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I. INTRODUCTION

The study of void formation in heavy-ion irradiated nickel has been aided by the use of an experimental technique which allows the irradiated foils to be viewed directly in cross-section.[1,2,3] With this technique, it is possible to study effects such as the void denuded zone at the front surface and the depth to which the damage extends. In addition, the microstructural state of the material along the ion path can be directly measured by properly interpreting this microstructural information, a better understanding of void formation under heavy-ion irradiation can be gained, leading to a better insight into the relationship between heavy-ion induced damage and displacement damage produced by fast neutrons.

The interpretation of the depth dependent microstructure in heavy-ion irradiated metals is aided if the depth profiles of the vacancy and interstitial concentrations are known. Previous calculations, both analytical and numerical,[4-9] have solved this problem in various forms, but none had solved the completely general case of heavy-ion bombardment. To fill this need, a computer code was written to calculate the steady-state vacancy and interstitial concentrations for any specified defect production profile with any general, depth dependent void and dislocation microstructure. For the specific case of heavy-ion irradiation, the excess interstitials introduced by the incoming ions can be included. If the incoming beam is of a different chemical species than the target, it is possible to estimate the final impurity distribution using a simple radiation enhanced diffusion code.

In this paper, the theoretical equations will be discussed in Section 2. Section 3 will discuss the numerical techniques, and Section 4 will present the various options of the code and some typical results. The code listing will be given in the Appendix.

II. THEORETICAL BACKGROUND

A. Steady-State Point Defect Concentrations

At temperatures sufficiently high enough to be of interest in studies involving void formation, the point defect concentration in the matrix can be found by solving the rate equations which determine the net rate of loss or gain of defects in the matrix. The equations are conservative equations formulated to describe the average defect concentrations in an irradiated material. These questions are found by integrating over a spatial distance greater than the average sink spacing and over a time interval greater than the cascade lifetime. The rate equations can be written in their steady-state form as:

$$\nabla \cdot (D_v \nabla C_v) + P_v - D_v K_v^2 (C_v - C_v^*) - \alpha C_i C_v = 0 \qquad (1)$$

and

$$\nabla \cdot (D_i \nabla C_i) + P_i - D_i K_i^2 (C_i - C_i^*) - \alpha C_i C_v = 0 \qquad (2)$$

where

$C_{v,i}$ are the average vacancy and interstitial concentrations,

$D_{v,i}$ the diffusion coefficients,

$P_{v,i}$ the point defect production rate,

$K^2_{v,i}$ the total sink strengths for the defects. $D_v C_v K_v^2$ is the total loss rate of vacancies to sinks, while $D_v C_v^* K_v^2$ is the vacancy emission rate from sinks,

α the bulk recombination coefficient, and

$C^*_{v,i}$ the thermal defect concentrations in the absence of irradiation.

D_i, D_v and α are temperature dependent material parameters and will not vary with depth unless large compositional gradients are present in the foil. For most cases of interest, the power input from the beam is so low that temperature gradients are negligible. For virtually all cases of experimental interest, Eqs. (1) and (2) will only depend on one spatial variable. Beam diameters are typically > 10^3 μm while beam penetration is ~ few μm. Hence, a one-dimensional treatment will be adequate for all of the irradiated area except the extreme beam edges.

The effective sink strength terms $K^2_{i,v}$ are found by modeling each type of sink as a single discrete sink in a homogeneous medium.[10] If there is no activation barrier for the transfer of defects across the sink boundary, these sink terms are given by

$$K^{2i,v}_{void} = 4\pi r_v C_v \tag{3}$$

for both interstitials and vacancies into a system of voids of average radius r_v and concentration C_v, and

$$K^{2i,v}_{dislocation} = Z^{i,v}\,\rho_D \tag{4}$$

where $Z^{i,v}$ is the bias term for interstitials or vacancies to dislocations and ρ_D is the total dislocation density. Note that it is postulated that dislocation will have a larger bias for interstitials than vacancies. This will

lead to a slightly larger number of vacancies free to migrate to the void sinks than interstitials and hence give void swelling.

The homogeneous recombination coefficient α is given by[11]

$$\alpha = Z_r V_i \tag{5}$$

where Z_r is the recombination volume and V_i the interstitial jump frequency. The recombination volume is defined as the volume of material surrounding a point defect that will always lead to the annihilation of any unlike defect. A typical recombination volume is about 40 atomic volumes. In general, α depends on both the vacancy and the interstitial jump frequency, but since the interstitial jump frequency is so much higher than the vacancy jump frequency, α can be rewritten as

$$\alpha = A * D_i \tag{6}$$

where A is a temperature independent material parameter on the order of 10^{15}.

The point defect production rates P_i and P_v are generally taken to be equal to the displacement rate calculated by an appropriate model. This is an obvious simplification of the actual process since the bulk of the displacements under neutron or heavy ion irradiation are created in displacement cascades. The high local density of defects in these cascades will lead to a certain amount of immediate recombination in the cascade and reduce the number of defects free to migrate into the bulk of the lattice. This process, which has been partially modeled by computer codes, is still poorly understood and at the present time, it is not feasible to attempt any refinement of the defect production rates.

The point defect diffusion coefficients are given by

$$D_{v,i} = D_o^{v,i} \exp(-E_m^{v,i}/kT)$$

where $D_o^{v,i}$ is the vacancy or interstitial pre-exponential, and

$E_m^{v,i}$ the motion energy of the defect.

The thermal point defect concentrations are given by

$$C_{v,i}^{eg} = \exp\ (S_f^{v,i}/k)\ \exp\ (-E_{v,i}^f/kT) \tag{7}$$

where $\exp\ (S_f^{v,i}/k)$ is the formation pre-exponential, and

$E_{v,i}^f$ is the vacancy or interstitial formation energy.

In most cases of interest, the formation energy for interstitials is so large that the equilibrium interstitial concentration can be neglected. If there exists non-equilibrium sinks in the system (i.e., voids or small dislocation loops) the point defect concentration at the sink boundary will have the form

$$C_{v,i}^* = C_v^{eg} \exp\ (\Delta E/kT) \tag{8}$$

where ΔE is the free energy change of the system when the sink emits a defect. For voids, ΔE is given by

$$\Delta E_{v,i}^{voids} = (Pb^3 + \gamma\ b^3/r_v) \tag{9}$$

where P is the gas pressure in the voids,

γ the surface energy,

b the nearest neighbor spacing of the material, and

r_v the void radius.

Generally, the thermal emission of interstitials can be neglected.

Once the point defect concentrations have been calculated for a given set of conditions, the net flux of vacancy into voids is given by

$$J_v = D_v C_v - D_i C_i - D_v C_v^* . \tag{10}$$

Hence, for a microstructure containing a void concentration of N_v with an average void radius r_{vg}, the swelling rate due to void growth will be

$$\frac{d}{dt}\left(\frac{\Delta v}{v}\right) = 4\pi N_v r_v J_v . \tag{11}$$

B. Radiation Enhanced Diffusion

In a material which is being bombarded by heavy ions, there are some peculiar effects that may occur in the end-of-range region. Heavy-ion irradiation generally involves the injection of a large atom that can take a substitutional site in the lattice, therefore a correct accounting of the interstitial production rate in the end-of-range will allow for the interstitials produced in excess of those produced by actual displacement reaction. These excess interstitials can be important in certain cases.[12]

If the bombarding ion is not the same chemical species as the target material, there may be interactions of the point defects with the impurity atoms in the end-of-range region. The initial distribution of the implanted ions can be estimated from calculated range and range distribution data. The final distribution of ions will be quite different, however, due to diffusion

of the impurity atoms out of the end-of-range region. This effect may be quite dramatic since the diffusion coefficients for most impurities will increase quite significantly during irradiation due to the increased concentration of mobile defects. In general, the concentration of an impurity of type A is described by[9]

$$\frac{\partial C_A}{\partial t} = \nabla \cdot [(D_A \nabla \mu_A) + D_{Av} \nabla C_v + D_{Ai} \nabla C_i] + S_A \qquad (12)$$

where μ_A is the chemical potential of the species A,

D_{Av} and D_{Ai} are coefficients relating the interaction of the flux of impurity atoms to the flux of vacancies and interstitials, and

S_A is a source term for the impurity A.

The diffusion coefficient D_A for impurities which diffuse substitutionally is given by

$$D_A = \sum_n F_n D_n C_n \qquad (13)$$

where the sum is over all mobile defects and defect clusters,

the F_n's are correlation factors, and

the C_n's are concentrations of the respective defects or defect clusters.

Under irradiation, one must learn how to relate the diffusion fluxes to the thermodynamic forces that cause these fluxes by studying the thermodynamics of irreversible processes. The large concentration of vacancies and interstitials during irradiation will modify the equilibrium values of the chemical potential[13] and may alter or even destroy the driving force for diffusion. Hence in lieu of an accurate solution of this problem one is

limited to modeling the enhanced mobility of the impurity due to the enhanced concentration of mobile defects and then making an assumption about the driving force for diffusion.

III. NUMERICAL METHODS

To solve Eqs. (1) and (2) for a case typical of heavy-ion bombardment where both the defect production rate and the sink density vary with depth, it was necessary to apply a numerical solution. To solve these equations, appropriate boundary conditions are needed. For a semi-infinite solid with a depth dependent defect production rate, these are:

$$C_v(o) = C_v^{th} \qquad C_v(x\to\infty) = C_v^{th}$$

$$C_i(o) = 0 \qquad C_i(x\to\infty) = 0 \tag{14}$$

For a solution of the problem for a foil with a constant defect production rate, the boundary condition at $(x\to\infty)$ is replaced by a reflecting boundary condition such that

$$\lim_{x\to\infty} \frac{\partial C_{i,v}}{\partial v} = 0 \ . \tag{15}$$

To solve these equations, the problem was formulated in a manner similar to Myers, et al.[9] By use of the method of lines, the partial derivatives in x were replaced by corresponding difference quotients on a grid of M points spaced at depths x_k:

$$\frac{\partial}{\partial x}\left(D\,\frac{\partial C}{\partial x}\right) \approx \frac{D_{k+1/2}\left(\frac{C_{k+1} - C_k}{\Delta x_k}\right) - D_{k-1/2}\left(\frac{C_k - C_{k-1}}{\Delta x_{k-1}}\right)}{(\Delta x_k + \Delta x_{k-1})/2}$$

$$= \alpha_k C_{k-1} - \beta_k C_k + \gamma_k C_{k+1} \tag{16}$$

where

$$D_{k+1/2} = \frac{D_{k+1} + D_k}{2} \tag{17}$$

$$\Delta x_k = x_{k+1} - x_k \tag{18}$$

$$\alpha_k = \frac{2D_{k-1/2}}{\Delta x_{k+1}\,(\Delta x_k + \Delta x_{k-1})} \tag{19}$$

$$\gamma_k = \frac{2D_{k+1/2}}{\Delta x_k\,(\Delta x_k + \Delta x_{k-1})} \tag{20}$$

$$\beta_k = \alpha_k + \gamma_k \tag{21}$$

For programming, these equations were formulated in terms of a vector $\underline{Y}$, where Y_1 is identified as $C_i(x_1)$, Y_2 as $C_v(x_2)$, Y_3 as $C_i(x_2)$, Y_4 as $C_v(x_2)$, etc. With this notation, the two equations to be solved are

$$\alpha_k^v\, Y_{3k-5} - \beta_k^v\, Y_{3k-2} + \gamma_k^v\, Y_{3k+1} + P_k^v - K_k^v\,(Y_{3k-2} - C_v^{th}) -$$

$$- \alpha Y_{3k-2}\, Y_{3k-1} = 0 \tag{22}$$

and

$$\alpha_k^i Y_{3k-4} - \beta_k^i Y_{3k-1} + \gamma_k^i Y_{3k+2} + P_k^i - K_k^i Y_{3k-1} - K^{iv} Y_{3k-2} Y_{3k-1} = 0 \qquad (23)$$

where $K_k^{v,i}$ is the total sink strength for vacancies or interstitials in interval k.

The equations were solved using a modified Gauss-Siedel iteration technique.[14] The initial values for $C_i(x)$ and $C_v(x)$ from which the iteration process proceeded were taken as the solutions of Eqs. (1) and (2) assuming no point defect diffusion out of each zone ($\nabla \cdot D_v \nabla C_v = 0$) and that $D_i C_i = D_v C_v$. From these initial values, Eqs. (22) and (23) were used to calculate new values of C_i and C_v until a specified convergence criterion was met. The rate of convergence of these equations was increased by allowing a relaxation coefficient a_k to increase if consecutive values of C_i^k or C_v^k both increased or both decreased, and by decreasing a_k if consecutive values oscillated.

Equation 12 was formulated to correspond to a case where C_A at time $t = 0$ was equal to zero, and where the source term $S_A(x)$ corresponded to the rate and spatial dependence of impurities that are the deposited ions. No solute drag was assumed (i.e., D_{Av} and $D_{Ai} = 0$) and the point defect concentrations needed for Eq. (13) were taken from the previously described steady-state solution. This solution of a time buildup and diffusion of impurities using point defect concentrations from a steady-state calculation will not be in large error if the time interval over which the integration is performed is not so long as to allow significant changes in the microstructure to occur. To integrate over long time periods, the point defect calculations should be

repeated several times using the appropriate sink strengths, and in this manner getting a quasi-time dependent D_A. The advantage of this procedure is that it allows the solution of Eq. (12) using experimentally determined sink strengths as opposed to a solution which used sink strengths calculated by integrating from some earlier time.

Equation (12) was formulated in a manner similar to Eq. (1) and (2) and integrated using a forward difference technique. The time step used in the integration was 0.45 of the smallest Fourier number $F_o(k)$ in the system, where

$$F_o(k) = \frac{(\Delta x_k)^2}{D_A(k)} . \tag{24}$$

The initial and boundary conditions were

$$\begin{aligned} C_A(\ t = 0) &= 0 \\ D_A \frac{\partial}{\partial x} C_A(x = 0) &= 0 . \end{aligned} \tag{25}$$

IV. RESULTS

The material parameters used in this study were those measured for nickel and are listed in Table 1. The vacancy and interstitial concentration profiles obtained from the code using the point defect production profile of 14 MeV nickel ions are shown in Fig. 1. In this case, the temperature was 525°C and the sink density was assumed to consist of dislocations at a uniform density of 5×10^9 cm/cm^3. Note that all of the curves except for the deposited ion curve are normalized to the peak values given in the figure.

Table 1

Input Parameters Used in Solving Eq. 1 and 2

Most Material Parameters are from Ref. 15

Temperature	525°C
Surface Energy	1000 J/m^2 (erg/cm^2)
Vacancy Migration Energy	1.38 eV
Interstitial Migration Energy	0.15 eV
Vacancy Formation Pre-Exponential	4.48
Interstitial Formation Pre-Exponential	5.0
Vacancy Diffusion Coefficient	
Pre-Exponential	0.062 cm^2/s
Interstitial Diffusion Coefficient	
Pre-Exponential	0.12 cm^2/s
Vacancy Formation Energy	1.39 eV
Interstitial Formation Energy	4.08 eV
Recombination Factor, α/D_i	1×10^{15} cm^{-2}
Dislocation Bias	2.0%
Ion Flux	2×10^{12} $ions/cm^2/s$

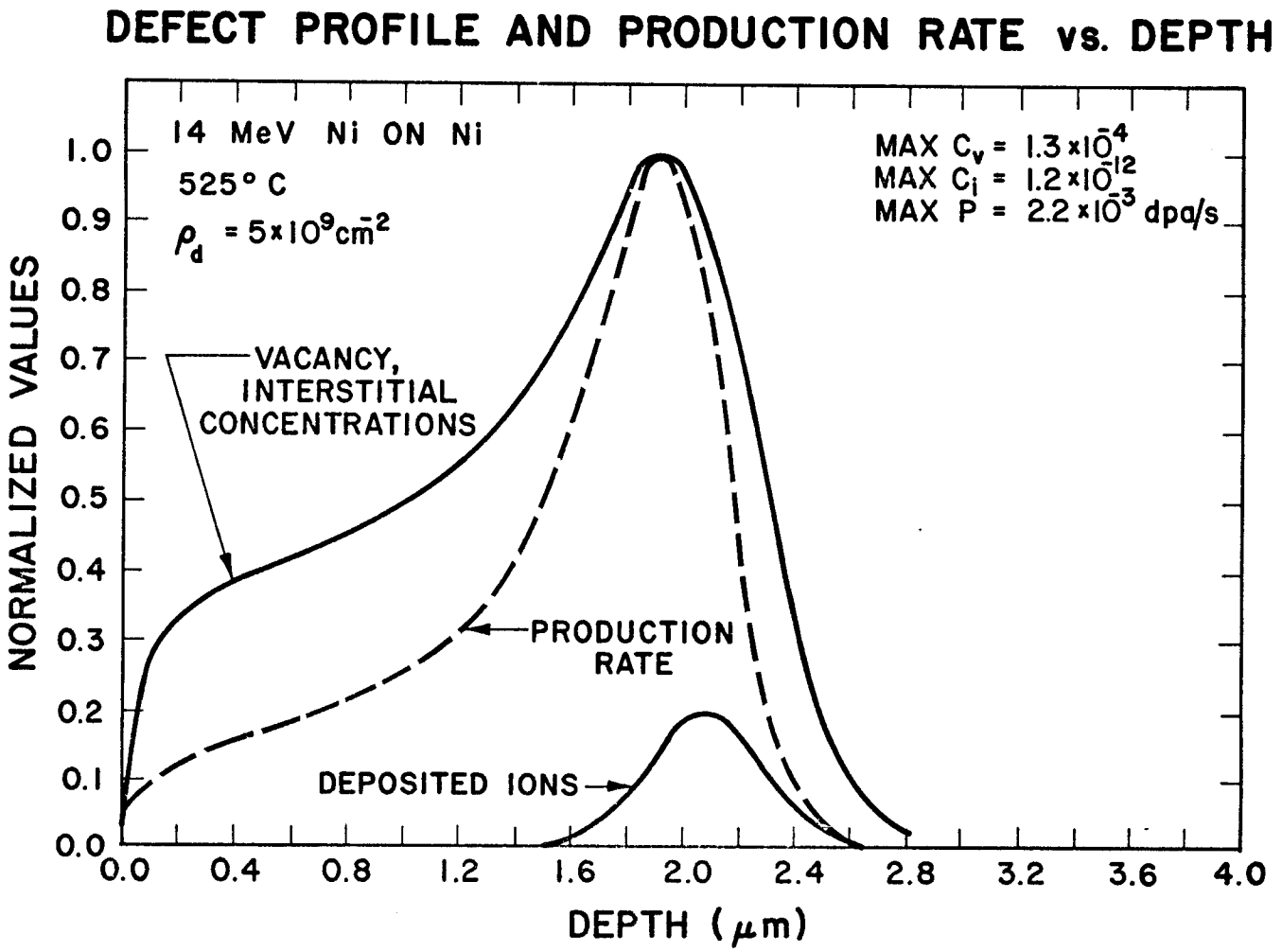

Fig. 1. Calculated vacancy and interstitial concentration profiles for 14 MeV nickel ions incident onto a nickel target. The curves are all normalized to the peak values shown in the figure.

There are several general features of these curves that are important in interpreting heavy-ion irradiated samples. First, the variation in the point defect concentrations is much less than the variation in the production rate curve. This is due to the increased recombination rate and the excess interstitials deposited in the end-of-range region. Second, there is a sharp dip in the concentration curves near the front surface. The front surface serves as a perfect defect sink and hence reduces the point defect concentrations near it. In this region, void growth will be impossible, leading to a void denuded zone. Finally, the diffusion of point defects beyond the production curve end-of-range gives a significant point defect concentration in this "undamaged" region. This effect could lead to observable defect clusters beyond the ion end-of-range.

Figure 2 shows the fraction of defects in each depth interval lost to sinks, by recombination, and by diffusion out of the interval. (Note that a negative diffusion fraction occurs when defects are diffusing into a depth interval.) In this particular case, the bulk of the defects are lost by recombination, with the fraction lost by recombinations increasing with depth. Beyond the end-of-range (i.e., ~ 2.6 μm) the point defect concentrations are low and they are annihilated predominately at the dislocation sinks.

In Figs. 3 and 4 the results of a similar run are shown except in this case, experimentally measured dislocation and void densities were used from Reference 3. The total sink strength increased with depth, having a peak value ~ 5 times the value at 0.5 μm. This increasing sink strength has depressed the peak concentration and increased the fraction of defects lost to sinks. The end-of-range region of this sample shows ~ 40% of the defects being lost by absorption at sinks.

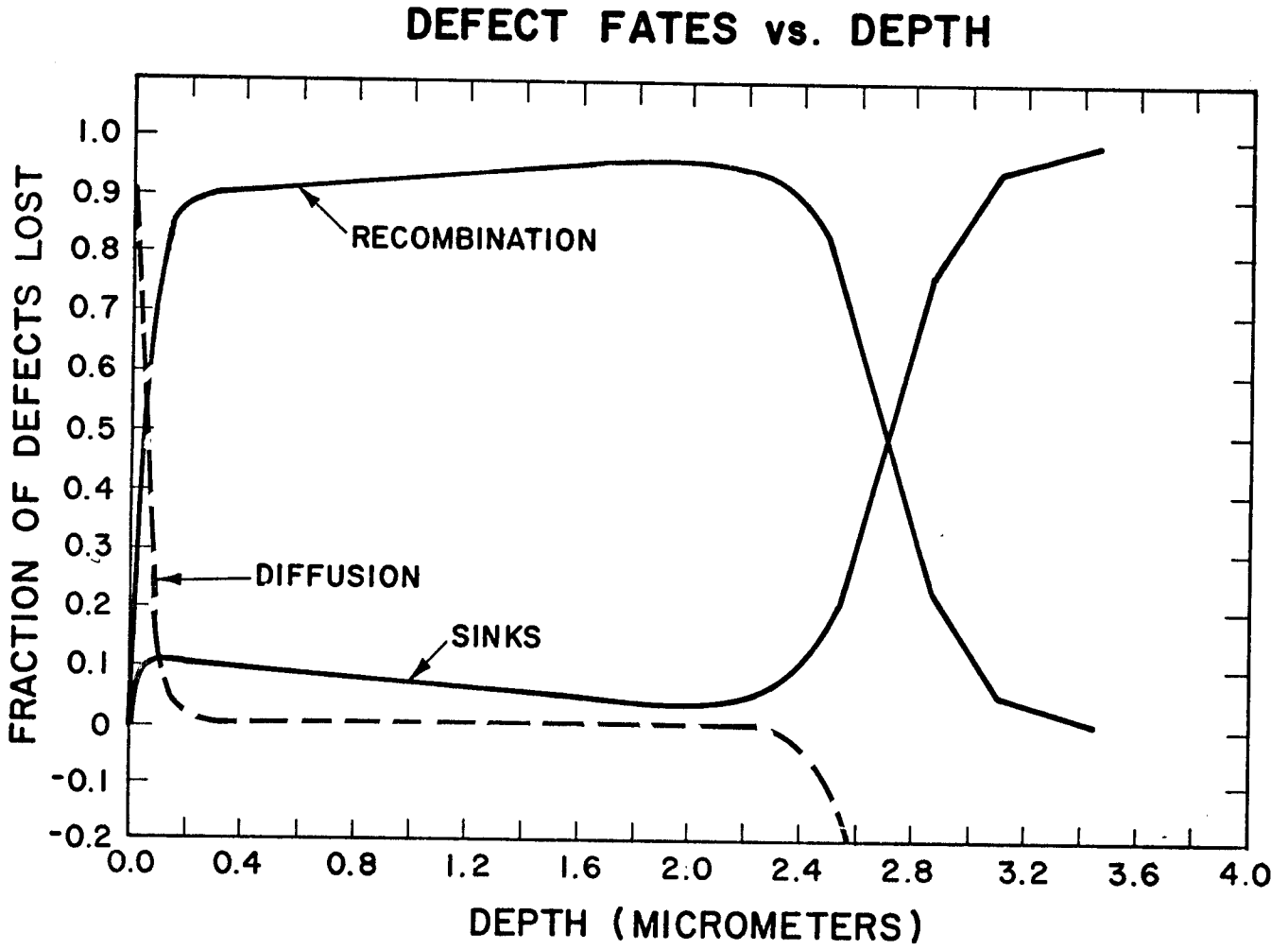

Fig. 2. The distribution of the defects produced by the calculation of Fig. 1 to their various sinks. A positive fraction for diffusion refers to a net loss of defects out of the depth interval while a negative fraction refers to a net gain of defects.

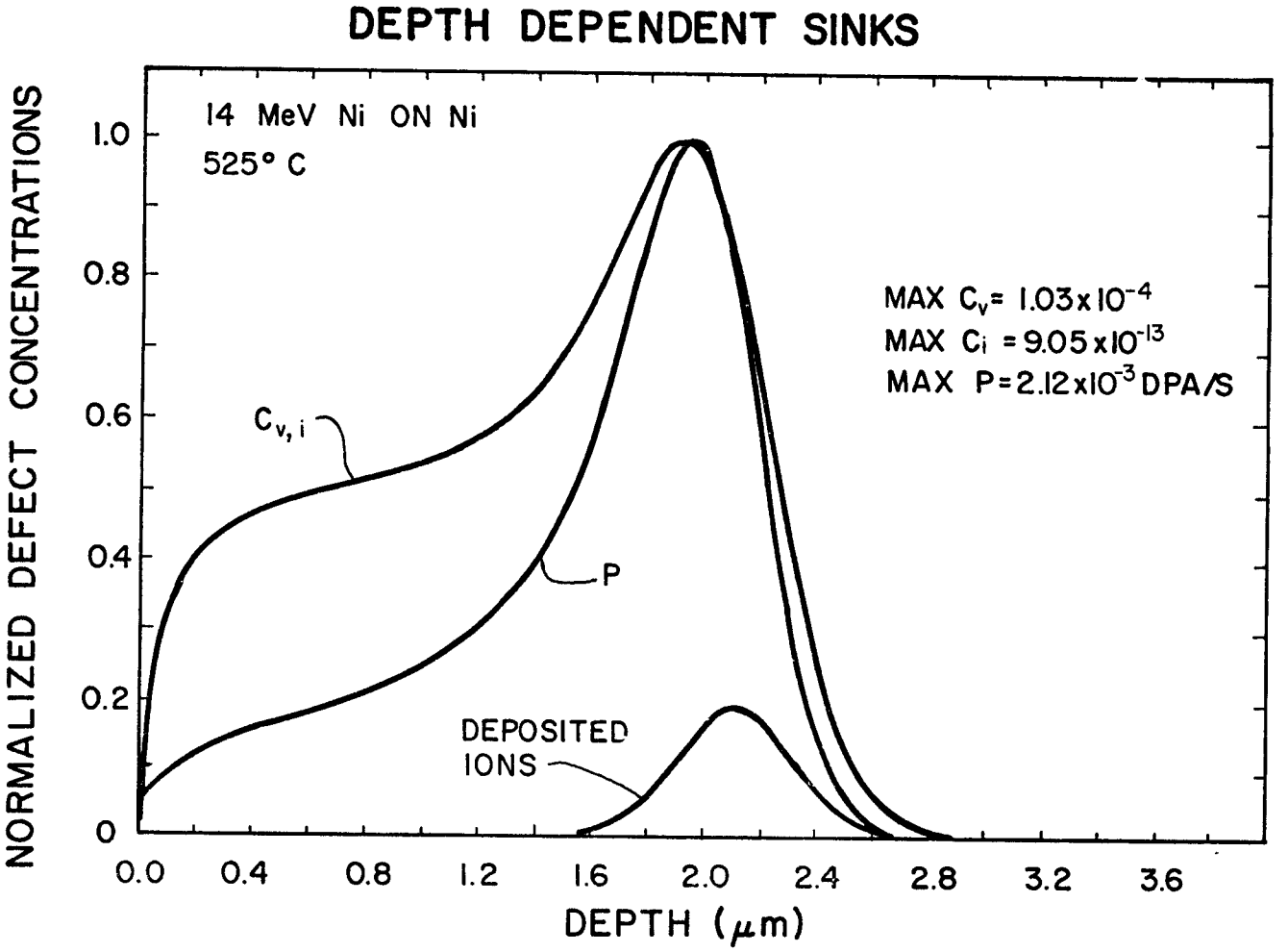

Fig. 3. Defect profiles for conditions identical to those of Fig. 1 except that an experimentally measured depth dependent dislocation density taken from Reference 3 was used.

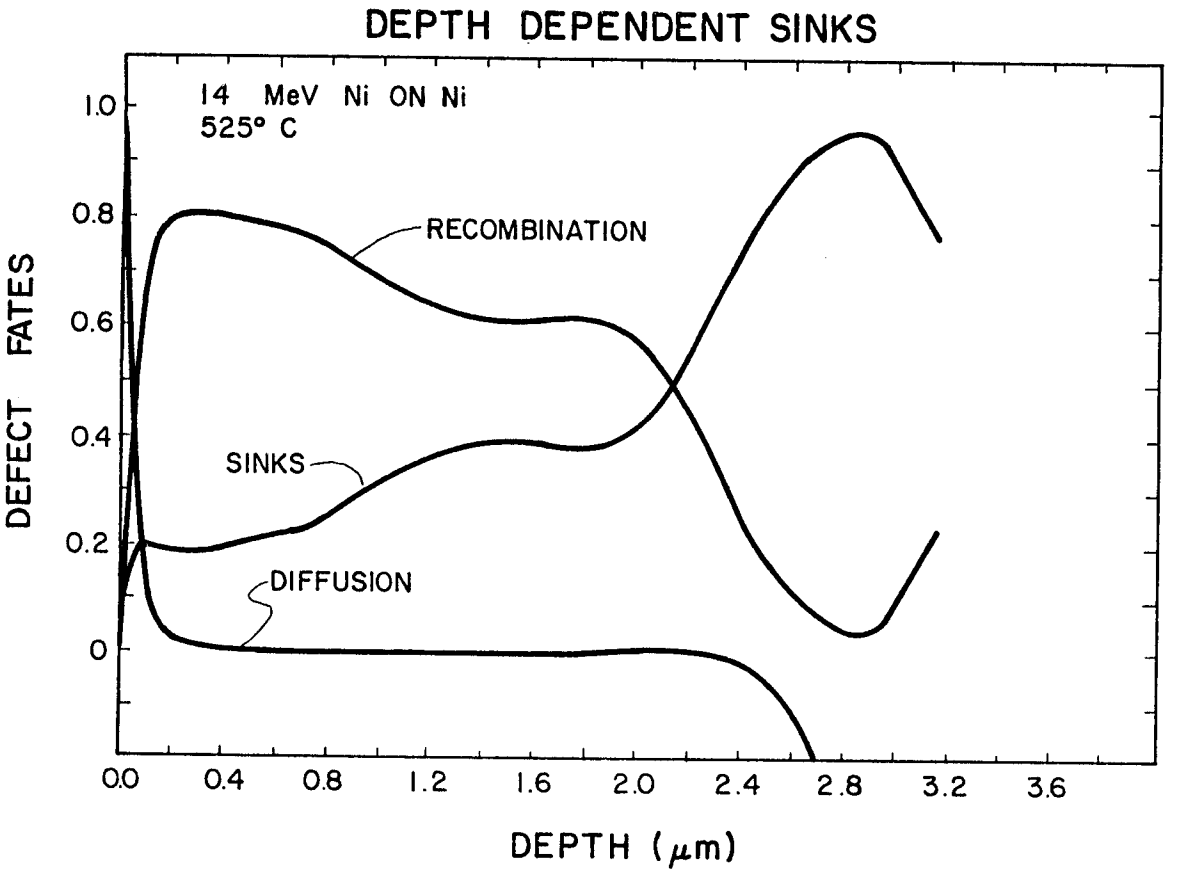

Fig. 4. The defect distribution to sinks from the calculation of Fig. 3.

The code also calculates the "growth fluid"[8] defined by Eq. (10) and, if voids are present in the microstructure, the void swelling rate is given by Eq. (11). The growth fluid is shown in Fig. 5, where a void radius of 1.0 nm was used to calculate C_v^* (Eq. 8). The swelling rate plot of Fig. 6 used the void size and densities input into the code to solve Eq. (11). In Fig. 7 the growth fluid calculated from the data of Fig. 1 is shown plotted with the experimentally measured swelling values of Reference 3. The reasonable match of the shapes of these curves shows that the growth fluid, with its inclusion of increasing recombination with depth, fits the experimental swelling profiles much better than does the displacement curve.

The concentration profiles in a foil with a uniform defect production is shown in Fig. 8. These profiles would correspond to grain boundary areas parallel to the foil surface in heavy ion irradiated foils or to grain boundaries and surfaces of neutron irradiated specimens. In this run, the dislocation density was 5×10^8 cm/cm^3 throughout the foil. Recombination dominates as is shown in Fig. 9, and defect loss to the surface is significant to a depth of 0.2 μm. The growth fluid curve of Fig. 10, however, shows that the "bulk" growth value is only achieved at depths greater than 1.0 μm.

The concentration profile of copper atoms introduced into the sample by irradiating with a high energy copper beam was also calculated. The point defect concentrations from the calculation of Fig. 3 were used to calculate a depth dependent radiation enhanced diffusion coefficient (Eq. 13). After 7200 seconds of irradiation (at an ion flux of $\sim 2 \times 10^{12}$ ions/cm^2), the copper has only diffused a small distance from its deposited position as is shown in Fig. 11. After 10^5 seconds (i.e., a peak dose of ~ 212 dpa) the copper has spread throughout the irradiated region, reaching a peak concentration of ~ 1.6

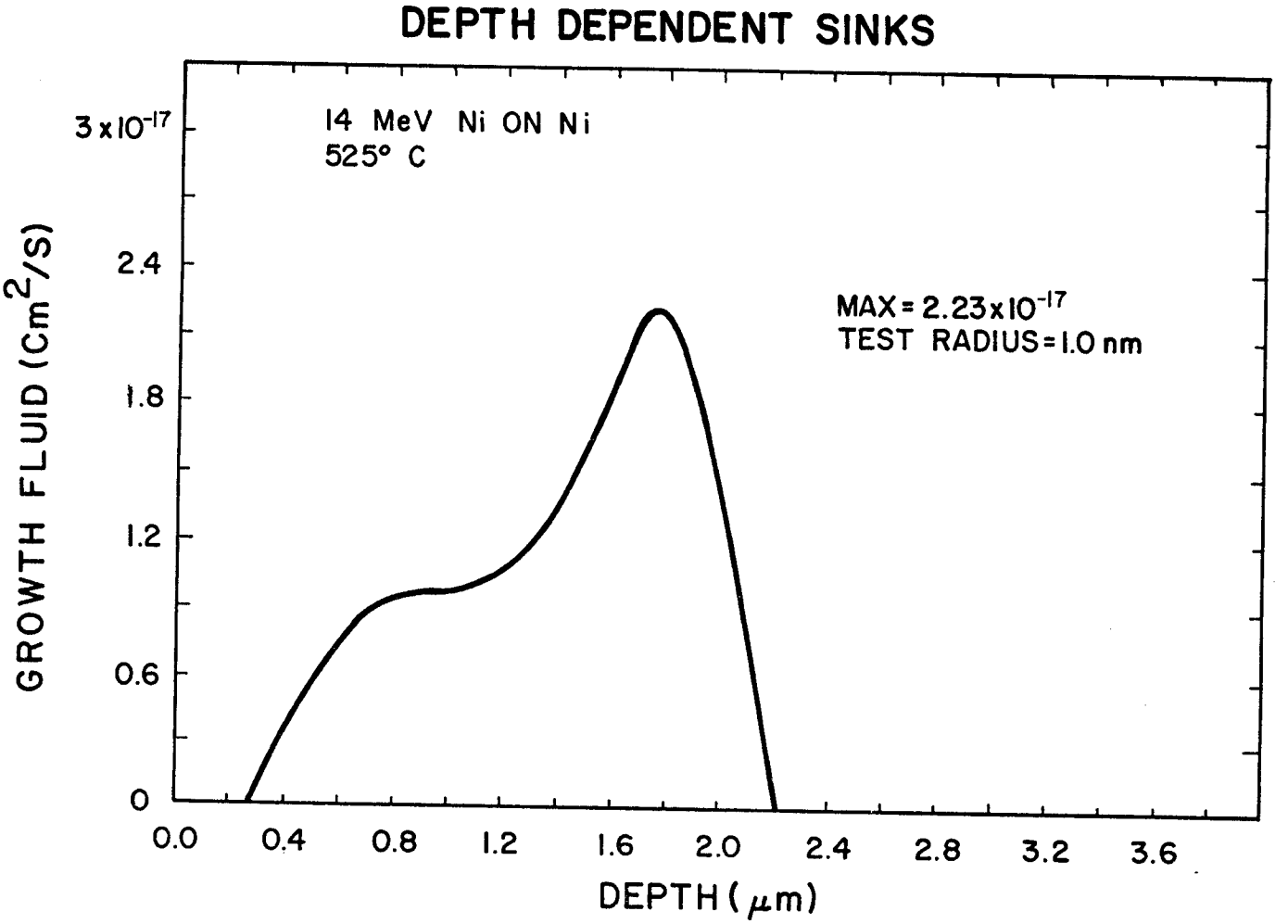

Fig. 5. The depth dependent growth fluid for a test radius of 1.0 nm using the defect concentration shown in Fig. 3.

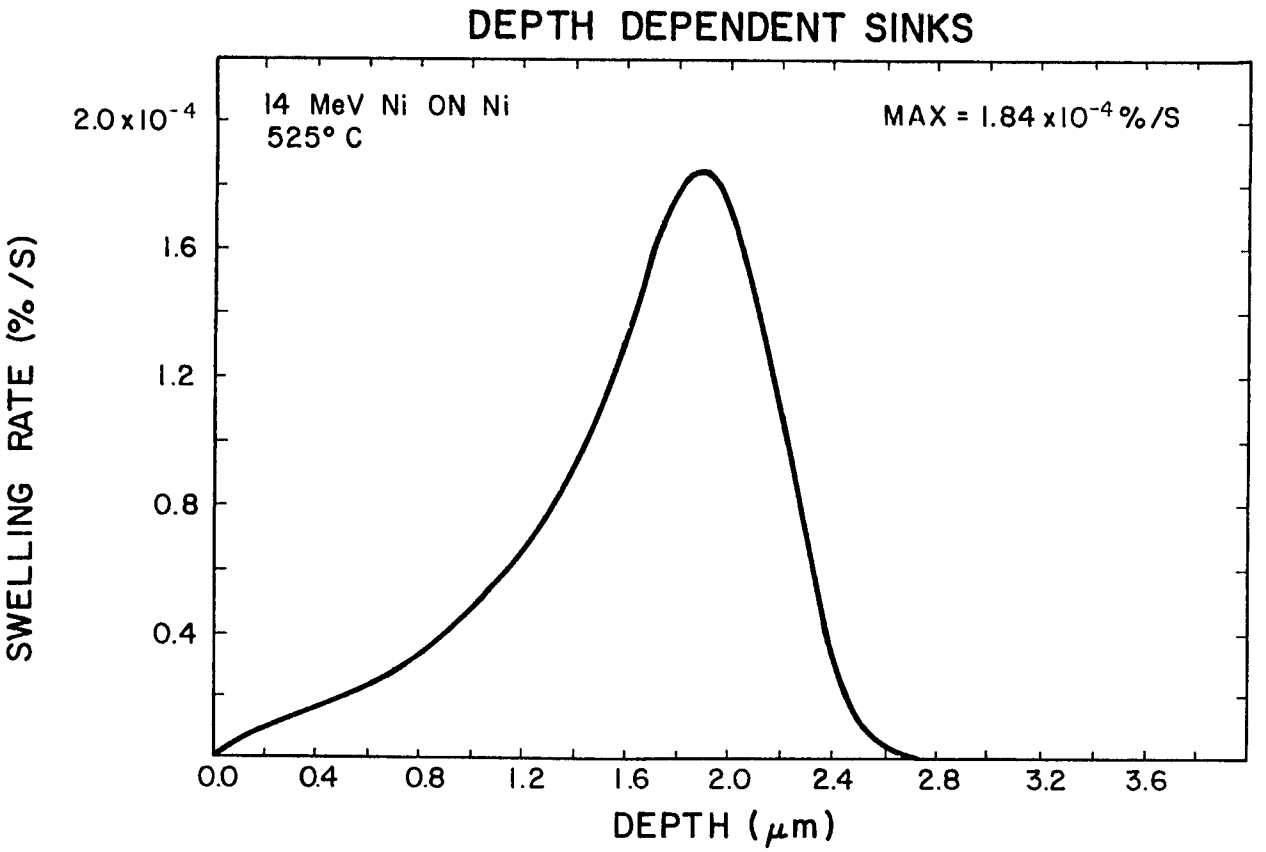

Fig. 6. The depth dependent swelling rate calculated using the defect concentrations of Fig. 3 and the experimentally measured void concentrations and sizes from Reference 3.

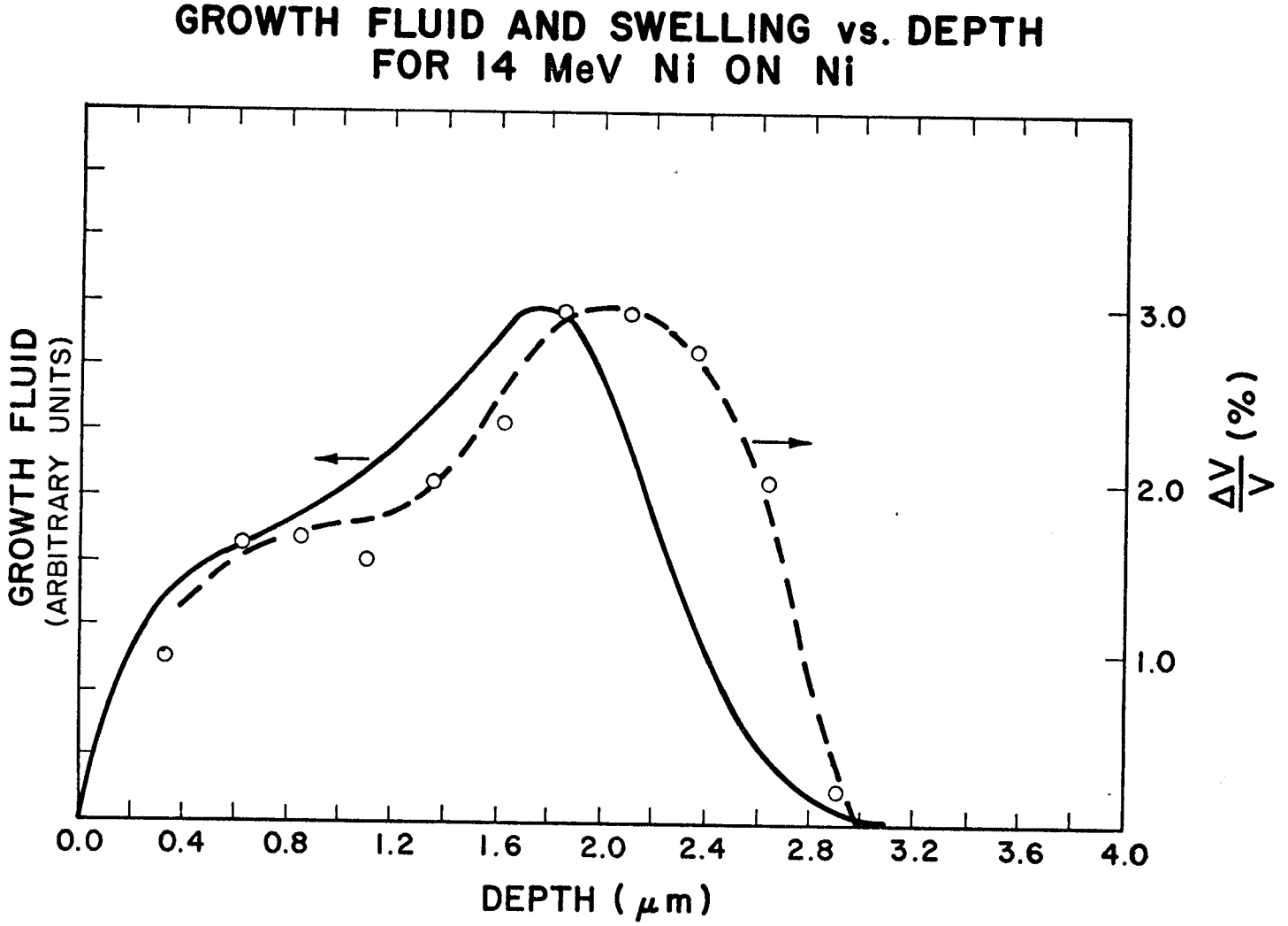

Fig. 7. A comparison of the growth fluid calculated using the defect concentrations shown in Fig. 1 to an experimentally measured swelling profile from Reference 3.

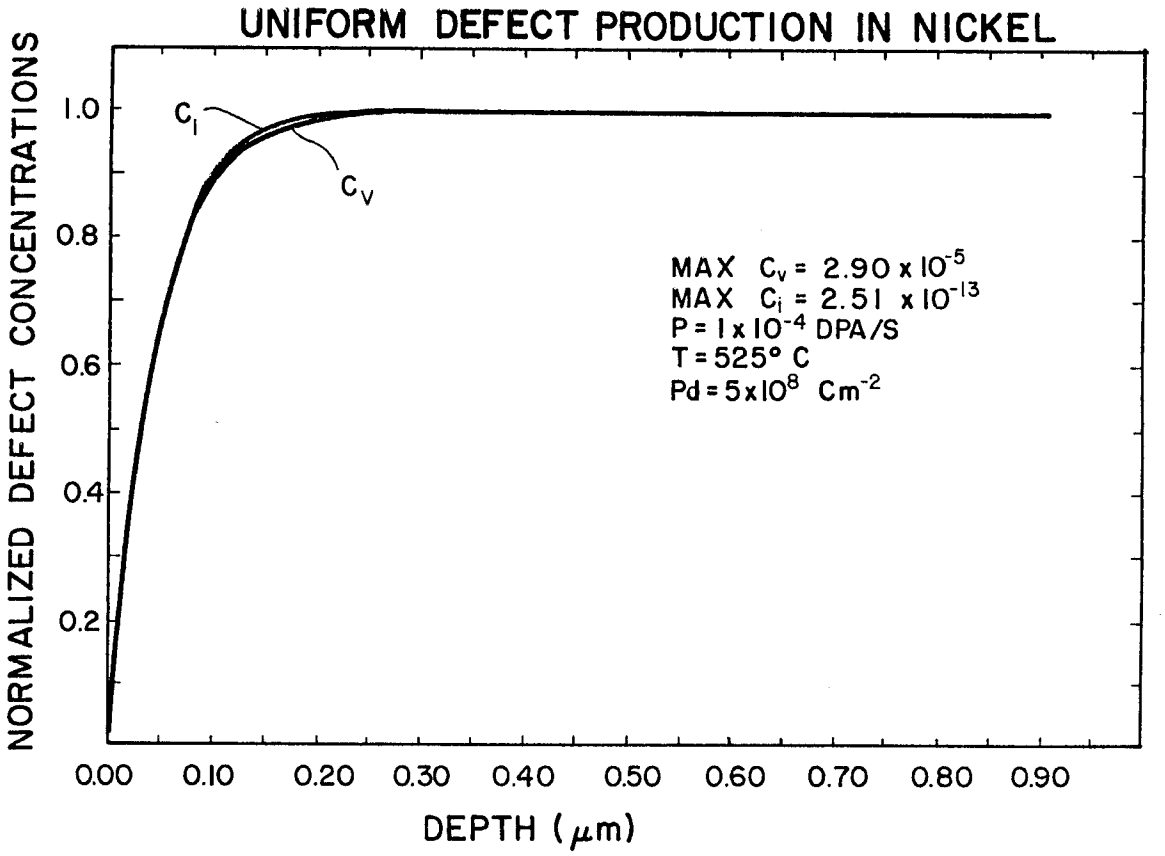

Fig. 8. The defect concentration profiles in a foil with uniform defect production and a uniform dislocation density of 5 x 10^{8} cm^{-2}.

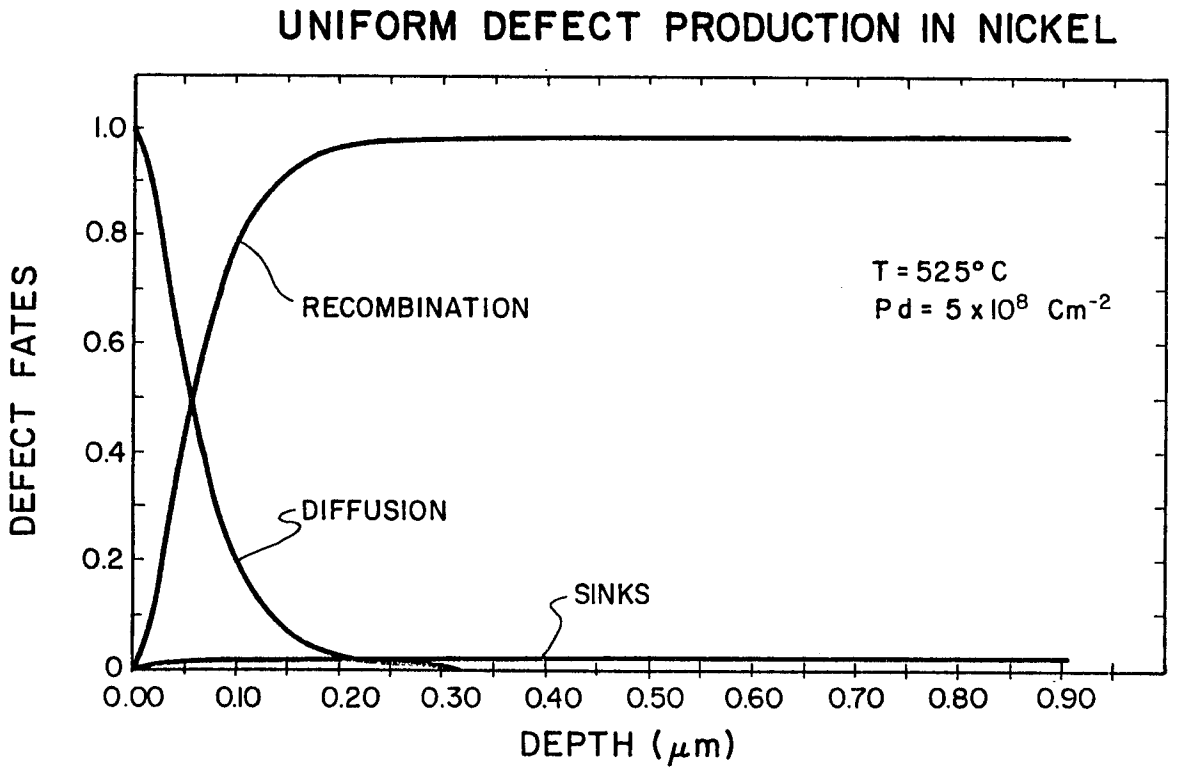

Fig. 9. The defect distributions from the calculations of Fig. 8. Note that diffusion of defects to the surface dominates over the first 0.1 μm for these conditions.

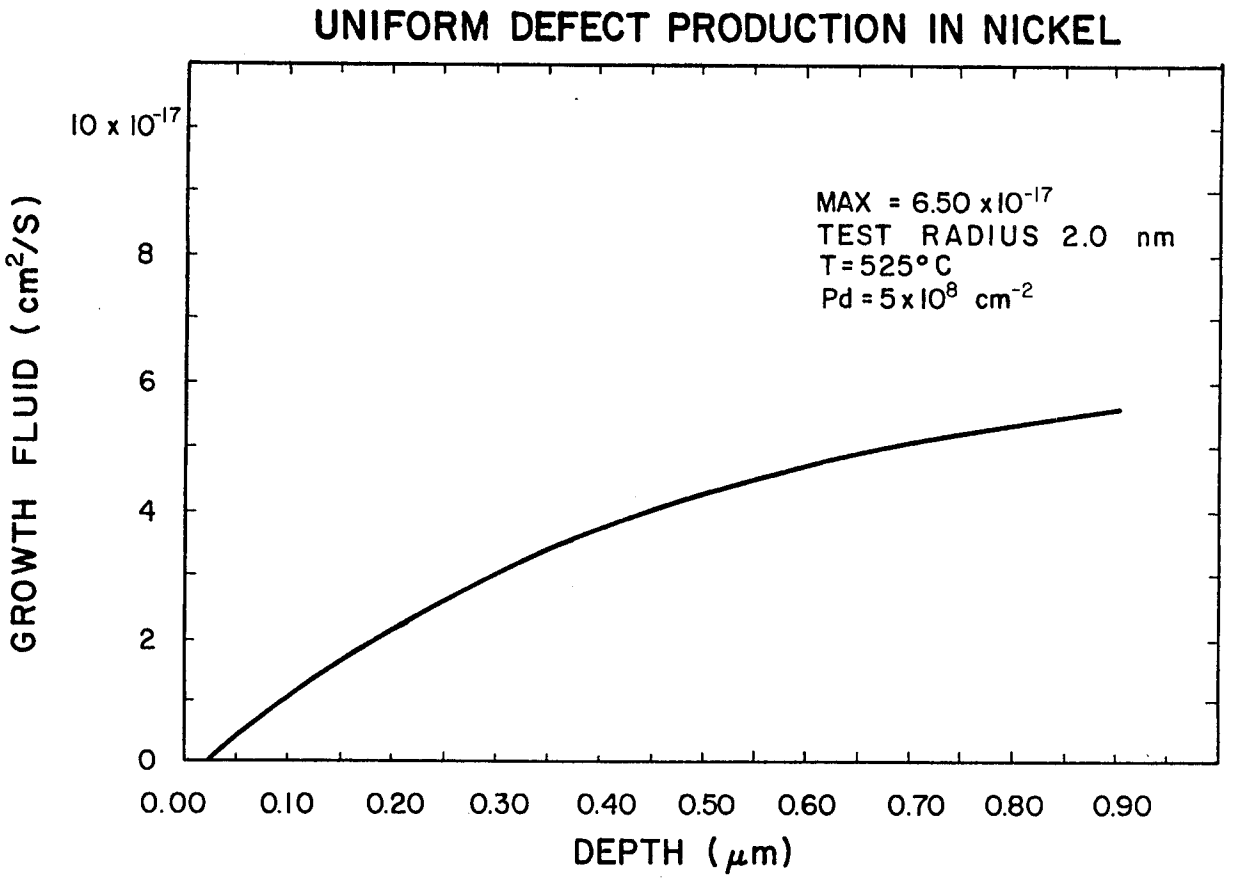

Fig. 10. The growth fluid calculated from the defect concentrations of Fig. 8.

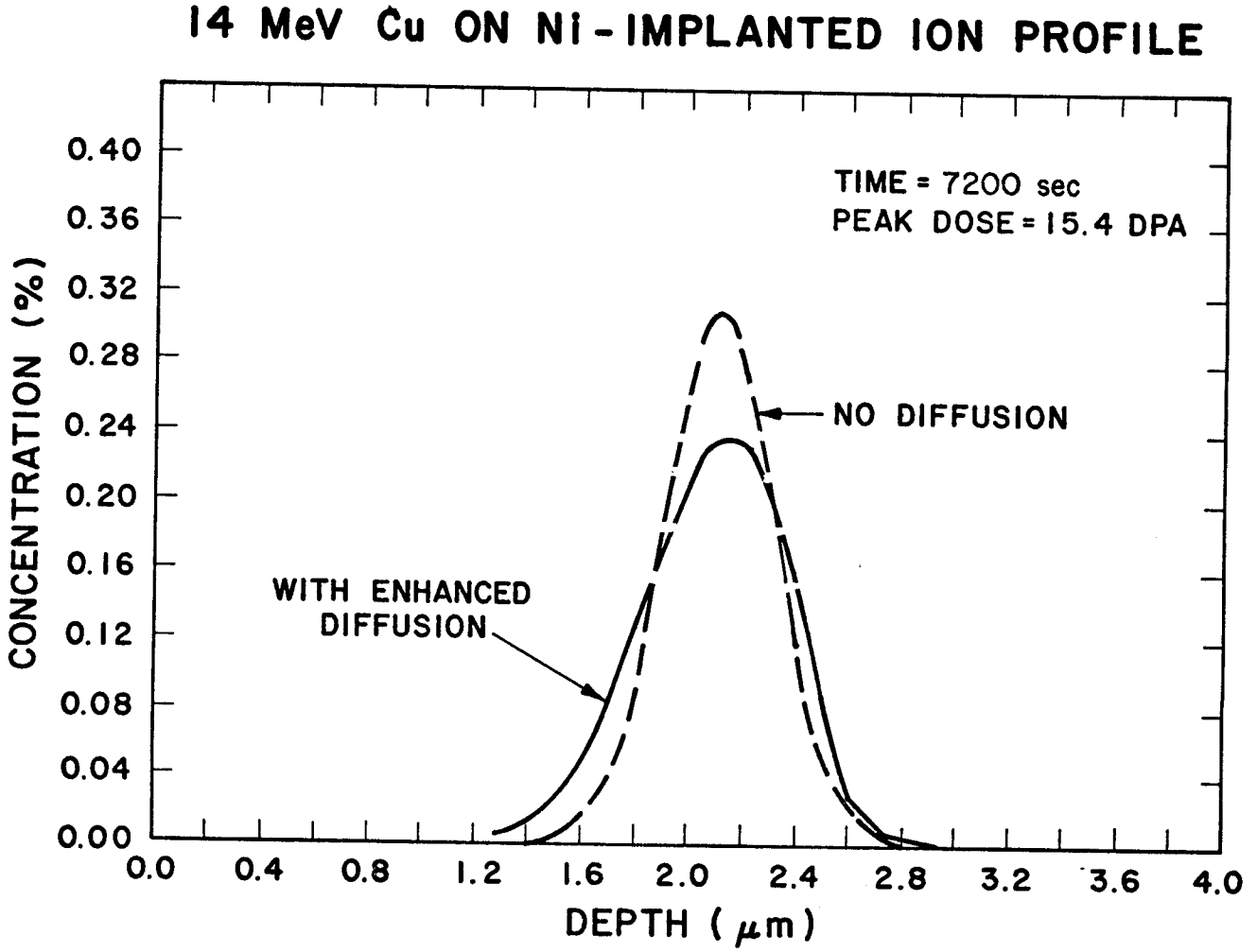

Fig. 11. The end-of-range distribution of copper ions incident on nickel after a total ion fluence of about 1.5×10^{16} ions/cm^2. The increased defect concentrations to the left of the ion end-of-range leads to a preferred migration of the copper toward the surface.

atomic percent (Fig. 12). The much larger defect concentrations in the irradiated zone to the left of the deposited ions have allowed much more diffusion of ions to the left. When irradiating with ions other than self-ions, this final impurity profile will determine in what depth regions of the sample one might expect point defect behavior to have been modified by interactions with impurities.

V. CONCLUSIONS

A computer code was developed which solves for the steady-state point defect concentrations in a thin foil under irradiation. Defect production in the foil can be any specified, depth dependent profile, as can the dislocation and void sink strengths. Using the steady-state defect concentration from this calculation, a depth dependent radiation enhanced diffusion coefficient is calculated, allowing the final distribution of incident "impurity" type atoms to be found.

Calculations were presented typical of a nickel foil irradiated at 525°C with 14 MeV nickel ions. The point defect profiles show less variation from mid-range to peak than does the displacement curve due to increased recombination in the end-of-range region.

Diffusion of point defects left a depleted zone near the front surface and also gave significant point defect concentrations beyond the ion end-of-range in the "undamaged" region. The void growth fluid calculated by the code was found to agree reasonably well with the experimentally measured void swelling profile.

Calculations of the final impurity concentration profile were carried out assuming an irradiating beam of 14 MeV copper ions into an initially pure nickel foil at 525°C. At times greater than $\sim 10^4$ seconds ($\sim$ 20 dpa at the

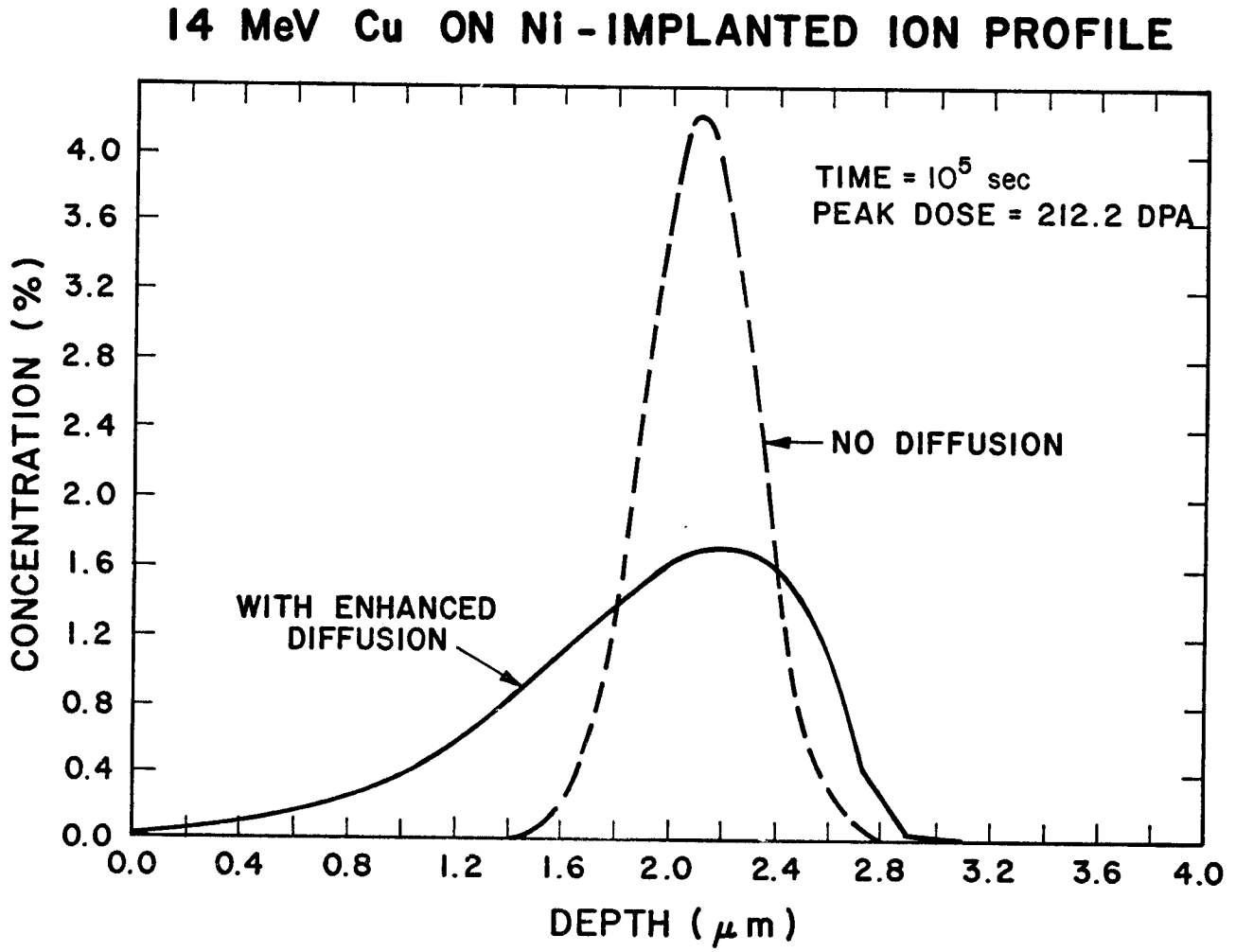

Fig. 12. The end-of-range distribution after a total ion fluence of about 2 x 10^{17} ion/cm^2. The copper has now distributed itself throughout the ion range.

peak), the copper has started to diffuse noticeable distances from the end-of-range region back into the irradiated region. After ~ 10^5 seconds (200 dpa at the peak), the copper has spread throughout the irradiated region and reached a peak concentration of ~ 1.6 atomic percent.

Acknowledgement

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Appendix A

The code was written in extended BASIC for use on a Tektronix 4051 desk-top computer with at least 16 K of user memory. Due to memory limitations, the code is written in four sections which are loaded from magnetic tape and executed segmentally. The four sections are (a) data and parameter input, (b) vacancy and interstitial concentration calculations, (c) data output, and (d) radiation enhanced diffusion calculation and output.

```
1 REM*****SPATIAL DISTRIBUTION OF POINT DEFECTS******FILE 4*
2 REM***** BY J.B. WHITLEY, 4/77 **************************
3 GO TO 90
4 REM***** UNIV. OF WISCONSIN, MADISON**********************
5 REM ODD LABELS OR SUBSCRIPTS REFER TO INTERSTITIALS,
6 REM EVEN LABELS OR SUBSCRIPTS TO VACANCIES
7 GO TO 2720
90 INIT
95 DIM E(11)
100 E=0
110 Z6=0
120 DIM M$(40),D$(30),W$(1)
130 PRINT "LENTER DATE,LABEL"
140 INPUT D$
150 PRINT "ENTER MATERIAL CODE:  1=NI, 0=OTHER"
160 INPUT Z5
170 RESTORE
180 GO TO Z5 OF 2190
190 IF E(1)=0 THEN 310
200 PRINT "DO YOU WANT ANY OF THE PREVIOUS VALUES? (Y or N)"
210 INPUT W$
220 IF W$="N" THEN 310
230 PRINT "PREVIOUS VALUES"
240 GOSUB 2250
250 PRINT "ENTER NUMBER OF PARAMETER TO CHANGE (0 IF NONE)"
260 INPUT Z5
270 IF Z5=0 THEN 360
280 GOSUB Z5 OF 2300,2320,2340,2360,2380,2400,2420,2440,2460,2480,2500
290 INPUT E(Z5)
300 GO TO 250
310 FOR I=1 TO 11
320    GOSUB I OF 2300,2320,2340,2360,2380,2400,2420,2440,2460,2480,2500
330    INPUT E(I)
340 NEXT I
```

```
350 GO TO 250
360 PRINT "ENTER CONVERGENCE CRITERION"
370 INPUT K1
380 PRINT "LENTER STORED DATA CODE_0=TO BE ENTERED"
390 PRINT "1=UNIFORM DEFECT PRODUCTION_2=5 MEV NI ON NI"
400 PRINT "3=18 MEV NI ON NI_4-6= OTHER ENTERED DATA"
420 INPUT Z5
430 GO TO Z5+1 OF 700,2520
440 IF Z6=0 THEN 510
450 PRINT "IS ORIGINAL PROGRAM DATA TAPE IN MACHINE? (Y or N)"
460 INPUT W$
470 IF W$="Y" THEN 510
480 PRINT "ENTER FILE NUMBER OF DESIRED DISPLACEMENT DATA"
490 INPUT Z5
500 Z5=Z5-6
510 FIND Z5+6
520 READ @33:M$,M
530 PRINT M$
540 DIM X(M),P(M),F1(M),P1(M)
550 READ @33:X,P,F1
560 PRINT "ADD EXCESS INTERSTITIALS? (Y or N)"
570 INPUT W$
580 PRINT "ENTER T (C), RECOMBINATION COEFFICIENT, FLUX (IONS/CM↑2/S)"
590 INPUT T1,A,F
600 IF W$="Y" THEN 620
610 F1=0
620 X2=X(1)
630 FOR I=1 TO M
640    P(I)=P(I)*F/1.0E+16
650    P1(I)=P(I)+F1(I)*F/(E(11)*2*X2*1.0E+22)
660    IF I=M THEN 680
670    X2=X(I+1)-X(I)-X2
680 NEXT I
690 GO TO 1280
700 PRINT "LENTER TITLE (UP TO 40 CHARACTERS)"
```

```
710 INPUT M$
720 PRINT "ENTER DEPTH (MICRONS TO MIDPOINT),DPA PER 1E16 IONS"
730 PRINT "ENTER NEGATIVE DEPTH TO TERMINATE ENTERIES"
740 DIM P5(80),X5(80)
750 FOR I=1 TO 80
760    PRINT I;"...  ";
770    INPUT X5(I),P5(I)
780    IF X5(I)<0 THEN 810
790    M=I
800 NEXT I
810 DIM P(M),X(M),F1(M),P1(M)
820 FOR I=1 TO M
830    P(I)=P5(I)
840    X(I)=X5(I)*1.0E-4
850 NEXT I
860 DELETE P5,X5
870 REM CALCULATE GAUSSIAN INTEGRAL
880 PRINT "MEAN RANGE (Microns)=  ";
890 INPUT U
900 U=U*1.0E-4
910 PRINT "STANDARD DEVIATION (Microns)=  ";
920 INPUT S
930 S=S*1.0E-4
940 F1=0
950 IF S=0 THEN 1220
960 X2=X(1)
970 P5=0.5
980 FOR I=1 TO M-1
990    X1=X2+X(I)
1000    Z=ABS((X1-U)/S)
1010    IF Z>4 THEN 1200
1020    T=0.7071068*Z
1030    S7=T
1040    Y2=Z↑2/2
1050    D=1
```

```
1060     D=D+2
1070     T=T*Y2*2/D
1080     S7=S7+T
1090     IF T/S7-1.0E-10>0 THEN 1060
1100     IF X1>U THEN 1140
1110     F1(I)=ABS(P5-0.5641896*S7*EXP(-Y2))
1120     P5=ABS(P5-F1(I))
1130     GO TO 1200
1140     IF (X1-U)/(X2*2)>1 THEN 1180
1150     F1(I)=P5+0.5641896*S7*EXP(-Y2)
1160     P5=0.5641896*S7*EXP(-Y2)
1170     GO TO 1200
1180     F1(I)=ABS(P5-0.5641896*S7*EXP(-Y2))
1190     P5=ABS(P5+F1(I))
1200     X2=X(I+1)-X(I)-X2
1210 NEXT I
1215 DELETE D,T,P5,U,S,Z,Y2,S7
1220 PRINT "ENTER FILE NUMBER TO STORE DATA (0 IF NOT TO BE STORED)"
1230 INPUT Z5
1240 IF Z5=0 THEN 560
1250 FIND Z5
1260 WRITE M$,M,X,P,F1
1270 GO TO 560
1280 DIM D(M),V(M),S(M)
1290 PRINT "LENTER DISLOCATION BIAS"
1300 INPUT B1
1310 PRINT "DO SINK STRENGTHS VARY WITH DEPTH ? (Y or N)"
1320 INPUT W$
1330 IF W$="Y" THEN 1400
1340 PRINT "ENTER VOID DENSITY(/cc),VOID SIZE (ANG),DISL DENSITY (/cm↑2)
     "
1350 INPUT V2,V3,V4
1360 V=4*PI*V2*V3*1.0E-8
1370 D=V4
1380 S=V3
```

```
1390 GO TO 1850
1400 D=0
1410 V=0
1420 I1=1
1430 I=1
1440 PRINT "ENTER DEPTH (MICRONS),VOID DENSITY (/cc),VOID SIZE (ANG)"
1450 PRINT "DISL DENSITY (/cm↑2)"
1460 PRINT I1;".. ";
1470 INPUT V1,V2,V3,V6
1475 IF V1<0 THEN 1400
1480 V5=4*PI*V2*V3*1.0E-8
1490 V1=V1*1.0E-4
1500 IF I1>1 THEN 1550
1510 V4=0
1520 V7=V5
1530 V9=V3
1540 V8=V6
1550 IF V1>V4 THEN 1580
1560 PRINT "**INTERVALS MUST BE ENTERED WITH INCREASING DEPTHS**GG"
1570 GO TO 1400
1580 V(I)=V7+(V5-V7)*(X(I)-V4)/(V1-V4)
1590 S(I)=V9+(V3-V9)*(X(I)-V4)/(V1-V4)
1600 D(I)=V8+(V6-V8)*(X(I)-V4)/(V1-V4)
1610 I=I+1
1620 IF I>M THEN 1700
1630 IF X(I)<V1 THEN 1580
1640 V4=V1
1650 V9=V3
1660 V7=V5
1670 V8=V6
1680 I1=I1+1
1690 GO TO 1460
1700 REM  SINK DATA SMOOTHING ROUTINE
1705 IF D(1)=SUM(D)/M AND V(1)=SUM(V)/M THEN 1850
1710 FOR I=2 TO M-1
```

```
1720     IF D(I)=D(M) THEN 1750
1730     I1=I
1740     D(I)=(D(I-1)+D(I+1))/4+D(I)/2
1750     IF V(I)=V(M) THEN 1790
1760     I1=I
1770     V(I)=(V(I-1)+V(I+1))/4+V(I)/2
1780     S(I)=(S(I-1)+S(I+1))/4+S(I)/2
1790 NEXT I
1800 FOR I=I1 TO 2 STEP -1
1810     D(I)=(D(I-1)+D(I+1))/4+D(I)/2
1820     V(I)=(V(I-1)+V(I+1))/4+V(I)/2
1830     S(I)=(S(I-1)+S(I+1))/4+S(I)/2
1840 NEXT I
1850 REM  CORRECT FOR DENSITY CHANGE DUE TO SWELLING
1855 IF SUM(V)=0 THEN 2120
1860 V4=0
1870 V6=0
1880 J=0
1890 V5=1+S(1)↑2*V(1)*1.0E-16/24
1900 FOR I=1 TO M
1910     V5=(X(I)-V4)*V5
1920     V4=X(I)
1930     X(I)=V6+V5
1940     V6=X(I)
1950     IF I=M THEN 2110
1960     IF X(I+J+1)>X(I) THEN 2030
1970     J=J+1
1980     IF I+J<M THEN 1960
1990     S(I)=S(M)
2000     V(I)=V(M)
2010     D(I)=D(M)
2020     GO TO 2070
2030     V3=V4*(J=0) MAX X(I+J)*(J>0)
2040     S(I)=S(I+J)+(S(I+J+1)-S(I+J))*(X(I)-V3)/(X(I+J+1)-V4)
2050     V(I)=V(I+J)+(V(I+J+1)-V(I+J))*(X(I)-V3)/(X(I+J+1)-V4)
```

```
2060    D(I)=D(I+J)+(D(I+J+1)-D(I+J))*(X(I)-V3)/(X(I+J+1)-V4)
2070    J=0
2080    V5=1+S(I)↑2*V(I)*1.0E-16/24
2090    P(I)=P(I)/V5
2100    P1(I)=P1(I)/V5
2110 NEXT I
2120 IF Z6>0 THEN 2890
2130 FIND 5
2140 DELETE 1,99
2150 DELETE 120,2140
2160 DELETE 2190,6000
2170 APPEND 100
2180 GO TO 120
2190 REM POINT DEFECT PARAMETERS;  DATA FOR MATERIALS OTHER THAN NI
2191 REM SHOULD BE ENTERED IN     DATA STATEMENTS FOLLOWING THE ONE
2192 REM FOR NICKEL (PRESENTLY FILLED WITH 0'S).
2195 FOR I=1 TO I
2200    READ E
2205 NEXT I
2210 DATA 0.15,1.38,4.08,1.39,0.12,0.062,5,4.48,1000,2.49,9.13
2215 DATA 0,0,0,0,0,0,0,0,0,0
2220 PRINT "FOLLOWING MATERIAL PARAMETERS ENTERED"
2230 GOSUB 2250
2240 GO TO 250
2250 FOR I=1 TO 11
2260    GOSUB I OF 2300,2320,2340,2360,2380,2400,2420,2440,2460,2480,
        2500
2270    PRINT USING "4D.3D":E(I)
2280 NEXT I
2290 RETURN
2300 PRINT "1...EMI=           EVBBBBBBBBBBBBB";
2310 RETURN
2320 PRINT "2...EMV=           EVBBBBBBBBBBBBB";
2330 RETURN
2340 PRINT "3...EFI=           EVBBBBBBBBBBBBB";
```

```
2350 RETURN
2360 PRINT "4...EFV=            EVBBBBBBBBBBBBBB";
2370 RETURN
2380 PRINT "5...DPEI=           CM↑2/SBBBBBBBBBBBBBBBBBB";
2390 RETURN
2400 PRINT "6...DPEV=           CM↑2/SBBBBBBBBBBBBBBBBB";
2410 RETURN
2420 PRINT "7...FPEI=  ";
2430 RETURN
2440 PRINT "8...FPEV=  ";
2450 RETURN
2460 PRINT "9...SURFACE ENERGY=            ERG/CM↑2BBBBBBBBBBBBBBBBBBB";
2470 RETURN
2480 PRINT "10..LATTICE SPACING          ANGSTROMSBBBBBBBBBBBBBBBBBBBB";
2490 RETURN
2500 PRINT "11..DENSITY=         *E22 /CM↑3BBBBBBBBBBBBBBBBBB";
2510 RETURN
2520 REM  UNIFORM DEFECT PRODUCTION
2530 PRINT "ENTER TEMP (C), RECOMBINATION A"
2540 INPUT T1,A
2550 PRINT "ENTER UNIFORM PRODUCTION RATE  (DPA/S)"
2560 M$="UNIFORM PRODUCTION RATE"
2570 M=42
2580 DIM X(M),P(M),F1(M),P1(M)
2590 X2=1.0E-6
2600 X(1)=5.0E-7
2610 FOR I=2 TO M
2620    X(I)=X(I-1)+X2/2+I*2.5E-7
2630    X2=I*5.0E-7
2640 NEXT I
2650 INPUT P6
2660 P=P6
2670 F=0
2680 F1=0
2690 P1=P
```

```
2700 GO TO 1280
2710 END
2720 REM  DATA ENTRY FOR MULTIPLE RUNS
2730 INIT
2740 DIM E(11)
2745 Z9=0
2750 E=0
2760 PRINT "A DATA TAPE SHOULD BE IN THE MACHINE WITH ENOUGH CONSECUTIVE
     "
2770 PRINT "NEW,  7K FILES MARKED TO HOLD THE ENTRIES"
2780 PRINT "ENTER NUMBER OF FIRST FILE FOR ENTRIES"
2790 INPUT Z6
2800 FIND Z6
2810 IF TYP(0)=0 THEN 2870
2820 PRINT "FILE ";Z6;"  IS NOT A NEW FILE"
2830 PRINT "DO YOU WANT TO WRITE OVER THE PRESENT DATA  (Y or N)"
2840 INPUT W$
2850 IF W$="Y" THEN 2870
2860 GO TO 2780
2870 DELETE X,P,F1,P1,D,V,S
2880 GO TO 120
2890 FIND Z6
2900 WRITE @33:M$,D$,E,K1,M,X,P,F1,P1,D,V,B1,T1,A,F,S
2910 CLOSE
2920 Z6=Z6+1
2925 Z9=Z9+1
2930 PRINT "MORE ENTRIES? (Y or N)"
2940 INPUT W$
2950 IF W$="Y" THEN 2800
2955 PRINT Z9;"  ENTRIES WERE MADE STARTING WITH FILE  ";Z6-Z9
2960 FIND 5
2970 OLD
2980 END
```

```
4 GO TO 1210
100 REM*****SPATIAL DISTRIBUTION OF POINT DEFECTS******FILE 5*
110 REM***** BY JOHN WHITLEY, 4/77 **************************
120 REM CALCULATION OF POINT DEFECT CONCENTRATIONS
130 REM USING DATA INPUT BY PROGRAM OF FILE 4
140 PRINT @32,26:2
150 DIM Y(2*M),U1(M-1),U2(M-1),U3(M-1),T3(2*M),T4(2*M)
160 U1(1)=2/(X(1)*X(2))
170 U3(1)=2/((X(2)-X(1))*X(2))
180 U2(1)=U1(1)+U3(1)
190 FOR I=2 TO M-1
200    U1(I)=2/((X(I)-X(I-1))*(X(I+1)-X(I-1)))
210    U3(I)=2/((X(I+1)-X(I))*(X(I+1)-X(I-1)))
220    U2(I)=U1(I)+U3(I)
230 NEXT I
240 T=T1+273
250 D1=E(5)*EXP(-E(1)/(T*8.6163E-5))
260 D2=E(6)*EXP(-E(2)/(T*8.6163E-5))
270 A2=A*D1/D2
280 C1=E(7)*EXP(-E(3)/(8.6163E-5*T))
290 C2=E(8)*EXP(-E(4)/(8.6163E-5*T))
300 FOR I=1 TO M
304    C4=C2
306    IF S(I)=0 THEN 320
310    C4=C2*EXP(2*E(9)*E(10)↑3/(1.3805*T*(S(I)/2)))
320    P(I)=P(I)/D2+C2*D(I)+C4*V(I)
330    P1(I)=P1(I)/D1+C1*D(I)+V(I)*C1*C4/C2
340 NEXT I
350 REM  MAKE INITIAL GUESS  (NO DIFFUSION, DiCi=DvCv)
360 IF A=0 THEN 450
370 FOR I=2 TO M*2 STEP 2
380    S1=V(I/2)+(1+B1)*D(I/2)
390    S2=V(I/2)+D(I/2)
400    Y(I-1)=(-S1*D1+((D1*S1)↑2+4*A2*P1(I/2)*D1↑2)↑0.5)/(2*A2*D1)+C1
```

```
410    Y(I)=(-S2*D2+((D2*S2)↑2+4*A*D2↑2*P(I/2))↑0.5)/(2*A*D2)+C2
420 NEXT I
430 GO TO 510
440 REM  INITIAL GUESS IF NO RECOMBINATION
450 FOR I=2 TO M*2 STEP 2
460    S1=V(I/2)+(1+B1)*D(I/2)
470    S2=V(I/2)+D(I/2)
480    Y(I-1)=P1(I/2)/S1+C1
490    Y(I)=P(I/2)/S2+C2
500 NEXT I
510 REMARK  **START CALCULATIONS*****
520 REM  EQUATIONS ARE SOLVED USING A MODIFIED GAUSS-SIEDEL ITERATION
530 REM  T3 IS A RELAXATION COEFFICIENT.  T3 WILL INCREASE IF THE
540 REM  SUCCESSIVE GUESSES ARE MOVING TOWARD A CONVERGED VALUE;
550 REM  T3 WILL DECREASE IF SUCCESSIVE GUESSES ARE OSCILLATING.
560 T3=1
570 FOR I1=1 TO 200
580    FOR I2=1 TO 4
590       S1=V(1)+(1+B1)*D(1)
600       T4(1)=(P1(1)+U3(1)*Y(3))/(U2(1)+S1+A*Y(2))-Y(1)
610       Y(1)=Y(1)+T3(1)*T4(1)
620       S2=V(1)+D(1)
630       T4(2)=(P(1)+U1(1)*C2+U3(1)*Y(4))/(U2(1)+S2+A2*Y(1))-Y(2)
640       Y(2)=Y(2)+T3(2)*T4(2)
650       FOR I=2 TO M-1
660          Q=2*I
670          S1=V(I)+(1+B1)*D(I)
680          S2=V(I)+D(I)
690          T4(Q)=(P(I)+U1(I)*Y(Q-2)+U3(I)*Y(Q+2))/(U2(I)+S2+A2*Y(Q-1))
700          T4(Q)=T4(Q)-Y(Q)
710          Y(Q)=Y(Q)+T3(Q)*T4(Q)
720          T4(Q-1)=(P1(I)+U1(I)*Y(Q-3)+U3(I)*Y(Q+1))/(U2(I)+S1+A*Y(Q))
             -Y(Q-1)
730          Y(Q-1)=Y(Q-1)+T3(Q-1)*T4(Q-1)
740       NEXT I
```

```
750        IF P(M)=0 THEN 790
760        REM USE REFLECTING BOUNDARY CONDITION IF UNIFORM DEFECT PRODUC
           TION
770        Y(2*M)=Y(2*M-2)
780        Y(2*M-1)=Y(2*M-3)
790     NEXT I2
800     G2=Y(2)
810     Y6=(P1(1)+U3(1)*Y(3))/(U2(1)+V(1)+(1+B1)*D(1)+A*Y(2))-Y(1)
820     T3(1)=T3(1)+0.1*SGN(T4(1)*Y6)*(T3(1)>0.4) MIN 1.8
830     Y(1)=Y(1)+T3(1)*Y6
840     S2=V(1)+D(1)
850     Y6=(P(1)+U1(1)*C2+U3(1)*Y(4))/(U2(1)+S2+A2*Y(1))-Y(2)
860     T3(2)=T3(2)+0.1*SGN(T4(2)*Y6)*(T3(2)>0.4) MIN 1.8
870     Y(2)=Y(2)+T3(2)*Y6
880     H3=ABS((Y(2)-G2)/G2)
890     FOR I=2 TO M-1
900        Q=2*I
910        G2=Y(Q)
920        S1=V(I)+(1+B1)*D(I)
930        S2=V(I)+D(I)
940        Y6=(P(I)+U1(I)*Y(Q-2)+U3(I)*Y(Q+2))/(U2(I)+S2+A2*Y(Q-1))-Y(Q)
950        T3(Q)=T3(Q)+0.1*SGN(T4(Q)*Y6)*(T3(Q)>0.4) MIN 1.8
960        Y(Q)=Y(Q)+T3(Q)*Y6
970        Y6=(P1(I)+U1(I)*Y(Q-3)+U3(I)*Y(Q+1))/(U2(I)+S1+A*Y(Q))-Y(Q-1)
980        T3(Q-1)=T3(Q-1)+0.1*SGN(T4(Q-1)*Y6)*(T3(Q-1)>0.4) MIN 1.8
990        Y(Q-1)=Y(Q-1)+T3(Q-1)*Y6
1000        H3=H3 MAX ABS((Y(Q)-G2)/G2)
1010    NEXT I
1020    IF P(M)=0 THEN 1050
1030    Y(2*M)=Y(2*M-2)
1040    Y(2*M-1)=Y(2*M-3)
1050    IF H3<K1 THEN 1080
1060    PRINT I1*5,H3
1070 NEXT I1
1080 PRINT @32,26:0
```

```
1090 FOR I=1 TO M
1094     C4=C2
1096     IF S(I)=0 THEN 1110
1100     C4=C2*EXP(2*E(9)*E(10)↑3/(1.3805*T*(S(I)/2)))
1110     P(I)=(P(I)-C2*D(I)-C4*V(I))*D2
1120     P1(I)=(P1(I)-C1*D(I)-C1*C4/C2*V(I))*D1
1130 NEXT I
1140 DELETE T3,T4,U2
1150 IF Z6>0 THEN 1300
1155 DELETE P1
1160 FIND 6
1170 DELETE 1,1160
1180 DELETE 1210,6000
1190 APPEND 1200
1200 END
1210 PRINT "ENTER NUMBER OF FIRST DATA FILE,NUMBER OF RUNS TO MAKE"
1220 INPUT Z6,Z5
1230 Z5=Z5+Z6
1240 DIM M$(40),D$(30),E(11)
1250 FIND Z6
1260 READ @33:M$,D$,E,K1,M
1270 DIM X(M),P(M),F1(M),P1(M),D(M),V(M),S(M)
1280 READ @33:X,P,F1,P1,D,V,B1,T1,A,F,S
1290 GO TO 120
1300 FIND Z6
1310 WRITE M$,D$,E,K1,M,X,P,F1,P1,D,V,B1,T1,A,F,Y,U1,U3,D1,D2,C1,C2
1320 WRITE H3,I1,S
1330 CLOSE
1340 PRINT Z5-Z6-1;" RUNS TO BE COMPLETED"
1350 DELETE Y,U1,U2,U3,X,P,F1,D,V,P1,T3,T4,S
1360 Z6=Z6+1
1370 IF Z6<Z5 THEN 1250
1380 END
```

```
3 GO TO 100
4 GO TO 2720
100 REM ******* SPATIAL DISTRIBUTION OF POINT DEFECTS **** FILE 6*
110 REM  ******  J.B. WHITLEY, 4/77**
120 REM  OUTPUT ROUTINE
130 Z6=0
140 T=T1+273
150 PRINT USING "P,40A,30A,1A,3D,/":M$,D$,"H",Z6
160 GOSUB 2280
170 PRINT USING 300:I1*5," STEPS TO CONVERGE WITHIN ",H3*100," PERCENT"
180 PRINT USING 190:"TEMPERATURE= ",T1,"C"
190 IMAGE13A,4D.,1A
200 PRINT USING "23A,2E":"RECOMBINATION FACTOR= ",A
210 PRINT USING " 6A,2E,12A":"FLUX= ",F," IONS/cm↑2/s"
220 IF SUM(V)+SUM(D)<>M*(D(1)+V(1)) THEN 260
230 PRINT USING 240:"SINK DENSITY THROUGHOUT SAMPLE= ";D(1)+V(1);" /cm↑2
    "
240 IMAGE 35A,2E,10A
250 GO TO 270
260 PRINT "SINK DENSITIES ARE DEPTH DEPENDENT"
270 PRINT USING "20A,2D.1D,1A":"DISLOCATION BIAS= ",B1*100,"%"
280 PRINT USING "/,10T,A,23T,A,39T,A,55T,A,/":"X","I","V","P"
290 Z5=0
300 IMAGE /,FD,26A,2E,8A
310 FOR I=1 TO 2*M-1 STEP 4
320    PRINT USING 330:X(I/2+0.5)*10000,Y(I),Y(I+1),P(I/2+0.5)
330    IMAGE 5X,3D.3D,5X,3E,5X,3E,5X,2E
340 NEXT I
350 PRINT USING "//,50A":"****OUTPUT DONE, COPY AND PUSH RETURN***GG"
360 INPUT W$
370 REM********BEGIN PLOTTING ROUTINE*
380 VIEWPORT 10,120,10,90
390 PRINT "ENTER MAXIMUM DEPTH TO BE PLOTTED (IN MICROMETERS)"
400 INPUT X9
```

```
410 X9=X9/10000
420 L1=0
430 L2=0
440 L3=0
450 L4=0
460 L5=0
470 M1=0
475 W$="N"
480 FOR I=1 TO M*2-1 STEP 2
490    L1=L1 MAX P(I/2+0.5)
500    L2=L2 MAX Y(I+1)
510    L3=L3 MAX Y(I)
520    L4=L4 MAX V(I/2)
530    L5=L5 MAX D(I/2)
540    M1=M1 MAX (I*(X(I/2+0.5)(X9)+1*(I(M))/2+0.5
550 NEXT I
555 IF M*(D(1)+V(1))=SUM(D)+SUM(V) THEN 580
560 PRINT "DO YOU WANT THE SINK STRENGTHS PLOTTED? (Y or N)"
570 INPUT W$
580 PRINT "L";Z6
590 WINDOW 0,100,0,110
600 MOVE 0,C2/L2*100
610 L9=L2
620 W=0
630 A$="V"
640 FOR E1=1 TO 2
650    W=W+INT(M1/7)+1
660    FOR I=2 TO M1+1
670       DRAW X(I-1)/X9*100,Y(2*I-E1-1)*100/L9
680       IF I<>W THEN 700
690       PRINT USING "A,A,S":A$,"H"
700    NEXT I
710    L9=L3
720    MOVE 0,0
730    A$="I"
```

```
740 NEXT E1
745 IF M*P(1)=SUM(P) THEN 880
750 MOVE 0,P(1)/L1*100
760 W=W+INT(M1/5)+1
770 FOR I=1 TO M1
780    DRAW X(I)/X9*100,P(I)*100/L1
790    IF I<>W OR X(I)>0.9*X9 THEN 810
800    PRINT USING "2A,S":"PH"
810 NEXT I
820 MOVE 0,0
830 X2=X(1)
840 FOR I=1 TO M1-1
850    DRAW X(I)/X9*100,F1(I)*1.0E-3/(2*X2)
860    X2=X(I+1)-X(I)-X2
870 NEXT I
880 IF W$<>"Y" THEN 1030
890 IF L4=0 THEN 960
900 MOVE 0,V(1)*100/L4
910 FOR I=1 TO M1
920    DRAW X(I)/X9*100,V(I)*100/L4
930    IF I<>INT(M1/2) THEN 950
940    PRINT USING "10A,S":"VOIDSHHHHH"
950 NEXT I
960 IF L5=0 THEN 1030
970 MOVE 0,D(1)*100/L5
980 FOR I=1 TO M1
990    DRAW X(I)*100/X9,D(I)*100/L5
1000    IF I<>INT(M1/1.3) THEN 1020
1010    PRINT USING " 8A,S":"DISLHHHH"
1020 NEXT I
1030 AXIS 5,10,0,0
1040 AXIS 5,10,100,110
1050 MOVE 70,100
1060 PRINT USING 1110:"MAX V= ",L2
1070 MOVE 70,95
```

```
1080 PRINT USING 1110:"MAX I= ",L3
1090 MOVE 70,90
1100 PRINT USING 1110:"MAX P= ",L1
1110 IMAGE 8A,2E
1120 IMAGE 7A,1D.3D,8A
1130 IF W$<>"Y" AND SUM(V)=0 THEN 1180
1140 MOVE 70,85
1150 PRINT USING 1110:"MAX VOID",L4
1160 MOVE 70,80
1170 PRINT USING 1110:"MAX DISL",L5
1180 L$="      DEFECT CONCENTRATIONS"
1190 GOSUB 2530
1200 INPUT W$
1210 GO TO Z5 OF 2410,2410,2410,2410
1220 REMARK***PLOT GROWTH FLUID = DvCv-DiCi*
1230 PRINT "L***PLOTTING OF GROWTH FLUID*****"
1240 PRINT "ENTER RADIUS OF TEST VOID (IN ANGSTROMS)"
1250 INPUT R
1260 C4=C2*EXP(2*E(9)*E(10)↑3/(1.3805*T*R))
1270 L4=-1
1280 Y6=0
1290 FOR I=2 TO M*2 STEP 2
1300    L4=L4 MAX D2*(Y(I)-C4)-D1*Y(I-1)
1310    IF S(I/2)>0 THEN 1340
1320    K=1
1330    GO TO 1350
1340    K=EXP(2*E(9)*E(10)↑3/(1.3805*T*(S(I/2)/2)))
1350    Y6=Y6 MAX (D2*(Y(I)-C2*K)-D1*Y(I-1))*V(I/2)
1360 NEXT I
1370 PRINT "MAXIMUM VALUE= ",L4
1380 PRINT "ENTER MAXIMUM VALUE FOR PLOT"
1390 INPUT L5
1400 PRINT "L";Z6
1410 IF L5>0 THEN 1430
1420 L5=L4
```

```
1430 WINDOW 0,100,0,110
1440 MOVE X(1)/X9*100,(D2*(Y(2)-C4)-D1*Y(1))*100/L5
1450 FOR I=2 TO M1
1460    DRAW X(I)/X9*100,(D2*(Y(2*I)-C4)-D1*Y(2*I-1))*100/L5
1470 NEXT I
1480 MOVE 70,95
1490 PRINT USING "6A,2E":"Y-TIC=",L5/10
1500 MOVE 70,90
1510 PRINT USING "5A,3E":"MAX= ",L4
1520 MOVE 70,85
1530 PRINT USING "13A,FD,A":"TEST RADIUS= ",R,"A"
1540 AXIS 5,10,0,0
1550 AXIS 5,10,100,110
1560 L$="           GROWTH FLUID"
1570 GOSUB 2530
1580 INPUT W$
1590 GO TO Z5 OF 2410,2410,2410,2410,2410
1600 IF Y6<=0 THEN 1910
1610 PRINT "LPLOTTING OF SWELLING RATE"
1620 PRINT "MAXIMUM VALUE =",Y6
1630 PRINT "ENTER MAXIMUM VALUE FOR PLOT"
1640 INPUT L5
1650 PRINT "L";Z6
1660 WINDOW 0,100,0,110
1670 IF L5>0 THEN 1690
1680 L5=Y6
1690 IF S(1)>0 THEN 1720
1700 C4=C2
1710 GO TO 1730
1720 C4=C2*EXP(2*E(9)*E(10)↑3/(1.3805*T*(S(1)/2)))
1730 MOVE X(1)*100/X9,(D2*(Y(2)-C4)-D1*Y(1))*100*V(1)/L5
1740 FOR I=2 TO M1
1750    IF S(I)>0 THEN 1780
1760    C4=C2
1770    GO TO 1790
```

```
1780    C4=C2*EXP(2*E(9)*E(10)↑3/(1.3805*T*(S(I)/2)))
1790    DRAW X(I)*100/X9,(D2*(Y(2*I)-C4)-D1*Y(2*I-1))*100*V(I)/L5
1800 NEXT I
1810 MOVE 70,95
1820 PRINT USING "5A,3E":"MAX=",Y6
1830 MOVE 70,90
1840 PRINT USING "7A,2E":"Y-TIC=",L5/10
1850 AXIS 5,10,0,0
1860 AXIS 5,10,100,110
1870 L$="           SWELLING RATE"
1880 GOSUB 2530
1890 INPUT W$
1900 GO TO 25 OF 2410,2410,2410,2410,2410
1910 REM **DEFECT FATE PLOTS
1920 PRINT "L";26
1930 WINDOW 0,100,-20,110
1940 MOVE X(1)/X9*100,A*D1*Y(1)*Y(2)/P(1)*100
1950 FOR I=4 TO 2*M1-1 STEP 2
1960    GOSUB 2240
1970    DRAW X(I/2)/X9*100,A*D1*Y(I)*Y(I-1)/L5
1980    IF I<>10 THEN 2000
1990    PRINT USING "2A,S":"RH"
2000 NEXT I
2010 AXIS 5,10,0,0
2020 AXIS 5,10,100,110
2030 MOVE X(1)/X9*100,D2*Y(2)*(D(1)+V(1))/P(1)*100
2040 FOR I=4 TO 2*M1-1 STEP 2
2050    GOSUB 2240
2060    DRAW X(I/2)/X9*100,D2*Y(I)*(D(I/2)+V(I/2))/L5
2070    IF I<>20 THEN 2090
2080    PRINT USING "2A,S":"SH"
2090 NEXT I
2100 U2=U1(1)+U3(1)
2110 MOVE X(1)/X9*100,-D2*(U1(1)*C2-U2*Y(2)+U3(1)*Y(4))/P(1)*100
2120 FOR I=4 TO 2*M1-1 STEP 2
```

```
2130    GOSUB 2240
2140    Y8=-D2*(U1(I/2)*Y(I-2)-(U1(I/2)+U3(I/2))*Y(I)+U3(I/2)*Y(I+2))
2150    Y8=Y8/L5
2160    DRAW X(I/2)/X9*100,Y8
2170    IF I<>30 OR X(I/2)>0.9*X9 THEN 2190
2180    PRINT USING "2A,S":"DH"
2190 NEXT I
2200 L$="           DEFECT FATES"
2210 GOSUB 2530
2220 INPUT W$
2230 GO TO 2410
2240 L5=A*D1*Y(I)*Y(I-1)+D2*Y(I)*(D(I/2)+V(I/2))
2250 Y8=-D2*(U1(I/2)*Y(I-2)-(U1(I/2)+U3(I/2))*Y(I)+U3(I/2)*Y(I+2))
2260 L5=(L5+Y8*(Y8>0))/100
2270 RETURN
2280 IMAGE 20A   ,4D.3D,10A
2290 PRINT USING 2280:"1...EMI=",E(1)," eV"
2300 PRINT USING 2280:"2...EMV=",E(2)," eV"
2310 PRINT USING 2280:"3...EFI=",E(3)," eV"
2320 PRINT USING 2280:"4...EFV=",E(4)," eV"
2330 PRINT USING 2280:"5...DPEI=",E(5)," cm↑2/s"
2340 PRINT USING 2280:"6...DPEV=",E(6)," cm↑2/s"
2350 PRINT USING 2280:"7...FPEI=  ",E(7)," "
2360 PRINT USING 2280:"8...FPEV=  ",E(8)," "
2370 PRINT USING 2280:"9...SURFACE ENERGY=",E(9)," erg/cm↑2"
2380 PRINT USING 2280:"10..LATTICE SPACING=",E(10),"*E-10 m"
2390 PRINT USING 2280:"11..DENSITY=",E(11),"*E22 /cm↑3"
2400 RETURN
2410 PRINT "LENTER_1 TO SEE OUTPUT _2 TO REPLOT DEFECT CONCENTRATIONS"
2420 PRINT "3 TO REPLOT GROWTH FLUID"
2430 PRINT "4 TO REPLOT DEFECT FATES_5 TO REPLOT SWELLING RATE"
2440 PRINT "6 TO RUN IMPURITY DIFFUSION CODE_7 TO PLOT NEW DATA"
2450 INPUT Z5
2460 GO TO Z5 OF 140,370,1220,1910,1610,2470,2720
2470 FIND 7
```

```
2480 DELETE 1,99
2490 DELETE 110,2470
2500 DELETE 2530,2640
2510 APPEND 100
2520 GO TO 100
2530 REM  AXIS LABELING ROUTINE
2540 HOME
2550 PRINT "   ";
2560 FOR I=1 TO 34
2570    W$=SEG(L$,I,1)
2580    PRINT W$;"HJ";
2590 NEXT I
2600 MOVE 50,0
2610 PRINT "JJJHHHHHHHHDEPTH (MICROMETERS)";
2620 MOVE 0,0
2630 FOR I=1 TO 10
2640    PRINT "JHH";
2650    IF X9<=2.0E-4 THEN 2680
2660    PRINT USING "2D.1D":(I-1)*X9*1000
2670    GO TO 2690
2680    PRINT USING "1D.2D":(I-1)*X9*1000
2690    MOVE I*10,0
2700 NEXT I
2710 RETURN
2720 REM  OUTPUT ROUTINE FOR DATA STORED ON TAPE
2730 INIT
2740 PRINT "ENTER FILE NUMBER OF STORED DATA"
2750 INPUT Z6
2760 DIM M$(40),D$(30),E(11)
2770 FIND Z6
2780 READ @33:M$,D$,E,K1,M
2790 DIM X(M),P(M),F1(M),P1(M),D(M),V(M),S(M)
2800 READ @33:X,P,F1,P1,D,V,B1,T1,A,F
2810 DELETE P1
2820 DIM Y(2*M),U1(M-1),U3(M-1)
```

```
2830 READ @33:Y,U1,U3,D1,D2,C1,C2,H3,I1,S
2840 GO TO 140
2850 END
```

```
3 GO TO 100
4 GO TO 1530
100 REM **** SPATIAL DISTRIBUTION OF POINT DEFECTS *****  FILE 7*
110 REM *** J.B. WHITLEY, 4/77*********************
120 REM *****CALCULATES RADIATION ENHANCED DIFFUSION IN ION ****
130 REM **   BOMBARDED FOILS.  USES INPUT FROM CODES IN FILES 5&6*
140 Z6=0
150 DELETE C3,P1,C4,S,D,V,U1,U2,U3
160 DIM D(M),C(M),C4(M),C6(M),U1(M-1),U2(M-1),U3(M-1),C3(M)
170 C=0
180 L8=0
190 C3=0
210 C6=0
220 C4=0
230 T6=100000
240 I5=0
250 Z5=0
260 PRINT "ENTER VACANCY CORRELATION FACTOR, INTERSTITIAL CORR. FACTOR"
270 INPUT V1,I1
280 PRINT "ENTER ACTIVITY GRADIENT"
290 INPUT A6
300 X2=X(1)
310 L1=0
320 REM  D(I) IS THE DEPTH DEPENDENT RADIATION ENHANCED DIFFUSION
330 REM  COEFFICIENT.  T6 IS THE MINIMUM TIME STEP ALLOWED USING
340 REM  A FOURIER NUMBER OF 0.45. L1 IS THE MAXIMUM DISPLACEMENT RATE
350 FOR I=1 TO M
360    L1=L1 MAX P(I)
370    D(I)=A6*(V1*D2*Y(2*I)+I1*D1*Y(2*I-1))
380    T8=(2*X2)↑2*0.45/D(I)
390    T6=T6 MIN T8
400    IF I=M THEN 420
410    X2=X(I+1)-X(I)-X2
420 NEXT I
```

```
430 PRINT "TIME STEP =  ";T6;"  SECONDS"
440 REM  C4 IS THE IMPURITY SOURCE TERM PER TIME STEP T6.
450 X2=X(1)
460 FOR I=1 TO M-1
470    C4(I)=F1(I)*F*T6/(2*X2)
480    X2=X(I+1)-X(I)-X2
490 NEXT I
500 U1(1)=(A6*V1*D2*C2+D(1))/(X(1)*X(2))
510 U3(1)=(D(2)+D(1))/((X(2)-X(1))*X(2))
520 U2(1)=U1(1)+U3(1)
530 FOR I=2 TO M-1
540    U1(I)=(D(I-1)+D(I))/((X(I)-X(I-1))*(X(I+1)-X(I-1)))
550    U3(I)=(D(I)+D(I+1))/((X(I+1)-X(I))*(X(I+1)-X(I-1)))
560    U2(I)=U1(I)+U3(I)
570 NEXT I
580 PRINT USING "28A,FD,15A":"PRESENT IRRADIATION TIME =  ";I5;"  SECOND
    S"
590 PRINT "ENTER OUTPUT TIME (SEC)   ";
600 INPUT T7
610 C6=C4*((T7-I5)/T6)
620 C3=C3+C6
630 L8=L1*(T7-I5)+L8
640 I5=I5+T6
650 C=C+C4
660 REM  C6 IS THE NET IMPURITY FLUX INTO AN INTERVAL PER TIME STEP
670 REM  C  IS THE IMPURITY LEVEL AT TIME I5.
680 C6(1)=2*D(1)*T6*(C(2)-C(1))/(X(2)-X(1))↑2
690 FOR I=2 TO M-1
700    C6(I)=(U1(I)*C(I-1)-U2(I)*C(I)+U3(I)*C(I+1))*T6
710 NEXT I
720 REM  THE IMPURITY FLUX FOR THE TIME STEP THAT EXCEEDS THE
730 REM  OUTPUT TIME IS FOUND BY INTERPOLATING BETWEEN THE LAST TWO
740 REM  TIME STEPS.
750 C6=C6*((I5<=T7)+(I5>T7)*(I5-T7)/T6)
760 C=C+C6
```

```
770 IF I5<T7 THEN 640
780 I5=T7
790 L4=0
800 FOR I=2 TO M-1
810    L4=L4 MAX C3(I)/(E(11)*1.0E+20)
820 NEXT I
830 PRINT USING "24A,2D.2D,4A":"MAXIMUM CONCENTRATION= ",L4,"%GG"
840 REM BEGIN OUTPUT**************************************************
850 PRINT "ENTER MAXIMUM CONCENTRATION TO PLOT (IN PERCENT)"
860 INPUT C5
870 IF C5<>0 THEN 890
880 C5=L4
890 IF Z5>0 AND Z5<>3 THEN 930
900 PRINT "ENTER MAXIMUM DEPTH TO PLOT (IN MICROMETERS)"
910 INPUT X9
920 X9=X9*1.0E-4
930 PAGE
940 VIEWPORT 15,120,10,90
950 WINDOW 0,100,0,110
960 MOVE 0,C(1)/(E(11)*1.0E+18*C5)
970 FOR I=1 TO M-1
980    DRAW X(I)/X9*100,C(I)/(E(11)*1.0E+18*C5)
990 NEXT I
1000 MOVE 0,C3(1)/(E(11)*1.0E+18*C5)
1010 FOR I=1 TO M-1
1020    DRAW X(I)/X9*100,C3(I)/(E(11)*1.0E+18*C5)
1030 NEXT I
1040 AXIS 5,10,0,0
1050 AXIS 5,10,100,110
1060 MOVE 65,100
1070 PRINT USING "16A":"IMPLANTED IONS"
1080 MOVE 65,95
1090 PRINT USING "5A,2E,4A":"TIME=",T7," SEC"
1100 MOVE 65,90
1110 PRINT USING "10A,FD.1D,3A":"PEAK DOSE=",L8,"DPA"
```

```
1120 MOVE 65,85
1130 PRINT USING "2D.2D,4D.2D,4D.2D":V1,I1,A6
1140 GOSUB 1210
1150 INPUT W$
1160 PRINT "LENTER_1 TO RUN AGAIN _2 TO CONTINUE TIME _3 TO PLOT AGAIN"
1170 PRINT "4 TO CONTINUE WITH NEW DEFECT CONCENTRATIONS"
1180 INPUT Z5
1190 GO TO Z5 OF 150,580,830,1550
1200 END
1210 REM  AXIS LABELING ROUTINE
1220 PRINT "↥";Z6
1230 HOME
1240 PRINT "  ";
1250 FOR I=1 TO 34
1260    W$=SEG("              CONCENTRATION",I,1)
1270    PRINT W$;"ʜ↓";
1280 NEXT I
1290 FOR I=1 TO 11
1300    MOVE 0,(I-1)*10-2
1310    IF C5>0.1 THEN 1340
1320    PRINT USING "5A,FD.3D":"ʜʜʜʜʜ",C5/10*(I-1)
1330    GO TO 1380
1340    IF C5>1 THEN 1370
1350    PRINT USING "5A,1D.2D":"ʜʜʜʜʜ",C5/10*(I-1)
1360    GO TO 1380
1370    PRINT USING "4A,FD.1D":"ʜʜʜʜ",C5/10*(I-1)
1380 NEXT I
1390 REM  HORIZONTAL AXIS LABELING ROUTINE
1400 MOVE 50,0
1410 PRINT "↓↓ʜʜʜʜʜʜʜʜDEPTH (MICROMETERS)";
1420 MOVE 0,0
1430 FOR I=1 TO 10
1440    PRINT "↓ʜʜ";
1450    IF X9<=1.0E-4 THEN 1480
1460    PRINT USING "2D.1D":(I-1)*X9*1000
```

```
1470     GO TO 1490
1480     PRINT USING "1D.2D":(I-1)*X9*1000
1490     MOVE I*10,0
1500 NEXT I
1510 RETURN
1520 REM  ROUTINE TO ENTER DEFECT CONCENTRATION DATA FROM TAPE
1530 INIT
1540 Z5=0
1550 PRINT "ENTER FILE NUMBER OF INPUT DATA"
1560 INPUT Z6
1570 DIM M$(40),D$(30),E(11)
1580 FIND Z6
1590 READ @33:M$,D$,E,K1,M
1600 DELETE X,P,F1,P1,V,Y,U1,U2,U3
1610 DIM X(M),P(M),F1(M),P1(M),V(M)
1620 READ @33:X,P,F1,P1,V,V,B1,T1,A,F
1630 DELETE P1,V
1640 DIM Y(2*M),U1(M-1),U2(M-1),U3(M-1)
1650 READ @33:Y,U1,U3,D1,D2,C1,C2
1660 T6=1000000
1670 GO TO SGN(Z5)+1 OF 150,300
1680 END
```

Table 2

Partial List of Variables Used in This Code

Name	Usual Notation	BASIC Notation	Units
Interstitial, Vacancy Concentrations	C_i, C_v	Y(i)	
Temperature	T	T1	°C
Recombination Factor	α/D_i	A	cm^2
Ion Flux	ϕ	F	ions/cm^2/s
Vacancy Production Rate	P_v	P(i)	dpa/s
Interstitial Production Rate	P_i	P1(i)	dpa/s
Ion Deposition Rate		F1(i)	atoms/atom/s
Net Interstitial Dislocation Bias	Z^i	B1	
Average Void Diameter in Interval i	$2*r_v$	S(i)	10^{-10} m
Void Density in Interval i	N_v	V(i)	cm^{-3}
Total Dislocation Line Length in Interval i	ρ_d	D(i)	cm^{-2}
Interstitial Diffusion Coefficient	D_i	D1	cm^2/s
Vacancy Diffusion Coefficient	D_v	D2	cm^2/s
Thermal Interstitial Concentration	C_i^{eq}	C1	
Thermal Vacancy Concentration	C_v^{eq}	C2	
Vacancy Concentration at Void Surface	C_v^*	C4	
Number of Depth Intervals		M	
Depth to Midpoint of Interval i	X	X(i)	μm
Interstitial Motion Energy	E_m^i	E(1)	eV
Vacancy Motion Energy	E_m^v	E(2)	eV
Interstitial Formation Energy	E_f^i	E(3)	eV
Vacancy Formation Energy	E_f^v	E(4)	eV
Interstitial Diffusion Pre-exponential	D_o^i	E(5)	cm^2/s
Vacancy Diffusion Pre-exponential	D_o^v	E(6)	cm^2/s
Interstitial Formation Pre-exponential	$e^{S_f^i/k}$	E(7)	

Table 2 (cont.)

Partial List of Variables Used in This Code

Name	Usual Notation	BASIC Notation	Units
Vacancy Formation Pre-exponential	$e^{S_f^v/k}$	E(8)	
Surface Energy	γ	E(9)	erg/cm^2
Lattice Spacing	b	E(10)	10^{-10} m
Atom Density	N	E(11)	cm^{-3}
Vacancy Correlation Factor		V1	
Interstitial Correlation Factor		I3	
Radiation Enhanced Diffusion Coefficient of Interval i	$D_A(x)$	Db(i)	cm^2/s

Table 3

X_i (μm)	P_i (dpa/10^{16} ions/cm^2)	X_i	P_i
0.005	0.581	1.670	7.511
0.015	0.622	1.710	8.206
0.030	0.685	1.750	8.922
0.050	0.767	1.790	9.607
0.075	0.868	1.830	10.200
0.110	1.004	1.870	10.633
0.155	1.168	1.910	10.844
0.210	1.339	1.950	10.788
0.275	1.493	1.990	10.445
0.350	1.625	2.000	9.823
0.430	1.737	2.070	8.968
0.510	1.842	2.110	7.917
0.590	1.952	2.150	6.768
0.670	2.072	2.195	5.448
0.750	2.206	2.250	3.923
0.830	2.756	2.315	2.462
0.910	2.524	2.390	1.269
0.990	2.716	2.475	0.513
1.075	2.936	2.570	0.153
1.150	3.193	2.690	0.024
1.230	3.500	2.860	0.000
1.310	3.875	3.110	0.000
1.390	4.348	3.460	0.000
1.465	4.919	3.960	0.000
1.530	5.559	4.660	0.000
1.585	6.221	5.560	0.000
1.630	6.868		

Mean Range = 2.08 μm