CONTENTS

D R A F T O P E R A T I N G M A N U A L

F O R

DFM290

A PROGRAM FOR CONSTRUCTING DEFORMATION MECHANISM MAPS

by

P.M. SARGENT

Cambridge University Engineering Department,
Trumpington Street, Cambridge CB2 1PZ, U.K.

JUNE 1993

The program DFM290 is based on current models for deformation mechanisms, and is supplied with data files for a number of crystalline materials. Every care has been taken in selecting the models and in critically assessing the data but further research will certainly improve on both. The program aims to assemble the best of current thinking into a useful package. No guarantee can be given, however, that all possible mechanisms and phenomena are included, or that inaccuracies do not exist in the data. The user must consult the sources and form his own judgement.

This document in 2024 is exactly as it was written in 1990 and edited in 1993, but with the index removed and some font formatting changed because Word is not exactly backwards compatible.

Note that these instructions assume that you are using floppy discs and running the MS-DOS operating system, not Windows.

Philip Sargent
https://www.researchgate.net/profile/Philip-Sargent-2
orcid.org/0000-0002-0968-4467
p.m.sargent.72@cantab.net

TABLE 1: NOMENCLATURE AND UNITS

acD0c	Dislocation core diffusion core diffusion: pre-exponential term (m$/s)
b	Burgers vector (m)
dD0b	Grain boundary diffusion Boundary diffusion: Boundary diffusion pre-exponential term (m/s) ob
Dv	Lattice diffusion Volume diffusion: Volume diffusion coefficient (m3/s)
D0v	Pre-exponentials for volume (lattice) diffusion (m2/s)
g	Grain size (microns)
	Shear strain rate (s-1)
k	Boltzmann's constant (1.38 x 10-26 J/K)
u0, u300	Shear modulus at O K, at 300 K (GPa)
n	Creep exponent
Qb	Activation energy for boundary diffusion (kJ/mol)
Qc	Activation energy for core diffusion (kJ/mol)
Qv	Activation energy for volume (lattice) diffusion (kJ/mol)
Qplc	Activation energy for power-law creep (kJ/mol)
R	Gas constant (8.314 J/mol.K)
T	Temperature, absolute (K)
Tm	Melting point temperature, absolute (K)
	Shear stress (MPa)
	Yield strength (MPa)
	Reference: Stress stress for creep: see text (MPa)
Omega	Atomic volume of diffusing species (m3)
Eo	Activation energy for obstacle-controlled glide (-)
Ep	Activation energy for Peierls stress-controlled glide (-)
	Temperature dependence of the shear modulus (-)

OPERATING MANUAL FOR DFM290

1. INTRODUCTION

This program constructs deformation mechanism maps for metals, ceramics and semiconductors. It uses models and rate equations devised by a very large number of researchers which have been rationalised and summarised in the book "Deformation Mechanism Maps" by Frost and Ashby (1982), and further work published by Sargent and Ashby (see references). Sections 2 to 5 of this manual explain how to load and run the program. Section 6 contains tutorial examples which introduce the user to the procedure for developing accurate maps. Section 7 lists some of the errors that can crop up in the use of the program, and how to fix them. The program code is written in Turbo Pascal version 5.5. No knowledge of Pascal, and no other software, is needed to run it. The disc contains everything.

2. HARDWARE

The program is designed to run on an IBM PC or PS/2, or a Compaq or equivalent, operating under MS-DOS: Version 2.11 or higher, with at least 640K of RAM and optionally, an 8087 math co-processor. It is a great help to have a hard-disc. The program is designed for a micro with a standard colour display (VGA, EGA or CGA), but will run perfectly well on a monochrome system (VGA or Hercules). The only required peripheral is a printer capable of graphics. The standard IBM dot-matrix printer or one of the Epson LX or LQ series printers is fine, but a Hewlett-Packard laserjet or equivalent will require extra software, which is not supplied with this package (see section 7.4). The compiled code is for a 286 or more recent processor, with a numeric coprocessor, but it can be recompiled for older machines without coprocessors very easily.

3. LOADING THE PROGRAM

The disc contains DFM290 in compiled form, together with a number of data files.

3.1 DATA SET: READING READING THE FILES ONTO A HARD-DISC

The best way to run the program is from a hard-disc. If your computer has one, then follow these steps.

(a) Make a DIRECTORY to put the files in. To do so, switch on the computer, wait for the C> prompt and type

```
MD \DFMAP                                    (R)
```

(The slash is a backslash \ , not a /. The (R) means "carriage" return" key). This creates a directory called DFMAP.

(b) Enter the new directory. To do so, type

```
CD \DFMAP                                    (R)
```

(c) Data set: ReadingRead the files into the directory. To do this, put the supplied floppy disc in Drive A and type

```
COPY A: *.*                                  (R)
```

with no spaces after the A. The discs sing for a bit, and finally you get the message

```
18 FILES COPIED.
```

Remove the disc and store it somewhere safe.

3.2 RUNNING THE PROGRAM FROM THE HARD-DISC

Make sure you are in DRIVE C: and in the DFMAP directory, type:

```
CD \DFMAP                                    (R)
```

Then type:

```
DFM                                          (R)
```

((R) means "carriage return").

The Batch files batchfile called DFM.BAT loads graphics memory-resident software (needed to print the maps on your printer, see 7.4) and runs the program DFM290. The opening screen appears. It is described in a moment.

3.3 RUNNING THE PROGRAM FROM THE FLOPPY DISC

(a) Insert the floppy disc in DRIVE A:

(b) Type

```
A:                                           (R)
```

(c) Wait for the A> prompt, and type:

```
DFM                                          (R)
```

The Batch files batchfile DFM.BAT loads GRAPHICS.COM memory-resident software (which you need to print the maps on the printerprinter, see 7.4) then it runs DFM290. The opening screen appears. Section 4 tells you what to do next.

3.4 COMMAND-LINE OPTIONS

The program has a number of options Command line which can be helpful if you are running a lot of data sets of data using your own MS-DOS batch files usage:

```
                                    DFM290 <matlname> <options>

e.g.                                DFMAP290 copper /f /w: \op\copper.lst /s-
```

where

<matlname> is the name of a set of materials parameters previously

loaded into the datafile, such as "copper"

<options> are as below:

/h or /?	brief help and information only - this text
/f	fast option, no interaction with user
/d	as /f above, but with a 10 s delay for each map on the screen
/e	display exit codes only
/s+	produce a strain-rate map (default values)
/s-	do not produce a strain-rate map
/t+	produce a temperature map (default values)
/t-	do not produce a temperature map
/l	write a listing: To a printer of the material parameters to the printer
/w: <fn>	writes the listing : To a fileto a file instead of the printer (<fn> denotes full path & filename)
/o	produce an Olivetti plot (640 x 400) on screen
/c	produce a CGA plot (640 x 200) on screen

Invalid or incomplete options are ignored.

4. RUNNING THE PROGRAM

The opening screen looks like this.

```
DFM290

              M E C H A N I S M  M A P S

      P. M. Sargent, Cambridge University

This program calculates and plots Deformation Mechanism
Maps. Details of the equations and of the models on
which they are based are given in:  H.J. Frost & M.F.
Ashby, "Deformation Mechanism Maps". Pergamon Press,
Oxford, UK. (1983).
    This software comes with NO WARRANTY.

Press W for warranty information
Press C for copying information
Press H for help, including some useful hints

               PRESS ANY KEY TO CONTINUE
```

If you select H you get two screens-full of HELP, outlining the function of the program. Press any other key, such as the space-bar, to proceed. The screen displays:

```
DFM290                                        30 Mar. 1990
CREATE OR READ A MATERIAL DATA SET

Press C to Create a data set for a new material. data
set: Creating
Press R to Read an existing data set: Reading.
Press D to Duplicate data and give it a new name.Data
set: Duplicating

Press H for help screen.
Press A for additional command-line information.
Command line
Press ^C at any prompt to quit (discarding data)

                     MAKE SELECTION
```

Selection 'C' allows you to Create a new data set for a material. Selection 'R' permits you to Read an existing data set. Selection 'H' gives a help screen which reminds you of requirements for a valid material name (a material name can have up to 9 letters or numbers, and certain other symbols and it must not contain any spaces).

The next two subsections detail the operation of the 'C' and 'R' options.

4.1 SELECTION 'C': DATA SET: CREATING A FILE

The program contains special features to help you create and check data sets of material parameters and of map variables. If you make the selection 'C' you will see:

```
DFM290
THE DATA FILE CURRENTLY CONTAINS

     FE-ALPHA       TI-ALPHA     ZR-ALPHA
   ALUMINA        TI-BETA        ZR-BETA
   COPPER       CO-EPSLON       GERMANIUM
    LEAD        MAGNESIA        MAR-M200
    SI3N4        MOLYBDM         NICKEL
  ROCKSALT          SIC         SILICON
   SILVER         SS-304          SS-316
  T-STEEL          TIN         TUNGSTEN
  URANIA        Y-Ba-CuO        ALUMINIUM
POTASSIUM

              Enter NAME of Material ...  copper
```

The upper part of the screen lists data set: Pre-existings of existing data. Do not reuse these names unless you mean to overwrite the existing data, if you do, you will be asked to confirm your decision. (The sets of data and names supplied may differ slightly from those listed here.)

Enter a new material data set name, following the rules (up to 9 characters beginning with a letter, no spaces). As an example: enter DUMMY. Press return.

To be legal, a material name must have one through nine characters (either letters of the alphabet or numbers 0 through 9), and the special characters # % - ( ) $! . Thus

COPPER MARBLE-5 TUNGSTEN and PMMA#1

are all legal names. The data sets are all stored in the same file MATLPARS.DAT. This file can be edited data set: Editingusing any plain-text editor or most word-processors in "non-document" mode. If you do edit the data file directly, it is sensible to do this on a copy and to keep a backup of your original.

Having given a material name, the list of material parameters appears:

```
DFM290                INPUT PARAMETERS FOR        DUMMY
0              Isomechanical Class:
1              Melting point Point          K
2              T-dependence of Modulus

3:             Shear Modulus @ O K          GPa
4:             OK Flow Stress (lattice)
5:             OK Flow Stress (obstacles)
6:             Lattice Glide Actv. Activation Energy
               (mu.b^3)
7:             Obstacle Glide Actv. Activation Energy
               (mu.b^3)
8:             Pre-exp. Volume diffusion Diffusionm^2/s
9:             Activ. energy, Vol. Diff.    kJ/mol
10:            Pre-exp. Bdry Diffusion
               m^3/sBoundary diffusion

11:            Activ. energy, Bdry.Diff.    kJ/mol
12:            Pre-exp. Core diffusionDiffusion   m^4/s
13:            Activ. energy, Diff.         kJ/mol
14:            Power Law Creep Exponent
15:            Reference:  Stress stress, P-L creep MPa
16:            Activ. energy for P-L creep  kJ/mol
17:            Burgers vector               m
18:            Atomic volume Volume         m^3

                  EDIT THE FILE ?  (Y/N)
```

The first parameter is the "Isomechanical Class" . Change the default ("unknown") by pressing the Tab key, you can go back by pressing the Shift and Tab key together. When you find the description that most closely describes your new material, press the Return key. All the rest are numeric. The PARAMETERS are more defined fully in Section 5.1. Enter the best estimates you

can, but put zeros (0) where you don't know a value. When you enter zero, the program calls up scaling relations to estimate values for the missing parameters, using methods which are described in APPENDIX B. When the table is full (it goes over two pages), you will be asked whether you wish to edit it. Answer "N" for "no" this time. You will then be asked whether you wish to save it, press "Y" for "yes" when prompted. Data set: Editing is discussed in a moment.

```
DFM290              Data set: Creating a new file for
                    DUMMY
17            Burgers vector              m    3.5E-10
18            Atomic volumeVolume         m^3
19            Phonon dragDrag Coefficient
20            Electron drag Drag Coefficient
21            Power-Law Breakdown Stress
22            Diffusion:  Cut-off stress
23            Phase Change Temperature    K
                    ENTER PARAMETERS
```

The list of VARIABLES now appears.

```
DFM290              INPUT VARIABLES FOR        COPPER
1             NumberofProgramSteps        =         25
2             Grainsizem                  =    3.OE-05
3             Lowerlimit,S/muaxis         =    1.OE-06
4             Upperlimit,S/muaxis         =       0.01
5             Lowerlimit,T/TMaxis         =          0
6             Upperlimit,T/TMaxis         =          1
7             Firststrain-ratecontour1/s  =    1.OE-14
8             Multiplier: strainrates     =        100
9             Numberstrain-ratecontours   =         10
10            Lowerlimit,StrainRateaxis1/s=     1.OE10
11            Upperlimit,StrainRateaxis1/s=     1.OE-4
12            HighestTemperaturecontourK  =       1356
13            TemperaturebetweencontoursK =        100
14            Numbertemperaturecontours   =         10
                  EDIT THE FILE  (Y/N)
```

These map VARIABLES govern the choice of plot, the range of the axes, the values of variables which are to be held constant in a given plot, and the number of program steps and they include also the grain size of the material. A full description is given in Section 5.2. If you already know some or all of these, enter them. If not, enter zeros (0). The program automatically replaces zeros by reasonable starting values. When the table is full, decline to edit it by pressing 'N' then save it by pressing 'Y'. Edit it if you wish, using the procedure described in Section 4.3). You are now given an opportunity to type a description of the data, your sources and comments. Type anything you like, and finish by pressing the 'Alt' key and the 'W' key at the same time. You will then be given an opportunity to edit your description.

```
DFM290 Data set: Creating a new reference for DUMMY
30 Mar. 1990

       Use the cursor keys, Finish with "Alt-W".
```

You now have a complete set of files for DUMMY. You are asked if you want a printout: See Listing: (a printed list) of the data.

```
DFM290   Immediate printout for   COPPER
SELECT TYPE OF PRINTOUT
Press  N  No Listing.
Press  O  an Ordinary Listing.
Press  E  an Epson dot-matrix REDUCED SIZE Listing.
Press  L  a Laser-printer REDUCED SIZE Listing.Laserjet
```

Press appropriate key (N/O/E/L) If you type 'O', 'E' or 'L' then the tables plus any data check DATA CHECK messages (see next paragraph) are printed.

The program now checks the files against known limits, using isomechanical scaling laws described in Appendix B. You will see

```
DFM290     CHECK ON INPUT DATA FOR COPPER
---------- DATA CHECK COMPLETE ----------


The RUN-TIME for this map is roughly =  61 seconds


        RE-EDIT FILES BEFORE PROCEEDING ? (Y/N)
```

Any parameter or variable which lies outside the expected, normal range is flagged: a message appears on the screen. A DATA-CHECK data check message does not necessarily mean that the datum is wrong, but it is suspect or very unusual. You should check it. Physically unreasonable data will cause the program to abort. If it does, start again by typing DFM and look hard at the DATA-CHECK data check messages when they appear.

Below this is an estimate of the run-time needed to plot one map it depends roughly linearly on the number of steps and on the number of contours (a map with 10 contours and 20 steps takes about 20 seconds one with 150 steps takes 6 minutes on a PS/2-50). Below this is the question

'RE-EDIT THE FILES BEFORE PROCEEDING?'. If you are happy with the files as they are, type 'N'. The program then calculates and plots the maps. They are described in Section 5. When a map is completed, pressing the space-bar will cause it to go on to the next. After the last map, an opportunity to finish is given (see section 4.7 below) and, if you wish to continue, the main menu reappears. If you wish to stop a map in the middle, press the 'Esc' key. This aborts the map. Then press space-bar to go on to the next as usual.

4.2 SELECTION 'R': READING A FILE

To read an existing data set: Reading(rather than create a new set), make the selection 'R' (instead of 'C') at the main menu. The list of available datasets data set appears, as on Page 7. You are asked for a name: enter one of the names on the screen. The name must appear exactly as on the screen (except that lower and upper case letters can be interchanged). If you enter an invalid name the program will ignore it and you will have to type it again correctly.

Enter a name (COPPER for instance) and press return. The name appears in white. If it is what you want, accept it by typing 'Y'. The table of material parameters for COPPER appears:

```
DFM290              INPUT PARAMETERS FOR      COPPER
0 Isomechanical Class:                      fcc
1 Melting point Point K                     =      1356
2 T-dependence of Modulus                   = 0.4823715
3 Shear Modulus @ O K GPa                   = 53.566593
4 OK Flow Stress (lattice)                  =   6.3E-03
5 OK Flow Stress (obstacles)                =   1.3E-03
6 Lattice Glide Actv. Activation Energy (mu.b^3)     =
             0.05
7 Obstacle Glide Actv. Activation Energy (mu.b^3)    =
             0.5
8 Pre-exp. Volume diffusion Diffusion m^2/s          =
             6.2E-05
9 Activ. energy, Vol. Diff. kJ/mo1          =       207
10 Pre-exp. Bdry Diffusion m^3/s            =  5.12E-15
11 Activ. energy, Bdry.Diff. kJ/mo1         =       105
12 Pre-exp. Core diffusionDiffusion m^4/s =   1.0E-24
13 Activ. energy, Core diffusionDiff. kJ/mo1         =
             117
14 Power Law Creep Exponent                 =       4.8
15 Reference: Stress stress, P-L creep MPa=        35
16 Activ. energy for P-L creep kJ/mo1       =       197


                 EDIT THE DATA ?  (Y/N)
```

```
DFM290              INPUT PARAMETERS FOR      COPPER

17            Burgers vector m              =  2.56E-10
18            Atomic volumeVolume m^3       =  1.18E-29
19            Phonon dragDrag Coefficient =   6.OE-10
20            Electron drag Drag Coefficient         =
              2.OE-08
21            Power-Law Breakdown Stress    =   1.OE-03
22            Diffusion:  Cut-off stress    =       0.3
23            Phase change Temperature K    =      1356
                                            PgUp for
more
                EDIT THE FILE ?  (Y/N)
```

and you are given the opportunity to edit it. this is followed by the map Variables, again with the edit option, and finally the 'reference' or comment text. Bibliographic Information

After the material 'Parameters' and the map 'Variables', there is an opportunity to add a textual reference: Text to the source of the information and perhaps a few comments. The text can be edited whenever it appears on the screen, and can be changed by overtyping:

```
 DFM290    REFERENCE DESCRIPTION FOR COPPER
COMMERCIAL PURITY COPPER

Data are from

Frost H.J. and Ashby M.F. "Deformation Mechanism Maps",
Pergamon Press, Oxford (1982) and from

Swinkels F.B. and Ashby M.F. Acta Metall. 29 (1981) 259
and

Helle A.S., Easterling K.E. and Ashby M.F. Acta Metall.
33 (1983) 2163.
                EDIT THE DATA ?   (Y/N)
```

Use the cursor (arrow) keys to move to where your wish to edit. Finish by pressing the <Alt><W> keys together ('W' stands for 'windup'. Again, the offer of editing. Decline in with an 'N' for the moment. You are asked whether you want a hard copy or not. Accepting ('O', 'L', or 'E') dumps the tables, plus any later DATA CHECKdata check messages, to the printer. printer The program then executes a DATA CHECKdata check and displays any material parameters or variables which lie outside the normally expected range. Take DATA CHECKdata check seriously. If one appears, make sure that the number you entered is in the right units and has the right sign. Physically unreasonable data cause the program to abort. If it does, you have to start again by typing DFM290.

```
DFM290     CHECK ON INPUT DATA FOR COPPER
---------- DATA CHECK COMPLETE ----------
The RUN-TIME for this map is roughly =  61 seconds
        RE-EDIT FILES BEFORE PROCEEDING ? (Y/N)
```

The words DATA CHECKdata check COMPLETE mean what they say. Below appears an estimate of the run time per map it depends on the number of steps and number of contours. If the run-time is too long, or you have second thoughts about other parameters or variables, accept the offer of re-edit. Otherwise press 'N'. The program then computes and displays the maps.

4.3 DATA SET: EDITING A SET OF DATA

Whenever a set of data is displayed, the message

```
                EDIT THE DATA (Y/N) ?
```

will appear, sooner or later, along the bottom line of the display. If you accept ('Y'), you are prompted for the line-number that you wish to edit. Enter the number and press (R). The descriptor for that line appears on the bottom line of the display. Enter the new value and press (R). It immediately appears in the table, and (on colour displays) the edited line is picked out in white. The bottom line now reads

```
              FINISHED EDITING (Y/N) ?
```

The response 'N' gives you another go. The response 'Y' terminates editing of that file and confronts you with

```
                SAVE THE DATA (Y/N) ?
```

It is usually best to save it - if you don't, you have no record of the values. If you do, you overwrite the previous version of that data set. Watch out for DATA CHECKdata check messages, and check any change that you have made with special care if one appears. You can get a hard copy of the edited files on the printerimmediately before the maps are calculated even if you haven't saved the data..

4.4 DELETING A SET OF DATA

If your disc gets too full, you may wish to delete some of the data data set: Deletings it contains. To delete a file, exit from the DFM290 program (press 'Q' for Quit when prompted, or press the <Ctrl>C keys at any prompt). The C: \DFMAP> or A: \> prompt appears. Use a word processor or text editor to edit the file MATLPARS.DAT and delete all files beginning with the name of the material you wish to discard. But be careful. Once they are gone, they are gone.

4.5 DUPLICATING A DATA SET

Selection 'D' on the main menu presents the list of existing material data sets and asks for the original material, and then a new name for the copy. It then leads directly in to the editing screens since the normal use for this option is to make some small number of changes to an already loaded data set.

4.6 SELECTION 'S': THE SAME MATERIAL

After all the maps have been produced, the main menu reappears - with an extra option, 'S': Data set: Same

```
DFM290                                          30 Mar. 1990
CREATE OR READ A MATERIAL DATA SET

Press S for the same material.
Press C to Create a data set: Creating for a new
material.
Press R to Read an existing data set: Reading.
Press D to Duplicate data and give it a new name.Data
set: Duplicating

Press H for help screen.
Press A for additional command-line information.Command
line
Press ^C at any prompt to quit (discarding data).^C
<Ctrl><Break>:

                      MAKE SELECTION
```

which, if selected, retains the same data as used in the previous maps without reloading it from disc. (Note that if the data had been edited and not saved to disc, then it is the edited data which will be used again).

4.7 THE END

After the maps are produced, an opportunity to finish quit exit the program is given:

```
                    TO QUIT TYPE  "Q"

              TO CONTINUE, PRESS ANY OTHER KEY
```

5. DATA SETS, PARAMETERS AND THE MAPS

5.1 DATA SETS

A number of data sets are provided with the program, and more can be created by using the Create and Duplicate options from the main menu. A Data Set for a material consists of a set of Parameter values, a set of Variable values, and some Bibliographic information which are described below. The Data Sets supplied with the program are listed in Table 5.1.

TABLE 5.1: DATA SETSdata set

DATA NAME	DESCRIPTION
COPPER	Commercial purity copper
LEAD	Commercial purity lead
NICKEL	Commercial purity nickel
SILVER	Commercial purity silver
TUNGSTEN	Commercial purity tungsten
MOLYBDM	Commercial purity molybdenum
FE-ALPHA	Commercial purity BCC iron
TI-ALPHA	Commercial purity alpha (HCP) titanium
TI-BETA	Commercial purity beta (BCC) titanium
ZR-ALPHA	Commercial purity alpha (HCP) zirconium
ZR-BETA	Commercial purity beta (BCC) zirconium
TIN	Commercial purity tin
MAR-M200	Superalloy MAR-M200
SS-304	Grade 304 stainless steel
SS-316	Grade 316 stainless steel
T-STEEL	Tool steel
ROCKSALT	Sodium chloride, rock salt
ALUMINA	Commercial aluminium oxide ceramic
MAGNESIA	Commercial magnesium oxide ceramic
URANIA	Uranium dioxide
CO-EPSLON	Epsilon phase cobalt
Y-BA-CUO	Yttrium-barium-copper oxideY-Ba-CuO
ZIRCONIA	Zirconium dioxide
GERMANIUM	Germanium, semiconductor purity
SILICON	Silicon, semiconductor purity
SIC	Alpha silicon carbide
SI3N4	Silicon nitride
INSB	Indium antimonite, semiconductor purity

These data provide a starting point only. They are derived from measurements on a wide variety of different batches of material and have not been checked. It is essential that the data are tuned to match the particular batch of material with which you are working. The procedure for doing this is outlined in Section 6. The DFM290 program corrects mistakes which were present in earlier Fortran programs so datasets from ref. (1) will require re-evaluation against even the old experimental data.

5.2 MATERIAL PARAMETERS

The material Parameter Parameter: parameters describe the properties of the material you wish to model. At the very least, you must know Parameter 0, the isomechanical class, and Parameter 1: The melting point. If you know no other (and enter zeros) the program makes sensible estimates for the rest (Appendix B), enters them and proceeds. But you cannot expect the maps to be of any real value if this is all you provide. As you add more data, the estimates for the remaining blanks become more accurate. The idea is to let you compute a first guess for the map it can then be refined by using data from actual yield and creep experiments.

The other MATERIAL PARAMETERS are the obvious ones that are needed to evaluate the models of deformation mechanisms: modulus, yield strength, diffusion Volume, Boundary, Core: coefficients, creep constants, etc. All are in SI units. Stresses are in MPa, shear modulus in GPa. The creep parameters need a bit more explanation, given below, and are discussed

fully in Appendix B. In slightly more detail, then:

Parameter 0: Isomechanical class.

Parameter 1: Melting point, Tm, of the solid, in units of degrees Kelvin (K).

Parameter 2: The temperature dependence of the shear modulus: it is entered as a positive number (e.g. 0.5).

Parameter 3: Shear modulus, , for the material at room temperature, in units of Giga-Pascals (GPa or GN/m2).

Parameter 8: The pre-exponential for lattice diffusion, D, in units of metres squared per second (m2/s).

Parameter 9: The activation energy for lattice diffusion, Q , in units of kilojoules per mole (kJ/mol).

Parameter 10: The pre-exponential for grain boundary diffusion, D the usual pre-exponential is multiplied here by the boundary thickness (usually about 2 atom diameters), so the units are metres cubed per second (m3/s).

Parameter 11: The activation energy for grain boundary diffusion, Q , in units of kilojoules per mole (kJ/mol).

Parameter 12: The pre-exponential for dislocation core diffusion, ac D0c , units of metres to the fourth per second (m4/s).

Parameter 13: The activation energy for core diffusion, Qc, in units of kilojoules per mole (kJ/mol).

Parameter 14: The power-law creep exponent, n. Is the dimensionless exponent in the power-law creep equation = A. (/) . exp (- Q /RT) where is the shear strain rate caused by a shear stress , and n, A and Q are creep constants.

Parameter 15: The reference: Stress stress for power-law creep, , an unfamiliar quantity. It is the stress required to cause a steady tensile creep rate of 10 /s at a temperature of one half of the absolute melting temperature. This way of characterising creep has a number of advantages. For details see Appendix B.

Parameter 16: The activation energy for power-law creep, Q , in units of kilojoules per mole (kJ/mol).

Parameter 17: Burger's vector, b: the dislocation slip distance (in metres).

Parameter 18: The atomic volume, Omega, in units of cubic metres (m).

Some of the parameters will need further adjustment to give an accurate map guidance in doing this is provided in Section 6. When modelling an alloy or a ceramic the atomic volume and the diffusion coefficients are those for the slowest diffusing species if this (as is usual) is rate-controlling in mass transport.

A listing of some of the Parameter data sets provided with the program is given in Appendix C. Tables of conversion factors for units are given in the inside covers of this manual.

5.3 THE MAP VARIABLES

The map Variable VARIABLES include everything that is not a material property.

Briefly, they are:

Variable 1: An important variable - the number of program steps. The value 30 gives a map very quickly, and is useful to check that the axes are set correctly. Increasing the number of steps increases the precision, but it also increases the run-time, roughly in proportion to the number of steps. Use 150 for a really precise

map. The program resets numbers less than 2 to 2 and it resets numbers greater than 300 to 300 (default : 40).

Variable 2: The grain size (in microns, 10 metres).

Variables 3 & 4 The end values of the range of normalised shear stress (/) axis. Default values: 10-6 and 10-2 .

Variables 5 & 6: The end values of the range of homologous temperature (T/Tm) axis. Defaults 0.0 and 1.0.

Variable 7: Lowest contours: Strain rate contour. Defaults 10 s .

Variable 8: The Contours: Multiplying factor by which the strain-rate increases between contours (default value : 100).

Variable 9: The number of contours : Number of(default : 10, giving, with the other default values, contours which span the range 10 to 10 s .

Variables 10 & 11 The range of strain rates for the axes of the strain-rate/stress plot

Variable 12: The temperature of the highest contours: Temperature contour (K).

Variable 13: The Contours: Temperature Difference between temperature contours (K).

Variable 14: The number of temperature contours: Temperature.

If you enter zeros when creating or editing a Parameter or Variable file, the program inserts the default values listed above. The quick way to get started with the program is to enter zeros for everything. Default values

5.5.THE MAPS

Three classes of mechanism contribute to the total strain: plastic yielding, power-law creep, and diffusion. The program uses rate equations for each mechanism, adding the rates when appropriate. The results are presented as Strain-rate-contour, Stress / Temperature axes maps, or as temperature-contour, Strain-Rate / Stress axes maps.

Examples of the two sorts of map are show in Figure 5.1 and 5.2. The left-hand and bottom axes show the normalised variables the right-hand and upper axes show the absolute values of the variables. The numbers at either end of the absolute scales correspond to the marker axis nearest to that end of the axis. If (as occasionally happens when scales are expanded) the axis has only one marker on it, the same number appears at both ends.

The box in the top-right corner shows, in order:

(a) The material name data name (as listed in Table 5.1).

(b) The grain size, in microns.

At the bottom left, the strain rates corresponding to the first and last strain rate contours are listed. The contours differ by a constant multiplying factor which you can set (Variable 15). Here it is 100. The current date is printed at the top right.

The axis can be chosen to cover any sensible range you like: you can, for instance, blow up the bit from T/Tm = 0.5 to T/Tm = 0.55 homologous temperature to fill the whole diagram by setting the range of the temperature axis to these values (Variables 6 and 7). As an example, the boxes marked on Figures 5.1a and 5.2a are shown, expanded by changing the appropriate variables, in Figures 5.1b and 5.2b.

Each map is divided by heavy broken lines into fields showing the range of dominance of a given mechanism. They are identified by abbreviations listed in Table 5.2.

The best way to develop a map is to use a small number of program steps (say 20) to start with, displaying the map on the screen quickly, until you have the axis ranges, contour numbers and spacing, and so on, to your satisfaction. Save the data sets at each stageData set: Saving. When you are happy, change the number of program steps to 150 and rerun. Print the map by pressing the print screen key <PRT SCR>. Examples which illustrate all these points are given in the next section.

TABLE 5.2 FIELD NAMES AND DESCRIPTIONS

FIELD	DESCRIPTION
PEIERLS	Yield, dislocation motion limited by Peierls stress drag
PHONON	Yield, dislocation motion limited by Phonon dragDrag (relativistic and non-relativistic)
RECRYST	Area of the map where dynamic recrystallization is expected
OBSTCLE	Deformation by plastic yielding when the dislocation glide is limited by obstacles
V-DIFF	Deformation by volume (lattice) diffusion of vacancies
B-DIFF	Deformation by grain-boundary diffusion of vacancies
PLC-LT	Low-temperature power-law creep (core diffusion)
PLC-HT	High-temperature power-law creep

6. TUNING THE DATA AND TUTORIAL EXAMPLES

[This section and the tutorial examples were never written in 1993]

6.1 DEVELOPING A DATA SET

6.2 TUNING THE PARAMETERS

6.3 TUTORIAL EXAMPLE 1: MAP FOR COPPER

6.4 TUTORIAL EXAMPLE 2: MAP FOR ALUMINA, AN OXIDE CERAMIC

7. THINGS THAT CAN GO WRONG

7.1 THE PROGRAM WON'T LOAD

(a) Disc in wrong disc drive.

Change to DRIVE A: if you are running from the floppy disc, or to C: \DFMAP if from the hard-disc.

(b) The system reports a Sector Read error, or complains that the DOS is wrong.

You have booted the system with an operating system which is not compatible with that used to make the DFM290 disc. Insert the DFM290 Disc in DRIVE A: and either switch the computer off and then on again, or press <Ctrl><Alt><Del> all at once. The computer will boot from your hard disc. The compiled version supplied was compiled using MS-DOS 6.0 but it has been tested (not extensively) with 3.3, 4.01 andd 5.0.

(c) The program appears to load, but aborts before the first screen appears.

Check that you are running the program from a directory which contains the appropriate Borland Graphics Interface file for your graphics system. This is EGAVGA.BGI for PS/2 computers. A full set is supplied on the disc. If you are a Turbo Pascal programmer, ensure that you are using the Turbo Pascal 6.0 versions with DFM290. Check also that you have sufficient memory, DFM290 requires 248K. Use the program MEMMAP.COM supplied on the floppy disc to check. (Documentation is in the file MEMMAP.DOC).

7.2 THE PROGRAM LOADS BUT REFUSES TO READ DATA OR ABORTS WHEN RUN

The program loads, and reads files, but the data sets they contain is blank or nonsense and the program aborts when you try to plot a map. It is probable that the file MATLPARS.DAT is corrupted. Recopy it from the original DFM290 floppy disc.

7.3 THE PRINTER WON'T PRINT PRINTER

(b) Printer not switched on, is not connected properly, or is out of paper.

(b) Printer set OFF LINE.

(c) Printer incorrectly set up. Go through setup procedure for printer given in the documentation of your computer and printer. Try using the MS-DOS MODE command:

```
MODE LPT1: 80,6                    (R).
```

7.4 THE PRINTER PRINTS TEXT OR RUBBISH BUT NOT GRAPHICS PRINTER

This is the most complex and difficult part of the system. It is nothing to do with DFM290, screen dumps are always difficult.

(a) The printer is of the wrong sort and won't handle graphics.

(b) You omitted to load .iGRAPHICS.COM before running DFM290. Press <Ctrl><Break> and run DFM290 by typing DFM <enter>.

(c) You loaded GRAPHICS.COM from some other hard or floppy disc, and it is for the wrong version of DOS. It is essential that the program GRAPHICS.COM which is loaded by DFM.BAT matches the version of MS-DOS that you use. either re-boot (press <Ctrl><Alt><Del>) with the floppy discsupplied in drive A: , and use GRAPHICS.COM supplied, or copy you own copy of GRAPHICS.COM from your MS-DOS disc into directory C: \DFMAP.

(d) Users of PS/2 and machines with EGA graphics adapters may need to run the program with the /c option to get the lower resolution CGA graphics on screen (type "DFM /c" to run the mapping program) which can be more easily printed. If you insist an using MS-DOS: Version 3.3. with a VGA display you will have to do this.

(e) If you have an Olivetti or AT&T computer then you can get higher resolution plots on the screen by using the /o option when you run the program, e.g. DFM /o. (This may also work with some Compaq computers.) If you want to do screen dumps of these plots you will need to read your MS-DOS documentation of the GRAPHICS command very carefully, and you will certainly need to use the GRAPHICS.COM program which came with your computer.

(f) If you have a Hercules graphics adapter then the appropriate dump program screen dump program is HGC.COM or MGC.COM, instead of GRAPHICS.COM and it should have been supplied with your computer. One solution to graphics dump problems is to purchase a commercial screen-capture utility which supports a wid range of printers - including HP LaserJets. We have found Graph-Plus to be effective. It can be ordered from "Grey Matter", 2 Prigg Meadow, Ashburton, Deven TG13 7DF, or see their regular advertisements in Byte magazine (tel. +44 (364) 53499). Alternatively, your word processor or desktop publishing program may have a screen-capture utiltiy with which you can dump screens into your word processor. MS Word 5.0 for DOS does this. Remember: run GRAPHICS before running DFM290 if you want to dump the plot to a dot-matrix printer. Do this by running the program GRAPHICS.COM supplied with the MS-DOS operating system which came with your computer. The batch file DFM.BAT does this automatically..

You can get a hard copy of the screen by pressing the <PRT SCR> key when the plot has finished and is labelled on the screen. This key may require the shift key to be pressed to be effective.

7.5 RUN-TIME ERRORS

Run-time errors halt the running of the program and abort it. To recover, you have to exit from the batch file DFM when prompted, then retype DFM and start again. (If you want to abort the program deliberately, press the <Ctrl><Break> keys. It only works when the program is paused, awaiting an instruction. When it is plotting, however, it checks the keyboard intermittently, so while it will stop, it may take a while to respond.) A run-time error gives an error message which looks like this:

Run-time error 160 at 0779: 6041

Run-time error 103 at 0DF1: 002E

The origins of run-time errors are these:

(a) The printer was not switched on when you tried to print (error 160) or it is out of paper (error 159).

(b) You pressed the <Ctrl><Break> Keys in the middle of the program run (error 103).

(c) You read a data set with wildly incorrect numbers in it.

Some parameters have to be positive (and, when properly chosen, always are) positive others, non-zero. Errors of this sort result in the program dividing by zero, or taking the square root of a negative number, and that gives Run-time errors 200 to 207 (but see 7.6 below).

Reload DFM290, check the data file MATLPARS.DAT, and look at the DATA CHECK data check messages when they appear. The program contains numerous checks, and inserts default values which, as far as possible, prevent this

happening. But you are much cleverer than it is, and you may find a way round the protection.

(d) Error 150 occurs if you try to save the data sets to a file on a disc which is write-protected. In all cases, the only solution is to abandon the batch file and type DFM to reload and start again. In extreme cases, you may have to turn off your computer, wait 10 seconds, and turn it back on again before you type DFM again. Floppy disc: Full Hard-disc: Full Data set: Saving Disc Hard-disc, Floppy disc:

7.6 SUBTLER PROBLEMS

There is always the possibility that "resident" programs which are loaded and stay in memory while DFM290 runs may cause problems. If a persistent error occurs, reboot your computer and run DFM290 as the first program you run. Examine your CONFIG.SYS and AUTOEXEC.BAT files for programs and device drivers. Use the program MEMMAP.COM (supplied on the disc) to investigate the memory use in your computer, documentation for this program is in the file MEMMAP.DOC. These problems can apperar as run-time errors of all kinds.

At this stage, the only additional problems I have encountered arise from faulty discs, which misread. A particular problem occurs with discs formatted as 360K but written-to using 1.2M (/AT compatible) floppy disc: Errordrives.Back-up

ALWAYS KEEP AT LEAST ONE BACK-UP COPY OF THE WHOLE DISC

APPENDIX A: THE MECHANISMS AND RATE EQUATIONS

A number of mechanisms contribute to deformation. They are fully-described in ref.1 by Frost and Ashby (1982).

Each mechanism can be modelled to give a rate-equation which defines the contribution of that mechanism to the current strain rate. they are central to the way the program works. rate equation consitutive equationEach has the form:

eps-dot = f(S, T, parameters) (1)

where eps-dot is the steady-state strain rate, S is the stress, and T the temperature. There are 12 rate equations in all.

The program evaluates the rate equations at each temperature step and several iterations are required to locate each strain-rate contour. the number of temperature steps is set by variable 17.

The equations for deformation are taken directly from the book by Frost and Ashby (1982). The five important mechanisms are:

(a) Obstacle controlled glide (OBSTCLE)

(b) Vacancy diffusion through the volume of the grains (V-DIFF)

(c) Vacancy diffusion along grain boundaries (B-DIFF)

(d) Power-law creep, both low-temperature and high-temperature varieties

(e) Harper-Dorn creep, another dislocation mechanism

(f) Phonon dragand electron drag controlled glide

(g) Peierl's stress controlled glide

(h) Dynamic recrystallization.

The equations are summarized here. There are a few slight changes and additions to the rate equations as published by Frost and Ashby and these are noted below in context. The rate equations are listed in Table A1, most have the form of equation (1). The symbols are defined in Table A2.

TABLE A1: Equations for Strain Rate

Obstacle controlled glide

Volume diffusion

Boundary Diffusion

Power-law creep high-temperature

Power-law creep low-temperature

Harper-Dorn creep

Phonon dragand electron drag controlled glide

Peierls stress controlled glide

Dynamic recrystallization

APPENDIX B: SCALING RELATIONS

The properties of a material are not independent of each other. Metals with high melting points have high moduli, high surface energies and (at a given absolute temperature) low rates of diffusion. Alloys with high yield strengths generally have high creep strengths. Detailed studies of these correlations lead to scaling relations which allow estimates to be made of some material properties when others are known. Scaling rlations are used in the program in two ways:

(a) To check all data entered by the user. If the data do not lie within the expected limits, a DATA CHECK data checkmessage is displayed on the screen, and is printed (with more details) when a printout is requested.

(b) To estimate data when real experimental values cannot be found. When a zero (0) is entered in teh table of material parameters when Creating or Editing a data set, the program automatically calls on these relations to estimate a value for the unknown datum.default values estimate data set: Creating data set: Editing The value is, of course, only an estimate, but it is of the right order of magnitude and it allows the user to get started. Then he or she can adjust the estimated parameters to give a good fit to experimental deformation data, as described in section 6. (If zeros are entered when creating or editing the map Variables the program again estimates sensible values indeed the best way to start is to enter zeros for all the Variables.)Variable Parameter

This appendix lists the scaling relations used in the program. The interested reader will find details of their origin, and more sophisticated methods, described in Frost and Ashby (1982, Chapter 18) and in Brown and Ashby (1980a, b).

The same scaling relations are used for all materials, but the scaling parameters are different for different isomechanical classes of materials.Parameter: Scaling

1. The melting point Tm, Young's modulus E and atomic volume Omega of metals and ceramics are related by:

$$E = 100\,k\,T_m / \Omega \qquad \textbf{(B1)}$$

where k is Boltzmann's constant (1.38 x 10-23 J/K). The error seldom exceeds 35%.

2. The temperature dependence of the modulus: Temperature-dependence of metals and ceramics, when normalised in the way shown in the next equation, almost always lies in the range -0.1 to -0.95. CHecking is based on this range estimation uses:

$$\frac{T_m}{\mu_0}\frac{d\mu}{dT} = -C_0 \qquad \textbf{(B2)}$$

(the minus sign is omitted in entering the data - the program inserts it automatically). Different isomechanical classes have different values for C0, e.g.

0.5 for body-centred cubic transition metals

0.1 for tetrahedrally-bonded semiconductors

3. The yield strengths of materials in comparable states of purity scale as the modulus, that isyielding

$$\sigma_y = C_1 E \qquad \textbf{(B3)}$$

For commercially pure metals (those with an impurity level of perhaps 0.1 atom %), C1 is about 1/1000. For heavily alloyed metals it can rise to 1/100 and for ceramics it can be as high as 1/50.alloying purity

4. The activation energy for volume diffusion, Qv, is related to the melting temperature by

$$\frac{Q_v}{RT_m} = C_2 \qquad \textbf{(B4)}$$

where R is the gas constant and C2 is about 18 for metals and 25 for ceramics. The value is quite well defined for quite subtle distinctions between isomechanical classes, and these are used in the program.

5. The pre-exponential, D0v, is found from the observation that the melting point : Diffusivitydiffusivity, for a given class of solid, is given approximately by:

Dv(Tm) / Omega2/3 = C3 (B5)

where C3 is about 10^7 s^{-1}.

6. Boundary diffusion parameters are estimated by a similar procedure. For the activation energy

Qb/RTm = C4 (B6)

where C4 is about 11 for metals about 15 for simple ceramics. This usually corresponds to the approximation

Qb = 0.6 Qv (B7)

The pre-exponential is estimated from

dD0b = 2 Omega1/3 D0v (B8)

6. Power-law creep is described in the following way. We start with the conventional description

eps-dot = A.Sn.exp -(Qplc/RT) (B9)

where n and A are creep constants. Define Sref as the stress which will cause a uniaxial strain rate of 10^{-6} s^{-1} at a temperature of exactly one half the absolute melting point (T=Tm/2):

106 = A.Srefn.exp -(2Qplc/RTm) (B9)

Dividing the first by the second gives

eps-dot = 10^{-6}.(S/Sref)n.exp -{(Qplc/RTm). (T/Tm - 2)} (B9)

This is the form of the creep equation used by the program for high-temperature power-law creep. Its great advantage is that it minimizes extrapolation errors (because creep testing, typically, is carried out at temperatures around or higher than Tm/2 and involves strain rates of 10-6 s^{-1}), and it makes checking simpler (because Sref is usually of the order of Sy/2).

The creep exponent, if unknown, is best estimated by

n = 3 (B10)

(but see Brown and Ashby (1980a, b) and Derby and Ashby (1987) for more information on this point.) The activation energy for creep is for many materials the same as that for volume diffusion

Qplc = Qv (B11)

The Stressstress Sref, defined as above, is conveniently read from a deformation mechanism map. (Remember to convert shear stress to uniaxial stress if necessary by multiplying by 1.732). When asked for a reference stress, if you reply with a zero (0), a secondary menu will appear in which you can enter a uniaxial stress, a uniaxial strain-rate and a temperature. This will calculate the reference stress for you. If you reply with zeros to all three of these, then the estimate of Sy/2 will be used, taking Sy from the obstacle-controlled flow stress.yielding

You should be aware that for certain creep-resistant alloys, particularly the superalloys, Sref can be greater than Sy. This is not as silly as it sounds: it is caused by the fact that creep is neglible at Tm/2 in these alloys.

APPENDIX C: DATA, DATA SETS AND SOURCES

Developing an accurate parameter data set : Sourcesreference: Text(that is, a set of the material parameters listing in section 5.2) for a material is an iterative process. The starting point is data for the properties of the bulk solid. For some materials (like pure copper) these are well-established, the problem is simply that of finding them. For others (like Y-Ba-CuO) the proerties have to be estimated by the methods outlined in Appendix B. But the data have to be "tuned" in the way described in Section 6 of the text, and illustrated in the case studies.

The data provided with the program gives starting point values for 22 materials. The data given here provides only a first estimate for a given material. No confidence should be placed in this data without first checking original sources yourself. It is supplied to show you what to expect, and tuning should involve only relatively small changes in the parameters.

This section gives the parameter data sets in the order given in Table C1, and gives sources. Often, once source lists most of the properties - then the single source is quoted. Where data have been assembled from several sources, details are given.

REFERENCES

data set : Sourcesreference: Text

American Institute of Physics Handbook (1972) 3rd edition, Am. Inst. of Phys. and McGraw-Hill.

[Ash75] Ashby, M.F. (1975) Acta Metall. 11 591.

ASM Metals Handbook (1975), Vol.8 8th edition, American Society for Metals, Metals Park, Columbus, Ohio, USA.

[Bro80a] Brown, A.M. and Ashby, M.F. (1980) Acta Metall. 28 1085.

[Bro80b] Brown, A.M. and Ashby, M.F. (1980) Scripta Metall. 14 1297

Diffusion Data (1968 to present) a journal taken by most science libraries.

[Fro82] Frost, H.J. and Ashby, M.F. (1982) "Deformation Mechanism Maps", Pergamon Press, Oxford.

Landholt-Bornstein Tables III-1 (1966) and III-2 (1969), SPringer-Verlag, Berlin.

[Mal80] Malakondaiah, G.A. (1980) Ph.D. thesis, Banares Hindu University, Varanesi, India.

Metals handbook (1961) Vol.1, ASM, Columbus, Ohio, USA.

[Sim71] Simmons, G. and Wang, H. (1971) "Single Crystal Elastic Constants and Calculated Aggregate properties", 2nd edition, MIT Press.