1 of 1

BNWL-SA-4114

CONF-711025--2

HYBRID COMPUTER SIMULATION OF RADIATION DAMAGE ANNEALING IN METALS*

by

R. A. Burnett

Battelle--Pacific Northwest Laboratory

Richland, Washington

October 22, 1971

*Based on work performed under United States Atomic Energy Commission Contract AT(45-1)-1830.

DISCLAIMER

INTRODUCTION

An important source of damage to a solid exposed to high energy neutrons (or ions) is the displacement of atoms from normal lattice sites. In a fast reactor, energies of tens of keV may be transferred to the primary knock-on atom (PKA), producing in medium and high atomic weight materials a displacement cascade comprising a localized high density of point defects in the atomic lattice. These defects will subsequently interact with one another to produce clusters and to reduce their density by mutual annihilation-- a process called short-term annealing in the present context.

The objective of this work was to study by computer simulation the defect clustering characteristics of γ-iron, a stand-in for the stainless steel used in fact reactors, under various simulated environmental conditions. An α-iron model has also been simulated. The technical results and implications of these studies have been reported in previous papers.[1,2] This paper presents a detailed description of the computer programs and simulation techniques which were applied.

POINT DEFECTS AND RADIATION DAMAGE IN METALS

A brief discussion of point defects in atomic lattices is presented in this section in order to introduce certain terms that will be used in the subsequent discussion. Reference 3 is a good source of additional information.

Several common metals crystallize in either the body-centered cubic (bcc) or face-centered cubic (fcc) structures. The former can be characterized by a cubic cell of size c with atoms at the corners and at the center of the cube; the latter has atoms at the corners and at the centers of the faces of the cube. The half-lattice unit (hlu), equal to the quantity c/2, is the unit of length used throughout this work. The symmetry of the lattice results in groups of atoms having equivalent positions with respect to a given atom. These neighbor shells are described in Table 1 for the fcc lattice.

Table 1.

FCC Neighbors

Neighbor	Relative Coordinates	Distance (Half-Lattice Units)	Number	
1	(110)	$\sqrt{2}$	12	
2	(200)	$\sqrt{4}$	6	
3	(211)	$\sqrt{6}$	24	
4	(220)	$\sqrt{8}$	12	
5	(310)	$\sqrt{10}$	24	
6	(222)	$\sqrt{12}$	8	
7	(321)	$\sqrt{14}$	48	
8	(400)	$\sqrt{16}$	6	
9	(330)	$\sqrt{18}$	12	36
9	(411)	$\sqrt{18}$	24	
10	(420)	$\sqrt{20}$	24	
11	(332)	$\sqrt{22}$	24	
12	(422)	$\sqrt{24}$	24	
13	(431)	$\sqrt{26}$	48	72
13	(510)	$\sqrt{26}$	24	
14	(521)	$\sqrt{30}$	48	
15	(440)	$\sqrt{32}$	12	
16	(433)	$\sqrt{34}$	24	48
16	(530)	$\sqrt{34}$	24	
17	(442)	$\sqrt{36}$	24	30
17	(600)	$\sqrt{36}$	6	
18	(532)	$\sqrt{38}$	48	72
18	(611)	$\sqrt{38}$	24	
19	(620)	$\sqrt{40}$	24	
20	(541)	$\sqrt{42}$	48	

There are two types of point defects which can occur in the lattice as a result of atoms being displaced from their normal positions. The absence of an atom at a normally occupied lattice site is called a vacancy. An atom which is located at an interstice rather than at a normal lattice site is termed an interstitial. Actually a displaced atom will cause an adjacent atom to move over and share its lattice site, thus creating a pair of atoms near and on opposite sides of the lattice site. The interstitial is then said to be located at the lattice site about which the two atoms are split. The line joining the two atoms defines the orientation of the split interstitial.

Although there are stable interstitial positions, they are of considerably higher energy than normal sites and therefore remain unoccupied in the absence of sufficient excitation; however, a metal placed in a fast reactor is bombarded by energetic neutrons that transfer much of their energy in collisions with the atoms. An atom receiving sufficient energy is displaced from its normal site, leaving behind a vacancy, and may in turn displace other atoms. When the energy of a moving atom becomes too low to cause further displacements, it will come to rest as an interstitial unless it finds a vacancy with which it can recombine. If the latter event occurs, both the interstitial and vacancy cease to exist and are said to be annihilated. The totality of interstitials and vacancies resulting from a single neutron-atom encounter is commonly called a "displacement cascade."

The formation of the cascade is very rapid, requiring perhaps 10^{-13} seconds. The process of formation is such that the spatial distribution of defects is characteristically a vacancy-rich central region surrounded by an interstitial-rich peripheral region. The vacancy concentration is sufficiently high that numerous vacancy clusters are formed, but essentially all interstitials are unclustered initially. A cluster is defined as two or more defects of the same

type in close proximity with one another so as to be rather tightly bound together. In the fcc model, first-neighbor separation constitutes clustering.

If the irradiation temperature is near absolute zero, no thermally activated processes can occur, but certain configurations of interstitial-vacancy pairs are expected to recombine spontaneously. For irradiation temperatures above perhaps 20°K, however, thermally activated processes will take place subsequent to cascade formation. These include, in order of increasing activation energy (and hence increasing characteristic temperature): additional recombination of interstitial-vacancy pairs, migration of interstitials, and migration of vacancies.

THE COMPUTER SIMULATION — HISTORICAL PERSPECTIVE

J. R. Beeler, Jr. and D. G. Besco developed a computer code to simulate the formation and short term annealing of an isolated displacement cascade.[4,5] Written in FORTRAN, it applied to a bcc lattice (nominally alpha-iron) at about room temperature--a temperature sufficiently low that vacancies were taken to be immobile. Some preliminary results of this code were published in 1966.[4] The code was extended by Doran to include vacancy migration and hence be applicable to higher simulated temperatures; results from the extended ANNEAL code (run on a UNIVAC 1108) have been published[1] for both low and high temperature simulated anneals in alpha-iron.

In early 1969 the Process Analysis and Simulation Section of Battelle-Northwest undertook a project to evaluate the comparative simulation capabilities of their small hybrid computer and the available big machine, a UNIVAC 1108, on a cross-section of scientific problems.[7] The ANNEAL code was one of the programs selected for comparison. ANNEAL was being run in three separate modes, two for interstitial motion (Mode 1--low temperature; Mode 2--high temperature) and one for vacancy motion (Mode 3); initially, only the interstitial modes were programmed on the hybrid computer. The program was rewritten in assembly

language directly from the model, rather than adapting the FORTRAN source program to the hybrid computer or attempting a direct translation of the FORTRAN code into assembly language instructions. This was done in order to maximize the efficiency of the hybrid program in terms of memory requirements and run time.

In order to validate the hybrid program, a deterministic run was made on both machines by replacing the random number routines with fixed sequences of numbers. This run also provided a direct comparison of run time. The outputs of both programs were identical, but the hybrid program was faster than the 1108 by a factor of 3.5. The average run time of several random runs also yielded a hybrid speed advantage of approximately 3.5. This advantage plus the much lower charge-out rate of the hybrid computer led to the decision to transfer the entire program to the hybrid.

The resulting program, called HAPBCC (Hybrid Anneal Program - BCC lattice), was completed in December 1969. The vacancy migration mode was added, and a new mode (Mode 4) permitted simultaneous vacancy and interstitial motion. This code has been employed to study the effect of variations in the parameters of the physical model and to study the overlap of several cascades. A display capability was added that permitted the production of stereo pair representations of cascades.[1] An electrostatic printer plotting program was later developed to generate 2-dimensional hard-copy plots of defect distributions.

The latest system of programs, the main annealing program of which is called HAPFCC, was developed in 1970 for fcc cascades and is the principal subject of this report. The simulation of point defects and small clusters in gamma-iron by Johnson[6] provided the physical model for the code.

The fcc code is more complex than the earlier bcc code in several respects: 1) There are more mobile species. 2) The orientations of the interstitials (the stress fields are not isotropic) are simulated and have an effect on interstitial

clustering, interstitial migration, and annihilation. 3) Periodic boundary conditions were included so that cascade interactions could be more effectively studied.

GENERAL DESCRIPTION OF THE FCC ANNEALING SIMULATION

The Computer System

The fcc annealing simulation was programmed on a small hybrid computer[8] consisting of a Digital Equipment Corporation PDP-7 computer (8K memory) interfaced to a Beckman EASE 2133 analog computer. Actually the only contribution from the analog side is a signal conditioning circuit which provides gain and dc drift stabilization for a noise signal from a random noise generator. This conditioned noise signal is then converted to digital form and used by the PDP-7 programs to generate random numbers.

A card reader and teletype provide inputs to the programs. Two Dectape magnetic tape units provide storage and retrieval of programs and data. Both numeric and graphic output are generated by an electrostatic printer. A CRT display program is capable of producing 3-dimensional stereo pair representations of cascades.

The primary reason for using the small computer is the high level of man-machine interaction it provides-- a significant consideration because the annealing runs are open-ended. Parameters can be changed through teletype entry at the beginning of a run, and several options can be exercised through console switches to control a run in progress. In addition, the program runs faster than an equivalent FORTRAN program on the available big machine (a UNIVAC 1108) and the charge rate is much lower on the small machine.

The annealing programs operate from the PDP-7 Relocatable Dectape Programming System, a software system designed especially for Battelle's hybrid computer.[9] The Relocatable System provides for simplified debugging and on-line program

changes and permits efficient use of the 8K memory through the relocatable loading feature. Core dump programs allow the user to save all (CORIT2) or selected blocks (CORIT) of core memory on Dectape.

The Simulation

Each point defect is initially described by its lattice position in terms of x, y, and z coordinates (half-lattice units) relative to an arbitrary origin, and its type (vacancy or interstitial). These data, normally the output of a UNIVAC 1108 cascade simulation program, are punched on cards and comprise the initial input to the annealing simulation. The pre-annealing program then determines or assigns additional information for each defect: its class (size of the cluster to which the defect belongs), its cluster number (identifying number of the cluster to which the defect belongs; zero if unclustered), and its orientation direction if an interstitial.

The mobility of a given defect is a function of its type and class. Each mobile defect executes a random walk on a three-dimensional lattice so long as it is sufficiently isolated from other defects. In the presence of other defects, the walk is no longer completely random but is correlated with the positions of nearby defects. Correlated configurations and the strengths of the correlations are necessary parameters of the simulation. Other parameters include the annihilation region (those configurations that result in mutual annihilation of vacancy-interstitial pairs) and clustering criteria.

The annealing is carried out in a series of time steps. In choosing the length of a time step, a compromise is made between the possible elimination of nearly simultaneous events through use of a long step, and the excessive use of computer time that results from using a short step. Each mobile defect is given an opportunity to jump with an assigned probability during each time step. The consequences of any jumps that occur-- clustering, dissociation, or annihilation--

are ascertained as they occur. The sequence is continued until defect interactions become rare.

Random numbers are used by the simulation in three major ways:

1) Determination of the order in which the mobile defects are selected for a jump opportunity;
2) Selection of the direction (jump vector) in which a given defect may jump in a given time step;
3) Determination of whether or not a mobile defect with a given jump probability actually executes the jump.

In addition, the random number routine is used in several ways by the pre-annealing program in preparing the input data for annealing.

Overall Program Flow

Figure 1 depicts the overall flow of programs and data, including control actions by the operator, during a typical annealing sequence. Program RANDOM is used to test and adjust the random noise generator to insure uniform distribution in the generation of random numbers. Defect data representing the initial radiation damage state are read from cards by program CARDIN and stored on magnetic tape. If keypunch errors are subsequently detected in the data listing, or if it is decided to add and/or delete certain defects from the data file, these operations can be accomplished by using the "edit" mode of CARDIN.

If the input deck contains more than the limit of 432 defects of either type, program IAP (Input Annihilation Program) can be used to reduce the first 864 defects (432 of each type) to a smaller number via 1st and 2nd neighbor annihilations. Then more defects can be added with CARDIN. This procedure can be repeated until all the cards have been read, or until no more annihilations occur.

Program INFACE prepares the input data for annealing by checking for illegal

Figure 1. Overall Operation of FCC System During the Processing and Annealing of a Typical Displacement Cascade.

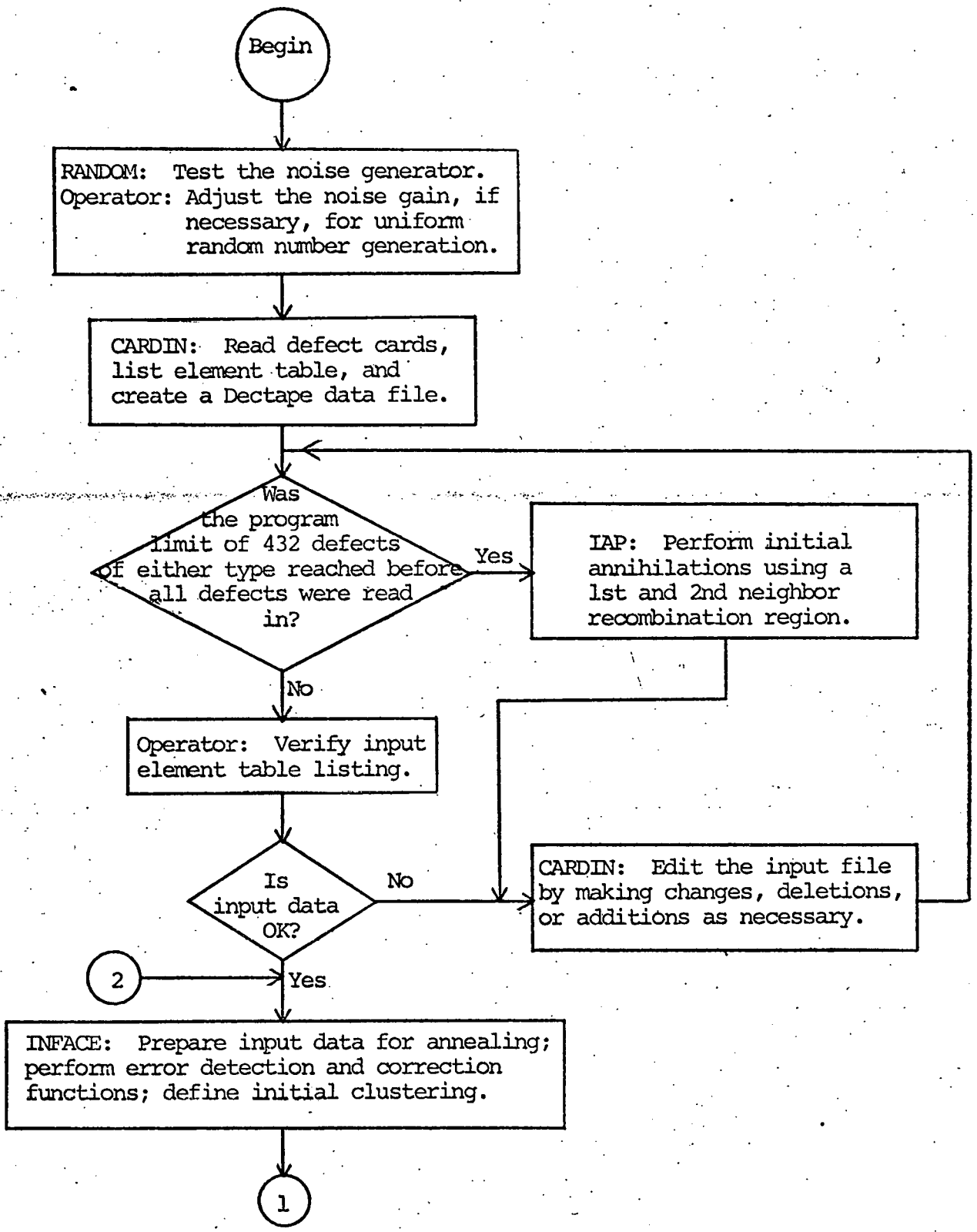
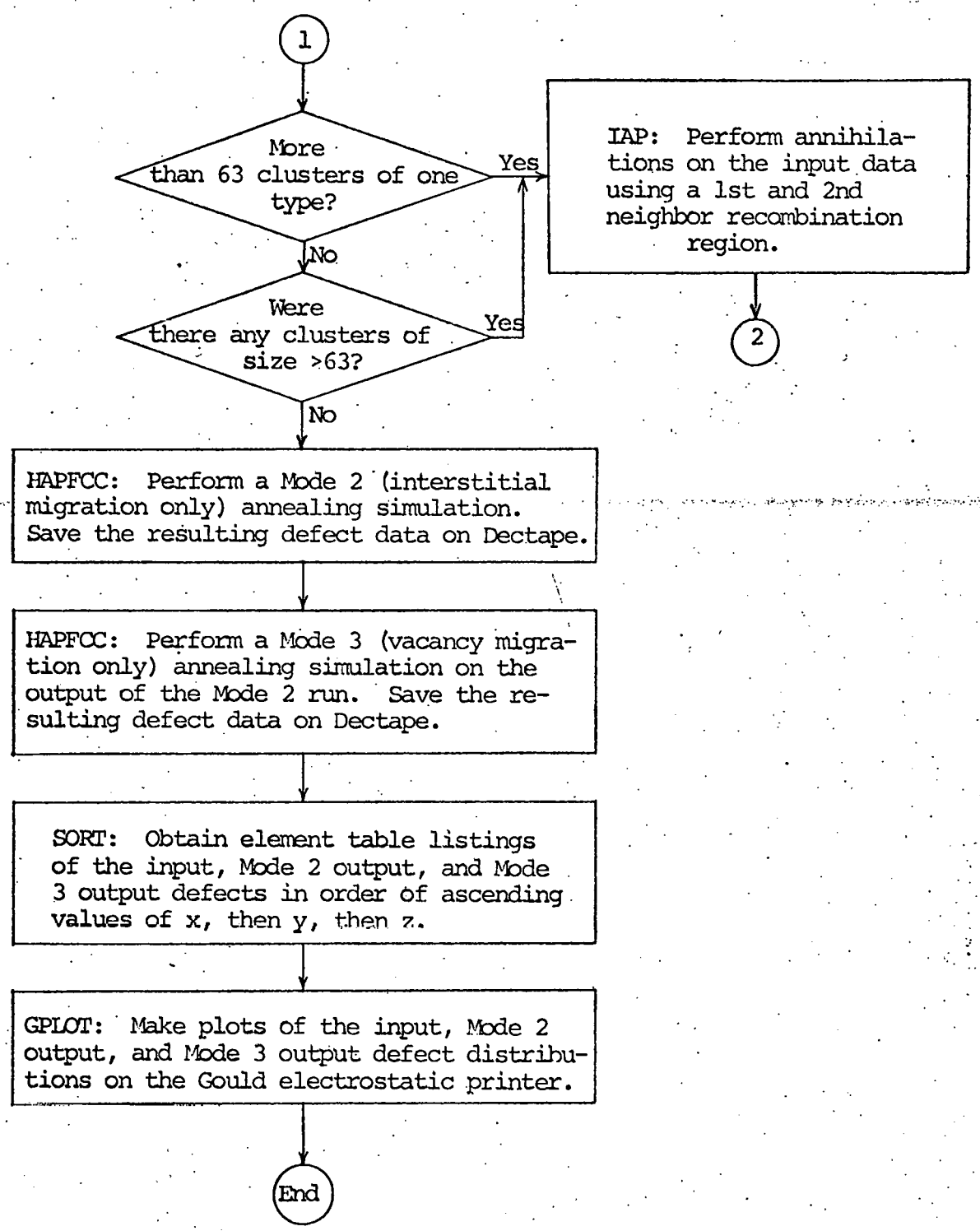


Figure 1 (cont.)



conditions and performing certain data initialization operations. Functions performed by INFACE include the following:

1) Check for defects at non-fcc sites (sum of coordinates must be even). A non-fcc defect is moved to one of the six adjacent fcc sites, chosen randomly.
2) Check for two or more defects occupying the same fcc site. If this occurs with like defects, one of the defects is allowed to remain, while the others are successively moved to 1st neighbor sites, chosen randomly, until a free site is found for each defect. If a pair of unlike defects occupy the same site, the pair is annihilated.
3) Check for defects lying outside the periodic boundaries. Such defects are systematically shifted into the periodic volume.
4) Define the initial clustering.
5) Assign orientations to interstitials. Single interstitials are randomly assigned, but the orientations of members of interstitial clusters are dependent upon the size and configuration of the cluster.
6) Put clusters of certain sizes and types into their "most stable" configurations.

The simulation is limited to no more than 63 clusters of either type, and to cluster sizes of 63 or less. If either of these limits is exceeded by INFACE, an error message is printed. Program IAP must then be used in an attempt to reduce the defects such that the exceeded clustering limit can be satisfied.

Program HAPFCC (Hybrid Annealing Program-- FCC lattice) performs the actual step-by-step annealing of the prepared displacement cascade. Before program execution begins, the user must enter from the teletype the appropriate set of parameter values for the run to be made. These parameters are listed in Appendix C .

When control is given to HAPFCC, a parameter information listing of the type shown in Figure 2 is printed. The data file is then read into memory, an initial element table listing and clustering summary are printed, and the annealing begins.

An element table listing provides complete information concerning the state of the cascade at the time the listing is made. Each defect's position, class, cluster number, and orientation direction (if an interstitial) are given. A sample listing is shown in Figure 3. A clustering summary, such as the one in Figure 4, provides a more concise indication of the state of the cascade. Clustering summaries are provided at pre-specified time step intervals as the run progresses. Element table listings are printed only at the beginning, at interval "breakpoints", and at the end of a simulation run unless requested by a console switch.

A run is terminated when either a pre-specified number of time steps have been completed or when a console switch is thrown. The annealed data are then saved on Dectape for plotting and possible further annealing.

As shown in Figure 1, the annealing process is normally carried out in two stages, a Mode 2 run (interstitial migration) followed by a Mode 3 run (vacancy migration). Due to the fact that interstitials are many times more mobile than vacancies, this method was chosen to conserve computer time. A Mode 4 simulation (simultaneous interstitial and vacancy migration) is also available.

With the program GPLOT, two-dimensional projections, such as the series of three plots shown in Figures 5-7, can be made for both the input cascade and the annealed cascade. Program SORT facilitates the specification of coordinate ranges for the plots by making three element table listings of the defects in a data file: first in order of ascending values of x, then y, then z.

```
HAPFCC---VERSION 1

DATE:  10-20-71
PROBLEM NO.  2051
RUN NO.  14

INPUT FILE:  2051-164

DIRECTION COSINES OF PKA:      DIRX = 25.66
                               DIRY = 8.07
                               DIRZ = 13.29

MODE 2 --- INTERSTITIAL MIGRATION ONLY

ANNIHILATIONS:
                (110) TYPE  EXCEPT WHEN DELTA B (INT'ST. ORIENT. DIRECTION) = + OR - 0
                (200) TYPE  EXCEPT WHEN DELTA B (INT'ST. ORIENT. DIRECTION) = + OR - 2
                (211) TYPE  EXCEPT WHEN DELTA B (INT'ST. ORIENT. DIRECTION) = + OR - 2
                (220) TYPE
                (310) TYPE  EXCEPT WHEN DELTA B (INT'ST. ORIENT. DIRECTION) = + OR - 0
                (222) TYPE
                (321) TYPE  EXCEPT WHEN DELTA B (INT'ST. ORIENT. DIRECTION) = + OR - 2
                (330) TYPE  EXCEPT WHEN DELTA B (INT'ST. ORIENT. DIRECTION) = + OR - 0

JUMP PROBABILITIES:

                INTERSTITIALS

PROBI1 = 0.500 (I1, UNCORRELATED)
ALPHA  = 1.000 (I1, JUMP FROM > OR = 5TH TO < OR = 4TH NABOR OF ANOTHER INT'ST)
PROBI2 = 0.063 (I2, UNCORRELATED)
PROBI3 = 0.006 (I3 MIGRATION JUMP)
AN I1 THAT IS 4TH, 3RD, OR 2ND NABOR TO ANOTHER I1 WILL MOVE TO FORM AN I2,
IF POSSIBLE, WITH UNITY PROBABILITY.  IF I2 FORMATION IS IMPOSSIBLE, I1 MOVES
TO INCREASE SEPARATION WITH UNITY PROBABILITY.
AN I1 THAT IS 4TH, 3RD, OR 2ND NABOR TO TWO OR MORE INTERSTITIALS WILL MOVE
TO DECREASE TOTAL SEPARATION WITH UNITY PROBABILITY.
THE APEX INTERSTITIAL OF AN I3(112)--2 PARALLEL WILL MAKE A "PLANE ROTATION"
JUMP WITH PROBABILITY = PROBI1.

PERIODIC BOUNDARIES:        XMIN = -500          XMAX =  3500
                            YMIN = -500          YMAX =  3500
                            ZMIN = -500          ZMAX =  3500
```

Figure 2. Typical HAPFCC Parameter Information Listing.

INPUT DATA

INT'ST. NUMBER	POSITION X	Y	Z	CLASS	CLUSTER NUMBER	VACANCY NUMBER	POSITION X	Y	Z	CLASS	CLUSTER NUMBER
1Y	239	159	190	1		38	220	208	208	3	15
26Z	230	157	145	3	6	57	208	202	204	1	
33Z	234	170	208	2	17	84	225	216	205	2	23
38	218	227	223	4	8	103	210	202	200	2	12
48	208	205	217	7	19	107	215	205	204	1	
50X	167	203	226	1		113	213	205	210	2	30
61Y	221	202	209	3	14	114	219	207	208	3	15
67X	147	220	221	1		122	203	195	220	1	
76X	230	155	145	3	6	131	210	203	203	1	
99	218	228	224	4	8	132	224	200	204	1	
101Z	220	189	191	2	5	137	209	202	209	3	35
107Y	250	235	195	1		140	210	202	210	3	35
126Z	231	156	145	3	6	152	209	201	200	2	12
127	225	199	198	4	18	153	210	204	200	2	18
154	227	198	199	4	18	156	230	211	203	2	40
155	227	199	198	4	18	157	230	212	204	2	40
160Z	233	179	208	2	17	160	220	207	209	3	15
180X	169	230	217	1		166	211	203	212	1	
198	207	204	217	7	19	177	224	207	197	1	
200Z	186	187	247	2	9	181	213	204	203	1	
201Z	221	188	191	2	5	182	222	209	205	1	
206X	197	248	183	1		185	222	207	207	2	28
214Y	222	202	208	3	14	192	212	205	213	1	
221Y	170	221	211	1		193	213	210	213	1	
224Z	192	197	255	1		194	209	192	215	1	
250Z	184	139	223	1		207	227	215	204	1	
251Z	199	228	155	1		221	208	192	220	1	
265X	229	211	216	3	16	230	204	207	201	1	
269	205	203	214	7	19	240	214	205	211	2	30
286X	229	212	215	3	16	253	209	205	200	3	18
299Y	158	215	225	1		257	223	217	204	1	
303Y	215	171	188	1		269	209	193	218	1	
322	220	228	224	4	8	284	223	208	207	2	28
329Y	239	207	210	2	13	285	223	222	207	1	
334Y	238	207	209	2	13	295	207	194	219	1	
345	219	227	224	4	8	300	223	203	196	1	
350	226	198	198	4	18	302	223	205	200	1	
363	204	203	215	7	19	331	224	215	205	2	23
364X	229	211	214	3	16	336	218	209	209	1	
368	204	203	213	7	19	339	210	193	213	1	
384Y	223	202	209	3	14	350	210	206	200	3	18
386	206	204	216	7	19	359	209	201	210	3	35
388	206	203	215	7	19	362	211	195	212	1	
395Z	187	188	247	2	9	381	231	210	207	1	

Figure 3. Typical HAPFCC Element Table Listing.

```
INT'ST. POPULATION:     44 TOTAL

     CLASS  NUMBER
       1      12
       2       4
       3       3
       4       2
       7       1

MOBILE FRACTION: .454

VACANCY POPULATION:     44 TOTAL

     CLASS  NUMBER
       1      25
       2       5
       3       3

INPUT DATA
```

Figure 4. Typical HAPFCC Clustering Summary Listing.

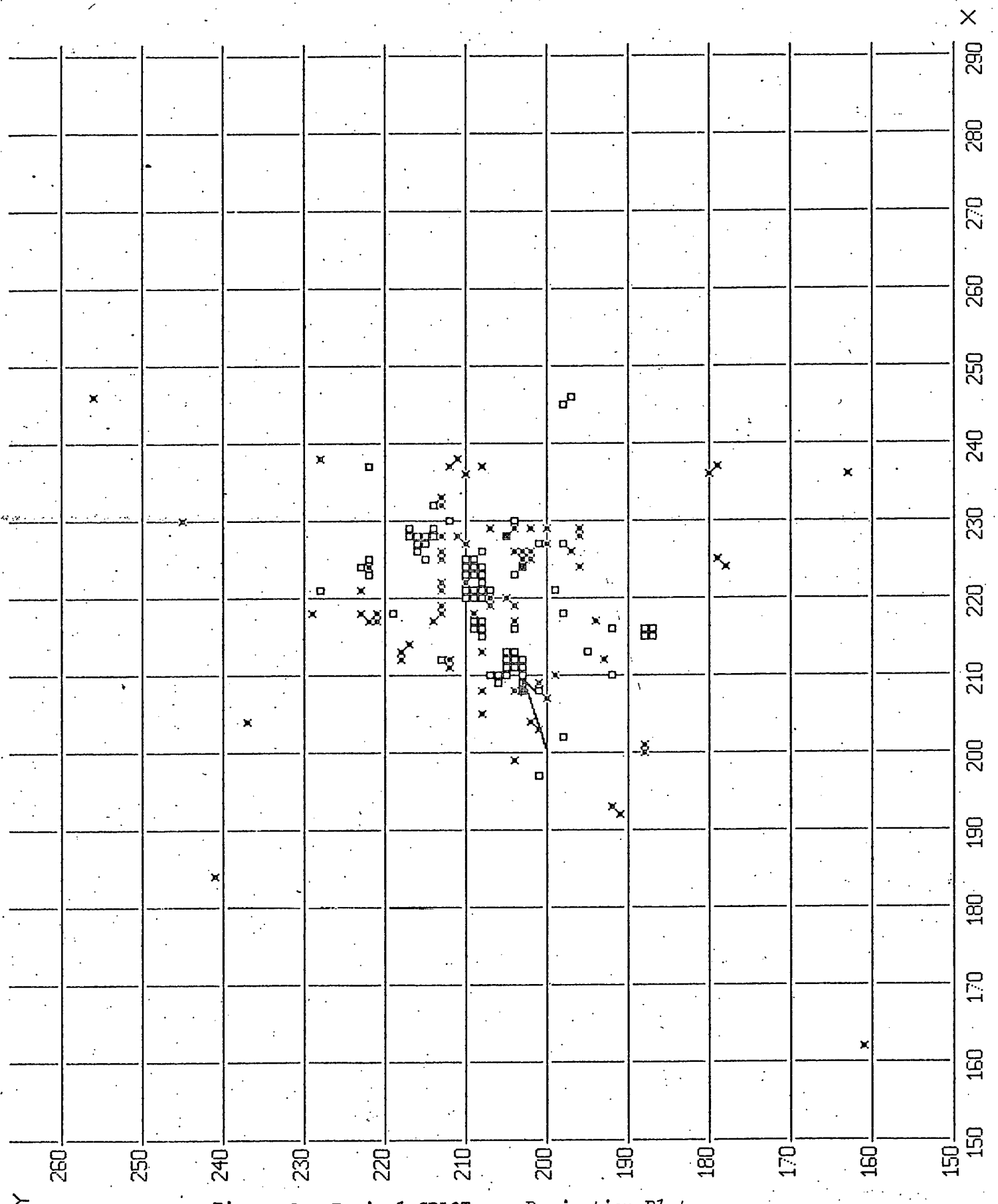


Figure 5. Typical GPLOT x-y Projection Plot

1000 TIME STEPS

DATA FILE 2051-565

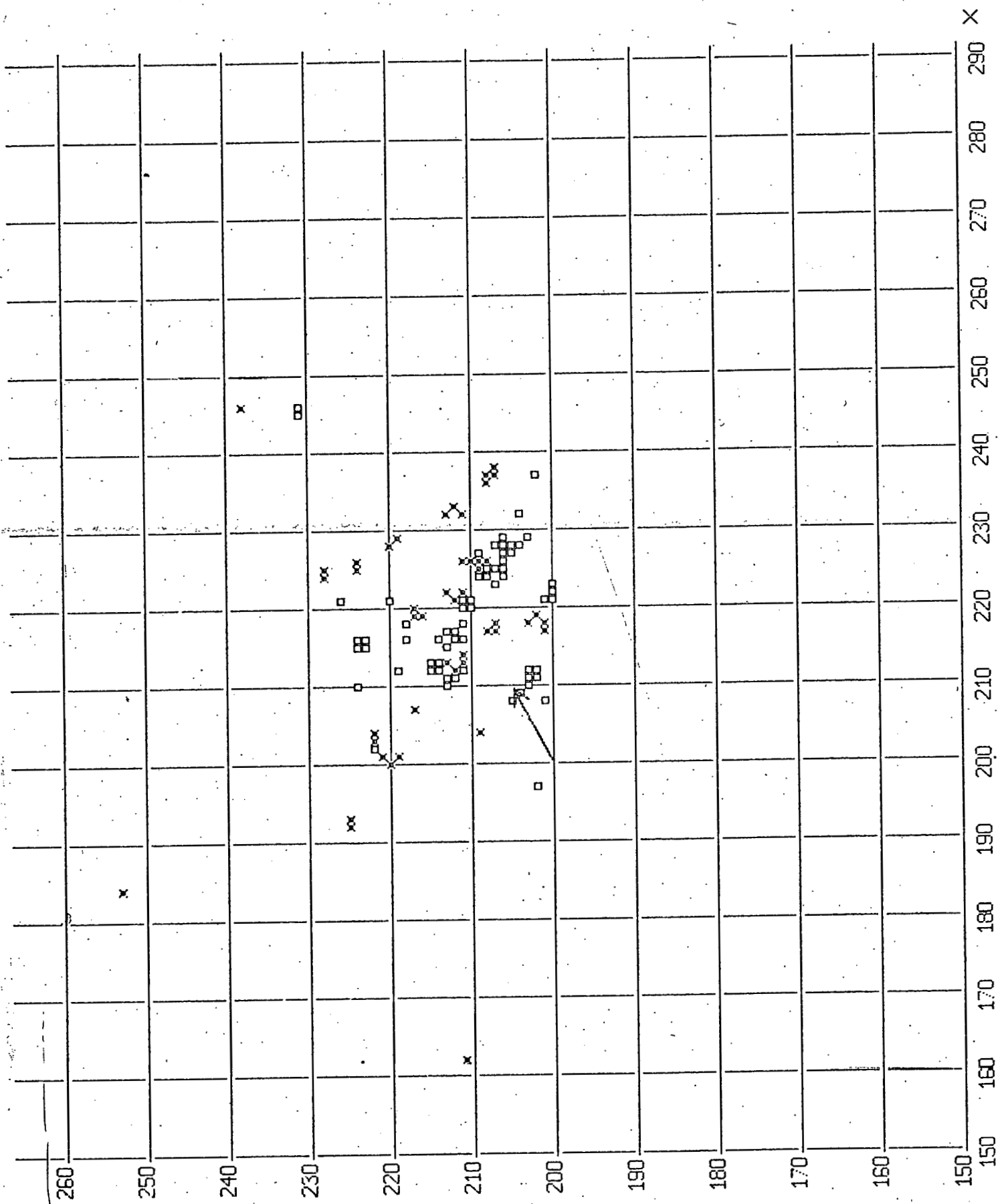


Figure 6. Typical GPLOT x-z Projection Plot

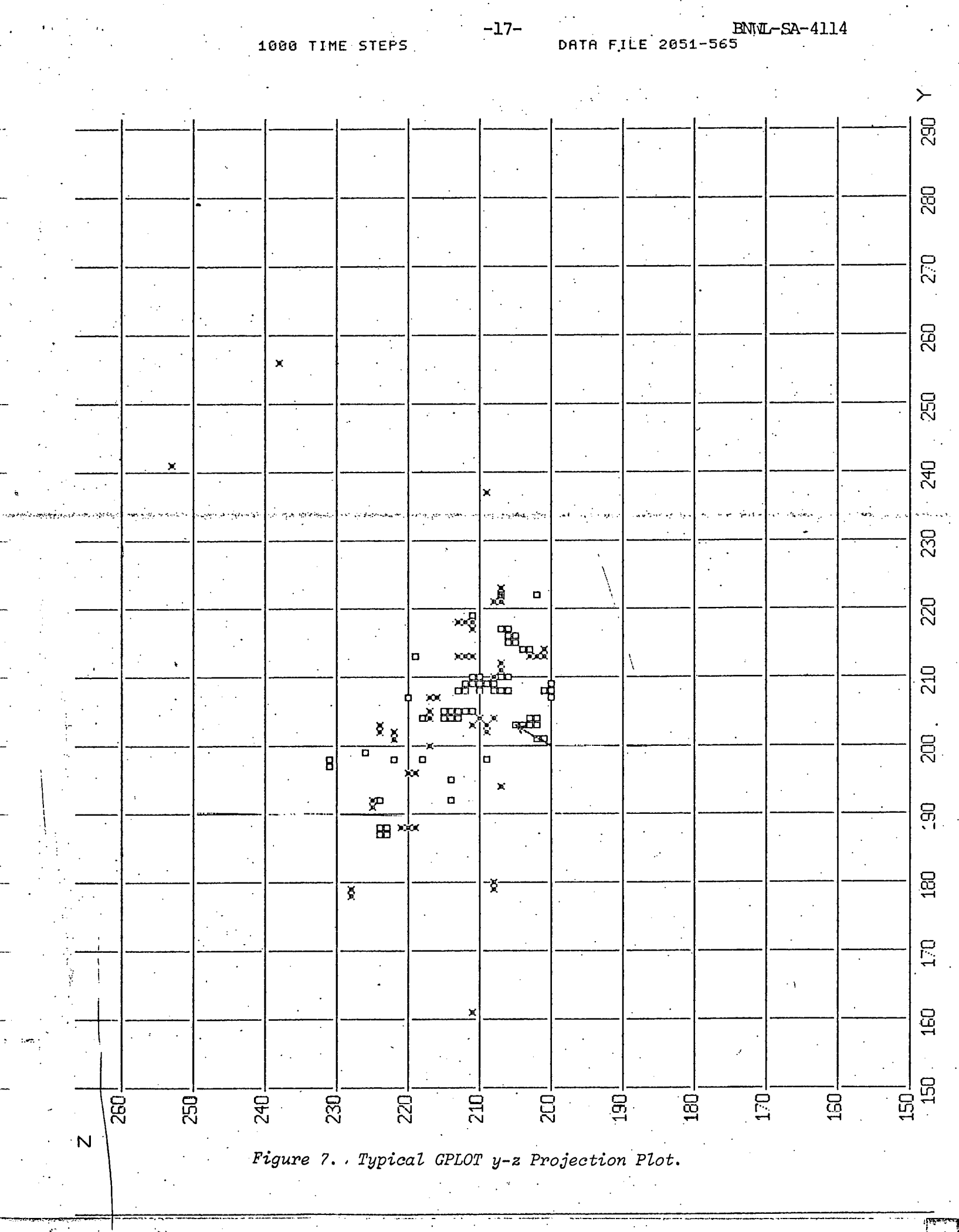


Figure 7. . Typical GPLOT y-z Projection Plot.

REFERENCES

1. D. G. Doran, Radiation Effects 2:249 (1970).

2. D. G. Doran and R. A. Burnett, The Simulation of Short-Term Annealing of Displacement Cascades in γ-Iron, U. S. Atomic Energy Commission Report HEDL-TME 71-110, August 1971.

3. A. C. Damask and G. J. Dienes, Point Defects in Metals, Gordon and Breach, 1963.

4. J. R. Beeler, Jr., Physical Review 150:470 (1966).

5. D. G. Besco, Computer Simulation of Point Defect Annealing in Metals, GEMP-644, October 1967.

6. R. A. Johnson, Physical Review 145:423 (1966).

7. Evaluation of Hybrid Computer Performance on a Cross-Section of Scientific Problems, edited by R. D. Benham, BNWL-1278, January 1970.

8. M. D. Erickson, The Pacific Northwest Laboratory Hybrid Computer System, BNWL-538, January 1968.

9. L. H. Gerhardstein, Hybrid PDP-7 Relocatable Dectape Programming System: Preliminary Report No. 1, BNWL-CC-1909, November 1968.

APPENDICES

APPENDIX A

CARDIN Parameters and Switch Functions

Symbolic Address	Typical Contents*	Description
IDELNO	3	Total no. of interstitials to be deleted from input file (applies only if AC switch Ø is up)
IOUT	7	Identification numbers of interstitials to be deleted. (Only the first IDELNO interstitials in the table will be deleted; applies only if AC switch Ø is up.)
IOUT+1	111	
IOUT+2	32	
⋮	⋮	
VDELNO	2	Total no. of vacancies to be deleted from input file (applies only if AC switch Ø is up.)
VOUT	49	Identification numbers of vacancies to be deleted. (Only the first VDELNO vacancies in the table will be deleted; applies only if AC Switch Ø is up.)
VOUT+1	38	
VOUT+2	⋮	
⋮		
PROBLM	2071	Problem (spike) identification number (applies only if AC Switch Ø is down).
DIRX	8298	PKA direction cosines $x10^4$ (applies only if AC Switch Ø is down).
DIRY	2076	
DIRZ	5185	
NEWPRO	2081	Replace problem no. with this no. (applies only if AC switches Ø and 2 are up.)
NEWDX	7071	Replace direction cosines with these values (applies only if AC switches Ø and 3 are up).
NEWDY	4242	
NEWDZ	5656	
YZBIAS	1000_8	Bias value added to each coordinate to insure a 12-bit positive number.
ILIMIT	400	Maximum number of interstitials desired (must not exceed program limit of 432).
VLIMIT	400	Maximum number of vacancies desired (must not exceed program limit of 432).
BLKIN	152	Dectape starting block number of input data file (applies only if AC switch Ø is up).
BLKØ	162	Dectape starting block number of output data file.

Numbers are decimal radix unless otherwise noted.

Accumulator Switch Functions

Switch No.	Meaning if up
Ø	Read data file from BLKIN and edit it. Examine AC switches 1, 2, and 3. (New data file is created from cards if switch Ø is down.)
1	Read defects from cards and add to input data file (applies only if switch Ø is up).
2	Change problem number to NEWPRO (applies only if switch Ø is up).
3	Change direction cosines to NEWDX, NEWDY, NEWDZ (applies only if switch Ø is up).

APPENDIX B

INFACE Run Parameters and Switch Functions

Symbolic Address	Typical Contents*	Description
XLOW	0	Lower and upper limits in x, y, and z for periodic boundary conditions.#
XHIGH	200	
YLOW	100	
YHIGH	300	
ZLOW	-500	
ZHIGH	3500	
BLKIN	100_8	Location (Dectape block) of input data file.
BLKØ	112_8	Location (Dectape block) of output data file.

Accumulator Switch Functions

Switch No.	Meaning if up
Ø	List the data file at block BLKIN, but do not operate on it.

Numbers are decimal radix unless otherwise noted.

#The boundary conditions must conform to the following:

- bHIGH - bLOW must be an even integer > 0
- bHIGH + YZBIAS < 4095 (7777_8)
- bLOW + YZBIAS > 1

where b = general coordinate representation (X,Y, or Z).

APPENDIX C

HAPFCC Run Parameters and Switch Functions

Symbolic Address	Typical Contents*	Description
MONTH DAY YEAR	6 1 71	Current date
RUNNO	2	Run number
SIMODE	2	Simulation mode: 2 = Interstitial migration only 3 = Vacancy migration only 4 = Both interstitial and vacancy migration
FMODE	1	Annihilation mode: 0 = Distance criterion (DMAXF) 1 = Specific sites (WASXXX)
WAS11Ø WAS2ØØ WAS211 WAS22Ø WAS31Ø WAS222 WAS321 WAS4ØØ WAS33Ø WAS44Ø WAS55Ø	CLA LAC TWO LAC TWO JMP KILL CLA JMP KILL LAC TWO JMP NOKILL CLA JMP NOKILL JMP NOKILL	If FMODE=1, set WASXXX to indicate annihilation condition for (XXX) site: CLA: Annihilate only if $\Delta b \neq 0$ LAC ONE (TWO, THREE, FOUR, or FIVE): Annihilate only if $\lvert\Delta b\rvert \neq 1$ (2,3,4,or 5). JMP KILL: Annihilate JMP NOKILL: Do not annihilate (Δb = Separation in direction of interstitial orientation.)
DMAXF	12	Maximum squared distance for recombination when FMODE = 0
TIMSET	DZM TIME	DZM TIME: Reset TIME to zero at beginning of run NOP: Continue counting from input file TIME value

**Numbers are decimal radix unless otherwise noted.*

Symbolic Address	Typical Contents	Description
BREAKS	20	Breakpoints (TIME values) for printout interval changes and program pauses
BREAKS+1	100	
BREAKS+2	500	
.	.	
.	.	
.	.	
.	.	
$BREAKS+11_8$	10000	
PRINTS	2	
PRINTS+1	10	Print intervals preceding the corresponding breakpoints above
PRINTS+2	100	
.	.	
.	.	
.	.	
.	.	
$PRINTS+11_8$	1000	
TLIMIT	20000	Maximum number of time steps (automatic run termination when TIME = TLIMIT)
LIGHT	HLT	HLT: Pause at each breakpoint. NOP: Do not pause at breakpoints.
PROBI1	500	
ALPHA	1000	
PROBI2	63	
PROBI3	6	
IP3A	500	Jump probabilities x 10^3
IP3B	11	
PROBVØ	0	
PROBV1	2	
PV1A	1000	
PV1B	86	
PV1C	7	
PV1D	4	
PROBV3	165	
PROBV4	24	
V2JMPS	10	Number of V_2 jumps per time step (Version 2 only)
BLKIN	120_8	Dectape starting block number of input data file (Unit 2)
BLKØ	127_8	Dectape starting block number of output data file (Unit 2)

Accumulator Switch Functions

Switch No.	Meaning if up
Ø	Print full element table listing if up at print time.
1	Print input data listing at beginning of run.
2	At end of current time step, print the time step number on the teletype and halt. Examine AC switch 8 when program is continued.
8	Terminate this run: Load CORITX, print annihilation report, and write output data file beginning at BLKØ of Unit 2. (Switch 8 is examined following the printout at each breakpoint, and after each "switch 2" interrupt.)