} = T_E - E_u V^{0.5}$$

where T_E is the eutectic temperature and T_{IE} is the eutectic growth temperature.

Using the expression for the dendrite undercooling (given in 7.2) gives

$$T_{ID} = T_o - \frac{GD}{V} - \left(\frac{\Gamma k \Delta T_o V}{D} \right)^{0.5}$$

where T_o is the liquidus temperature for alloy C_o and T_{ID} is the dendrite tip growth temperature. At the transition condition $T_{IE} = T_{ID}$ so that

$$T_o - T_E = \frac{GD}{V} + \left(\frac{\Gamma k \Delta T_o V}{D} \right)^{0.5} - E_u V^{0.5} \quad \text{dividing both sides by the liquidus slope } m$$

gives the eutectic range on one side of the eutectic composition C_E .

$$C_o - C_E = \frac{1}{m} \left[\frac{GD}{V} + \left(\frac{\Gamma k \Delta T_o V}{D} \right)^{0.5} - E_u V^{0.5} \right]$$

The eutectic range can be understood in terms of the relatively size of the three terms. In fact 'Alloy' uses the full expression for dendrite undercooling given in appendix B.

7.6 Peritectic growth:

Various aspects of peritectic growth are easily demonstrated using the 'Alloy' program. Choose a peritectic system such as BiPb. Adjust the velocity so that there is a reasonably large dendrite undercooling; then use the arrow keys to slowly move the composition past the change in liquidus slope at the peritectic temperature and note the phase which forms first. The lower temperature, β , phase will remain for some time after the composition line passes the change in liquidus slope. The change does not occur at the break because the phase selected is the one which grows at the highest temperature. In general, the dendrite tip undercooling will be less for the β phase than for the higher temperature α phase. Note that the GD/V is the same for both phases but that the $k\Delta T_o$ (which is the liquidus slope times the difference in liquid and solid composition) will be larger for the α phase.

The peritectic reaction $L + \alpha \rightarrow \beta$ will only occur if the high temperature α phase is present. The amount of transformation of α to β depends on a number of factors. An important factor is the solid state diffusion in the β phase. This may be examined by altering the diffusion coefficient. Run the program observe the amount of reaction, then go to Editor F2 select the β phase using the right mouse button (see section 3.3) change the constant part of D_o by an order of magnitude and run again (the changes in D_o will not become permanent unless the save option is accepted at the end of a session). The amount transformed also depends on how rapidly the β single phase expands with decreasing temperature. This may be checked by using the Editor F2 to alter the points on the phase diagram using the left mouse button. Another important factor is the difference in composition between the α and β phase at the peritectic composition. This cannot be changed using the mouse but can be changed by changing the β peritectic composition in both the $\alpha + \beta$ and the $\beta + L$ two phase regions using the F2 editor.

8. Limitations:

Every effort has been made to make the present treatment as complete as is reasonably possible. Despite this the limitations of the program should not be glossed over.

Probably the major difficulty is the choosing of the relevant diffusion distance. This has already been discussed in section 6.1. An alternative might be to measure the effective diffusion distance empirically but clearly this would mean that it would not be possible to rapidly examine the effect of phase diagram shape, growth conditions etc. It is felt that the use of a fraction of the primary spacing which depends on dendrite morphology is a serious attempt to treat a difficult problem.

Another difficulty is that, as in almost all solidification theory, it is implicitly assumed that all the phases have the same average atomic volume and that this volume is not a function of composition. That is, as a phase transforms there is no physical flow of material. This will sometimes not be true.

Another obvious limitation is the lack of detailed physical data. The database has been filled with the data that could easily be obtained from references. When a reference has been used it is noted in the database. When no reference is included the data has been 'estimated'. The majority of the data has had to be estimated. Users are responsible for ensuring the data is suitable for their purposes.

During dendritic growth it is known that solid formed at a high temperature is remelted by coarsening of dendrite arms and even by the migration of dendrite arms by TGZM (temperature gradient zone melting)[16]. Both of these effects will reduce the microsegregation. As a first approximation these effects could be allowed for a slightly modified diffusion distance.

Equilibrium has been assumed to occur at all boundaries. This is probably a reasonable approximation for boundaries involving a liquid for velocities up to many cm/sec. In principle it would not be difficult to incorporate a kinetic model such as Aziz [17] but this does not appear to be worthwhile at the present time since it would just involve another set of unknown physical constants.

Another important limitation is that all reactions after the initial growth of a primary phase are assumed to take place by layers of new phases and diffusion within phases. Clearly many solid state reactions actually take place by the nucleation of stable or metastable phases within an existing phase. This type of process cannot at the moment be treated in the present model which only treats one length scale. A similar limitation at present occurs when a phase boundary is crossed from a single to a two phase region. In addition checks are not made to determine the limit of a single phase region except for the formation of the first solid from the liquid.

9. References:

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Appendix A.

The ASCII file 'DATA0' stores all the data associated with a phase diagram. The format is as follows:

The first three lines are

*

AlCu

Al

The * signals a new phase diagram; the next line is the two elements in the binary diagram and should consist of two characters for each element (that is C_Fe is the iron carbon phase diagram). The order of the phase diagrams in 'DATA0' is not important but they have been sorted in the conventional alphabetical order. The symbol on the third line is the element which is the solute (that is the compositions in the AgAu system are expressed in wt % Au).

After the first three lines each of the single phase regions are listed. The first should be the liquid. Each single phase uses six lines eg.

liquid phase 1

0. 3e-9

0. 0.

2.0e6

9.5e8

95.

These are the six lines discussed earlier for the single phase in section 3.3.

Line 1 is the phase here 'liquid'. Only the first word will be read; the phase number is taken from the order in 'DATA0'.

Line 2 two numerical entries which give D_0 (see section 6.3) this with q is used to give the diffusion coefficient.

Line 3 two numerical entries which give q (see section 6.3).

Line 4 The specific heat in $J/m^3 K$

Line 5 The excess heat H_o in J/m^3 . The heat content $H = H_o + C_p T$ (see section 6.3)

Line 6 The conductivity in $W/m K$.

All the single phases are then entered each having six lines. The end of the single phase region is signalled by

end

After the single phases, the two phase regions are entered eg.

Liquid-Aluminium

1 9

6

660 100 100

642.91 91.84 99.36

614.70 82.09 98.05

587.43 75.04 96.50

566.74 70.49 95.20

548 67.0 94.3

1 13 1 30.

0 0.900E-07

The first line gives the two phases in words, the second the number representing the two phases. The number of a phase is the number of the single phases in the list of single phases. Liquid is the first and solid aluminium is the ninth. The third line gives the number of points in the two phase region, here 6. The next 6 lines have three numbers representing temperature, composition of the first and composition of the second phase. The compositions are in the same order as the phases in line 1 and 2.

The penultimate line has four numbers which indicate to the program details of the reaction which occurs after the lowest temperature.

'Reactn' means reaction type. Peritectic (peritectoid) =2, eutectic (eutectoid) =1 and end of diagram (no reaction)= 0. The latter occurs at the lowest phase diagram temperature. In the example given above a eutectic occurs at 548 C.

'nphase' means new phase. This is the phase number of the phase which will appear below the 548 C, in the example above it would be CuAl_2 which has the number 13.

'ophase' this means old phase and is the phase which should disappear below the lowest temperature. This would be liquid (ie. phase 1) for a eutectic.

'eute' means eutectic coefficient. This is the constant E_u which appears in the eutectic undercooling equation $\Delta T_E = E_u \sqrt{V}$. At present the same value **must** be entered in both of the two phase regions which occur above the eutectic (it is really the only piece of three phase data). If 'Reactn' has been entered as a zero none of the other terms have any meaning and can be entered as zeros.

The last line contains two numbers. The first 'Faceting' is a flag which indicates whether faceting occurs. Non faceting=0, faceting=1 and highly faceting (ie needles)=2.

The second number is the Gibbs Thomson coefficient. This is needed to calculate dendrite spacing and undercooling.

Each two phase region should be entered in a similar way. The end of the two phase regions is signalled by an

end

A number of minor complications arise. At a particular temperature there must be only one pair of compositions referring to a particular two phases. This means an intermetallic, which has a maximum in temperature such as AlLi shown below, must appear twice in the single phase list as AlLi(r) and AlLi(l). The (r) and (l) refers to right and left side of the AlLi phase. This means that there is a separate Liquid-AlLi(r) and a Liquid-AlLi(l) region. Another minor complication is that the minimum phase diagram temperature is taken to be the lowest temperature two phase temperature. To show a lower temperature in a diagram which has complete solid solubility an imaginary two phase region is added at the lowest temperature see the AgAu phase diagram.

Appendix B.

In the numerical work on the array growth of dendrites [6] it was found that the dimensionless undercooling $\Delta T' = \Delta T / \Delta T_o$ could be calculated as a function of four parameters. The four dimensionless parameters were chosen to be.

$$G' = \frac{G\Gamma k}{\Delta T_o^2}, \quad V' = \frac{V\Gamma k}{D\Delta T_o}, \quad \lambda = \frac{\lambda\Delta T_o}{\Gamma k} \quad \text{and} \quad k = \frac{C_s}{C_L}.$$

where G , V , Γ , D , m , C_o and k are respectively the temperature gradient, tip velocity, Gibbs Thomson coefficient, liquid diffusion coefficient, liquidus slope, bulk composition and the distribution coefficient, and where $\Delta T_o = mC_o(k-1)/k$. These parameters were chosen because $\Delta T_o = 1$ for a planar front, $V' = 1$ at the absolute stability limit (see section 4) and $V' = G'$ at the constitutional undercooling limit. The form of λ' was chosen so that $V'\lambda' = V\lambda/D$ which is a Peclet number.

It was found that there was a minimum array spacing which was termed the 'array stability limit'. Using the array stability limit as a condition removes one of the four degrees of freedom. The dimensionless undercooling (or primary spacing) can now be calculated as a function of G' , V' and k . The undercooling as a function of G' and V' is shown below in figure 10. Because each distribution coefficient k , gives a simple surface it was possible to give analytical expressions which approximated the numerical results for the undercooling and for spacing and these were presented in [6]. Although the original curve fitting considered distribution coefficients varying from 0.0685 to 0.6975, it later became apparent that the analytic expressions were a poor fit as the distribution coefficient approached zero. The dimensional numerical calculations showed that the tip undercooling and spacing approached a limiting value as $k \rightarrow 0$. This result would seem to be intuitively correct; it is not reasonable to expect a different undercooling and spacing for $k = 10^{-6}$ and $k = 10^{-9}$, since in both effectively all the solute is rejected by the solid. The need for a better expression is particularly important for the 'Alloy' program where the distribution coefficient approaches zero in many systems.

The dendrite solute undercooling:

The difficulty in the analytic expressions arise because of the k in the numerator of G' and V' (also in the denominator of λ'). Note that because of the ΔT_o there is a k^3 in the G' and a k^2 in the V' terms. These powers of k are necessary to line up the undercooling curves so that $\Delta T'$ approaches one at the absolute stability limit and the constitutional undercooling condition. It should be noted that as $k \rightarrow 0$ the dimensional absolute velocity becomes infinity

and the dimensional constitutional undercooling velocity approaches zero.

What is necessary is analytic expressions which have G' and V' as before but the terms are arranged so that powers of k are not left in the final dimensional expressions of undercooling and spacing as $k \rightarrow 0$. Clearly there is no problem with expressions which contain $(1 - k)$.

The search for a suitable undercooling expression provided a good tie in to the earlier analytic expressions. In the earlier analytical work [eg. 15,16] the solute undercooling is assumed to be given by a GD/V term and that necessary to get rid of solute from an isolated dendrite tip. Diffusion of solute from an isothermal (isolated) dendrite tip is given by the Ivantsov solution (see for example [2]). The Ivantsov function

$$I(p) = p \exp(p) E_1(p) = \frac{C_L - C_o}{C_L(1-k)}$$

where p is the tip radius Peclet number given by $p = VR/2D$ and E_1 is the exponential integral function. The equation relates the tip composition C_L , to the tip radius R (or more precisely the Peclet number). The equation can be rearranged to give the dimensional solute undercooling;

$$\Delta T_s = m(C_L - C_o) = \frac{mC_o I(p) (k-1)}{1 + I(p) (k-1)}$$

Provided p approaches a limiting value as $k \rightarrow 0$, this equation approaches a limiting value. Making dimensionless by dividing by ΔT_o gives

$$\Delta T_s' = \frac{\Delta T_s}{\Delta T_o} = \frac{k I(p)}{1 - I(p) (1-k)}$$

The earlier workers proceed by assuming the marginal stability condition. As discussed in [6], the application of the marginal stability condition is not necessary and indeed should not be applied when surface energy is correctly included in the problem (despite this, the dendrite tip always grows with a radius which is similar to the marginal stability condition).

Numerically it was found that the dimensionless curvature undercooling was given by

$$\Delta T_o' = \frac{\Delta T_o}{\Delta T_o} = a(V' - G')^b$$

where $a \sim 0.33$ and $b \sim 0.5$. It is difficult to give precise values for a and b , since various pairs of values give a similar fit. The objective is thus to find a value for b which would make p approach a limiting value as $k \rightarrow 0$ and then to find whether the value of b fitted the numerical results.

Noting that the definition of $\Delta T_o = 2\Gamma/R$ and $R' = R\Delta T_o/\Gamma k$ is the dimensionless tip radius, gives

$$\Delta T_o' = \frac{2}{kR'} = a(V' - G')^b$$

So that $p = \frac{V'R'}{2} = \frac{VR}{2D} = \frac{V^{(1-b)}}{ak\left(1 - \frac{G'}{V'}\right)}$.

When $k \rightarrow 0$, $G' \gg V'$ and $p = \frac{V'^{(1-b)}}{ak}$

Since V' contains k^2 means that if b is precisely 0.5, the Peclet number becomes

$$p = \frac{1}{a} \left(\frac{V\Gamma}{DmC_o(k-1)} \right)^{0.5}$$

and now p only depends only on the $(k - 1)$ term.

The dimensionless solute undercooling (including the GD/V term) now becomes

$$\Delta T'_s = \frac{G'}{V'} + \frac{k I(p)}{1 - I(p) (1 - k)} \quad \text{where } p = \frac{V'^{0.5}}{0.33k(1 - G'/V')}.$$

In section 6.1 $a_1 = G'/V'$ and $a_2 = (k I(p))/(1 - I(p) (1 - k))$. A comparison between the numerical work and the analytic expression is shown in figure 10. The fit is reasonably good and the new expression behaves suitably as $k \rightarrow 0$.

Figure 10. The numerical work is shown by lines and the analytic expression by points for the solute undercooling. Three distribution coefficients are shown 0.6975, 0.14 and 0.00715. It was not possible to get numerical results for all conditions.

The total undercooling becomes

$$\Delta T' = \frac{G'}{V'} + \frac{k I(p)}{1 - I(p) (1 - k)} + 0.33(V' - G')^{0.5}$$

The dimensional form of the equation is used in 'Alloy'.

The primary dendrite spacing:

In the original numerical work it was predicted [6] and later shown experimentally [7] that there is a different relationship between the minimum spacing and velocity at low velocities/high gradient conditions and high velocity/low gradient conditions. In the low velocity region there is a strong interaction between the dendrites and the minimum spacing is determined by the array stability limit. As the velocity increases the interaction between adjacent dendrites becomes smaller and eventually the minimum spacing can only be determined by the spacing where interaction first takes place between adjacent dendrites. The numerical results for the minimum spacing were fitted using two different analytic expressions. Experimentally the measured minimum spacing will be the smallest of the two spacings.

In the low velocity region (high gradient region) region the numerical results were fitted by an expression of the form

$$\lambda' = aV^b \left(1 - \frac{G'}{V'}\right)^c G'^d \quad \text{where } a, c \text{ and } d \text{ were constants and } b \text{ was a function of } G'.$$

The fit was reasonably good for a value of k between 0.068 and 0.69. Unfortunately, as for the undercooling expression, the analytic expression for spacing does not behave well as $k \rightarrow 0$. Dimensional numerical calculations showed that the predicted spacing approached a limiting value as $k \rightarrow 0$ even though the approximate analytic expression does not.

Figure 11. The figure shows a plot of dimensionless spacing against velocity. The lines are the numerical work and the points the new analytic expressions. All the different distribution coefficients are superimposed.

An attempt was made to devise a new relationship but maintain the form of the previous expression. The term $(1 - G'/V')$ goes to one as $k \rightarrow 0$ so that the power of k in λ' , V' and G' should be modified to cancel out any dependence on k in the dimensional expression. An expression which does this is

$$\lambda' = 2.5V'^{-b} \left(1 - \frac{G'}{V'}\right)^{0.5} G'^{-\frac{2(1-b)}{3}}.$$

A good fit of the data is obtained when $b = 0.3 + 1.9G'^{0.18}$ and typically b varies from about 0.3 to 0.6. A comparison between the numerical results and the analytic expression is shown in figure 11.

In the earlier work, the first interaction spacing was taken to the spacing there was a 2% overlap in the dendrite diffusion fields [6]. The numerical results were fitted by

$$\lambda' = 12V'^{-0.94}$$

This is almost a constant spacing Peclet number of 12. When made dimensional the expression is slightly dependent on k . The term in k is eliminated if the equation becomes

$$\lambda' = 12V'^{-1}$$

The fit of the numerical data is almost as good.

An average spacing is required in the program 'Alloy' and this is taken to be 1.5 times the minimum spacing calculated using the array stability limit. When the first interaction spacing is less than the expression for the array stability limit a larger range of spacings on the specimen is indicated by the 'irregular structure' label.

Dendritic growth in any part of the phase diagram:

In the numerical work on dendritic growth it is assumed that the liquidus and solidus are straight lines and cross at the pure material axis. In 'Alloy' any liquid-solid system is treated by extrapolating the local liquidus and solidus line to the point that they cross C_θ . In general the point will not be the zero composition. The term C_o which goes in the dendrite equations then becomes $(C_o - C_\theta)$. The distribution coefficient becomes $k = (C_s - C_\theta)/(C_L - C_\theta)$ and the liquidus slope is unchanged.

Alloy

Solidification Modeling

Alloy

Solidification Modeling

“Alloy is a computer program which predicts the way a material solidifies. The present version considers two components although more than two components can be created by the underlying numerical code. The program is based on the extensive theoretical and experimental studies of solidification that have occurred over the last thirty years. Much of the theory that has been developed has been gathered into the present program. The program itself is designed to be a research tool and a teaching aid. At present, about fifty binary systems are included in the data base but any system can be added and thus treated.”

J.D. Hunt
G. Antipas
R.W. Thomas

Oxford 1996