TRANSWELL (Version I) Computer Code Documentation

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TRANSWELL (Version I): A Computer Code for Metal Swelling and Creep Under Transient, Pulsed or Steady Irradiation Conditions

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Abstract

TRANSWELL (Version I) is a FØRTRAN IV based computer code based on the rate theory approach to the response of a metal under irradiation. It is the first in a series of codes that will be made available for the purpose of studying metal swelling and creep under irradiation. The present version of the code is designed to simulate irradiation of metals under 8 different conditions. It solves time dependent coupled rate equations for metals under electron, heavy ion or neutron irradiation. External uniaxial stress effects are also included and the transient, pulsed or quasi-steady state irradiation modes are analyzed within the code. Programming considerations such as efficiency, economy, simplicity and versatility have been emphasized.

I. Introduction

The TRANSWELL code solves the kinetic rate equations for single vacancies and single interstitials in a homogeneous medium (spacially averaged concentrations). Coupled rate equations are solved for an average void radius, average aligned and non aligned interstitial loop radii, the concentration of aligned and non aligned vacancy loops, the concentration of vacancies tied up in aligned and non aligned vacancy loops, and finally strain and strain rate equations. The code is built on the theoretical ideas in the rate formulation developed by Harkness and Li[1]; Wiedersich[2]; Brailsford and Bullough[3]; Bullough, Eyre and Krishan[4]; and Ghoniem and Kulcinski[5] It is written with the objective of standardizing transport kinetic calculations of point defects and their effect on the response of metals under different irradiation conditions.

TRANSWELL (VEROI) is designed to help the experimentalist as well as the theoritician to parametrically study the effect of input material properties on the final experimental observations. The sophistication of the code is moderate at this point in time but its structure facilitates the modification of the inherent physics in the future.

Time dependent computations in the rapidly developing radiation damage field are fairly recent and have been discussed in previous documents (5,6,7,8). Given the present fluidity of conceptual developments it was felt that the existence of a flexible code that can easily accomodate new additions and changes can be very useful.

Part II of this report briefly describes the theory and numerical analysis of the solutions of a Stiff System of Ordinary Differential Equations (ØDE). Part III describes in detail a generalized formulation of the rate theory and some remarks on the qualitative time dependent

properties and characteristics of the system. Part IV is a description of the TRANSWELL code itself and it is useful for future changes and modifications. The users manual is well documented in part V and part VI contains test problems for the users benefit.

II. Method of Solution

Many physical systems give rise to ordinary differential equations in which the magnitudes of the eigenvalues vary greatly. Such situations arise in the study of point defects in metals using the rate theory as described in references (5,6).

For example, the production of highly mobile interstitials and relatively immobile vacancies at moderate temperatures present a situation where the interstitials migrate quickly to their 'final' configuration while the vacancies have not begun to move. Later when the vacancies are annealing the interstitials are relatively fixed. It is common to refer to the equations describing the behavior of such systems as stiff.

The TRANSWELL code contains a FØRTRAN subroutine collection called the GEAR package.[9] It is based on a program written by C. W. Gear[10], for the solution of the initial value problem for systems of ordinary differential equations (ØDE's). Such a system has the form

$$\dot{y} = f(y,t)$$

or more specifically,

$$\frac{dy_i(t)}{dt} = f_1 \left(y_1(t), \ldots, y_N(t), t\right) \qquad (1)$$

where y, $\dot{y}$ and f are vectors of length $N \geq 1$. Given an initial value of the vector

$$y(t_0) = y_0,$$

and a subroutine for the calculation of f, the GEAR package computes a numerical solution to Eq. (1) at values of the independent variable t in some interval $[t_0, T]$, as desired by the user. (The endpoint T may not be known in advance).

The basic methods used for the solution are of implicit linear multistep type. There are two classes of such methods available to the user. The first is the implicit Adams methods (up to order 12), and the second is the back-

ward differentiation formula (BDF) methods (up to order 5), also called Gear's stiff methods. In either case the implicitness of the basic formula then requires an algebraic system of equations be solved at each step. A variety of corrector-iteration methods is available for this, such as described in reference (9).

A prime feature of GEAR (or of the methods of C. W. Gear on which it is based) is its ability to solve stiff ODE problems. Roughly speaking, an ODE system is called stiff if it involves both very rapidly changing terms and very slowly changing terms, all of a decaying nature. More precisely, we consider the eigenvalues λ_i of the N x N Jacobian matrix.

$$J = \frac{\partial f}{\partial y} = \left(\frac{\partial f_i}{\partial y_j}\right)_{i,j=1}^{N} \qquad (2)$$

and suppose that the λ_i all have negative real parts. The "time constants" of the problem are then $\tau_i = 1/|\mathrm{Re}(\lambda_i)|$ and the decaying nature (locally) of the solution is given by the exponentials e^{-t/τ_i}. If the N time constants τ_i are widely spread, and those terms with the smaller τ_i have already decayed to an insignificant level while those with large value of τ_i are still active, then the system is stiff. (Actually, some of the $\mathrm{Re}(\lambda_i)$ may be non-negative, meaning that some solution components are non-decaying, and the system would still be called stiff if the negative $\mathrm{Re}(\lambda_i)$ values have a relatively large magnitude), The property of stiffness is local in time; a problem may be stiff in some regions of t and not in others. It is also relative, the ratio max τ_i/min τ_i being a measure of the stiffness.

The difficulty with stiff problems is that most conventional methods for solving ODE's require incremental values of t commensurate with min τ_i, while the size $|T - t_0|$ of the problem range is commensurate with max τ_i. As a result, the problem cannot be run to completion in a reasonable number of steps. With Gear's methods, however, the increment h is restricted to small values, by the

requirements of accuracy, only where the solution is relatively active. By definition, the problem is not stiff in such regions, and accuracy is achieved at minimum cost by allowing both h and the order of the method to vary with time. Then in regions of stiffness, where the solution is inactive, Gear's methods have the property of "stiff stability," which assures that h is no longer restricted by the small time constants, unless or until the corresponding rapidly decaying terms become active again. This property necessitates, among other things, that the methods be implicit, and therefore that a system of (generally) nonlinear algebraic equations be solved at each step. Moreover, stiffness dictates that a fairly powerful iteration method be used to solve this system, and the GEAR package contains variants of Newton's method (called chord methods) for this purpose. Both the stiff and non-stiff methods are implemented in a manner which allows the step size and the order to vary in a dynamic way throughout the problem. This variability is now widely recognized as highly desirable for efficiency in using linear multistep methods.

The GEAR package is a collection of seven subroutines, one of which is the single-step core integrator routine, STIFF. Subroutine STIFF is a heavily revised version of a routine written and published by GEAR[9].

The methods used in the GEAR package are documented in considerable detail elsewhere[10]. Hence, only a brief summary of them will be given here.

The basic methods involved are linear multipoint methods of the form

$$y_n = \sum_{j=1}^{K_1} \alpha_j y_{n-j} + h \sum_{j=0}^{K_2} \beta_j \dot{y}_{n-j} , \qquad (3)$$

where y_k is an approximation to $y(t_k)$, $\dot{y}_k = f(y_k,t_k)$ is an approximation to $\dot{y}(t_k)$, and h is a constant step size: $h = t_{k+1} - t_k$. In the case of the Adams method of order q, we have $K_1 = 1$ and $K_2 = q-1$. In the case of the backward differentiation formula (BDF) of order q, we have $K_1 = q$ and $K_2 = 0$. The BDF's are so called because, on dividing through by $h\beta_0$, they can be regarded as approximation formulas for $\dot{y}_n$ in terms of y_n, y_{n-1}, ..., y_{n-q}. In either case, the α_j and β_j are constants associated with the method, and $\beta_0 > 0$. The latter means that Eq. (2) is an implicit equation for y_n and is in general a nonlinear algebraic system that

must be solved on every step. The fact that the order of a given method is q means that, if Eq. (2) is solved for y_n with all past values being exact, then y_n will differ from the correct solution of the ODE by a local truncation error that is order of (h^{q+1}) for small h.

If Eq. (2) is written in the form

$$g(y_n) \equiv y_n - h\beta_o f(y_n,t_n) - \sum_1^{K_1} \alpha_j\, y_{n-j} - h \sum_1^{K_2} \beta_j\, \dot{y}_{n-j} = 0, \qquad (4)$$

then the nonlinear system $g(y_n) = 0$ can be solved, for example, by Newton's method.

In all of the iteration methods, a first approximation $y_n(0)$ is required. This is computed from the existing information corresponding to saved past values of y_k and $\dot{y}_k$. This prediction is such that $y_n(0)$, as well as the final value y_n, is accurate to q^{th} order.

Following a step of size h at order q, the GEAR package, at intervals of q+2 steps, attempts to choose a larger step size by estimating the local truncation errors at orders q-1, q, and q+1. The largest value h' of the three step sizes obtained is then chosen, and the order reset accordingly. Also, the Nordsieck array must be rescaled by powers of h'/h. The data used to take the subsequent steps of size h' is in effect obtained by interpolating with the data at a spacing of h.

III. Generalized Rate Theory for Metal Swelling

The TRANSWELL code is designed to deal with a variety of irradiation conditions. It is constructed in such a way that one can add (or delete) parts depending on the particular aspect of the problem that is of interest. In this version of TRANSWELL, the following situations can be analyzed and studied for a metal;

(1) Ion or neutron irradiation* in a transient or pulsed mode of operation with a uniaxial stress applied.

(2) Ion or neutron irradiation at a steady rate or annealing of voids after a long irradiation at the same or different temperature, with uniaxial stress applied.

*The grouping here is associated with the ability to produce vacancy clusters in displacement cascades.

(3) Ion or neutron irradiation in a transient or pulsed mode of operation with no stress applied.

(4) Electron irradiation in a transient or pulsed mode of operation with a uniaxial stress applied.

(5) Electron irradiation at a steady rate, or annealing of voids after a long irradiation time at the same or different temperature, with uniaxial stress applied.

(6) Electron irradiation in a transient or pulsed mode of operation with no stress applied.

(7) Ion or neutron irradiation at a steady rate, or annealing of voids after a long irradiation time at the same or different temperature, with no stress applied.

(8) Electron irradiation at a steady rate, or annealing of voids after a long irradiation time at the same or different temperature, with no stress applied.

The cases described above are classified according to the number of equations in each case. Case (1) is the most general and all other cases are subsets of this first case. Instead of lumping all the previous studies in one huge core subroutine, we chose to construct eight different subroutines. The main reason is to alleviate computational bottle necks and to give the code greater flexibility and to save computer time. For example, if one decided to study the growth behavior of a void size or dislocation loop size distribution, he might add other core subroutines for this study.

In the following, a descritpion of the variables and equations used in the first case are given. The other cases are well described within the code once one is familiar with the general notation. To help the interested reasearcher, comment cards are liberally dispersed throughout the code.

As stated previously, we have used vector notation to describe the kinetic behavior of the system. The various components are defined as follows:

$Y(1)$ = average void radius in cm. (D1)*

$Y(2)$ = average non-aligned interstitial loop radius in cm. (D2)

$Y(3)$ = concentration of non-aligned vacancy loops per cm^3. (D3)

$Y(4)$ = concentration of single vacancies tied up in non-aligned vacancy loops in at./at. (D4)

$Y(5)$ = total single vacancy concentration in at./at. (D5)

$Y(6)$ = total single interstitial concentration in at./at. (D6)

$Y(7)$ = average aligned interstitial loop radius in cm. (D7)

$Y(8)$ = concentration of aligned vacancy loops per cm^3. (D8)

$Y(9)$ = concentration of single vacancies tied up in aligned vacancy loops in at./at. (D9)

$Y(10)$ = network creep strain in cm/cm. (D10)

Following the notations of References 4, 5 and 11, the following processes are analyzed.

Dislocation Densities

$$\rho_d^{i\ell n} = 2\pi Y(2) N_{i\ell n} \tag{5}$$

$$\rho_d^{i\ell a} = 2\pi Y(7) N_{i\ell a} \tag{6}$$

$$\rho_d^{v\ell n} = 2\sqrt{\pi Y(3) Y(4)/b} \tag{7}$$

$$\rho_d^{v\ell a} = 2\sqrt{\pi Y(8) Y(9)/b} \tag{8}$$

$$\rho_d = \rho_d^e + \rho_d^{i\ell n} + \rho_d^{i\ell a} + \rho_d^{v\ell n} + \rho_d^{v\ell a} \tag{9}$$

where

*Equations with the prefix "D" refer to definitions.

- $\rho_d^{i\ell n}$ is the non-aligned dislocation loop line density; cm^{-2}. (D11)
- $N_{i\ell n}$ is the non-aligned dislocation loop concentration; cm^{-3}. (D12)
- $\rho_d^{i\ell a}$ is the aligned dislocation loop line density; cm^{-2}. (D13)
- $N_{i\ell a}$ is the aligned dislocation loop concentration; cm^{-3}. (D14)
- $\rho_d^{v\ell n}$ is the non-aligned vacancy loop line density; cm^{-2}. (D15)
- $\rho_d^{v\ell a}$ is the aligned vacancy loop line density; cm^{-2} (D16)
- ρ_d^e is the deformation produced edge dislocation line density; cm^{-2}. (D17)
- ρ_d is the total dislocation line density produced by both deformation and radiation; cm^{-2}. (D18)

Vacancy Emission from Voids

$$P_V^e = 4\pi Y(1) N_V D_V C_V^e \exp\left\{ \left(\frac{2\gamma}{Y(1)} - P_g(Y(1), N_g) b^3/kT\right)\right\} \quad (10)$$

where

- P_V^e is the vacancy emission rate from the surface of all voids, s^{-1} (D19)
- N_V is the temperature dependent void concentration, cm^{-3} (D20)
- D_V is the temperature dependent vacancy diffusion coefficient, $cm^2\ s^{-1}$ (D21)
- C_V^e is the equilibrium vacancy concentration, at./at. (D22)
- γ is the surface energy of the void surface, ev/cm^2 (D23)
- P_g is the gas pressure inside the void, ev/cm^3 (D24)
- N_g is the number of gas atoms in a void. (D25)

Vacancy Emission from Deformation Produced Dislocations

$$P_d^{ea} = Z_v^a D_v C_v^e \exp(\sigma\Omega/kT)\, \rho_d^{ea} \quad (11)$$

$$P_d^{en} = Z_v^n D_v C_v^e\, \rho_d^{en} \quad (12)$$

$$P_d^e = P_d^{ea} + P_d^{en} \quad (13)$$

where

- P_d^{ea} is the rate of vacancy emission from all aligned edge dislocations, s^{-1} (D26)
- P_d^{en} is the rate of vacancy emission from all nonaligned edge dislocations, s^{-1} (D27)
- P_d^e is the total rate of vacancy emission from edge dislocations (D28)
- σ is the uniaxial externally applied stress, eV/cm^3 (D29)
- Ω is the atomic volume, cm^3 (D30)
- k is Bolzmann's constant, $eV\ ^oK^{-1}$ (D31)
- ρ_d^{ea} is the aligned edge dislocation density, cm^{-2} (D32)
- ρ_d^{en} is the nonaligned edge dislocation density, cm^{-2} (D33)
- Z_v^a is the vacancy-aligned dislocation bias factor (D34a)
- Z_v^n is the vacancy non-aligned dislocation bias factor (D34b)
- T is the temperature, ^oK

Vacancy Emission from Interstitial Loops

$$P_d^{i\ell a} = D_v C_v (Y(7)) Z_v^a \exp(\sigma\Omega/kT)\, \rho_d^{i\ell a} \quad (14)$$

$$P_d^{i\ell n} = D_v C_v (Y(2)) Z_v^n\, \rho_d^{i\ell n} \quad (15)$$

$$P_d^{i\ell} = P_d^{i\ell a} + P_d^{i\ell n} \quad (16)$$

$$C_v(Y(7)) = C_v^e \exp - \left(\frac{\{\gamma_{sf} + F_{el}(Y(7))\} b^2}{kT} \right) \tag{17}$$

$$F_{el}(Y(7)) = \frac{\mu b^2}{(1-\nu) 4\pi (Y(7)+b)} \ell n \left(\frac{Y(7)+b}{b} \right) \tag{18}$$

where

- $P_d^{i\ell a}$ is the rate of vacancy emission from aligned interstitial loops, s^{-1} (D35)
- $P_d^{i\ell n}$ is the rate of vacancy emission from nonaligned interstitial loops, s^{-1} (D36)
- $P_d^{i\ell}$ is the total rate of vacancy emission from all interstitial loops, s^{-1} (D37)
- γ_{sf} is the stacking fault energy, ev cm^{-2} (D38)
- $F_{el}(Y(7))$ is the elastic energy of a dislocation loop of radius $Y(7)$, eV cm^{-2} (D39)
- b is the Burger's vector, cm (D40)
- μ is the shear modulus, ev cm^{-3} (D41)
- ν is the Poisson's ratio (D42)

In (17), $C_v(Y(7))$ is the equilibrium vacancy concentration at the edge of a dislocation loop of radius Y(7)

Vacancy Emission from Vacancy Loops

$$P_d^{v\ell a} = D_v C_v (r_{v\ell}^a) Z_v^a \exp(\sigma\Omega/kT) \rho_d^{v\ell a} \tag{19}$$

$$P_d^{v\ell n} = D_v C_v (r_{v\ell}^n) Z_v^n \rho_d^{v\ell n} \tag{20}$$

$$P_d^{v\ell} = P_d^{v\ell a} + P_d^{v\ell n} \tag{21}$$

$$r_{v\ell}^{n} = \sqrt{Y(4)/\pi b Y(3)} \tag{22}$$

$$r_{v\ell}^{a} = \sqrt{Y(9)/\pi b Y(8)} \tag{23}$$

$$C_v(r_{v\ell}) = C_v^e \exp\left\{\frac{\{\gamma_{sf}+F_{el}(r_{v\ell})\}b^2}{kT}\right\} \tag{24}$$

and $F_{el}(r_{v\ell})$ is as defined in (18) before

where

- $P_d^{v\ell a}$ is the rate of vacancy emission from aligned vacancy loops, s^{-1} (D43)
- $P_d^{v\ell n}$ is the rate of vacancy emission from nonaligned vacancy loops, s^{-1} (D44)
- $P_d^{v\ell}$ is the total rate of vacancy emission from all vacancy loops, s^{-1} (D45)
- $r_{v\ell}^{a}$ is the aligned vacancy loop radius, cm (D46)
- $r_{v\ell}^{n}$ is the nonaligned vacancy loop radius, cm (D47)
- $\rho_d^{v\ell a}$ is the aligned vacancy loop line dislocation density, cm^{-2} (D48)
- $\rho_d^{v\ell n}$ is the nonaligned vacancy loop line dislocation density, cm^{-2} (D49)

Total Rate of Vacancy Emission

$$P^e = P_V^e + P_d^e + P_{v\ell}^e + P_{i\ell}^e \tag{25}$$

where P^e is the total vacancy emission rate, s^{-1}. (D50)

Single Point Defect Time Constants

$$\lambda_i = \lambda_i^d + \lambda_i^V \tag{26}$$

$$\lambda_v = \lambda_v^d + \lambda_v^V \tag{27}$$

$$\lambda_i^d = \rho_d D_i Z_i \tag{28}$$

$$\lambda_i^V = 4\pi N_V Y(1) D_i \tag{29}$$

$$\lambda_v^d = \rho_d D_v Z_v \tag{30}$$

$$\lambda_v^V = 4\pi N_V Y(1) D_v \tag{31}$$

where $\cdot\lambda_i$ is the total single interstitial time constant, s^{-1} (D51)

$\cdot\lambda_v$ is the total single vacancy time constant, s^{-1} (D52)

$\cdot\lambda_i^d$ is the single interstitial time constant due to all dislocations, s^{-1} (D53)

$\cdot\lambda_i^V$ is the single interstitial time constant due to all voids, s^{-1} (D54)

$\cdot\lambda_v^d$ is the single vacancy time constant due to all dislocations, s^{-1} (D55)

$\cdot\lambda_v^V$ is the single vacancy time constant due to all voids, s^{-1} (D56)

Removal Rates

$$P_{si} = \lambda_i \, Y(6) \tag{32}$$

$$P_{sv} = \lambda_v \, Y(5) \tag{33}$$

$$P_r = \alpha \, Y(5) \, Y(6) \tag{34}$$

$$\alpha = g \left(\nu_i \exp\left(-E_i^m/kT\right) + \nu_v \exp\left(-E_v^m/kT\right)\right) \tag{35}$$

where

$\cdot P_{si}$ is the total sink removal rate for interstitials, s^{-1} (D57)

$\cdot P_{sv}$ is the total sink removal rate for vacancies, s^{-1} (D58)

- P_r is the total recombination rate of vacancies and interstitials, s^{-1} (D59)
- α is the recombination coefficient, s^{-1} (D60)
- g is the number of unstable sites around a vacancy. (D61)
- $\nu_i \exp(-E_i^m/kT)$ is the interstitial jump frequency, s^{-1} (D62)
- $\nu_v \exp(-E_v^m/kT)$ is the vacancy jump frequency, s^{-1} (D63)

Vacancy Loops

$$\kappa_1^n = \frac{2}{3}(1-f)\frac{\varepsilon P}{\pi r_{v\ell}^2(o)b} \tag{36}$$

$$\kappa_1^a = \frac{1}{3}(1+2f)\frac{\varepsilon P}{\pi r_{v\ell}^2(o)b} \tag{37}$$

$$\kappa_2^n = \frac{2}{3}(1-f)\,\varepsilon P \tag{38}$$

$$\kappa_2^a = \frac{1}{3}(1+2f)\,\varepsilon P \tag{39}$$

$$\Lambda_1^n = Y(3)(Z_iD_iY(6) - Z_vD_vY(5) + D_vC_v^eZ_v \times \exp\{(\gamma_{sf} + F_{el}(r_{v\ell}(o)))b^2kT\}/(r_{v\ell}(o)b) \tag{40}$$

$$\Lambda_1^a = Y(3)(Z_i^aD_iY(6) - Z_v^aD_vY(5) + D_vC_v^eZ_v^a \times \exp\{(\gamma_{sf} + F_{el}(r_{v\ell}(o)))b^2/kT\}\exp(\sigma\Omega/kT)/(r_{v\ell}(o)b) \tag{41}$$

$$\Lambda_2^n = (Z_i^nD_iY(6) - Z_v^nD_vY(5) + Z_v^nD_vC_v^e \times \exp\{(\gamma_{sf} + F_{el}(r_{v\ell}^n))b^2/kT\}) \times \sqrt{4\pi Y(4)Y(3)/b} \tag{42}$$

$$\Lambda_2^a = (Z_i^a D_i Y(6) - Z_v^a D_v Y(5) + Z_v^a D_v C_v^e \exp\{(\gamma_{sf} + F_{el}(r_{v\ell}^n))b^2/kT\} \times \exp(\sigma\Omega/kT)) \sqrt{4\pi Y(9)Y(8)/b} \quad (43)$$

where

- κ_1^n is the production rate of nonaligned vacancy loops, $cm^{-3}\ s^{-1}$ (D64)
- κ_1^a is the production rate of aligned vacancy loops, $cm^{-3}\ s^{-1}$ (D65)
- κ_2^n is the production rate of vacancy fraction tied up in non aligned vacancy loops, s^{-1} (D66)
- κ_2^a is the production rate of vacancy fraction tied up in aligned vacancy loops, s^{-1} (D67)
- Λ_1^n is the decay rate of nonaligned vacancy loops, $s^{-1}\ cm^{-3}$ (D68)
- Λ_1^a is the decay rate of aligned vacancy loops, $s^{-1}\ cm^{-3}$ (D69)
- Λ_2^n is the decay rate of vacancy fraction tied up in non-aligned vacancy loops, $s^{-1}\ cm^{-3}$ (D70)
- Λ_2^a is the decay rate of vacancy fraction tied up in aligned vacancy loops, $s^{-1}\ cm^{-3}$ (D71)
- ε is the fraction of vacancies formed in vacancy loops. (D72)
- P is the production rate of point defects. (D73)
- $r_{v\ell}(o)$ is the initial radius of a vacancy loop formed in a cascade, cm (D74)
- f is the fraction of total interstitial loop population that are aligned perpendicular to applied stress (D75)

$$f = \frac{\exp(\sigma\Omega n/kT)-1}{\exp(\sigma\Omega n/kT)+2} \quad (44)$$

- $n \simeq 10$ is the number of interstitials defining a planar nucleus. (D76)

Swelling

$$S\% = \frac{\Delta V}{V}\% = \frac{4}{3}\pi Y(1)^3 N_V \ . \tag{45}$$

State Space Representation

In state space there is one and only one point at a particular time that defines completely the state of the metal under irradiation. The dimensions of this space depend on the system of equations chosen to simulate the metal's response to irradiation. In this version of the code, the following dimensions (number of equations) are used:

CASE	CORE SUBROUTINES	STATE SPACE DIMENSIONS
1	DERV1, JACK1	10
2	DERV2, JACK2	8
3	DERV3, JACK3	6
4	DERV4, JACK4	6
5	DERV5, JACK5	6
6	DERV6, JACK6	4
7	DERV7, JACK7	4
8	DERV8, JACK8	2

We will only give the equations in the first case since it is the most general.

$$\dot{Y}(1) = (D_v Y(5) - D_i Y(6) - D_v C_v^e \exp\{(\frac{2\gamma}{Y(1)} - P_g(Y(1),N_g))\frac{\Omega}{kT}\})/Y(1) \tag{46}$$

$$\dot{Y}(2) = (D_i Z_i Y(6) - D_v Z_v Y(5) + D_v Z_v C_v(Y(2)))/b \tag{47}$$

$$\dot{Y}(3) = \kappa_1^n - \Lambda_1^n \tag{48}$$

$$\dot{Y}(4) = \kappa_2^n - \Lambda_2^n \tag{49}$$

$$\dot{Y}(5) = (1 - \varepsilon)P + P^e - P_{sv} - P_r \tag{50}$$

$$\dot{Y}(6) = P - P_{si} - P_r \tag{51}$$

$$\dot{Y}(7) = (D_i Z_i^a Y(6) - D_v Z_v^a Y(5) + D_v Z_v^a C_v(Y(7)) \exp(\Omega\sigma/kT))/b \tag{52}$$

$$\dot{Y}(8) = \kappa_1^a - \Lambda_1^a \tag{53}$$

$$\dot{Y}(9) = \kappa_2^a - \Lambda_2^a \tag{54}$$

$$\dot{Y}(10) = \rho_d^{ea} \{((Z_i^a - Z_i^n)D_i Y(6) + (Z_v^n - Z_v^a)D_v Y(5)) + Z_v^a D_v C_v^e \exp(\sigma\Omega/kT) - Z_v^n D_v C_v^e\} \tag{55}$$

Irradiation Creep Strain

$$\varepsilon_{i\ell} = \pi b N_{i\ell}\{(1 + 2f)[Y(7)]^2 - (1 - f)[Y(2)]^2\}/3 \tag{56}$$

$$\varepsilon_{vl} = -(Y(4) - Y(9)/2) \tag{57}$$

where

- $\dot{\varepsilon}_{i\ell}$ is the irradiation induced creep due to interstitial loops, cm/cm (D77)
- $\dot{\varepsilon}_{vl}$ is the irradiation induced creep due to vacancy loops, cm/cm (D78)

Jacobian Matrix for the System

We will list here the nonzero elements of the Jacobian matrix for the full system. P(i,j) would mean the local time constant of element i due to the presence of element j.

Let us define the following:

$$\frac{\partial F_{el}}{dx} = \frac{\mu b^2}{4\,(1-\nu)(x+b)^2}\,(1-\ell n(\frac{b+x}{b})) \tag{58}$$

$$\phi_i = Z_i D_i Y(6) \tag{59}$$

$$\phi_v = Z_v D_v Y(5) \tag{60}$$

$$\phi_v^e = Z_v D_v C_v^e \tag{61}$$

$$\beta = 1/(kT)$$

$$\frac{\partial r_{vl}^n}{\partial Y(3)} = -\frac{Y(4)}{(2\pi r_{vl}^n b[Y(3)]^2)} \tag{62}$$

$$\frac{\partial r_{vl}^n}{\partial Y(4)} = \frac{1}{(2\pi r_{vl}^n b Y(3))} \tag{63}$$

$$\frac{\partial r_{vl}^a}{\partial Y(8)} = -\frac{Y(9)}{(2\pi r_{vl}^n b[Y(8)]^2)} \tag{64}$$

$$\frac{\partial r_{vl}^a}{\partial Y(9)} = \frac{1}{(2\pi r_{vl}^a b Y(8))} \tag{65}$$

where

- ϕ_i is the biased interstitial flux. (D79)
- ϕ_v is the biased vacancy flux. (D80)
- ϕ_v^e is the thermal equilibrium biased vacancy flux. (D81)

First Row

$$P(1,1) = 2\gamma\beta\,\frac{\Omega}{[Y(1)]^3}\,\phi_v^e\,\exp\{(\frac{2\gamma}{Y(1)} - P_g)\,\frac{\Omega}{kT}\} - (D_v Y(5) - D_i Y(6) - \phi_v^e\,\exp\{(\frac{2\gamma}{Y(1)} - P_g)\,\frac{\Omega}{kT}\})/[Y(1)]^2 \tag{66}$$

$$P(1,5) = D_v/Y(1) \tag{67}$$

$$P(1,6) = - D_i/Y(1) \tag{68}$$

Second Row

$$P(2,2) = \phi_v^e \exp\left\{\frac{-(\gamma_{sf}+F_{el}(Y(2))b^2}{kT}\right\} b\beta \frac{\partial F_{el}}{\partial Y(2)} \tag{69}$$

$$P(2,5) = - Z_v D_v/b \tag{70}$$

$$P(2,6) = Z_i D_i/b \tag{71}$$

Third Row

$$P(3,3) = - (\phi_i - \phi_v + \phi_v^e \exp\left\{\frac{\gamma_{sf}+F_{el}(r_{vl}(o))b^2}{kT}\right\})/br_{vl}(o) \tag{72}$$

$$P(3,5) = Y(3)Z_v D_v/br_{vl}(o) \tag{73}$$

$$P(3,6) = - Y(3)Z_i D_i/br_{vl}(o) \tag{74}$$

Fourth Row

Define $T_2^n = \sqrt{4\pi Y(4)Y(3)/b}$ (75)

$$T_3^n = \phi_i - \phi_v + \phi_v^e \exp\left\{\frac{(\gamma_{sf}+F_{el}(r_{vl}^n))b^2}{kT}\right\} \tag{76}$$

Then

$$P(4,3) = - 2\pi Y(4)T_3^n/T_2^n b - T_2^n b^2 \beta \frac{\partial F_{el}}{\partial r_{vl}^n} \cdot \frac{\partial r_{vl}^n}{\partial Y(3)} \times \phi_v^e \exp\left\{\frac{(\gamma_{sf}+F_{el}(r_{vl}^n))b^2}{kT}\right\} \tag{77}$$

$$P(4,4) = - 2\pi Y(3)T_3^n/T_2^n b - T_2^n b^2 \beta \frac{\partial F_{el}}{\partial r_{vl}^n} \cdot \frac{\partial r_{vl}^n}{\partial Y(4)} \times \phi_y^e \exp\left\{\frac{(\gamma_{sf}+F_{el}(r_{vl}^n))b^2}{kT}\right\} \tag{78}$$

$$P(4,5) = T_2^n Z_v D_v \tag{79}$$

$$P(4,6) = - T_2^n Z_i D_i \tag{80}$$

Fifth Row

$$P(5,1) = 4\pi N_V D_v \{C_v^e \exp\left[\left(\frac{2\gamma}{Y(1)} - Pg\right)\frac{\Omega}{kT}\right]\left(1 - 2\,\frac{\gamma\Omega\beta}{Y(1)}\right) - Y(5)\} \tag{81}$$

$$P(5,2) = 2\pi Z_v N_{i\ell}^n D_v \{C_v^e \exp\left[\frac{(\gamma_{sf}+F_{el}(Y(2)))b^2}{kT}\right] x\ (1 - Y(2)b^2\beta$$

$$\frac{\partial F_{el}}{\partial Y(2)}) - Y(5)\} \tag{82}$$

$$P(5,3) = 2\pi Z_v D_v \{C_v^e \exp\left[\frac{(\gamma_{sf}+F_{el}(r_{vl}^n))b^2}{kT}\right] x\ (\frac{\partial r_{vl}^n}{\partial Y(3)} \cdot Y(3)$$

$$+ r_{vl}^n + r_{vl}^n\ Y(3)b^2\beta\ \frac{\partial F_{el}}{\partial r_{vl}^n} \cdot \frac{\partial r_{vl}^n}{\partial Y(3)}) - Y(5)\ (r_{vl}^n + Y(3)$$

$$\frac{\partial r_{vl}^n}{\partial Y(3)}\} \tag{83}$$

$$P(5,4) = 2\pi Z_v D_v \{C_v^e \exp\left[\frac{(\gamma_{sf}+F_{el}(r_{vl}^n))b^2}{kT}\right] x\ (\frac{\partial r_{vl}^n}{\partial Y(4)} + r_{vl}^n b^2\beta$$

$$\frac{\partial F_{el}}{\partial r_{vl}^n} \cdot \frac{\partial r_{vl}^n}{\partial Y(4)}) - Y(5)\ \frac{\partial r_{vl}^n}{\partial Y(4)}\} Y(3) \tag{84}$$

$$P(5,5) = - D_v(4\pi Y(1)N_V + Z_v\rho_d^{en} + Z_v^a\rho_d^{ea} + 2\pi Y(2)N_{i\ell}^n + 2\pi Y(7)N_{i\ell}^a + 2\pi r_{vl}^n$$

$$Y(3) + 2\pi r_{vl}^a\ Y(8)) - \alpha Y(6) \tag{85}$$

$$P(5,6) = - \alpha Y(5) \tag{86}$$

$$P(5,7) = 2\pi Z_v^a N_{i\ell}^a D_v \{C_v^e \exp\left(\frac{\sigma\Omega}{kT}\right) \exp\left[\frac{-(\gamma_{sf}+F_{el}(Y(7)))b^2}{kT}\right]$$

$$x\ (1 - Y(7)b^2\beta\ \frac{\partial F_{el}}{\partial Y(7)}) - Y(5)\} \tag{87}$$

$$P(5,8) = 2\pi Z_v^a D_v \{C_v^e \exp\left(\frac{\sigma\Omega}{kT}\right) \exp\left[\frac{(\gamma_{sf}+F_{el}(r_{vl}^a))b^2}{kT}\right]$$
$$\times \left(\frac{\partial r_{vl}^a}{\partial Y(8)}\, Y(8) + r_{vl}^a + r_{vl}^a\, Y(8) b^2 \beta \frac{\partial F_{el}}{\partial r_{vl}^a} \cdot \frac{\partial r_{vl}^a}{\partial Y(8)}\right)$$
$$- Y(5)\left(r_{vl}^a + Y(8)\frac{\partial r_{vl}^a}{\partial Y(8)}\right)\} \tag{88}$$

$$P(5,9) = 2\pi Z_v^a D_v \{C_v^e \exp\left(\frac{\sigma\Omega}{kT}\right) \exp\left[\frac{(\gamma_{sf}+F_{el}(r_{vl}^a))b^2}{kT}\right]$$
$$\times \left(\frac{\partial r_{vl}^a}{\partial Y(9)} + r_{vl}^a\, b^2 \beta \frac{\partial F_{el}}{\partial r_{vl}^a} \cdot \frac{\partial r_{vl}^a}{\partial Y(9)}\right) - Y(5)\frac{\partial r_{vl}^n}{\partial Y(9)}\} Y(8) \tag{89}$$

Sixth Row

$$P(6,1) = -4\pi N_V D_i Y(6) \tag{90}$$

$$P(6,2) = -2\pi Z_i N_{i\ell}^n D_i Y(6) \tag{91}$$

$$P(6,3) = -2\pi Z_i D_i Y(6) \left[r_{vl}^n + Y(3)\frac{\partial r_{vl}^n}{\partial Y(3)}\right]$$

$$P(6,4) = -2\pi Z_i D_i Y(6) Y(3) \frac{\partial r_{vl}^n}{\partial Y(4)} \tag{92}$$

$$P(6,5) = -\alpha Y(6) \tag{93}$$

$$P(6,6) = -D_i(4\pi Y(1) N_V + Z_i \rho_d^{en} + Z_i^a \rho_d^{ea} + 2\pi Z_i Y(2) N_{i\ell}^n$$
$$+ 2\pi Z_i^a Y(7) N_{i\ell}^a + 2\pi Z_i r_{vl}^n Y(3) + 2\pi Z_i^a r_{vl}^a Y(8))$$
$$- \alpha Y(5) \tag{94}$$

$$P(6,7) = -2\pi Z_i^a N_{i\ell}^a D_i Y(6) \tag{95}$$

$$P(6,8) = -2\pi Z_i^a D_i Y(6)\left[r_{v1}^a + Y(8)\frac{\partial r_{v1}^a}{\partial Y(8)}\right] \quad (96)$$

$$P(6,9) = -2\pi Z_i^a D_i Y(6)Y(8)\frac{\partial r_{v1}^a}{\partial Y(9)} \quad (97)$$

Seventh Row

$$P(7,5) = -Z_v^a D_v/b \quad (98)$$

$$P(7,6) = Z_i^a D_i/b \quad (99)$$

$$P(7,7) = \phi_v^e \exp\left(\frac{\sigma\Omega}{kT}\right)\exp\left\{\frac{-(\gamma_{sf}+F_{e1}(Y(7)))b^2}{kT}\right\} b\beta\frac{\partial F_{e1}}{\partial Y(7)} \quad (100)$$

Eighth Row

$$P(8,5) = Y(8)Z_v^a D_v/br_{v1}(o) \quad (101)$$

$$P(8,6) = -Y(8)Z_i^a D_i/br_{v1}(o) \quad (102)$$

$$P(8,8) = -\left(Z_i^a D_i Y(6) - Z_v^a D_v Y(5) + Z_v^a D_v C_v^e \exp\left(\frac{\sigma\Omega}{kT}\right) x \right.$$
$$\left. \exp\left\{\frac{[\gamma_{sf}+Fe_1(r_{v1}(o))]b^2}{kT}\right\}\right)/br_{v1}(o) \quad (103)$$

Ninth Row

Define $T_2^a = \sqrt{4\pi Y(8)Y(9)/b}$ (104)

$$T_3^a = Z_i^a D_i Y(6) - Z_v^a D_v Y(5) + Z_v^a D_v C_v^e \exp\left(\frac{\sigma\Omega}{kT}\right) x$$
$$\exp\frac{[\gamma_{sf}+F_{e1}(r_{v1}^a)]b^2}{kT} \quad (105)$$

$$P(9,5) = T_2^a Z_v^a D_v \quad (106)$$

$$P(9,6) = -T_2^a Z_i^a D_i \quad (107)$$

$$P(9,8) = -2\pi Y(8)T_3^a/T_2^a b - T_2^a b^2 \beta \frac{\partial F_{el}}{\partial r_{vl}^a} \cdot \frac{\partial r_{vl}^a}{\partial Y(8)} \times Z_v^a D_v C_v^e \exp\left(\frac{\sigma\Omega}{kT}\right)$$

$$\exp\left\{\frac{[\gamma_{sf}+F_{el}(r_{vl}^a)]b^2}{kT}\right\} \tag{108}$$

$$P(9,9) = -2\pi Y(8)T_3^a/T_2 b - T_2^a b^2 \beta \frac{\partial F_{el}}{\partial r_{vl}^a} \cdot \frac{\partial r_{vl}^a}{\partial Y(9)} \times Z_v^a D_v C_v^e \exp$$

$$\left(\frac{\sigma\Omega}{kT}\right) \exp\left\{\frac{[\gamma_{sf}+F_{el}(r_{vl}^a)]b^2}{kT}\right\} \tag{109}$$

Tenth Row

$$P(10,5) = \rho_d^{ea} (Z_v - Z_v^a) D_v \tag{110}$$

$$P(10,6) = \rho_d^{ea} (Z_i^a - Z_i) D_i \tag{111}$$

IV. TRANSWELL I Program Structure

IV-A. Introduction

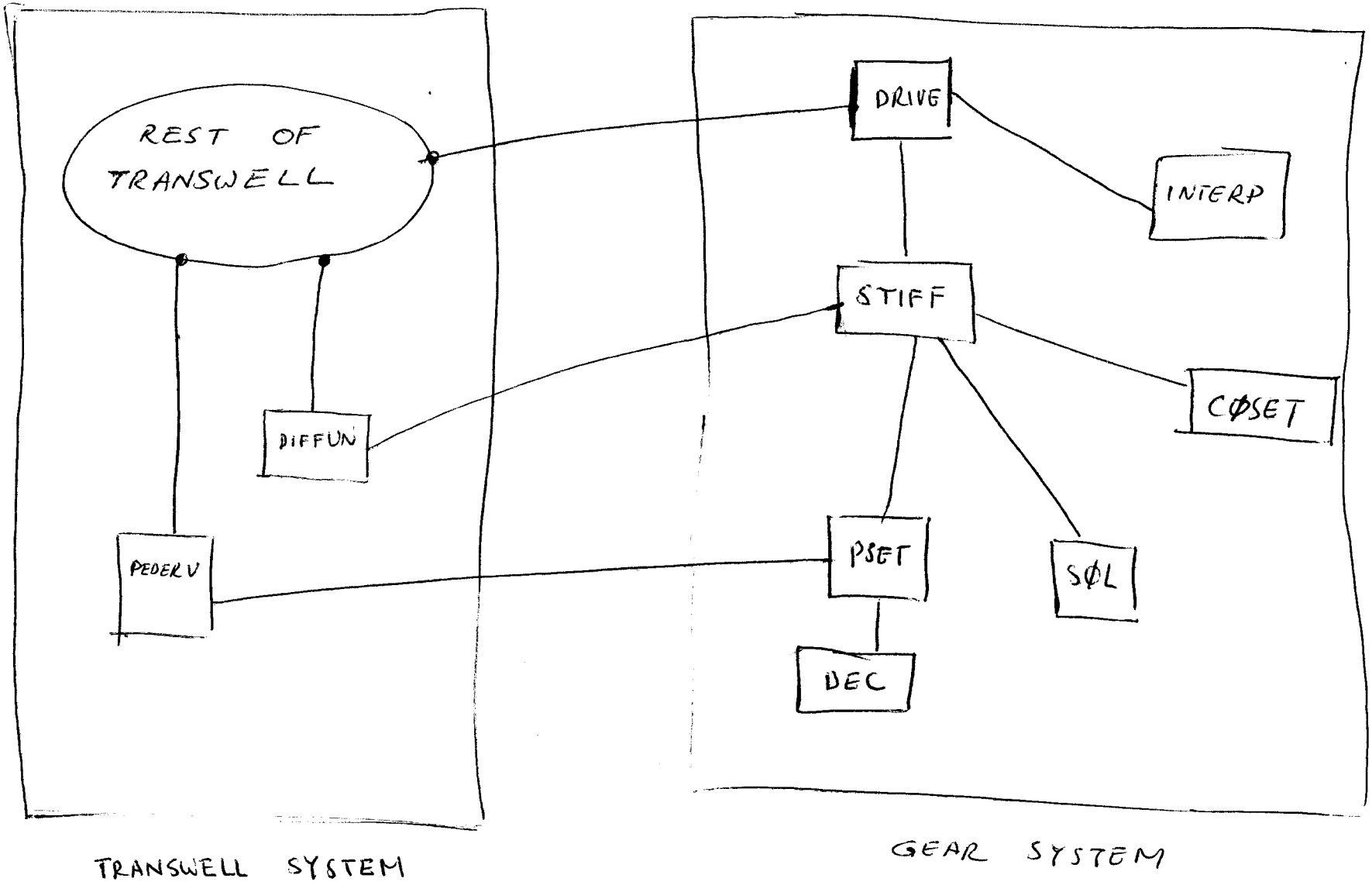
TRANSWELL I is structured with the following considerations:

(1) Minimizing the number of rate equations used in a specific condition. This is mainly to alleviate using more equations than necessary. It was noticed in previous versions that using redundant equations increases computation time dramatically.

(2) Computing the minimum number of variables. Thus time invariant quantities are computed once at the beginning. Time dependent equations contain "almost" the minimum number of time invariant arithmetic operations.

(3) Ease of accessibility to most of the variables through the use of common areas as will be described.

(4) Since basic applications of this code are expected to be in the area of time dependent analysis, special attention was given to methods of reducing computation time.



STRUCTURE OF THE GEAR PACKAGE AND COMMUNICATION WITH TRANSWELL

FIG-(1)

(5) Minimum programming ambiguity with forward branching and abundance of comment cards to guide the interested researcher for future changes.

(6) Logical separation of different irradiation conditions. This slightly increases the storage requirements of the object code, but it will be extremely valuable when one wants to add more physics to the code.

IV-B Subroutines

TRANSWELL subroutines are written with the idea of affixing calculational as well as logical functions to each subroutine. 'Arguments' are avoided from most subroutines with only a few exceptions. All information is handled and passed between subroutines through the CØMMØN blocks. This section is concerned with describing all subroutines and functions in a general sense. Comments on the logic and method of calculation are amply dispersed in all of the subroutines. This provides detailed information on each of the separate subroutines.

MAIN

The main program masters and manipulates the logic of any specific problem. It calls 10 subroutines for setting up the input and initial conditions, performing time independent calculations; and calling the core integrator subroutines.

Called from: N.A. (Not Applicable)

Calls to: ZERØ, INPUT, ØUTKEY, PARAM, BURGER, INITIA, SPLIT, CØNCERN, DRIVE.

CØMMON Blocks: NAMES, CØNST, IRRAD, ANNEAL, INTEG, PULSE, BTEMP, INITL, MAT, ØUTCØN, VECTØR, DØT, ØUT.

ZERØ

This subroutine sets all of the CØMMØN blocks to zero. It uses double precision zeroes (0.D0) for all the variables. Having this done, it sets up some default values of input parameters as will be explained later.

Called from: MAIN

Calls to: N.A.

CØMMØN Blocks: INTEG, NAMES, CØNST, IRRAD, ANNEAL, PULSE, BTEMP, INITL, MAT, BKDAT, STRESS, BURG, CØNC, JACK, METDAT, ØUTCØN, ØUT.

INPUT

This is the main input subroutine. It is called only once after ZERØ and reads in numeric and alphanumeric input. Thus it supercedes default values set up by ZERØ. Description of input variables and their default values is given in V.

Called from: MAIN

Calls to: ØUTKEY, ERROR, TITLE

COMMON Blocks: NAMES, INTEG, MAT, IRRAD, ANNEAL, PULSE, STRESS, METDAT, CØNST, BKDAT, DPLØT

NAMELISTS: INDATA

ERROR (NAME, ERRFLG)

It prints misspelled input characters, and/or indicates if the input is in incorrect order.

Called from: INPUT

Calls to: N.A.

CØMMØN Blocks: N.A.

TITLE

It reads numeric data using NAMELIST, then it reads alphanumeric input for each graph.

It is called only once when plotting option is specified.

Called from: INPUT

Calls to: N.A.

CØMMØN Blocks: INTEG

Namelists: PINFO

ØUTKEY

This subroutine is designed merely to give full explanations (ENTRY TABLE) of output quantities. If one is familiar with the output notation, he can omit it from the output stream by introducing a suitable data card as explained later.

Called from: MAIN

Calls to: N.A.

CØMMØN Blocks: N.A.

PARAM

This subroutine picks up metal parameters under consideration. Best available data are stored at the compilation time in element BDATA. Metals and their ID numbers available now are:

Metal	ID
Nickel	1
Stainless Steel	2
Aluminum	3
Niobium	4
Vanadium	5

The following quantities are defined for a metal from a 5 x 15 matrix.

Parameter	Matrix Element	Unit	Meaning
E_v^f	A(1,ID)	ev	vacancy formation energy
E_i^f	A(2,ID)	ev	interstitial formation energy
E_v^m	A(3,ID)	ev	vacancy migration energy
E_i^m	A(4,ID)	ev	interstitial migration energy
D_v^o	A(5,ID)	$cm^2\ sec^{-1}$	vacancy diff. coef. preexpon.
D_i^o	A(6,ID)	$cm^2\ sec^{-1}$	interstitial diff. coef. preexpon.
b	A(7,ID)	cm	Burger's vector
γ	A(8,ID)	ev cm^{-2}	surface energy
Z_v	A(9,ID)	dimensionless	vacancy bias factor
Z_i	A(10,ID)	dimensionless	interstitial bias factor
Ω	A(11,ID)	cm^3	atomic volume
γ_{sf}	A(12,ID)	ev cm^{-2}	stacking fault energy
μ	A(13,ID)	ergs cm^{-3}	shear modulus
ν	A(14,ID)	dimensionless	Poisson's ratio
e_i^o	A(15,ID)	dimensionless	Ratio of interstitial relaxation volume to atomic volume

Called from: MAIN

Calls to: N.A.

COMMON Blocks: BKDAT, METDAT, INTEG.

BDATA

This is the BLØCK DATA of the program. Information is stored at the compilation time in CØMMØN Blocks CONST and METDAT.

Called from: N.A.

Calls to: N.A.

CØMMØN Blocks: CØNST, METDAT.

BURGER

This subroutine is called only once and it calculates all time independent quantities and stores them in CØMMØN Block /BURG/.

Called from: MAIN

Calls to: SPLIT

CØMMØN Blocks: NAMES, CØNST, IRRAD, MAT, BKDAT, STRESS, BURG.

TEMPER

This subroutine is called only once and it calculates and prints out the temperature dependent information.

Called from: MAIN

Calls to: N.A.

CØMMØN Blocks: CØNST, BTEMP, MAT, IRRAD, BKDAT.

INITIA

This subroutine is called only once before starting the time dependent calculations. It sets up the initial value of the vector components Y(NEQ) and stores them in CØMMØN Block INITL. It also selects the number of equations (NEQ), and the initial time step used in the core integrator (GEAR).

Called from: MAIN

Calls to: N.A.

CØMMØN Blocks: INITL, PULSE, BTEMP, MAT, BKDAT, INTEG.

SPLIT

This is called only when input variable TYPE (5) = 'STRESS'. It calculates the fraction f of the total interstitial loop population that are aligned perpendicular to the applied stress as given by Equation (57) and as defined in (D75). It also calculates the concentration of aligned and non-aligned interstitial loops per cm^3.

Called from: MAIN, BURGER

Calls to: N.A.

COMMON Blocks: CØNST, IRRAD, BTEMP, BKDAT, STRESS.

CONCEN

This subroutine calculates the steady state vacancy and interstitial concentrations (CV and CI) and their fluxes (DV*CV and DI*CI). It solves simultaneously Equations (49) and (50) for the special case: $\dot{Y}(5) = \dot{Y}(6) = 0.D0$.

Called from: MAIN

Calls to: DIFFUN

CØMMØN Blocks: INTEG, IRRAD, BTEMP, INITL, MAT, CØNC, ØUTCØN.

GEAR PACKAGE

A full description of the theory and practice of this package is given in reference (9). However, we will repeat only the means of communication with the package.

To use the GEAR package, the user must provide: (a) routines which define the problem and which are called by the package (primarily Subroutine DIFFUN defining f(y,t)), and (b) a calling program which makes calls to Subroutine DRIVE. The routines called by the package are discussed below under External Names. The calling program must set the initial values, method parameters, and output values of t, and make calls to DRIVE. DRIVE in turn calls other routines for the solution of the problem. Since the integration process uses step sizes determined internally and dynamically, it will not generally hit the output values of t exactly. Normally, it will go slightly beyond each output point, and values of y at the output point are computed by interpolation.

Communication with DRIVE

The calling sequence to Subroutine DRIVE is as follows:

CALL DRIVE (N, TO, HO, YO, TOUT, EPS, MF, INDEX).

The arguments to DRIVE are defined as follows:

N = the number of first-order ordinary differential equations. N is limited to 20, unless dimensions are altered in DRIVE. N can be decreased on any call to DRIVE after the first call, with INDEX = -1 on input, but can never be increased.

TO = the initial value of the independent variable t, and is used only on the first call.

HO = the step size, h. Normally, HO is used on input only for the step size to be attempted for the first step, on the first call (see Usage Note 2, below). The sign of h is arbitrary but will not be changed during a problem. On output, HO is the step size last used, whether successfully or not.

YO = a vector of length N for the dependent variable y. On input, YO is the vector of initial values, and is used only on the first call. On output, YO is the vector of values of y at t = TOUT (normally computed by interpolation).

TØUT = the next output value of t. TOUT is used for input on every call. On output, TØUT is unchanged if reached successfully (it is altered slightly if INDEX = 2 on input), and is the farthest value of t reached otherwise.

EPS = the local error tolerance parameter. It is used only for input, and used only on the first call, unless INDEX = -1. Estimates of the single-step error in y_i, divided by YMAX(i), are kept less than EPS in root-mean-square (RMS) norm (i.e., Euclidean norm divided by $\sqrt{N}$). The vector YMAX of weights is computed in DRIVE. EPS should be at least an order of magnitude larger than the unit roundoff (URØUND) but generally not larger than about 10^{-3}.

MF = the method flag. It is used only for input, and used only on the first call, unless INDEX = -1. The allowed values of MF are 10, 11, 12, 13, 20, 21, 22, and 23. MF has two decimal digits, METH and MITER (MF = 10*METH + MITER). METH is the basic method indicator, with the following values and meanings:

1 for implicit Adams methods;

2 for BDF methods, or Gear's stiffly stable methods.

MITER is the corrector iteration method indicator, with the following values and meanings:

0 for functional (fixpoint) iteration;

1 for chord method with user-supplied Jacobian from PEDERV;

2 for chord method with Jacobian generated internally;

3 for chord method with diagonal approximation to Jacobian (See Usage Note 1, below).

INDEX = an integer flag used for both input and output. On input, it indicates the type of call to DRIVE, with the following values and meanings:

1 for the first call for the problem;

0 for a call other than the first, with normal continuation;

-1 for a call other than the first, in which the user has reset N, EPS, and/or MF;

2 for a call other than the first, with integration to continue so as to hit t = TOUT exactly, and not interpolate for output values; this assumes TOUT is beyond the current value of t;

3 for a call other than the first, with control to return to the calling program after one step; TOUT is ignored on input and set to the current value of T on output.

On output, INDEX indicates the results of the last call, with the following values and meanings:

0 if integration was completed successfully as requested;

-1 if integration was halted after failing to pass the error test even after reducing the step size, h, by a factor of 10^{10} from its initial value;

-2 if integration was halted after some initial success either by repeated error test failures or by a direct test indicating that EPS is too small;

-3 if integration was halted after failing to achieve corrector convergence even after reducing h by a factor of 10^{10} from its initial value;

-4 if an input value was found to be illegal; either EPS $\leq$ 0., N $\leq$ 0, (TO-TØUT)*HO $\geq$ 0., or the input value of INDEX was illegal;

-5 if INDEX was -1 on input, but TOUT was not beyond the current t; the desired changes of parameters were, therefore, not made; to continue, simply reset TOUT and INDEX and call DRIVE again.

Notice that, since the normal output value of INDEX is 0, it need not be reset for a normal continuation.

Additional communication between the user and the package can be gained by reference to the Common Blocks used by the package. For blocks GEAR1 to GEAR7, descriptions of the variables can be found in the comment cards of Subroutine STIFF, and for GEAR8, descriptions are given in Subroutine PSET. The block GEAR9 is used for statistical quantities, and is probably the one most likely to be of interest to the user. Its contents are as follows:

HUSED = the step size h last used (successfully);

NQUSED = the order last used (successfully);

NSTEP = the cumulative number of steps taken;

NFE = the cumulative number of f evaluations (DIFFUN calls);

NJE = the cumulative number of Jacobian evaluations, and hence also of matrix LU decompositions.

External Names

Besides Subroutine DRIVE, the following six routines are supplied as part of the GEAR package. Their calling sequences and functions are described below, although this information is not essential for use of the package.

- Subroutine INTERP (TØUT, Y, NO, YO) is called by Drive. It computes interpolated values for y at t = TOUT, using the data in the Y array.
- Subroutine STIFF (Y,NO) is called by DRIVE. It performs a single step of the integration, and does the control of local error (which entails selection of step size and order) for that step.
- Subroutine COSET (METH, NQ, EL, TQ, MAXDER) is called by STIFF, and sets coefficients that are used there, both for the basic integration step and for error control.
- Subroutine PSET (Y, NO, CON, MITER, IER) is called by STIFF if MITER is 1 or 2. It sets up the matrix $P = I - h\beta_0 J$, where I is the identity matrix, β_0 is a scalar related to the method, and J is the Jacobian matrix. It then processes P for subsequent solution of linear algebraic systems with P as coefficient matrix, as part of the chord iteration methods.
- Subroutine DEC (N, NDIM, A, IP, IER) is called by PSET, and performs an LU decomposition of a matrix.
- Subroutine SOL (N, NDIM, A, B, IP) is called by STIFF if MITER is 1 or 2, and solves linear algebraic systems for which the matrix was processed by DEC.

PEDERV (N, X, Y, PD, NO)

This subroutine directs the path of calculation to one of the eight subroutines JACK1 through JACK8. It also receives the Jacobian matrix P(10,10) in COMMON area /JACK/ and puts it in the matrix PD(NEQ,NEQ).

It is called by PSET if MITER = 1. It is to supply the partial derivates of f(y,x) with respect to y, evaluated at x = t and Y = y. It must form a two dimensional array PD, stored as NOxNO array, according to

$$PD(i,j) = \frac{\partial f_i}{\partial y_j} , \quad 1 \leq i, j \leq N . \tag{112}$$

N here is the number of equations used = NEQ.

Called from: PSET

Calls to: JACK1, JACK2, JACK3, JACK4, JACK5, JACK6, JACK7, JACK8

CØMMØN Blocks: JACK, INTEG.

JACK1

This subroutine computes elements of the Jacobian matrix P(10,10) for case (1).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK2

This subroutine computes elements of the Jacobian matrix P(8,8) for case (2).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK3

This subroutine computes elements of the Jacobian matrix P(6,6) for case (3).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK4

This subroutine computes the elements of the Jacobian matrix P(6,6) for case (4).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK5

This subroutine computes the elements of the Jacobian matrix P(6,6) for case (5).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK6

This subroutine computes the elements of the Jacobian matrix P(4,4) for case (6).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK7

This subroutine computes the elements of the Jacobian matrix P(4,4) for case (7).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

JACK8

This subroutine computes the elements of the Jacobian matrix P(2,2) for case (8).

Called from: PEDERV

Calls to: GEØML, GEØMV

CØMMØN Blocks: JACK, CONST, IRRAD, STRESS, BTEMP, MAT, BKDAT, BURG, BVECT, DØT.

DIFFUN (N, X, Y, YDØT)

This subroutine is called by STIFF, and also by PSET if MITER = 2. It is to compute the vector YDØT = $\dot{y}$ = f(y,t) of length N for given values x = t and the vector Y = y of length N. It is required regardless of the value of MF chosen. It actually directs the path of computation to one of the DERV subroutines.

Called from: CØNCEN, PSET, STIFF

Calls to: DERV1, DERV2, DERV3, DERV4, DERV5, DERV6, DERV7, DERV8

CØMMØN Blocks: INTEG, DØT, BVECT, BTEMP, NAMES, INITL.

DERV1

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (10) for given values x = t and the vector Y = y of length (10). The derivatives are those of case (1).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CONST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, OUT.

DERV2

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (8) for given values x = t and the vector Y = y of length (8). The derivatives are those of case (2).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CONST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, OUT.

DERV3

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (6) for given values x = t and the vector Y = y of length (6). The derivatives are those of case (3).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CONST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, ØUT.

DERV4

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (6) for given values x = t and the vector Y = y of length (6). The derivatives are those of case (4).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CØNST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, ØUT.

DERV5

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (6) for given values x = t and the vector Y = y of length (6). The derivatives are those of case (5).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CØNST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, ØUT.

DERV6

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (4) for given values x = t and the vector Y = y of length (4). The derivatives are those of case (6).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CØNST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, ØUT.

DERV7

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (4) for given values x = t and the vector Y = y of length (4). The derivatives are those of case (7).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CØNST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, ØUT.

DERV8

This subroutine computes the vector YDØT = $\dot{y}$ = f(y,x) of length (2) for given values x = t and the vector Y = y of length (2). The derivatives are those of case (8).

Called from = DIFFUN

Calls to = GEØMV, GEØML

CØMMØN Blocks = NAMES, CØNST, IRRAD, BTEMP, MAT, BKDAT, STRESS, BURG, ØUTCØN, VECTØR, DØT, ØUT.

DELTA

This subroutine calculates for a delta function response of a metal under irradiation. Theory for this subroutine is in reference (12). It computes the vacancy and interstitial concentrations as well as average void and interstitial loop radii as a function of time.

Called from: MAIN

Calls to: DRIVE

CØMMØN Blocks: CØNST, BTEMP, IRRAD, PULSE, INITL, BKDAT, STRESS, ØUTCØN, BVECT.

EXPØN

This is one of the external functions in the program. It calculates double precision exponentials and guards against overflow and underflow.

Called from: GEØMV, GEØML, PRESS, DELTA

Calls to: N.A.

CØMMØN Blocks: N.A.

GEØMV (RV)

This external function calculates the exponential part in Equation (10). It is defined as

$$\text{GEØMV(RV)} = \frac{c_v(r_v)}{c_v^e} \tag{113}$$

where $c_v(r_v)$ is the vacancy concentration at the surface of a void of radius r_v, and c_v^e is the thermal equilibrium vacancy concentration.

Called from: DERV1, DERV2, DERV3, DERV4, DERV5, DERV6, DERV7, DERV8, JACK1, JACK2, JACK3, JACK4, JACK5, JACK6, JACK7, JACK8, DIFFUN

Calls to: EXPØN

CØMMØN Blocks: CØNST, IRRAD, BKDAT.

GEØML (RL)

This internal function calculates the exponential part in Equation (17). It is defined as

$$\text{GEØML(RL)} = \frac{c_v(r_\ell)}{c_v^e} \tag{114}$$

where $c_v(r_\ell)$ is the vacancy concentration at the surface of an interstitial loop of radius r_ℓ, and c_v^e is the thermal equilibrium vacancy concentration.

The corresponding geometry function for vacancy loops is obtained as the inverse of GEØML.

Called from: DERV1, DERV2, DERV3, DERV4, DERV5, DERV6, DERV7, DERV8, JACK1, JACK2, JACK3, JACK4, JACK5, JACK6, JACK7, JACK8

Calls to: EXPØN

CØMMØN Blocks: CØNST, IRRAD, BURG, BKDAT, BTEMP.

PRESS(RV)

This internal function calculates the internal pressure in a void of radius (RV) and containing (GAS) number of gas atoms.

Called from: GEØMV

Calls to: N.A.

CØMMØN Blocks: CØNST, IRRAD, MAT, BKDAT.

ØUTDET

This subroutine merely choses a suitable output path according to the irradiation particle, mode of irradiation and stress state.

Called from: MAIN

Calls to: ØUTP1 ØUTP2, ØUTP3, ØUTP4, ØUTP5, ØUTP6, ØUTP7, ØUTP8

COMMON Blocks: INTEG

ØUTP1

This subroutine is designed for output quantities of case (1). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP2

This subroutine is designed for output quantities of case (2). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP3

This subroutine is designed for output quantities of case (3). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP4

This subroutine is designed for output quantities of case (4). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP5

This subroutine is designed for output quantities of case (5). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP6

This subroutine is designed for output quantities of case (6). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

COMMON Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP7

This subroutine is designed for output quantities of case (7). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

ØUTP8

This subroutine is designed for output quantities of case (8). It gives detailed output, brief output, plotted output or a combination of detailed and plotted output. This depends on the input parameter TYPE (13) as will be described later.

Called from: ØUTDET

Calls to: JACKPR, TMPLØT, PLPLØT, STØRE

CØMMØN Blocks: ØUT, ØUTCØN, BVECT, DØT, JACK, INITL, INTEG, CØNC.

TMPLØT

This subroutine gives an approximate plot on the printer or the terminal using the GRAPH2 routine.

Called from: ØUTP1, ØUTP2, ØUTP3, ØUTP4, ØUTP5, ØUTP6, ØUTP7, ØUTP8

Calls to: GRAPH2, GRAPH2V, GRAPHND

CØMMØN Blocks: DPLØT, INTEG.

PLPLØT

This subroutine plots graphs using the plotter and the GRAPH and GRAPHM routines.

Called from: ØUTP1, ØUTP2, ØUTP3, ØUTP4, ØUTP5, ØUTP6, ØUTP7, ØUTP8

Calls to: INITPL, SCALRV, GRAPH, GRAPHM, ENDPLT

CØMMØN Blocks: DPLØT, INTEG.

STØRE

This subroutine stores the values for each variable to be plotted and also the time values.

Called from: ØUTP1, ØUTP2, ØUTP3, ØUTP4, ØUTP5, ØUTP6, ØUTP7, ØUTP8

Calls to : N.A.

CØMMØN Blocks: BVECT, DØT, ØUTCØN, CØNC, ØUT, INTEG, DPLØT, INITL.

DUMP

This subroutine dumps out the values of all parameters stored in CØMMØN areas. It is very useful as a debugging aid throughout the code since it could be easily called at any point in the code. However, for normal computations, it prints out the contents of all CØMMØN blocks at the end of the run.

This subroutine also writes the contents of pertinent CØMMØN Blocks on unit 2 using FØRTRAN unformatted write statements. Thus, once the CØMMØN blocks have been saved, the calculation can be restarted by reading them back into core and starting again as if the calculation never stopped.

Called from: MAIN

Calls to: N.A.

CØMMØN Blocks: INTEG, NAMES, CØNST, IRRAD, ANNEAL, PULSE, TEMP, INITL, MAT, BKDAT, STRESS, BURG, CØNC, JACK, METDAT, ØUTCØN, ØUT, VECTØR, DØT.

BIAS

This subroutine calculates the aligned dislocation loop-vacancy bias factor and the aligned dislocation loop - interstitial bias factor.

Called from: SPLIT

Calls to: N.A.

CØMMØN Blocks: STRESS, BKDAT.

IV-C TRANSWELL I Computer Code Variables

All TRANSWELL real variables are implicit double precision giving **14 decimal places** of accuracy on an IBM or a UNIVAC computer. For a CDC computer the statement "IMPLICIT DØUBLE PRECISION (A-H, O-Z)" has to be deleted from the beginning of all subroutines.

Variable names were chosen to indicate the actual names used in current literature on rate theory applied to point defects. This facilitates understanding of the different subroutines for further development. The following conventions were used throughout the Computer Code:

i) If the character (E) is attached to the end of a temperature dependent variable name, the thermal equilibrium value of this variable is meant.

ii) The character (0) "ZERO" is used at the end of some variable names to indicate their initial values.

iii) The character (A) is used at the end of some variable names to indicate their stress aligned values.

iv) The character (N) is used at the end of some variable names to indicate their stress non-aligned values.

The variables are grouped such that a subroutine will find most of the variables that it needs in few CØMMØN Blocks. We now list all of the variables (by CØMMØN Blocks) along with their meaning and units.

COMMON/INTEG/

1) NTØT; total number of pulses to be studied.

2) MF; the method flag as described in subroutine DRIVE.

3) INDEX; integration continuation index as in subroutine DRIVE.

4) NEQ; number of equations solved.

5) IPATH; integer determining a suitable path leading to subroutines pertinent to one of the eight cases described.

6) JØUT; integer determining the method of output desired.

7) ID; integer determining the ID number of a metal as described in subroutine PARAM.

8) IRESET; integer to reset the calculations.

9) JPLØT(5,3); 15 integers corresponding to a maximum of 15 plots in a particle run. Each one can assume the values 1-300 corresponding to a certain output quantity to be plotted. This will be described in Section V.

10) NPLØT(5); 5 integers determining the number of overlayed plots in a maximum of 5 graphs.

11) IGRID(5); 5 integers for the grid desired in each of the 5 plots.

12) NGRAPH; total number of graphs to be plotted.

13) NØUT; output counter for number of output intervals.

14) NWAIT; integer determining how many output intervals plotting routines will skip before they store a value for plotting.

15) NTIME; plotting counter for number of plotted points.

CØMMØN/CØNST/

1) BK; Bolzmann's constant eV/^{o}K.

2) PI = π.

3) BVAN; Vander Waal's constant.

4) FREQ, Debye frequency, sec^{-1}.

5) SITES; number of unstable sites around a vacancy.

6) FST; steady state divisor determining the number of output points. Default value = 100.D0.

7) FPL1; pulsed divisor for number of output points inside the pulse. Default value = 10.D0.

8) FPL2; } pulsed divisors for number of output points

9) FPL3; } in between pulses. Default values are 10.D0 and 10.D0.

10) FAC; factor to terminate computations before the pulse is ended to alleviate sharp derivative changes. Default value = 0.9999999D0.

CØMMØN/IRRAD/

1) PROD, production rate of point defects in dpa/sec.

2) DPA, total DPA accumulated during irradiation.

3) TEMP, irradiation temperature in ^{o}K.

4) DØSE, accumulated dpa at any current time.

CØMMØN/ANNEAL/

1) TIRR, irradiation time in seconds.

2) TANN, annealing time in seconds.

3) TEMPAN, annealing temperature in ^{o}K.

CØMMØN/PULSE/PW, TP, RS, EPS

1) PW; pulse width in seconds.

2) TP; pulse period in seconds.

3) RS; multiplier in the order of 10^{-10} for HO.

4) EPS; relative accuracy normally between 10^{-4} - 10^{-9}.

CØMMØN/BTEMP/

1) DV, vacancy diffusion coefficient at a certain temperature, cm^2/sec.

2) DI, interstitial diffusion coefficient at a certain temperature, cm^2/sec.

3) CVE, equilibrium vacancy concentration in at./at.

4) CIE, equilibrium interstitial concentration in at./at.

5) XNV, concentration of voids in cm^{-3}.

6) XNIL, concentration of interstitial loops in cm^{-3}.

7) TAUV, vacancy lifetime in seconds.

8) TAUI, interstitial lifetime in seconds.

9) ALFA, recombination coefficient in sec^{-1}.

10) BETA = $\frac{1}{kT}$ in eV^{-1}.

CØMMØN/INITL/

1) TO, initial integration time in seconds.

2) TIME, current time in seconds.

3) TØUT, output time in seconds.

4) YO(10), a vector of length 10 double precision words for the initial values of the components of the $\vec{Y}$ vector.

5) HS, initial step size for steady state calculations, sec.

6) HP, initial step size for pulsed or transient calculations, sec.

CØMMØN/MAT/

1) CASC, cascade efficiency as defined in (D72).
2) PRØDV, production rate of free vacancies in dpa/sec.
3) XNVO, void density preexponential for nucleation in cm^{-3}.
4) EVØID, void density energy for nucleation in eV.
5) XNILO, interstitial loop density preexponential for nucleation in cm^{-3}.
6) ELØØP, interstitial loop density energy for nucleation in eV.
7) RØDE, deformation produced dislocation density in cm^{-2}.
8) RØDO, total initial dislocation density in cm^{-2}.
9) RVLO, initial vacancy loop radius in cm. In the order of 15.D-8 cm.
10) RILO, initial interstitial loop radius in cm.
11) RVO, initial void radius in cm.
12) GAS, the number of gas atoms in a void.

CØMMØN/NAMES/TYPE(20)

1) TYPE(1) and TYPE(2); 2A4 alphanumeric input variables indicating irradiation particle. They assume the values: 'ELECTRON', 'IØNbbbbb' and 'NEUTRONb' for electron irradiation, ion irradiation or neutron irradiation, respectively. b here means a blank.

2) TYPE(3) and TYPE(4); 2A4 alphanumeric input variables indicating irradiated metal. They assume the values: 'NICKELbb', 'STEELbbb', 'ALUMINUM', NIØBIUMb' and 'VANADIUM'.

3) TYPE(5) and TYPE(6); 2A4 alphanumeric input variables for irradiation mode. They assume the values: 'PULSEDbb', 'STEADY' and 'ANNEAL'.

4) TYPE(7) and TYPE(8); 2A4 alphanumeric input variables for pulsed analysis method of solution. They assume the values: 'EXACTbbbb' and 'DELTAbbb'.

5) TYPE(9) and TYPE(10); 2A4 alphanumeric input variables for stress state. They assume the values: 'STRESSbb' and 'NØbSTRES'.

6) TYPE(11) and TYPE(12); 2A4 alphanumeric input variables for creep studies. They assume the values: 'CREEPbbb' and 'NØbCREEP'.

7) TYPE(13) and TYPE(14); 2A4 alphanumeric input variables for method of output desired. They assume the values: 'PLØTbbbb', 'PRINTbbb', FULLbbbb' and 'PARTPRIN'.

8) TYPE(15) and TYPE(16); 2A4 alphanumeric input variables for calling subroutine ØUTKEY. They assume the value 'ENTRYbbb' if one wants an ENTRY TABLE for output quantities and the value 'NØbENTRY' if one doesn't want it.

9) TYPE(17) and TYPE(18); 2A4 alphanumeric input variables for requesting graphics on a certain device. They assume the value 'TERMINAL' for terminal or printer graphs and the value 'PLØTTERb' for plotter graphs.

10) TYPE(19) and TYPE(20); 2A4 alphanumeric input variables reserved for possible expansions.

CØMMØN/BKDAT/

1) EVF, vacancy formation energy in eV.

2) EIF, interstitial formation energy in eV.

3) DVE, vacancy diffusion coefficient preexponential in cm^2/sec.

4) DIE, interstitial diffusion coefficient preexponential in cm^2/sec.

5) EVM, vacancy migration energy in eV.

6) EIM, interstitial migration energy in eV.

7) BU, Burger's vector in cm.

8) GAMA, surface energy in eV/cm^2.

9) ZV, vacancy-nonaligned dislocation loop bias factor.

10) ZI, interstitial-nonaligned dislocation loop bias factor.

11) ØMEGA, atomic volume in cm^3.

12) STACK, stacking fault energy in eV/cm^2.

13) SHEAR, shear modulus in $ergs/cm^3$.

14) XNEW, Poisson's ratio.

CØMMØN/STRESS/

1) SIGMA, uniaxial stress applied on the sample in eV cm^{-3}.
2) XPLAN, the number of atoms defining an atomic plane, in the order 10.
3) ZVA, the vacancy-aligned interstitial loop bias factor.
4) ZIA, the interstitial-aligned interstitial loop bias factor.
5) RVGAS, equilibrium bubble radius in cm.
6) FACTØR, the fraction of total interstitial loop population that are aligned perpendicular to applied stress.
7) XILA, the number density of aligned interstitial loops in cm^{-3}.
8) XILN, the number density of non-aligned interstitial loops in cm^{-3}.

CØMMØN/BURG/

This common areas contain constants that are calculated once before integration starts. Explicit expressions for different variables are written.

1) QUAN = $\pi\,[r_{v\ell}(o)]^2 b$

2) BUSQ = b^2

3) GEØME = exp $\{\frac{\sigma\Omega}{kT}\}$

4) GEØVLO = GEØML (RVLO)

5) STARTN = $\frac{2}{3}(1 - f)\ \varepsilon P/\pi[r_{v\ell}(o)]^2 b$

6) DRIVEN = $\frac{2}{3}(1 - f)\ \varepsilon P$

7) STARTA = $\frac{1}{3}(1 + 2f)\ \varepsilon P/\pi[r_{v\ell}(o)]^2 b$

8) DRIVEA = $\frac{1}{3}(1 + 2f)\ \varepsilon P/\pi[r_{v\ell}(o)]^2 b$

9) RØDEN = $\frac{2}{3}\,\rho_d^e$

10) RØDEA = $\frac{1}{3}\,\rho_d^e$

11) PI2 = 2π

12) PI4 = 4π

13) PI400 = $\frac{400\pi}{3}$

14) BURVL = $b\ r_{v\ell}(o)$

CØMMØN/CØNC/

1) CV; Vacancy concentration in at./at.

2) CI; Interstitial concentration in at./at.

3) FLUXV; vacancy flux in cm^2/sec.

4) FLUXI; interstitial flux in cm^2/sec.

CØMMØN/JACK/

1) P(10, 10); 100 element matrix where values of the pertinent Jacobian elements are stored.

CØMMØN/METDAT/

1) A(15, 5); 75 element matrix where 15 physical parameters for each of 5 metals are stored as described before in subroutine PARAM

CØMMØN/ØUTCØN/

1) XLAMI; interstitial time dependent time constant in sec^{-1}.

2) XLAMV; vacancy time dependent time constant in sec^{-1}.

3) EMIT; total rate of vacancy emission in at./at./sec.

CØMMØN/BVECT/

This common area is used with a maximum dimension of 10. It contains different elements of the vector $\vec{Y}$ at different conditions. We will describe here the elements stored in each of the previous 8 cases

In all cases the following applies

1) Y(1); Average void radius, cm.

2) Y(2); Average non-aligned interstitial loop radius, cm.

CASE (1)

1) Y(3); Number density of non-aligned vacancy loops, cm^{-3}.

2) Y(4); Fraction of vacancies in non-aligned vacancy loops, at./at.

3) Y(5); Vacancy concentration, at./at.

4) Y(6); Interstitial concentration, at./at/

5) Y(7); Average aligned interstitial loop radius, cm.

6) Y(8); Number density of aligned vacancy loops, cm^{-3}.

7) Y(9); Fraction of vacancies in aligned vacancy loops, at./at.

8) Y(10); Network creep strain, cm/cm.

CASE (2)

1) Y(3); Number density of non-aligned vacancy loops, cm^{-3}.

2) Y(4); Fraction of vacancies in non-aligned vacancy loops, at./at.

3) Y(5); Average aligned interstitial loop radius, cm.

4) Y(6); Number density of aligned vacancy loops, cm^{-3}.

5) Y(7); Fraction of vacancies in aligned vacancy loops, at./at.

6) Y(8); Network creep strain, cm/cm.

CASE (3)

1) Y(3); Number density of vacancy loops, cm^{-3}.

2) Y(4); Fraction of vacancies in vacancy loops, at./at.

3) Y(5); Vacancy concentration, at./at.

4) Y(6); Interstitial concentration, at./at.

CASE (4)

1) Y(3); Vacancy concentration, at./at.

2) Y(4); Interstitial concentration; at./at.

3) Y(5); Average aligned interstitial loop radius, cm.

4) Y(6); Network creep strain, cm/cm.

CASE (5)

1) Y(3); Average aligned interstitial loop radius, cm.

2) Y(4); Network creep strain, cm/cm.

CASE (6)

1) Y(3); Vacancy concentration, at./at.

2) Y(4); Interstitial concentration, at./at.

CASE (7)

1) Y(3); Number density of vacancy loops, cm^{-3}.

2) Y(4); Fraction of vacancies in vacancy loops, at./at.

CASE (8)

No extra equations are used in this case.

This CØMMØN block contains the time derivatives of vector elements $\vec{Y}(i)$, $2 \leq 10$. The contents of this CØMMØN block are always the time derivatives of the foregoing 8 cases discussed in CØMMØN/BVECT/.

CØMMØN/ØUT/

1) RØDILN; Non-aligned dislocations loop line density, cm^{-2}.

2) RØDILA; Aligned dislocation loop line denstiy, cm^{-2}.

3) RØDVLN; Non-aligned vacancy loop line density, cm^{-2}.

4) RØDVLA; Aligned vacancy loop line density, cm^{-2}.

5) RØD; Total line dislocation density, cm^{-2}.

6) EMITV; Vacancy emission rate from voids, at./at./sec.

7) EMITDA; Vacancy emission rate from aligned edge dislocations, at./at./sec.

8) EMITDN; Vacancy emission rate from non-aligned edge dislocations, at./at./sec.

9) EMITD; Vacancy emission rate from all edge dislocations, at./at./sec.

10) EMITIA; Vacancy emission rate from aligned interstitial loops, at./at./sec.

11) EMITIN; Vacancy emission rate from non-aligned interstitial loops, at./at./sec.

12) EMITIL; Total rate of vacancy emission from interstitial loops, at./at./sec.

13) EMITVA; Vacancy emission rate from aligned vacancy loops, at./at./sec.

14) EMITVN; Vacancy emission rate from non-aligned vacancy loops, at./at./sec.

15) EMITVL; Total rate of vacancy emission from vacancy loops, at./at./sec.

16) SDISV; Vacancy time constant due to dislocation sinks, sec^{-1}.

17) SDISI; Interstitial time constant due to dislocation sinks, sec^{-1}.

18) SVØIDV; Vacancy time constant due to void sink, sec^{-1}.

19) SVØIDI; Interstitial time constant due to void sink, sec^{-1}.

20) SINKI; Total interstitial sink removal rate, sec^{-1}.

21) SINKV; Total vacancy sink removal rate, sec^{-1}.

22) RECØM; Rate of vacancy-interstitial recombination, sec^{-1}.

23) SWELL; Swelling percent, %.

24) DELRV; Change in void radius (RV-RVO), cm.

25) DELRIL; Change in interstitial loop radius (RIL-RILO), cm.

V. Users Manual

V-A. Implementing the TRANSWELL Code

A great deal of effort has been directed towards optimization of both CPU time and core storage requirements. The necessity for pulsed and transient irradiation analysis with a great number of time steps imposes strict efficiency requirements on any code for such studies.

Approximately 62000 decimal words on a UNIVAC 1110 computer are needed for total program storage. Certain irradiation cases are very inexpensive to study using TRANSWELL. A typical case of electron irradiation, steady production of point defects and no stress applied requires an average of 0.23 seconds of CPU time per simulated dpa over a wide range of temperatures.

TRANSWELL reads two NAMELIST inputs from I/Ø unit and writes BCD output to logical unit six. If it is requested, subroutine DUMP writes, in unformatted FØRTRAN statements, to logical I/Ø number 2. This is read into CØMMØN blocks by subroutine BINARY using FØRTRAN unformatted read statements.

There should be no language compatibility problems, but the implicit double precision statements should be removed from all subroutines when using a CDC 6600 or 7600. The code was initiated on the Engineering Computing Laboratory (ECL) of the University of Wisconsin, and then developed on a UNIVAC 1110 using the FØRTRAN V compiler. Gear Package includes approximately 1200 card images while TRANSWELL (including GEAR) contains approximately 6000 card images.

V-B. Using the TRANSWELL Code

TRANSWELL is designed with 2 NAMELIST inputs. The first NAMELIST is /INDATA/ for all input quantities, while NAMELIST/PINFØ/ is for plotting information.

NAMELIST/INDATA/

1) XNVO
2) EVØID
3) XNILO
4) ELØØP
5) PRØD
6) DPA
7) TEMP
8) TIRR
9) TANN
10) TEMPAN
11) NTØT
12) PW
13) TP
14) CASC

---

15) A(1,1), A(1,2),..., A(14,5)
16) SITES
17) RVO
18) GAS
19) SIGMA
20) XPLAN
21) RS
22) MF
23) EPS
24) RVLO
25) IRESET
26) FST
27) FPL1
28) FPL2
29) FPL3
30) FAC
31) DIVP

(1)-(14) are required as input. (15)-(31) have present default values and may be changed if they are included as input.

NAMELIST/PINFØ/

1) IXSCAL (1,1), ..., IXSCAL (5,3)

2) IYSCAL (1,1), ..., IYSCAL (5,3)

3) ISXSCAL

4) ISYSCAL

5) REFY (1,1), ..., REFY (5,2)

6) REFX (1,1), ..., REFX (5,2)

7) IGRID (1), ..., IGRID (5)

8) JPLØT (1,1), ..., JPLØT (5,3)

9) NPLØT (1), ..., NPLØT (5)

10) NGRAPH

11) NWAIT

When the plotting of output is required, some of the previous NAMELIST variables have to be suppled as described below.

Input Description

The most general form of input to TRANSWELL would be as follows:

b$INDATA var1 = value 1, var2 = value 2, ..., varn = value n

b$END

TYPE (1) & TYPE (2)

TYPE (3) & TYPE (4)

TYPE (5) & TYPE (6)

TYPE (7) & TYPE (8)

TYPE (9) & TYPE (10)

TYPE (11) & TYPE (12)

TYPE (13) & TYPE (14)

TYPE (15) & TYPE (16)

TYPE (17) & TYPE (18)

b$PINFØ var1 = value 1, var2 = value 2, ..., varn = value n

b$END

Other sets of data could follow according to IRESET. The (b) here means a blank.

In the following, we will describe the /INDATA/NAMELIST variables, the ALPHANUMERIC input variables, the /PINFØ/NAMELIST and then the ALPHANUMERIC titling input. Finally we will describe how one can set an input Run Stream.

NUMERIC INPUT

1-XNVO Default = 0.D0

Preexponential for void number density (Nucleation Condition), cm^{-3}.

2-EVØID Default = 0.D0

Energy used for determining void number density (Nucleation Condition) ev.

3-XNILO Default = 0.D0

Preexponential for interstitial loop number denstiy (Nucleation Condition), cm^{-3}.

4-ELØØP Default = 0.D0

Energy used for determining interstitial loop number density (Nucleation Condition), ev.

5-PRØD Default = 0.D0

Production rate of point defects in steady state or during square pulses, dpa sec^{-1}.

6-DPA Default = 0.D0

Total accumulated dose at the end of irradiation; at./at.

7-TEMP Default = 0.D0

Irradiation temperature, ^{o}K.

8-TIRR Default = 0.D0

Irradiation time when an irradiation-annealing procedure is studied, sec.

9-TANN Default = 0.D0

Annealing time when an irradiation-annealing procedure is studied, sec.

10-TEMPAN Default = 0.D0

Annealing temperature, ^{o}K.

11-NTØT Default = 1

Total number of pulses.

12-PW Default = 0.D0

Pulse width in a square pulse generation of point defects, sec.

13-TP Default = 0.D0

Pulse period, sec.

14-CASC Default = 0D.0

Cascade efficiency

15-A(I,J); $1 \leq I \leq 14$, $1 \leq J \leq 5$

A 14 x 5 matrix for metal data of 5 different metals. Best available data are stored in this matrix prior to calling the INPUT subroutine. Therefore any input of a particular element in this matrix supercedes previous stored value. Default values are listed in the following table:

		Metal				
	Parameter	Ni	S.S.	Al	Nb	Va
		1	2	3	4	5
1	E_v^f	1.39D0	1.6D0	0.7D0		
2	E_i^f	4.08D0	4.0D0	3.2D0		
3	E_v^m	1.38D0	1.3D0	0.57D0		
4	E_i^m	.15D0	.2D0	0.1D0		
5	D_v^o	.06D0	.58D0	0.045D0		
6	D_i^o	.12D0	1.D-3	0.08D0		
7	b	2.5D-8	2.0D-8	2.D-8		
8	γ	6.2415D14	1.25D15	6.2415D14		
9	Z_v	1.00D0	1.00D0	1.00D0		
10	Z_i	1.01D0	1.08D0	1.01D0		
11	Ω	1.5625D-23	0.8D-23	0.8D-23		
12	γ_{sf}	2.496D14	9.4D12	1.248D14		
13	μ	9.47D11	2.836D11	2.65D11	4.73D11	3.96D11
14	ν_o	0.276D0	0.291D0	0.347D0	9.35D0	0.392D0
15	e_i	1.40D0	1.40D0	1.40D0	1.40D0	1.40D0

16-SITES Default = 100.D0

Number of unstable atomic sites around a vacancy.

17-RVO Default = 1.0 D-7

Initial void radius, cm.

18-GAS Default = 10.D0

Number of gas atoms in a void.

19-SIGMA Default = 0.D0

Stress applied on the sample, ev cm^{-3}.

20-XPLAN Default = 10.D0

Number of atoms defining an atomic plane.

21-RS Default = 1.D-10

Multiplier used to determine the initial time step. For steady state calculations HS = RS * TAUV is used, while HP = RS * TAUI is used for pulsed and transient calculations. TAUV and TAUI are the vacancy and interstitial lifetimes in sec, respectively.

22-MF Default = 21

Method flag determining method used in integrations as described in DRIVE subroutine.

23-EPS Default = 1.0D-5

Relative accuracy of calculations as described in DRIVE subroutine.

24-RVLO Default = 15.D-8

Initial vacancy loop radius, cm.

25-IRESET Default = 0

Integer for restarting the calculations with the following possible values:

0 Start all over again and read numeric and alphanumeric data.

1 Read a following numeric input only.

2 Read a following alphanumeric input only.

3 Write all CØMMØN blocks in binary form on unit 2 for purpose of continuing computations.

4 Last input to be supplied. Data Set with IRESET=4 should include all numeric and alphanumeric data.

5 Read all CØMMØN blocks in binary form from unit 2 for continuation of computations to a longer integration time.

6 Gives a dump of all common areas after certain subroutines as a debugging aid.

26-FST Default = 100.D0

Number of output points desired in steady state calculations.

27-FPL1 Default = 10.D0

Number of output points desired inside a pulse of width PW.

28-FPL2 Default = 10.D0

Multiplier giving logarithmic output starting from time t = PW to t = TLIMIT

29-FPL3 Default = 10.D0

Divisor giving linear output starting from time t = TLIMIT to t = TP at intervals of TP/FPL3 each.

30-FAC Default = .9999999Do

Factor to give last output at time t = FAC * PW inside the pulse.

31-DIVP Default = 2.D0

Divisor to determine TLIMIT in above. TLIMIT = TP/DIVP.

ALPHANUMERIC INPUT

First Card

This 2A4 alphanumeric input card is for type of irradiation particle. It only takes one of the three values (starting column 1):

ELECTRON for electron irradiation

ION for ion irradiation

NEUTRON for neutron irradiation

Second Card

This 2A4 alphanumeric input is for the metal under irradiation. It takes one of the five values (starting from column 1):

NICKEL

STEEL

ALUMINUM

NIØBIUM

VANADIUM

Third Card

This 2A4 alphanumeric input is for mode of irradiation. It only takes one of the three values (starting column 1):

PULSED for pulsed or transient irradiation modes.

STEADY for steady rate of point defect production by irradiation

ANNEAL for zero rate of point defect production by irradiation (annealing)

Fourth Card

This 2A4 alphanumeric input is for the method used in pulsed analysis. It is contingent on card 3 taking the value PULSED. If the mode is not pulsed, this card should be omitted. It takes one of the two values (starting from first column):

EXACT for exact treatment within the Rate Theory

DELTA for approximate treatment to the Rate Theory using a delta function input

Fifth Card

This 2A4 alphanumeric input is for stress state of the irradiated metal. It only takes the two values (starting column 1):

STRESS for a uniaxial stress applied

NØbSTRESS for no stress applied

Sixth Card

This 2A4 alphanumeric input is for creep studies. It only takes the two values (starting column 1):

CREEP for creep studies desired

NØbCREEP for no creep studies desired

Seventh Card

This 2A4 alphanumeric input is for method of output desired. It only takes one of the four values (starting column 1):

PLØT	for plotted output either on the terminal, printer or plotter
PRINT	for a full printed output at each time step
PARTPRINT	for a partial printed output at each time step
FULL	for a full printed output at each time step as well as a plotted output on the terminal, printer or plotter

Eighth Card

This 2A4 alphanumeric input is for an ENTRY TABLE to define and describe all abbreviations and notations used in the printout. It only takes the values (starting column 1):

ENTRY	for ENTRY TABLE desired on output
NØbENTRY	for no ENTRY TABLE desired on output

Ninth Card

This 2A4 alphanumeric input is for requesting graphics on a certain device. It is contingent on card 7. If card 7 has the value PLØT or FULL, this card should be supplied, otherwise it should be deleted from the Run Stream. It only takes the values (starting column 1):

TERMINAL	for output plotted on a terminal or a printer
PLØTTER	for output plotted on the standard plotter

PLØTTING NUMERIC INPUT

Plotted output from TRANSWELL is designed to conform with the following rather arbitrary conditions:

1. A maximum of 5 graphs in one run.

2. A maximum of 3 overlayed plots in each graph. Thus we have a maximum of 15 plots in the same run. One can imagine we have a matrix of places, 5 x 3. In each place one can choose to plot any variable by giving a certain integer (JPLØT), which define this variable as described later.

1. IXSCAL(I,J); $1 \leq I \leq 5$, $1 \leq J \leq 3$.

Hollerith or equivalent INTEGER scale transformation control for TIME or DØSE axis.

IXSCAL(I,J) = 6HDØUBLE or 2; DØUBLE PRECISIØN data, linear scaling.

IXSCAL(I,J) = 6HLØGDBL or 6; DØUBLE PRECISIØN data, logarithmic scale.

IXSCAL(I,J): $1 \leq I \leq 5$, J = 2 or 3.

IXSCAL(I,J) = -1; Use same scale as defined by a CALL to GRAPH.

(i.e., 2nd overlay with scale as used by first graph).

= -2; Use same scale as defined by a call to GRAPHM.

(i.e., 3rd overlay with scale defined by a second overlay).

2. IYSCAL(I,J,); $1 \leq I \leq 5$, $1 \leq J \leq 3$.

Hollerith or equivalent INTEGER scale transformation control for any output quantity to be plotted.

IYSCAL(I,J) = 6HDØUBLE or 2; DØUBLE PRECISIØN data, linear scaling.

IYSCAL(I,J) = 6HLØGDBL or 6; DØUBLE PRECISIØN data, logarithmic scale.

IYSCAL(I,J); $1 \leq 1 \leq 5$, J = 2 or 3

IYSCAL(I,J) =-1; Use same scales as defined by a call to GRAPH (i.e., 2nd overlay with scale as used by first graph).

= -2; Use same scale as defined by a call to GRAPHM.

(i.e., 3rd overlay with scale defined by a second overlay.

Default Values:

IXSCAL (1-5, 1)
IYSCAL (1-5, 1) } = 2 (Double precision - Linear)

IXSIAL (1-5, 2-3)
1YSCAL (1-5, 2-3) } = -1 (Same scale used for a CALL to GRAPH, i.e. same scale as first graph)

3. REFX(I,J); $1 \leq I \leq 5$, $1 \leq J \leq 3$. Default = 0.DO.

DØUBLE PRECISIØN reference value for the TIME axis.

4. REFY(I,J); $1 \leq I \leq 5$, $1 \leq J \leq 3$. Default = 0.DO.

DØUBLE PRECISIØN reference value for any plotted quantity axis.

5. IGRID(I); $1 \leq I \leq 5$. Default = 2.

Hollarith or equivalent INTEGER graphing coordinate axis or grid control:

IGRID = 4HNØNE or -3; neither of the axes nor a grid is drawn. Labels are written if specified by 1XLABL or IYLABL.

IGRID = 5HXØNLY or -2; a single axis is drawn along the bottom edge of the graphing rectangle. Y-axis label is written if specified by IYLABL.

IGRID = 5HYØNLY or -1; a single axis is drawn along the left edge of the graphing rectangle. X-axis label is written if specified by IXLABL.

IGRID = 4HAXES or 0; single set of axes along bottom and left edges of graphing rectangle.

IGRID = 6HNØRMAL or 1; a set of axes is drawn along the bottom and left edges of the graphing rectangle, which is then completed on the opposite sides by simple straight lines.

IGRID = 5HFRAME or 2; axes are drawn as for

IGRID = 4HAXES, and the graphing rectangle is completed on the opposite sides by duplicate axes (without labels).

IGRID = 4HGRID or 3; graphing coordinate system depicted by a complete grid.

6. JPLØT(I,J); $1 \leq I \leq 5$, $1 \leq J \leq 3$. Default = N.A.

An integer determining the output variable desired for plotting in the I'th graph and J'th overlay.

For contents of CØMMØN block /BVECT/:

$1 \leq$ JPLØT(I,J) ≤ 100.

For contents of CØMMØN block /DØT/:

$101 \leq$ JPLØT(I,J) ≤ 200.

For contents of CØMMØN block /ØUTCØN/:

$201 \leq$ JPLØT(I,J) ≤ 210.

For contents of CØMMØN block /CØNC/:

$211 \leq$ JPLØT(I,J) ≤ 220.

For contents of CØMMØN block /ØUT/:

$221 \leq JPLØT(I,J) \leq 300.$

A full table of this numeric code will be given below.

7. NPLØT(I); $1 \leq I \leq 5$. Default = 2.

Number of overlayed plots in I'th graph.

8. NGRAPH. Default = N.A.

Total number of graphs desired on output.

9. ISXREF(I,J); $1 \leq J \leq 5$, $1 \leq J \leq 2$.

ISYREF(I,J); $1 \leq I \leq 5$, $1 \leq J \leq 2$.

Used in calls to scaling subroutines to indicate how reference values are to be used.

Values

0 = No reference value used in scaling (i.e. scaled on maximum and minimum of data)

1 = Reference values used as minimum values.

2 = Reference values used as center values.

3 = Reference value used as maximum value.

Default values

ISYREF(I,J)
ISXREF(I,J) } = 1 (minimum)

PLØTTING TITLES

These are supplied in sets of card images with a maximum of 80 characters in each. There are 3 cards per desired graph. The first card is for general TITLE, the second is for X-LABLE and the third is for Y-LABLE.

ORDER OF INPUT

All numeric data different from default values are to be inputted in the $PINFØ NAMELIST. Then the title, x label and y label for each graph.

Table (1) JPLØT(I,J) Code

JPLØT name	JPLØT equivalent integer	JPLØT name	JPLØT equivalent integer
RV	1	CV	211
RIL	2	CI	212
Y(3)	3	FLUXV	213
Y(4)	4	FLUXI	214
Y(5)	5	RØDILN	221
Y(6)	6	RØDILA	222
Y(7)	7	RØDVLN	223
Y(8)	8	RØDVLA	224
Y(9)	9	RØD	225
Y(10)	10	EMITV	226
DRVT	101	EMITDA	227
DRILT	102	EMITDN	228
YDØT(3)	103	EMITD	229
YDØT(4)	104	EMITIA	230
YDØT(5)	105	EMITIN	231
YDØT(6)	106	EMITIL	232
YDØT(7)	107	EMITVA	233
YDØT(8)	108	EMITVN	234
YDØT(9)	109	EMITVL	235
YDØT(10)	110	SDISV	236
XLAMI	201	SDISI	237
XLAMV	202	SVØIDV	238
EMIT	203	SVØIDI	239
		SINKI	240
		SINKV	241
		RECØM	242
		SWELL	243
		DELRV	244
		DELRIL	245
		EPSIL	246
		EPSVL	247
		RØVØID	248

VI. Example Problems

VI-A. Example Problem (1)

STAINLESS STEEL UNDER ELECTRON IRRADIATION IN A STEADY IRRADIATION MODE:

The first example shows a steady state application of TRANSWELL. Electron irradiated steel in a steady irradiation mode is chosen because it is an easy system to study. It also shows the agreement between swelling values predicted by the code and those measured experimentally by the choice of suitable input parameters[13].

Details of input parameters are given at the beginning of output, while meanings of abbreviations used are given in the ENTRY TABLE.

Complete output was desired which gives all the time varying quantities and the elements of the Jacobian at each time step. A 100 time steps were used (which is the minimum number of points to generate a plot), and a final accumulated dose of 50 dpa was obtained.

At the end of output, a dump of all CØMMØN blocks is given to aid in evaluating the calculations. The last order used was the first order, the total number of steps taken were 1013, the total number of DIFFUN calls were 1326 and the total number of Jacobian evaluations were 280.

4 different graphs were plotted on the line printer for the removal rates, void radius, interstitial loop radius and swelling. The input for this problem is reported on the next page.

INPUT DATA FOR EXAMPLE (1)

```
@ RUN, 11162,9000151022, 2M
@ XQT TRANS*WELL.SWELL
  $INDATA  XNVO = 6.5D8, XNILO = 6.7D-3, EVØID = 1., ELØØP = 2.8,
   DPA = 50., PRØD = 5.D-3, TEMP = 773., IRESET = 4,
  $END
 ELECTRØN
 STEEL
 STEADY
 NØ STRESS
 NØ CREEP
 FULL
 ENTRY
 TERMINAL
  $PINFØ NGRAPH = 4, NPLØT(1) = 1, NPLØT(2) = 1, NPLØT (3) = 3,
   NPLØT(4) = 1,
   JPLØT(1,1) = 1, JPLØT(2,1) = 2, JPLØT(3,1) = 240, JPLØT(3,2) = 241,
   JPLØT(3,3) = 242, JPLØT(4,1) = 243,
  $END
              ** RV  ** ..
              TIME      ..
              YAXIS     ..
              ** RIL ** ..
              TIME      ..
              YAXIS     ..
              ** RECØM, SINKV AND SINKI ** ..
              TIME      ..
              YAXIS     ..
@ FIN
```

Output of selected time steps follows.

```
**********************************************************************

** TRANSWELL CODE TO FIND MATERIALS REPONCE TO IRRADIATION **  N. GHONIEM .

**********************************************************************
```

(1)STEEL UNDER ELECTRON IRRADIATION IN A STEADY IRRADIATION MODE
*NO STRESS EFFECTS ARE BEING STUDIED *
** NO CREEP BEHAVIOR OF THE METAL IS STUDIED **

(2)MATERIAL CHARACTERISTICS

CASCADE EFFICIENCY	=	.00000+000	
VOID PREEXPONENTIAL	=	.65000+009	
VOID ENERGY (NUCLEATION)	=	.10000+001	EV
INTER-LOOP PREEXPONENTIAL	=	.67000-002	
INTER-LOOP ENERGY (NUCLEATION)	=	.28000+001	EV
INITIAL DISLOCATION DENSITY	=	.10000+009	CM/CM3
INITIAL AVERAGE VOID RADIUS	=	.10000-006	CM
NUMBER OF GAS ATOMS IN A VOID	=	.10000+002	

(3)IRRADIATION CHARACTERISTICS

PRODUCTION RATE	=	.50000-002	DPA/SEC
TOTAL DOSE	=	.50000+002	DPA
IRRADIATION TEMPERATURE	=	.77300+003	KELVIN

(4) STRESS AND PLANNAR ATOM INPUT

MAGNITUDE OF UNIAXIAL STRESS	=	.00000+000
NUMBER OF PLANNAR ATOMS	=	.00000+000

(5)METHOD OF OUTPUT IS FULL

TIME IN SEC=TIME DOSE IN DPA=DOSE

(1) AVERAGE CONCENTRATIONS OF POINT DEFECTS

AVERAGE CONCENTRATION OF VACANCIES	*CV
AVERAGE CONCENTRATION OF INTERSTITIALS	*CI

(2) FLUXES OF VACANICES AND INTERSTITIALS

VACANCY FLUX(DV*CV)	*FLUXV
INTERSTITIAL FLUX(DI*CI)	*FLUXI

(3) LEAKAGE RATES OF FRENKEL PAIRS TO DIFFERENT SINKS

(3-A) LEAKAGE RATES OF VACANCIES TO SINKS

LEAKAGE RATE OF VACANCIES TO TOTAL SINKS	*SINKV
LEAKAGE RATE OF VACANCIES TO DISLOCATIONS	*SDISV
LEAKAGE RATE OF VACANCIESTO VOIDS	*SVOIDV

(3-B) LEAKAGE RATES OF INTERSTITIALS TO SINKS

LEAKAGE RATE OF INTERSTITIALS TO TOTAL SINK	*SINKI
LEAKAGE RATE OF INTERSTITSALS TODISLOCATIONS	*SDISI
LEAKAGE RATE OF INTERSTITIALS TO VOIDS	*SVOIDI

(4) EMISSION RATES OF VACANCIES

EMISSION RATE FROM VACANCY LOOPS	*EMITVL
EMISSION RATE FROM INTERSTITIAL LOOPS	*EMITIL
EMISSION RATE FROM VOIDS	*EMITV
EMISSION RATE FROM DISLOCATIONS	*EMITD
TOTAL EMISSION RATE OF VACANCIES	*EMITT

(5) RATE OF RECOMBINATION OF VACANCIES AND INTERSTITIALS *RECOM

(6) DISLOCATION DENSITIES IN CM**-2

INTERSTITIAL LOOP DISLOCATION DENSITY	*RODIL
VACANCY LOOP DISLOCATION DENSITY	*RODVL
INITIAL DISLOCATION DENSITY	*RODO
TOTAL DISLOCATION DENSITY	*ROD
EQUIVALENT VOID SINK DENSITY	*ROVOID

(7) RADII OF VOIDS AND LOOPS IN ANGSTROMS

VOID RADIUS *RV

VACANCY LOOP RADIUS	*RVL
INTERSTITIAL LOOP RADIUS	*RIL
RATE OF CHANCE OF VOID RADIUS	*DRVT
RATE OF CHANGE OF INTERSTITIAL LOOP RADIUS	*DRILT

(9) NUMBER OF VACANCY LOOPS AND FRACTION OF VACANCIES RETAINED IN THEM

NUMBER OF VACANCY LOOPS	*NVL
FBACTION OF VACANCIES IN LOOPS	*QVL

(10) CHANGES IN INITIAL RADII OF VOID AND INTERSTITIAL LOOP IN ANG.

CHANGE IN LOOP RADIUS(RIL-RILO)	*DELRIL
CHANGE IN VOID RADIUS(RV-RVO)	*DELRV

(11) PERCENT SWELLING *SWELL

IN THE CASE OF PRESENCE OF AN EXTERNAL STRESSTHE LETTER...(N)...WILL BE ATTACHED TO NON-ALLIGNED QUANTIES, AND THE LETTER...(A)...WILL BE ATTACHED TO ALLIGNED QUANTIES.

I	TIME DOSE	RODIL SINKV CV	ROD RECOM CI	EMITV SWELL FLUXV	EMITD XLAMI FLUXI	EMITIL XLAMV DELRV	SDISV EMIT DELRIL	SDISI RV	SVOIDV RIL	SVOIDI DRVT	SINKI DRILT
1	.1000+03 .5000+00	.1643+12 .5248-02 .1496-04	.1644+12 .4072-02 .5481-09	.1939-08 .2074+00 .2900-13	.7168-11 .9640+07 .2722-13	.1005-07 .3508+03 .5056-06	.3186+03 .1199-07 .2007-05	.8817+07 .6056-06	.3212+02 .2116-05	.8231+06 .2910-08	.5284-02 .1970-07

Jacobian Matrix Elements =

	1	2
1	-.6255-02	.0000
2	.0000	-.3945-18

2	.2000+03 .1000+01	.2140+12 .4410-02 .9656-05	.2141+12 .1685-02 .3514-09	.2249-08 .4537+00 .1872-13	.7168-11 .1255+08 .1745-13	.1334-07 .4568+03 .6891-06	.4151+03 .1560-07 .2685-05	.1148+08 .7891-06	.4170+02 .2794-05	.1068+07 .1593-08	.4411-02 .6454-08

	1	2
1	-.2397-02	.0000
2	.0000	-.1968-18

3	.3000+03 .1500+01	.2559+12 .4518-02 .8298-05	.2560+12 .1244-02 .3019-09	.2477-08 .7088+00 .1608-13	.7168-11 .1497+08 .1499-13	.1612-07 .5445+03 .8176-06	.4961+03 .1861-07 .3237-05	.1373+08 .9176-06	.4838+02 .3346-05	.1240+07 .1181-08	.4519-02 .5481-08

	1	2
1	-.1542-02	.0000
2	.0000	-.1501-18

4	.4000+03 .2000+01	.2915+12 .4587-02 .7413-05	.2916+12 .9927-03 .2697-09	.2658-08 .9619+00 .1437-13	.7168-11 .1701+08 .1339-13	.1850-07 .6188+03 .9189-06	.5652+03 .2117-07 .3717-05	.1564+08 .1019-05	.5357+02 .3826-05	.1373+07 .9551-09	.4588-02 .4766-08

	1	2
1	-.1029-02	.0000
2	.0000	-.1104-18

5	.5000+03 .2500+01	.3368+12 .4823-02 .6768-05	.3369+12 .8274-03 .2462-09	.2873-08 .1330+01 .1312-13	.7168-11 .1960+08 .1222-13	.2153-07 .7126+03 .1003-05	.6530+03 .2441-07 .4142-05	.1807+08 .1103-05	.5967+02 .4251-05	.1529+07 .7847-09	.4824-02 .4237-08

	1	2
1	-.7392-03	.0000
2	.0000	-.8407-19

6	.6000+03	.3539+12	.3540+12	.2951-08	.7168-11	.2268-07	.6862+03	.1899+08	.6188+02	.1585+07	.4695-02

	.3000+01	.4694-02 .6275-05	.7111-03 .2282-09	.1483+01 .1216-13	.2057+08 .1133-13	.7481+03 .1078-05	.2564-07 .4543-05	.1178-05	.4652-05	.7030-09	.3836-08

	1	2
1	-.6223-03	.0000
2	.0000	-.7491-19

7	.7000+03 .3500+01	.3961+12 .4899-02 .5866-05	.3962+12 .6213-03 .2133-09	.3139-08 .1893+01 .1137-13	.7168-11 .2297+08 .1059-13	.2551-07 .8351+03 .1143-05	.7680+03 .2865-07 .4895-05	.2125+08 .1243-05	.6713+02 .5004-05	.1720+07 .6070-09	.4900-02 .3507-08

	1	2
1	-.4740-03	.0000
2	.0000	-.5854-19

8	.8000+03 .4000+01	.4097+12 .4786-02 .5545-05	.4098+12 .5552-03 .2016-09	.3197-08 .2035+01 .1075-13	.7168-11 .2374+08 .1001-13	.2642-07 .8631+03 .1203-05	.7944+03 .2962-07 .5236-05	.2198+08 .1303-05	.6877+02 .5345-05	.1762+07 .5610-09	.4787-02 .3255-08

	1	2
1	-.4347-03	.0000
2	.0000	-.5633-19

9	.9000+03 .4500+01	.4327+12 .4792-02 .5264-05	.4328+12 .5002-03 .1914-09	.3295-08 .2287+01 .1020-13	.7168-11 .2504+08 .9503-14	.2796-07 .9104+03 .1256-05	.8389+03 .3126-07 .5543-05	.2321+08 .1356-05	.7150+02 .5652-05	.1832+07 .5129-09	.4792-02 .3036-08

	1	2
1	-.3877-03	.0000
2	.0000	-.5214-19

10	.1000+04 .5000+01	.4553+12 .4814-02 .5032-05	.4554+12 .4571-03 .1829-09	.3390-08 .2549+01 .9753-14	.7168-11 .2632+08 .9083-14	.2948-07 .9567+03 .1305-05	.8826+03 .3287-07 .5832-05	.2442+08 .1405-05	.7413+02 .5941-05	.1899+07 .4735-09	.4815-02 .2860-08

	1	2
1	-.3472-03	.0000
2	.0000	-.4807-19

11	.1100+04 .5500+01	.4728+12 .4795-02 .4831-05	.4729+12 .4212-03 .1756-09	.3462-08 .2761+01 .9363-14	.7168-11 .2731+08 .8719-14	.3065-07 .9927+03 .1350-05	.9166+03 .3412-07 .6106-05	.2536+08 .1450-05	.7613+02 .6215-05	.1951+07 .4430-09	.4796-02 .2709-08

	1	2
1	-.3050-03	.0000

				2 | .0000	| -.4303-19						
12	.1200+04	.4926+12	.4927+12	.3543-08	.7168-11	.3199-07	.9550+03	.2643+08	.7837+02	.2008+07	.4809-02
	.6000+01	.4809-02	.3908-03	.3012+01	.2843+08	.1033+04	.3554-07	.1492-05	.6473-05	.4149-09	.2578-08
		.4653-05	.1691-09	.9019-14	.8398-14	.1392-05	.6364-05				
					1	2					
				1	-.2831-03	.0000					
				2	.0000	-.4104-19					
13	.1300+04	.5135+12	.5136+12	.3627-08	.7168-11	.3339-07	.9955+03	.2755+08	.8069+02	.2067+07	.4839-02
	.6500+01	.4839-02	.3649-03	.3287+01	.2961+08	.1076+04	.3702-07	.1532-05	.6720-05	.3898-09	.2463-08
		.4497-05	.1634-09	.8715-14	.8115-14	.1432-05	.6611-05				
					1	2					
				1	-.2533-03	.0000					
				2	.0000	-.3723-19					
14	.1400+04	.5286+12	.5287+12	.3686-08	.7168-11	.3440-07	.1025+04	.2835+08	.8234+02	.2109+07	.4823-02
	.7000+01	.4822-02	.3424-03	.3493+01	.3046+08	.1107+04	.3810-07	.1570-05	.6958-05	.3703-09	.2362-08
		.4356-05	.1583-09	.8443-14	.7861-14	.1470-05	.6849-05				
					1	2					
				1	-.2358-03	.0000					
				2	.0000	-.3539-19					
15	.1500+04	.5528+12	.5529+12	.3781-08	.7168-11	.3603-07	.1072+04	.2965+08	.8494+02	.2176+07	.4890-02
	.7500+01	.4890-02	.3226-03	.3835+01	.3183+08	.1157+04	.3982-07	.1605-05	.7185-05	.3487-09	.2270-08
		.4228-05	.1536-09	.8195-14	.7630-14	.1505-05	.7076-05				
					1	2					
				1	-.2152-03	.0000					
				2	.0000	-.3272-19					
16	.1600+04	.5699+12	.5700+12	.3847-08	.7168-11	.3718-07	.1105+04	.3057+08	.8676+02	.2223+07	.4901-02
	.8000+01	.4901-02	.3052-03	.4086+01	.3279+08	.1192+04	.4104-07	.1640-05	.7408-05	.3323-09	.2188-08
		.4113-05	.1494-09	.7971-14	.7421-14	.1540-05	.7299-05				
					1	2					
				1	-.2008-03	.0000					
				2	.0000	-.3100-19					
17	.1700+04	.5822+12	.5823+12	.3893-08	.7168-11	.3801-07	.1129+04	.3123+08	.8805+02	.2256+07	.4873-02
	.8500+01	.4873-02	.2895-03	.4271+01	.3348+08	.1217+04	.4191-07	.1672-05	.7622-05	.3191-09	.2113-08
		.4005-05	.1455-09	.7763-14	.7227-14	.1572-05	.7513-05				
					1	2					

:	1	:	-.1900-03	:	.0000	:
:	2	:	.0000	:	-.2986-19	:

18	.1800+04	.6115+12	.6116+12	.4004-08	.7168-11	.3998-07	.1185+04	.3280+08	.9108+02	.2334+07	.4987-02
	.9000+01	.4987-02	.2754-03	.4728+01	.3514+08	.1277+04	.4399-07	.1703-05	.7828-05	.3011-09	.2044-08
		.3907-05	.1419-09	.7572-14	.7049-14	.1603-05	.7719-05				

:	1	:	2	:
:	1	:	-.1733-03	:	.0000	:
:	2	:	.0000	:	-.2738-19	:

19	.1900+04	.5943+12	.5944+12	.3939-08	.7168-11	.3882-07	.1152+04	.3188+08	.8931+02	.2288+07	.4850-02
	.9500+01	.4849-02	.2754-03	.4457+01	.3416+08	.1241+04	.4277-07	.1734-05	.8033-05	.3070-09	.2044-08
		.3816-05	.1387-09	.7397-14	.6886-14	.1634-05	.7924-05				

:	1	:	2	:
:	1	:	-.1733-03	:	.0000	:
:	2	:	.0000	:	-.2738-19	:

20	.2000+04	.6273+12	.6274+12	.4062-08	.7168-11	.4104-07	.1216+04	.3365+08	.9269+02	.2375+07	.4882-02
	.1000+02	.4882-02	.2511-03	.4983+01	.3602+08	.1309+04	.4511-07	.1763-05	.8226-05	.2828-09	.1922-08
		.3731-05	.1355-09	.7231-14	.6731-14	.1663-05	.8117-05				

:	1	:	2	:
:	1	:	-.1599-03	:	.0000	:
:	2	:	.0000	:	-.2618-19	:

21	.2100+04	.6409+12	.6410+12	.4113-08	.7168-11	.4196-07	.1242+04	.3438+08	.9408+02	.2410+07	.4882-02
	.1050+02	.4882-02	.2407-03	.5210+01	.3679+08	.1337+04	.4608-07	.1790-05	.8414-05	.2729-09	.1869-08
		.3653-05	.1327-09	.7080-14	.6590-14	.1690-05	.8305-05				

:	1	:	2	:
:	1	:	-.1521-03	:	.0000	:
:	2	:	.0000	:	-.2520-19	:

22	.2200+04	.6528+12	.6529+12	.4156-08	.7168-11	.4276-07	.1265+04	.3502+08	.9528+02	.2441+07	.4872-02
	.1100+02	.4871-02	.2312-03	.5412+01	.3746+08	.1361+04	.4692-07	.1817-05	.8597-05	.2643-09	.1820-08
		.3580-05	.1301-09	.6939-14	.6459-14	.1717-05	.8488-05				

:	1	:	2	:
:	1	:	-.1477-03	:	.0000	:
:	2	:	.0000	:	-.2488-19	:

23	.2300+04	.6768+12	.6769+12	.4243-08	.7168-11	.4438-07	.1312+04	.3630+08	.9767+02	.2502+07	.4951-02
	.1150+02	.4950-02	.2225-03	.5830+01	.3880+08	.1410+04	.4863-07	.1843-05	.8775-05	.2530-09	.1775-08

				: 1 : -.3318-04 : .0000 :							
				: 2 : .0000 : -.7707-20 :							
92	.9200+04	.1253+13	.1253+13	.6100-08	.7168-11	.8323-07	.2428+04	.6719+08	.1483+03	.3801+07	.4962-02
	.4600+02	.4962-02	.6686-04	.2043+02	.7099+08	.2577+04	.8934-07	.2827-05	.1648-04	.9247-10	.8009-09
		.1926-05	.6990-10	.3733-14	.3471-14	.2727-05	.1637-04				
				: 1 : 2 :							
				: 1 : -.3268-04 : .0000 :							
				: 2 : .0000 : -.7599-20 :							
93	.9300+04	.1258+13	.1258+13	.6116-08	.7168-11	.8359-07	.2438+04	.6747+08	.1488+03	.3812+07	.4960-02
	.4650+02	.4960-02	.6624-04	.2060+02	.7129+08	.2587+04	.8971-07	.2837-05	.1656-04	.9179-10	.7960-09
		.1917-05	.6958-10	.3716-14	.3455-14	.2737-05	.1645-04				
				: 1 : 2 :							
				: 1 : -.3268-04 : .0000 :							
				: 2 : .0000 : -.7599-20 :							
94	.9400+04	.1267+13	.1267+13	.6141-08	.7168-11	.8417-07	.2455+04	.6794+08	.1495+03	.3829+07	.4970-02
	.4700+02	.4970-02	.6563-04	.2089+02	.7177+08	.2605+04	.9032-07	.2846-05	.1664-04	.9096-10	.7911-09
		.1908-05	.6926-10	.3699-14	.3439-14	.2746-05	.1653-04				
				: 1 : 2 :							
				: 1 : -.3199-04 : .0000 :							
				: 2 : .0000 : -.7475-20 :							
95	.9500+04	.1271+13	.1271+13	.6153-08	.7168-11	.8447-07	.2464+04	.6817+08	.1498+03	.3838+07	.4964-02
	.4750+02	.4964-02	.6503-04	.2103+02	.7201+08	.2613+04	.9063-07	.2855-05	.1672-04	.9034-10	.7864-09
		.1900-05	.6894-10	.3682-14	.3424-14	.2755-05	.1661-04				
				: 1 : 2 :							
				: 1 : -.3199-04 : .0000 :							
				: 2 : .0000 : -.7475-20 :							
96	.9600+04	.1279+13	.1280+13	.6178-08	.7168-11	.8504-07	.2480+04	.6863+08	.1505+03	.3855+07	.4974-02
	.4800+02	.4974-02	.6445-04	.2132+02	.7248+08	.2631+04	.9123-07	.2864-05	.1680-04	.8954-10	.7817-09
		.1891-05	.6863-10	.3665-14	.3408-14	.2764-05	.1669-04				
				: 1 : 2 :							
				: 1 : -.3199-04 : .0000 :							
				: 2 : .0000 : -.7475-20 :							
97	.9700+04	.1284+13	.1284+13	.6191-08	.7168-11	.8533-07	.2488+04	.6886+08	.1508+03	.3864+07	.4968-02
	.4850+02	.4968-02	.6387-04	.2146+02	.7272+08	.2639+04	.9153-07	.2873-05	.1688-04	.8895-10	.7771-09
		.1883-05	.6832-10	.3649-14	.3393-14	.2773-05	.1677-04				

	1	2
1	-.3199-04	.0000
2	.0000	-.7475-20

98	.9800+04	.1288+13	.1288+13	.6203-08	.7168-11	.8561-07	.2497+04	.6908+08	.1511+03	.3872+07	.4962-02
	.4900+02	.4962-02	.6331-04	.2161+02	.7295+08	.2648+04	.9182-07	.2882-05	.1696-04	.8837-10	.7725-09
		.1874-05	.6802-10	.3633-14	.3378-14	.2782-05	.1685-04				

	1	2
1	-.3199-04	.0000
2	.0000	-.7475-20

99	.9900+04	.1296+13	.1296+13	.6227-08	.7168-11	.8618-07	.2513+04	.6953+08	.1518+03	.3889+07	.4972-02
	.4950+02	.4972-02	.6276-04	.2189+02	.7342+08	.2665+04	.9241-07	.2890-05	.1703-04	.8760-10	.7680-09
		.1866-05	.6772-10	.3617-14	.3363-14	.2790-05	.1692-04				

	1	2
1	-.3199-04	.0000
2	.0000	-.7475-20

```
100  .1000+05   .1301+13   .1301+13   .6239-08   .7168-11   .8646-07   .2521+04   .6976+08   .1521+03   .3898+07   .4967-02
     .5000+02   .4967-02   .6221-04   .2203+02   .7365+08   .2673+04   .9271-07   .2899-05   .1711-04   .8704-10   .7637-09
                .1858-05   .6743-10   .3601-14   .3348-14   .2799-05   .1700-04
```

	1	2
1	-.3199-04	.0000
2	.0000	-.7475-20

CONTENTS OF COMMON AREA /INTEG/

```
     0    21     0     2     8     3     2     1   242   243
     1     2     0   241     0     0     0     0   240     0
     0     0     0     3     1     1     1     0     0     0
     0     0     0     4   100     1   101     2
```

CONTENTS OF COMMON AREA /NAMES/

ELECTRON STEEL STEADY @@@@@@@@ NO STRES NO CREEP FULL NO ENTRY TERM@@@@

CONTENTS OF COMMON AREA /CONST/

```
     .8617-04   .3142+01   .8300-22   .1000+15   .1000+03   .1000+03   .1000+02   .1000+02   .1000+02   .1000+01
.0000
```

CONTENTS OF COMMON AREA /IRRAD/

```
     .5000-02   .5000+02   .7730+03
.5000+02
```

CONTENTS OF COMMON AREA /ANNEAL/

```
     .0000      .0000      .0000
```

CONTENTS OF COMMON AREA /PULSE/

```
     .0000      .0000      .1000-09   .1000-04
```

CONTENTS OF COMMON AREA /TEMP/

```
     .1938-08   .4966-04   .3698-10   .8316-26   .2152+16   .1208+17   .6162-01   .2227-05   .4966+12   .1501+02
```

CONTENTS OF COMMON AREA /INITL/

```
     .0000      .1003+05   .1010+05   .1000-06   .1090-06   .0000      .0000      .0000      .0000      .0000
     .0000      .0000      .0000      .7202+02   .2227-15
```

CONTENTS OF COMMON AREA /MAT/

```
     .0000      .5000-02   .6500+09   .1000+01   .6700-02   .2800+01   .1000+09   .8373+10   .1500-06   .1090-06
     .1000-06   .1000+02
```

CONTENTS OF COMMON AREA /BKDAT/

```
     .1600+01   .4000+01   .5800+01   .1000-02   .1300+01   .2000+00   .2000-07   .1250+16   .1000+01   .1080+01
     .8000-23   .9400+13   .4000+12   .3000+00
```

CONTENTS OF COMMON AREA /STRESS/

```
     .0000      .0000      .0000      .0000      .5000-07   .0000      .0000      .0000
```

CONTENTS OF COMMON AREA /BURG/

```
     .1414-20   .4000-15   .1000+01   .4700+00   .0000      .0000      .0000      .0000      .6667+08   .3333+08
     .6283+01   .1257+02   .4189+03   .3000-14
```

CONTENTS OF COMMON AREA /CONC/

```
     .1858-05   .6743-10   .3601-14   .3348-14
```

CONTENTS OF COMMON AREA /OUTCON/

```
     .7365+08   .2673+04   .9271-07
```

CONTENTS OF COMMON AREA /VECTOR/

```
     .2899-05   .1711-04   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
```

CONTENTS OF COMMON AREA /DOT/

```
     .8704-10   .7637-09   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
```

CONTENTS OF COMMON AREA /OUT/

```
     .1301+13   .0000      .0000      .0000      .1301+13   .6239-08   .0000      .0000      .7168-11   .0000
     .0000      .8646-07   .0000      .0000      .0000      .2521+04   .6976+08   .1521+03   .3898+07   .4967-02
     .4967-02   .6221-04   .2203+02   .2799-05   .1700-04
```

CONTENTS OF COMMON AREA /GEAR9/

```
     .7202+02        1     1013     1326      280
```

** RV **

Figure 3

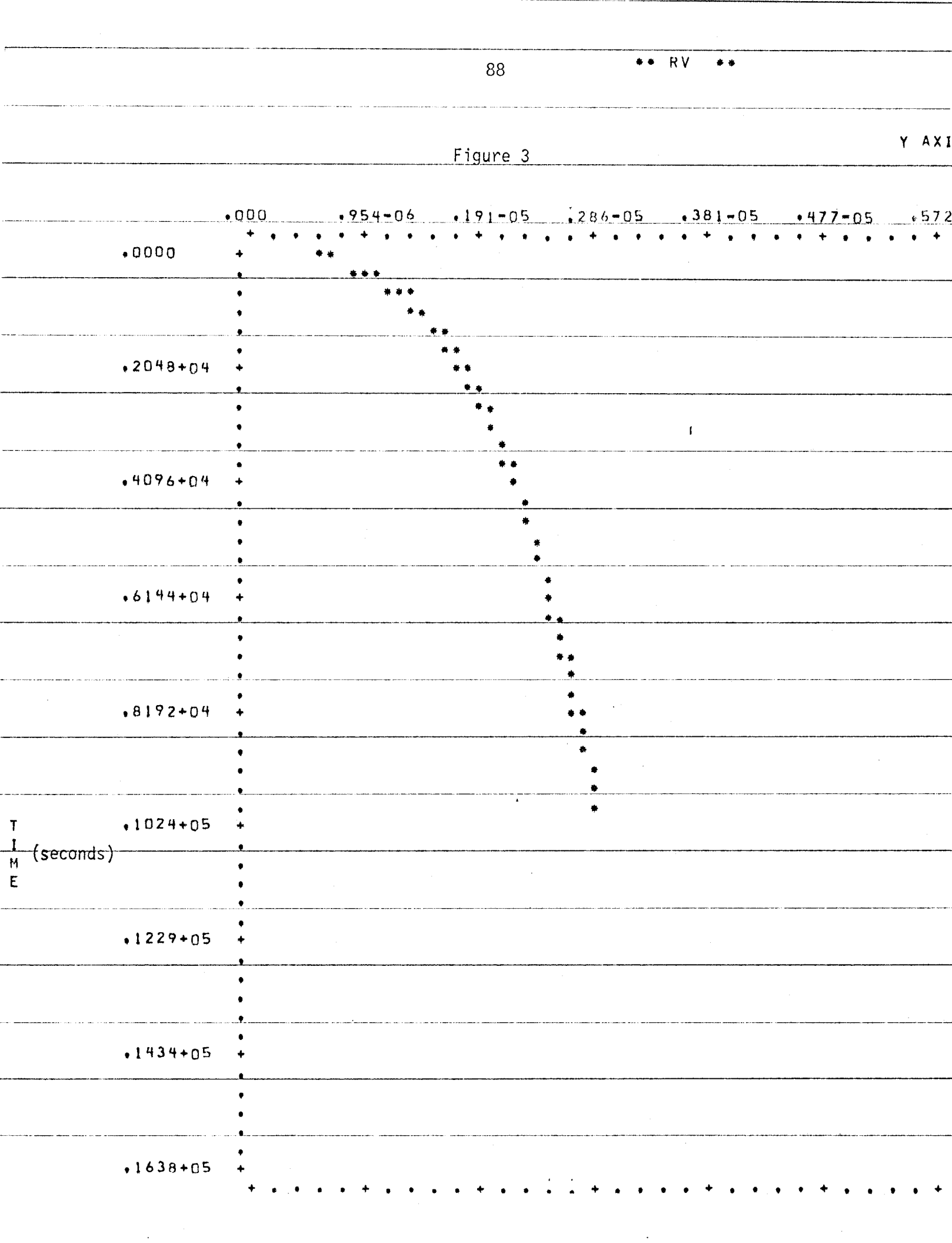

Y AXI
.000
.954-06
.191-05
.286-05
.381-05
.477-05
.572
.0000
.2048+04
.4096+04
.6144+04
.8192+04
.1024+05
.1229+05
.1434+05
.1638+05
TIME (seconds)

Figure 4

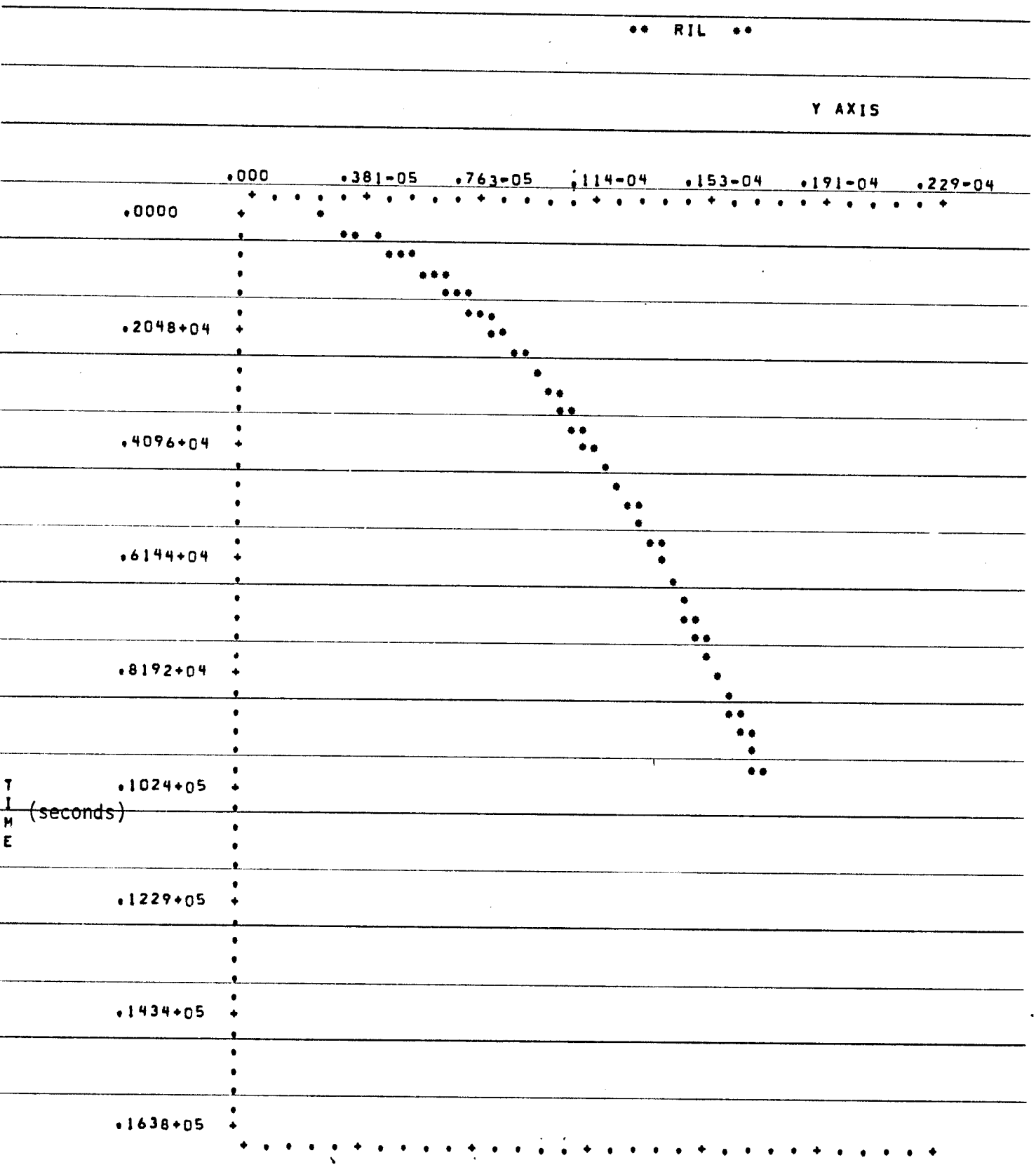

** RIL **
Y AXIS
.000
.381-05
.763-05
.114-04
.153-04
.191-04
.229-04
.0000
.2048+04
.4096+04
.6144+04
.8192+04
.1024+05
.1229+05
.1434+05
.1638+05
TIME (seconds)

Figure 5

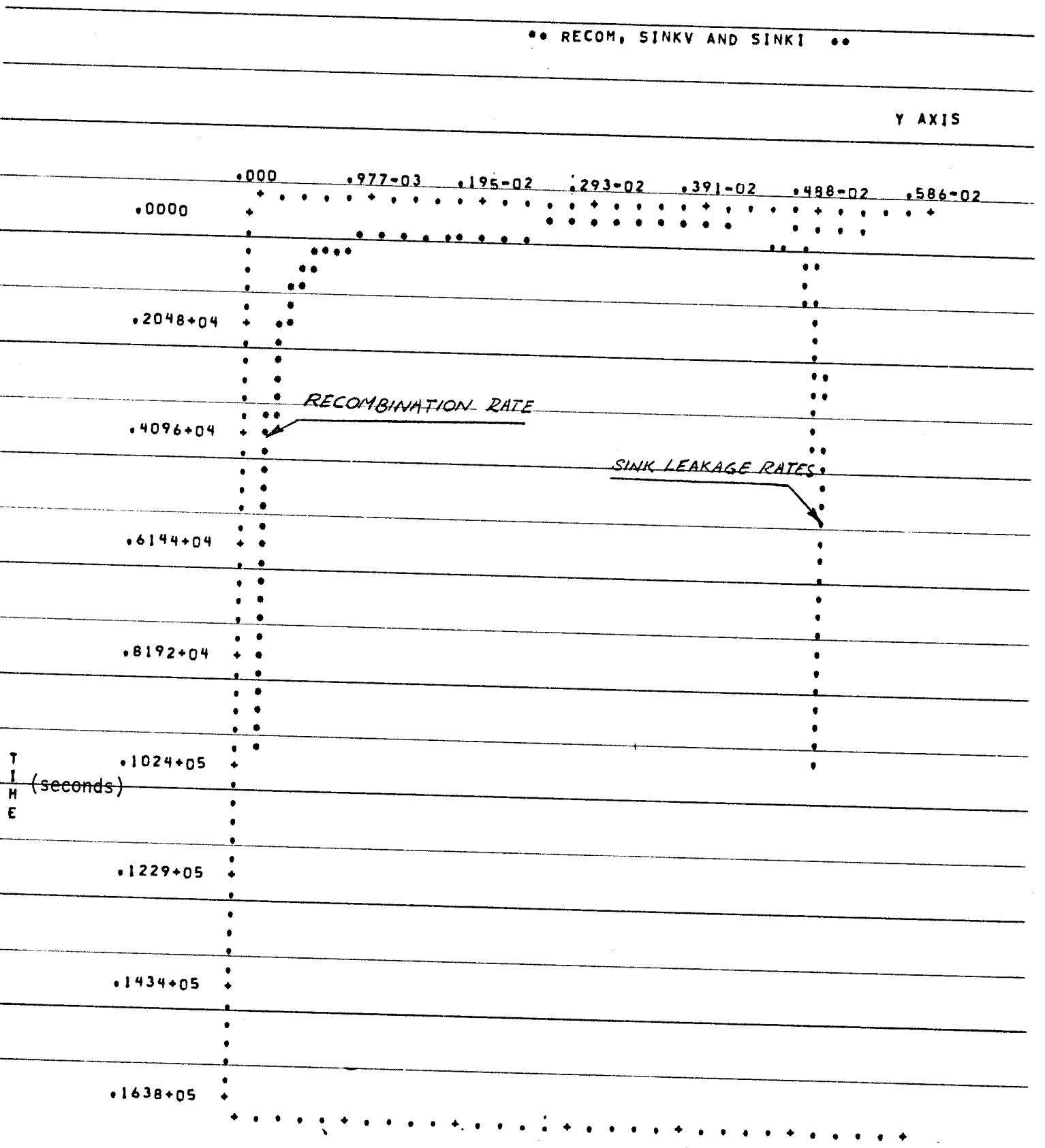
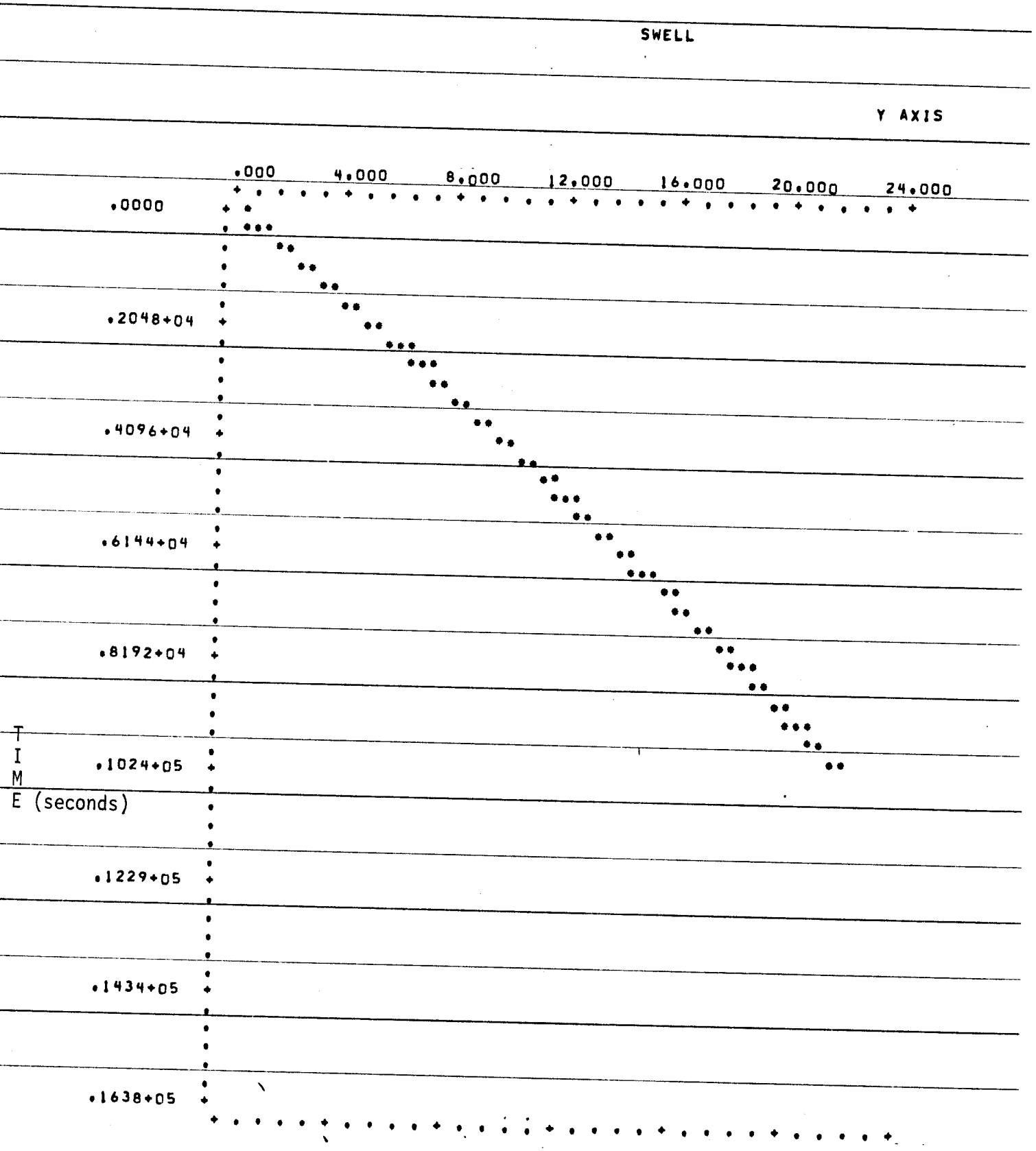

** RECOM, SINKV AND SINKI **
Y AXIS
.000
.977-03
.195-02
.293-02
.391-02
.488-02
.586-02
.0000
.2048+04
.4096+04
.6144+04
.8192+04
.1024+05
.1229+05
.1434+05
.1638+05
RECOMBINATION RATE
SINK LEAKAGE RATES
TIME (seconds)

Figure 6


SWELL
Y AXIS
.000
4.000
8.000
12.000
16.000
20.000
24.000
.0000
.2048+04
.4096+04
.6144+04
.8192+04
.1024+05
.1229+05
.1434+05
.1638+05
TIME (seconds)

EXAMPLE PROBLEM (2)

STAINLESS STEEL UNDER NEUTRON IRRADIATION IN A PULSED IRRADIATION MODE

This example shows an application of the code to pulsed irradiation. A damage pulse of 10^{-8} seconds pulse width and 10 dpa/sec. damage rate is analyzed. The analysis is requested with the following scheme:

1. Five time steps inside the pulse at equal intervals. Therefore, we use FPL1 = 5.D0.
2. Logarithmic steps from time pulse ends to $\leq \frac{1}{2}$ of total pulse period (50 seconds here). Base 10 is chosen for the log scale. Hence we use FPL2 = default and DIVP = default.
3. Equal time steps from t = 10 seconds to t = 100 seconds with step size = 1 second. So use FPL3 = 100.D0.
4. Output is required in the form of plots only for three different temperatures: 400°C, 500°C, 600°C.
5. Changes in void radius and interstitial loop radius as a function of time are overlayed on one graph.
6. Vacancy and interstitial concentrations as a function of time are overlayed on another graph. This gives us 6 graphs for a certain void radius.
7. Steps 4-6 are implemented for initial void radii: 100 Å, 40 Å and a 10 Å to give a total of 18 graphs.

The reader finds the input for this example in the next page. Notice how IRESET is used in different situations, and that graphs are not smooth enough because of the small number of points used for plotting.

INPUT DATA FOR EXAMPLE (2)

```
@RUN, 11162, 9000151622,4M
@GSP,X
 PLØTTER PEN/LIQ
@XQT TRANS*SWELL.SWELL
 $INDATA XNVO = 3.15 D11, XNILO = 1.3 D-4, EVØID = .625, ELØØP = 2.8,
    PRØD = 10., DPA = 1.D-7, CASC = .044,
     FPL1 = 5., FPL3 = 100.,
     TP = 100., PW = 1.D-8, NTØT = 1,
     TEMP = 673., RVO = 100.D-8,
 $END
IØN
STEEL
PULSED
EXACT
NØ STRESS
NØ CREEP
PLØT
NØ ENTRY
PLØTTER
 $PINFØ NGRAPH = 2, NPLØT(1) = 2, NPLØT(2) = 2,
    IXSCAL(1,1) = 6, IXSCAL(1,2) = -1, IYSCAL(1,2) = -1,
    ISYREF(1,1) = 2, ISYREF(1,2) = 2, REFX(1,1) = 1.D-10,
    REFX(1,2) = 1.D-10,
    JPLØT(1,1) = 244, JPLØT(1,2) = 245,
    IXSCAL(2,1) = 6, IXSCAL(2,2) = 6, IYSCAL(2,1) = 6, IYSCAL(2,2) = 6,
    REFX(2,1) = 1.D-10, REFX(2,2) = 1.D-10, REFY(2,1) = 1.D-14,
```

```
      REFY(2,2) = 1.D-14,
      JPLØT(2,1) = 5, JPLØT(2,2) = 6,
  $END
CHANGES IN VØID AND LØØP RADII  $$
TIME (SEC.)  $$
CHANGE IN RADIUS (CM)  $$
PØINT DEFECT CØNC. IN AN IRRADIATIØN PULSE  $$
TIME (SEC.)  $$
CØNCENTRATION (AT./AT.)  $$
  $INDATA  TEMP = 773., IRESET = 1, $END
  $INDATA  TEMP = 873., $END
  $INDATA  TEMP = 673., RVO = 40.D-8, $END
  $INDATA  TEMP = 773., $END
  $INDATA  TEMP = 873., $END
  $INDATA  TEMP = 673., RVO = 10.D-8, $END
  $INDATA  TEMP = 773., $END
  $INDATA  TEMP = 873., $END
@FIN
```

The output computer plots are shown in the following pages.

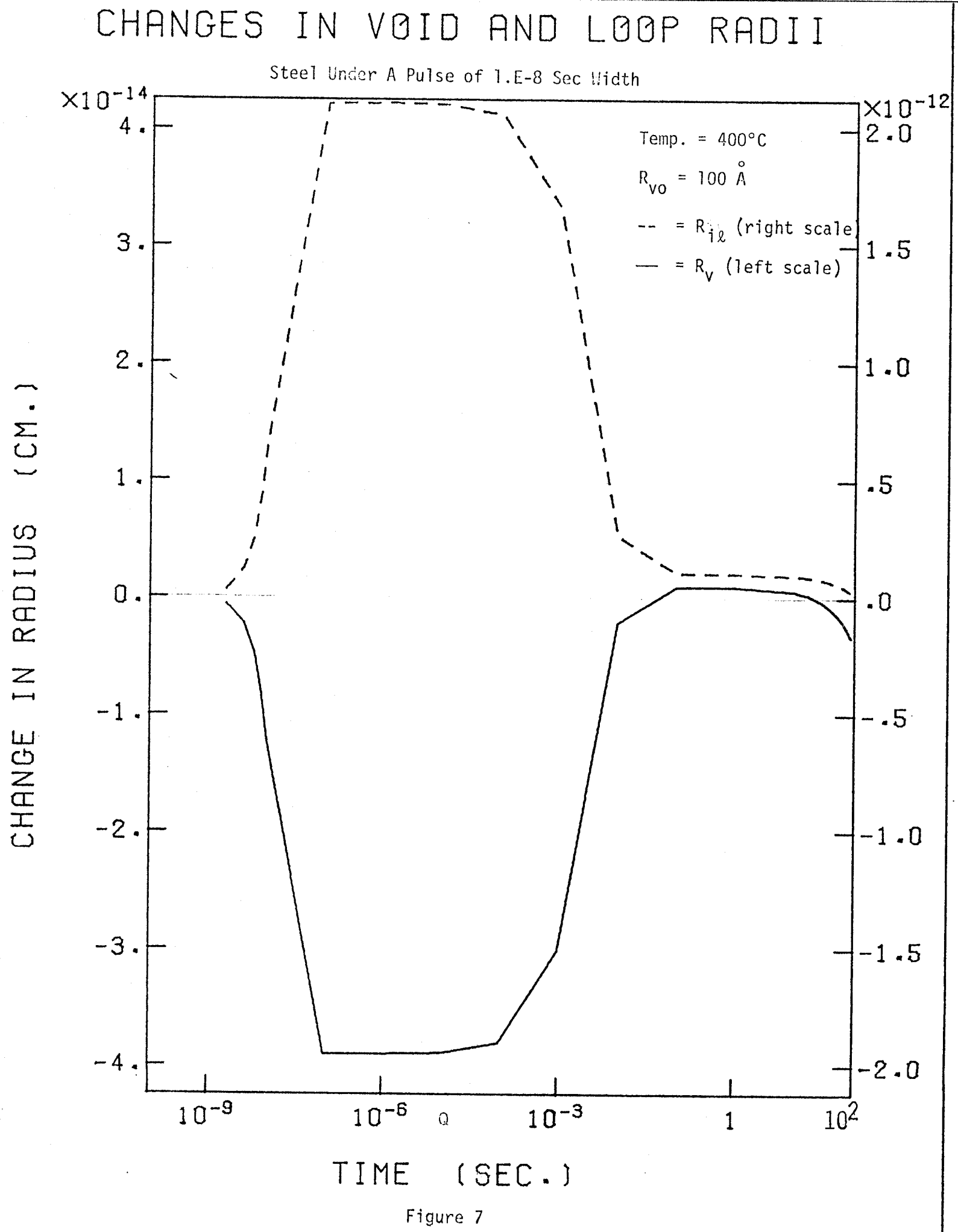

CHANGES IN VOID AND LOOP RADII
Steel Under A Pulse of 1.E-8 Sec Width
X10-14
4.
3.
2.
1.
0.
-1.
-2.
-3.
-4.
X10-12
2.0
1.5
1.0
.5
.0
-.5
-1.0
-1.5
-2.0
Temp. = 400°C
Rvo = 100 Å
-- = Ril (right scale)
— = Rv (left scale)
CHANGE IN RADIUS (CM.)
10-9
10-6
10-3
1
102
TIME (SEC.)

Figure 7

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width

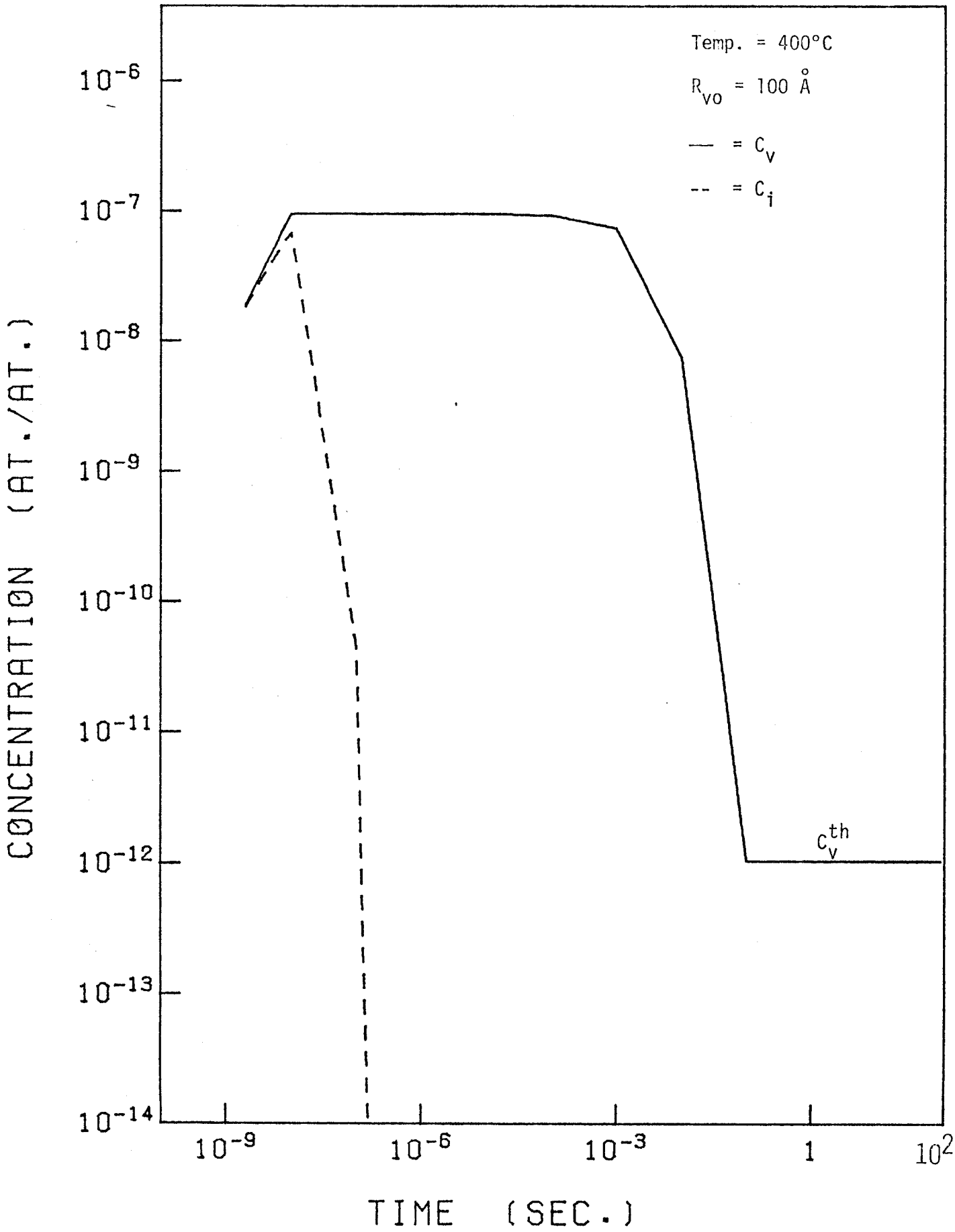


Figure 8

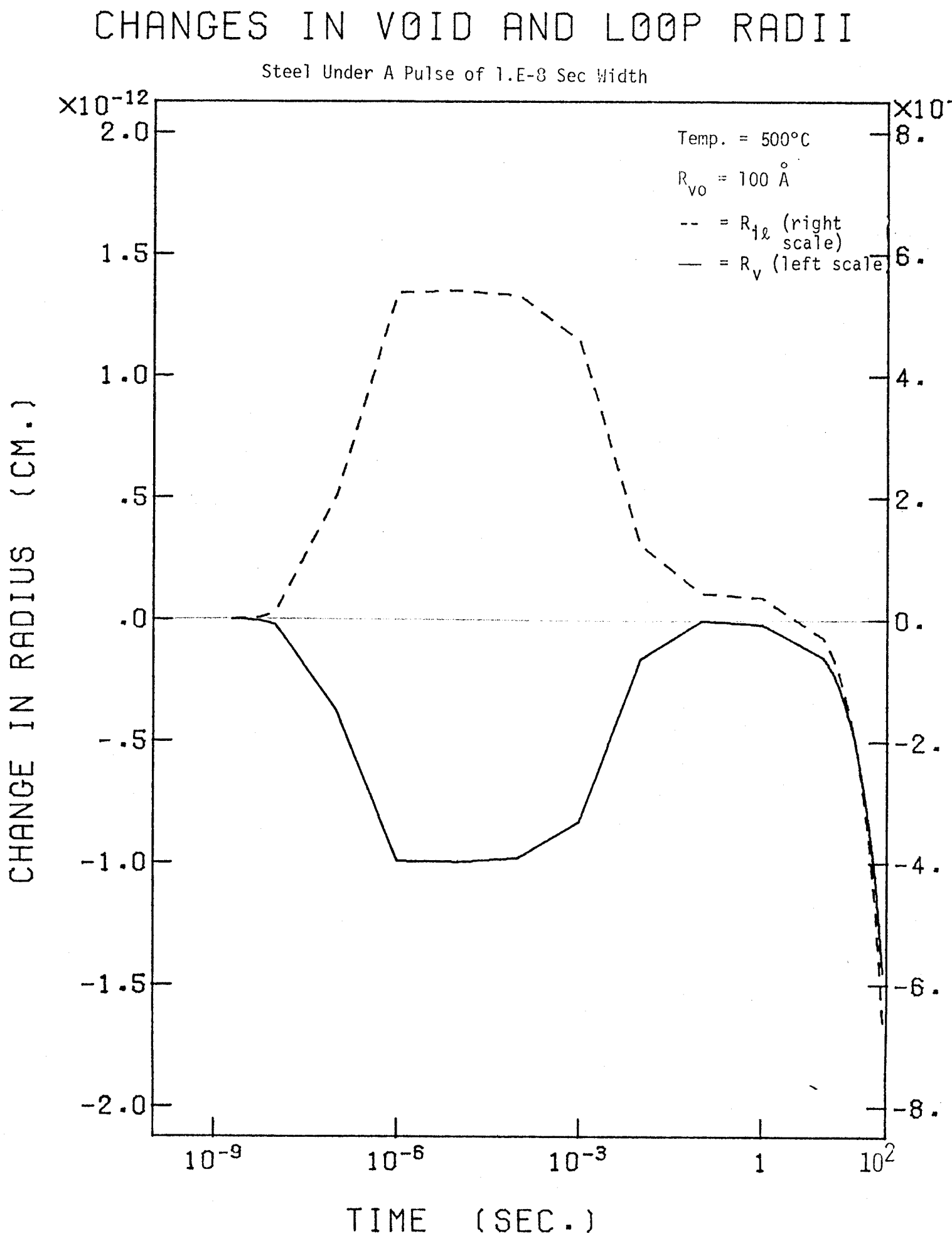

CHANGES IN VOID AND LOOP RADII
Steel Under A Pulse of 1.E-8 Sec Width
Temp. = 500°C
R_{vo} = 100 Å
-- = $R_{i\ell}$ (right scale)
— = R_v (left scale)
CHANGE IN RADIUS (CM.)
TIME (SEC.)
X10⁻¹²
X10
2.0
1.5
1.0
.5
.0
-.5
-1.0
-1.5
-2.0
8.
6.
4.
2.
0.
-2.
-4.
-6.
-8.
10⁻⁹
10⁻⁶
10⁻³
1
10²

Figure 9

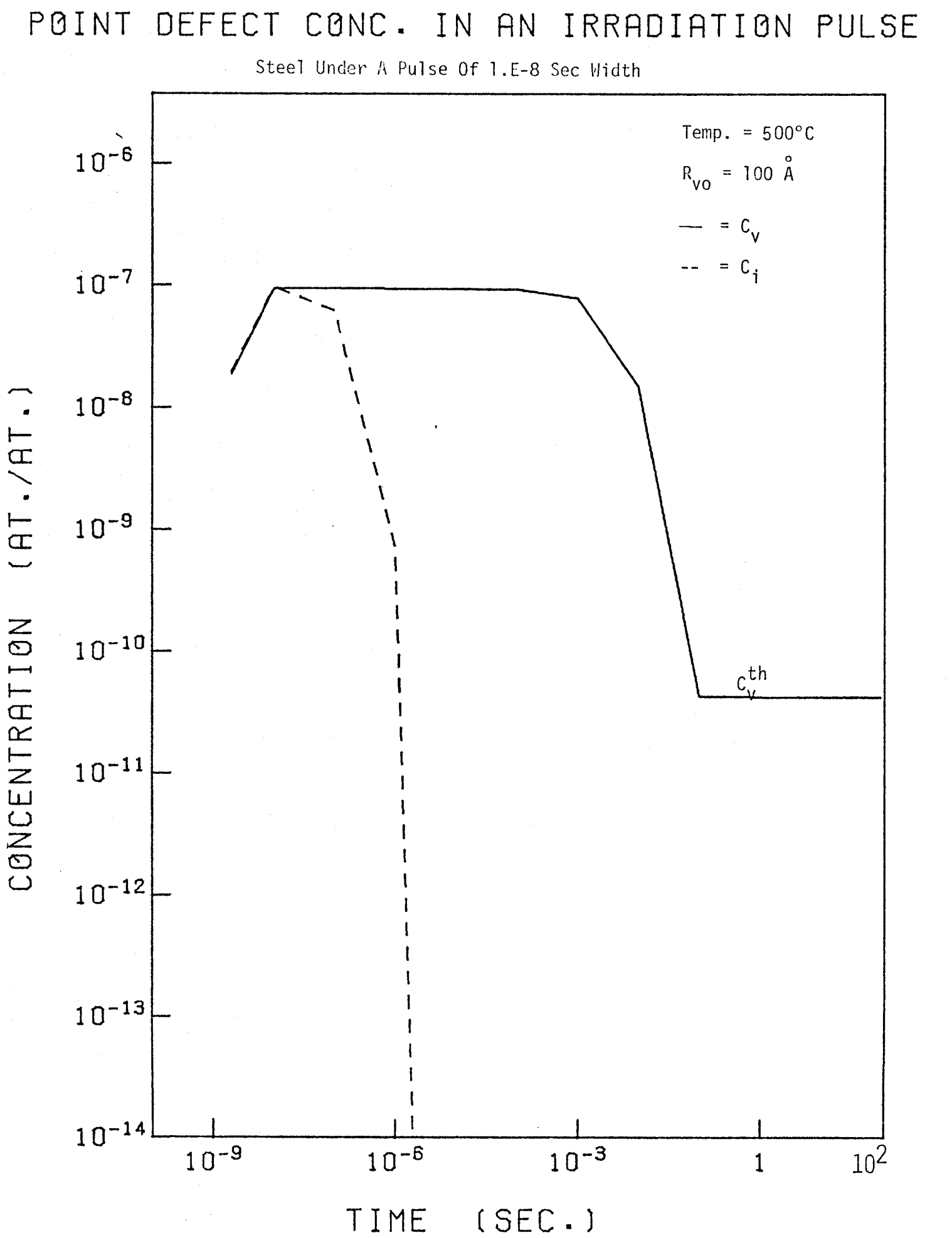

POINT DEFECT CONC. IN AN IRRADIATION PULSE
Steel Under A Pulse Of 1.E-8 Sec Width
Temp. = 500°C
R_{vo} = 100 Å
— = C_v
-- = C_i
C_v^{th}
CONCENTRATION (AT./AT.)
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-9}
10^{-6}
10^{-3}
1
10^{2}
TIME (SEC.)

Figure 10

CHANGES IN VOID AND LOOP RADII

Steel Under A Pulse Of 1.E-8 Sec Width

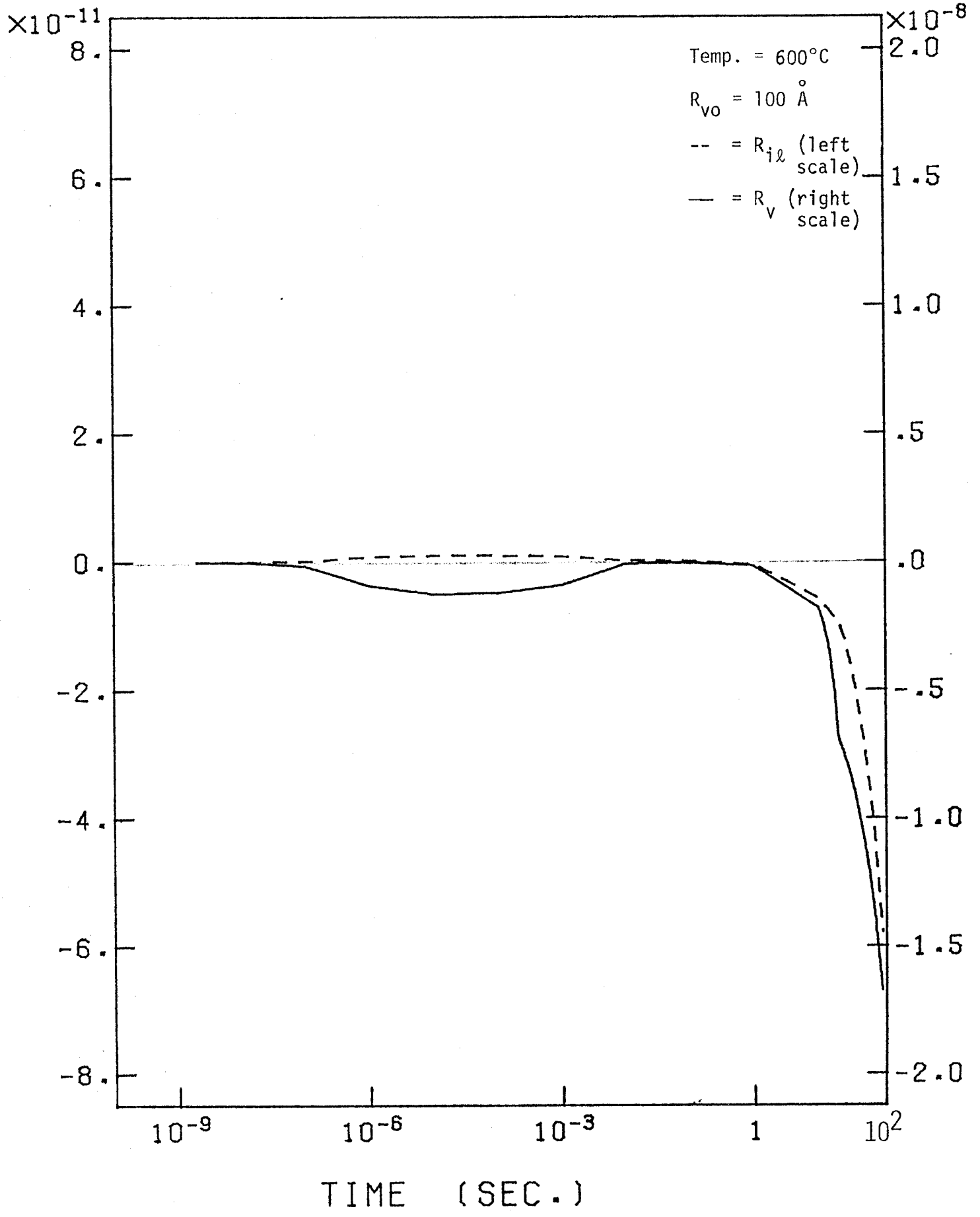


Figure 11

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width

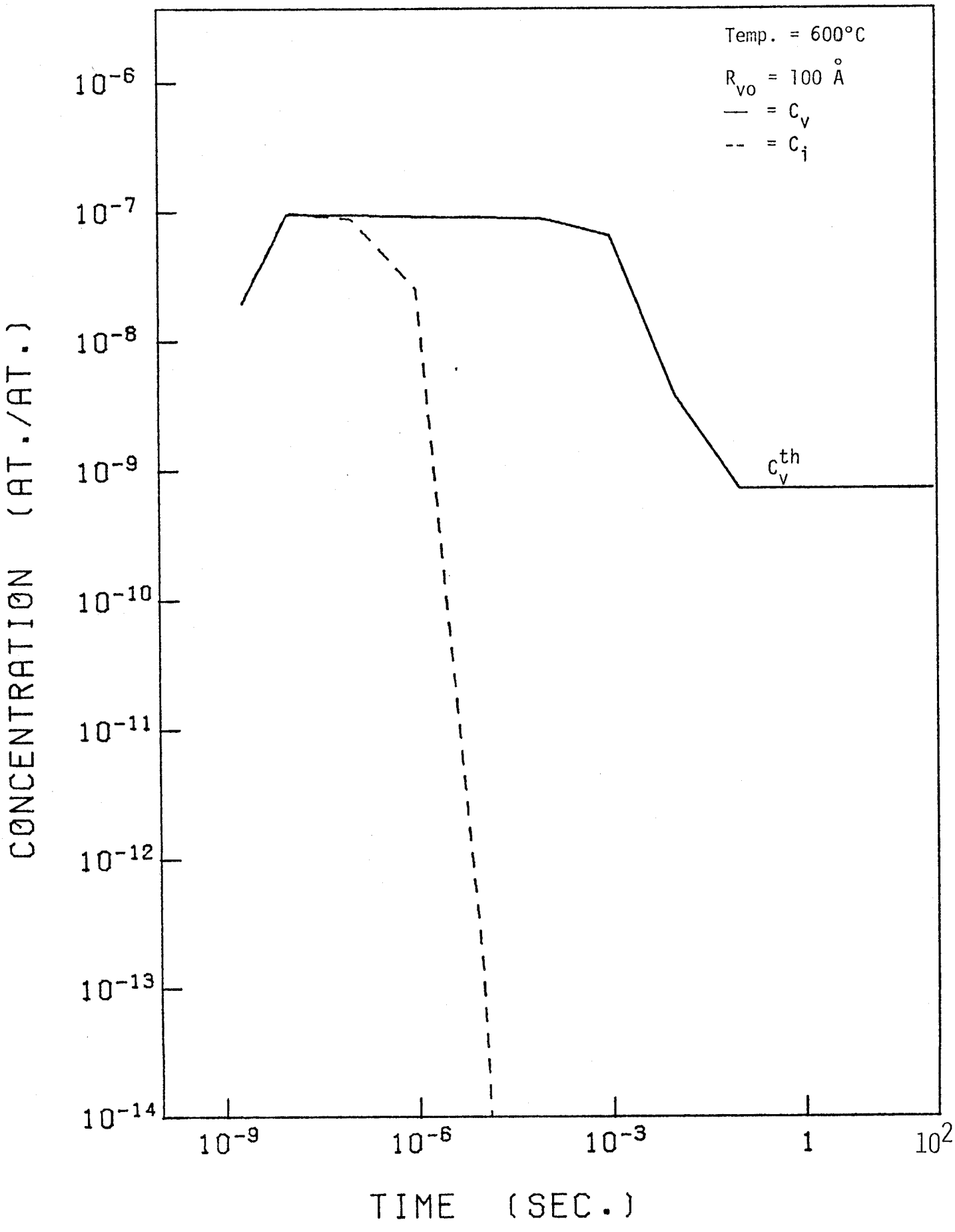


Figure 12

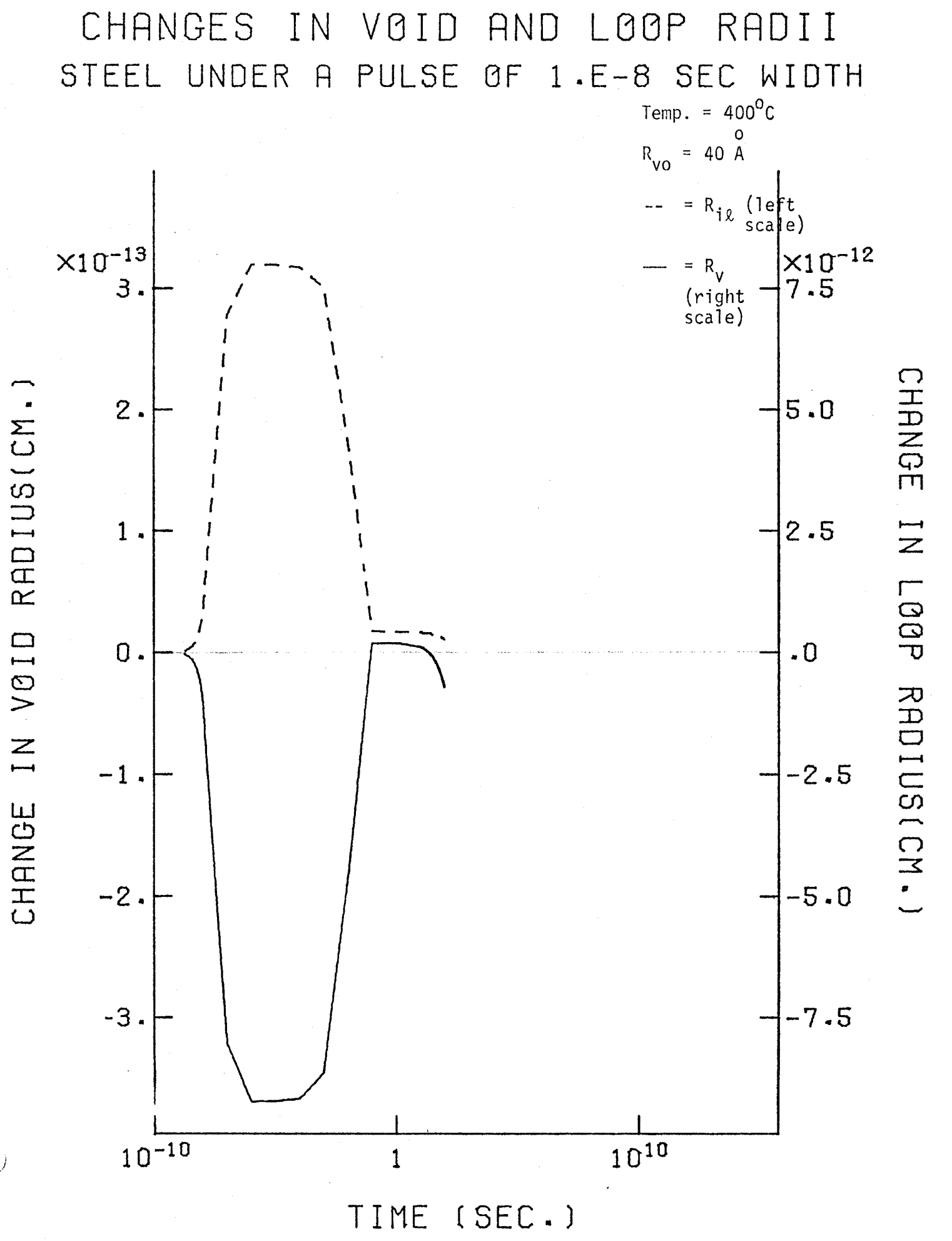

CHANGES IN VOID AND LOOP RADII
STEEL UNDER A PULSE OF 1.E-8 SEC WIDTH
Temp. = 400°C
R_{vo} = 40 Å
-- = $R_{i\ell}$ (left scale)
— = R_v (right scale)
X10^-13
3.
2.
1.
0.
-1.
-2.
-3.
X10^-12
7.5
5.0
2.5
.0
-2.5
-5.0
-7.5
CHANGE IN VOID RADIUS(CM.)
CHANGE IN LOOP RADIUS(CM.)
10^-10
1
10^10
TIME (SEC.)

Figure 13

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width

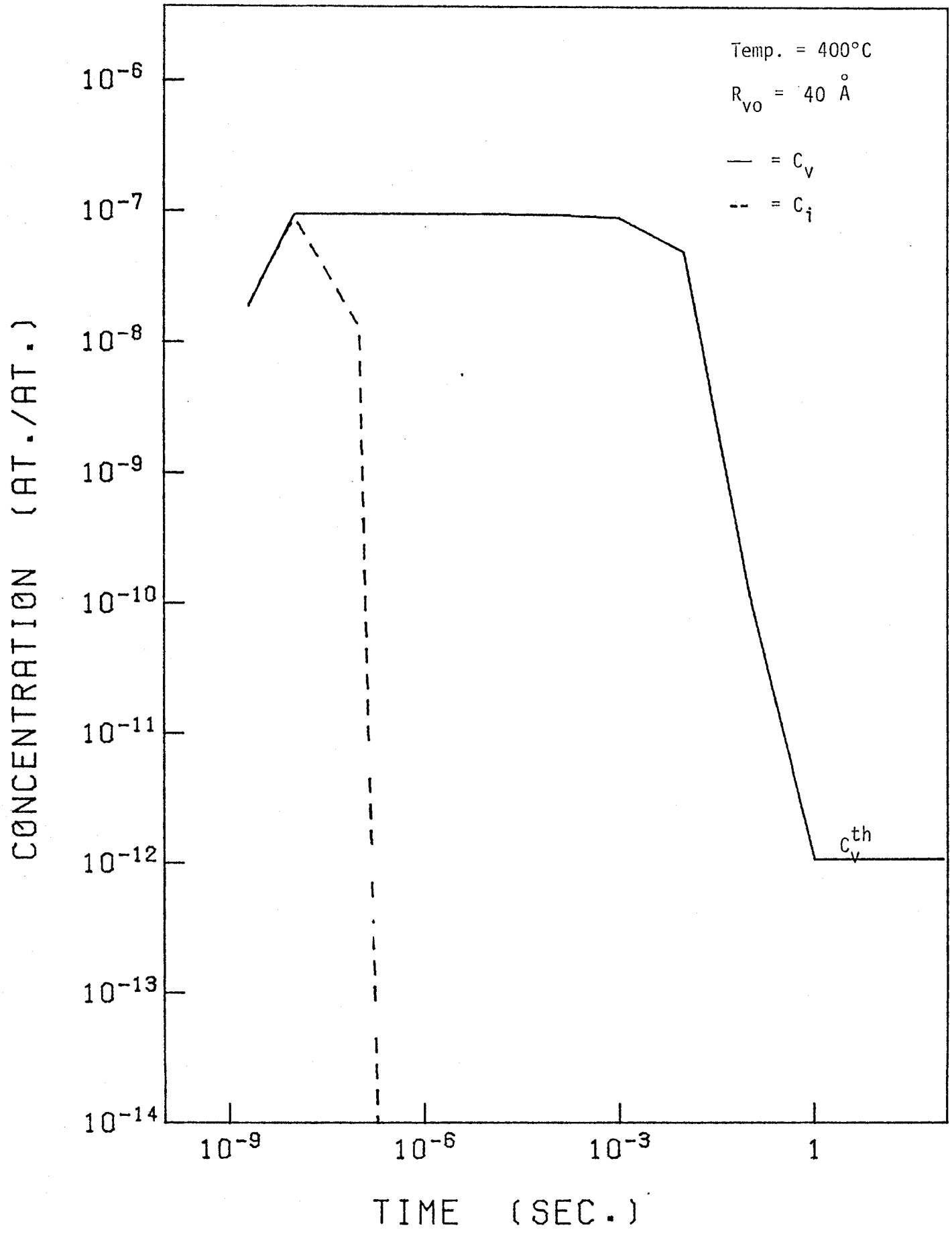


Figure 14

CHANGES IN VOID AND LOOP RADII

STEEL UNDER A PULSE OF 1.E-8 SEC WIDTH

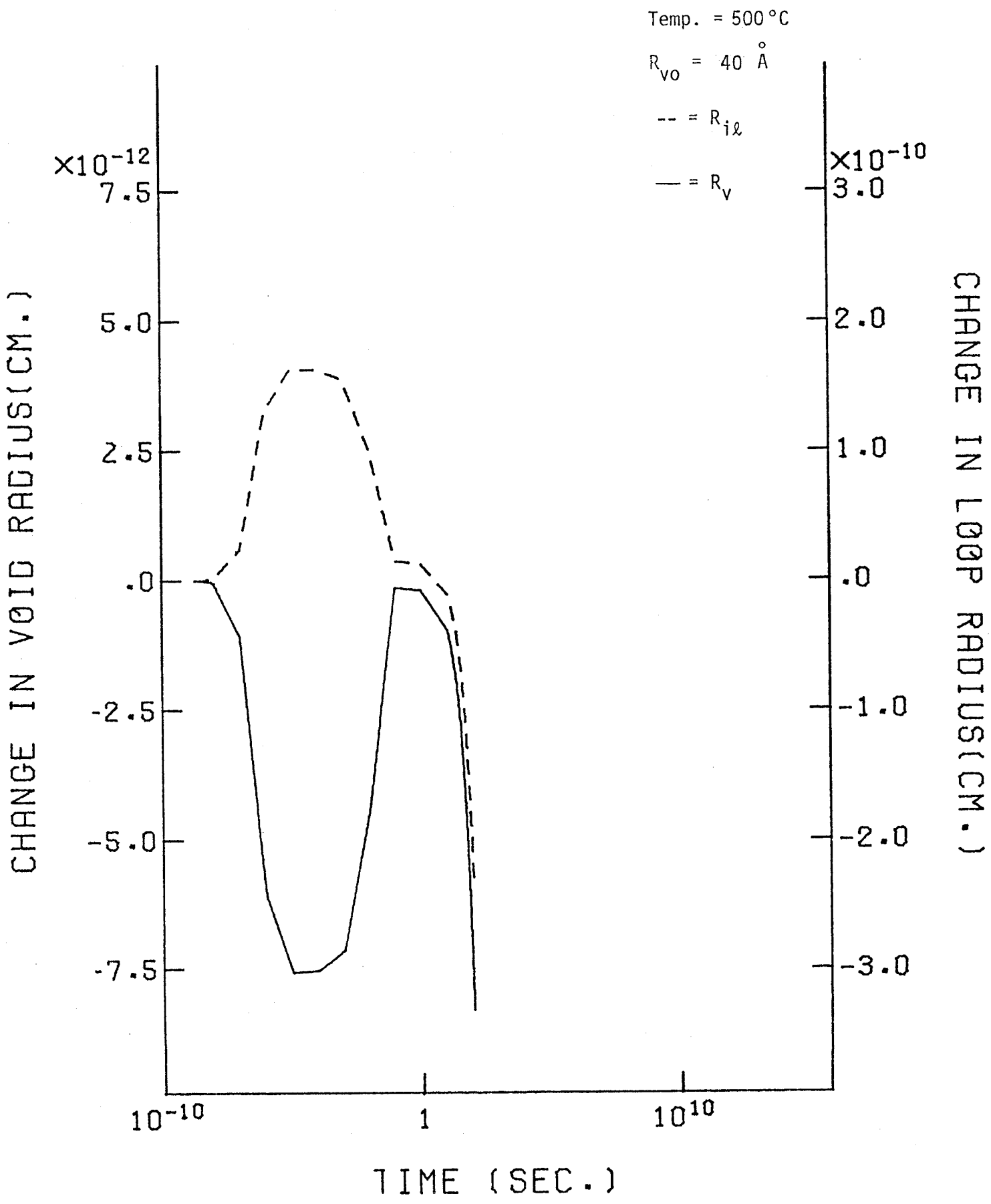


Figure 15

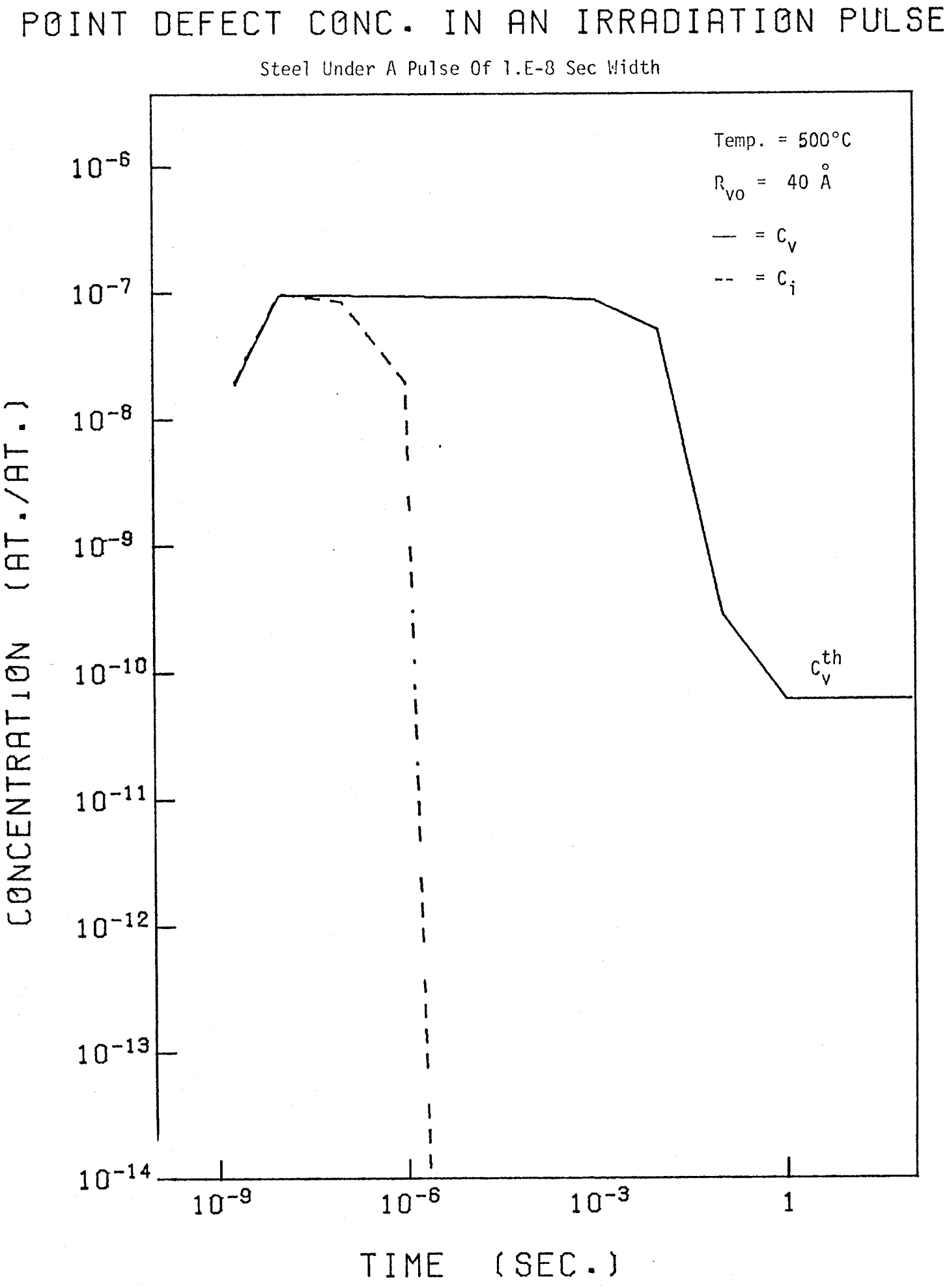

POINT DEFECT CONC. IN AN IRRADIATION PULSE
Steel Under A Pulse Of 1.E-8 Sec Width
Temp. = 500°C
R_{vo} = 40 Å
— = C_v
-- = C_i
C_v^{th}
CONCENTRATION (AT./AT.)
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-9}
10^{-6}
10^{-3}
1
TIME (SEC.)

Figure 16

CHANGES IN VOID AND LOOP RADII
STEEL UNDER A PULSE OF 1.E-8 SEC WIDTH

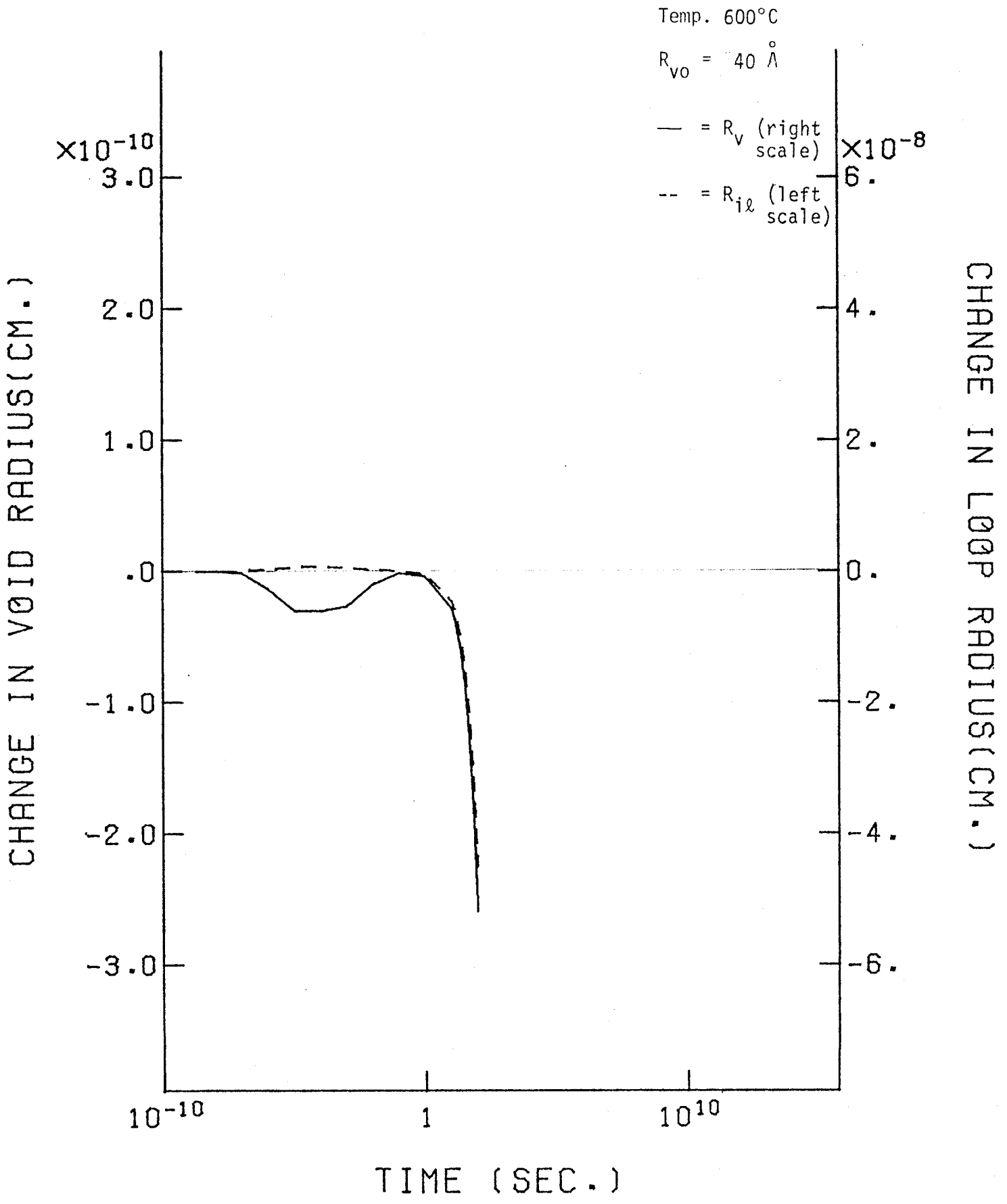


Figure 17

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width

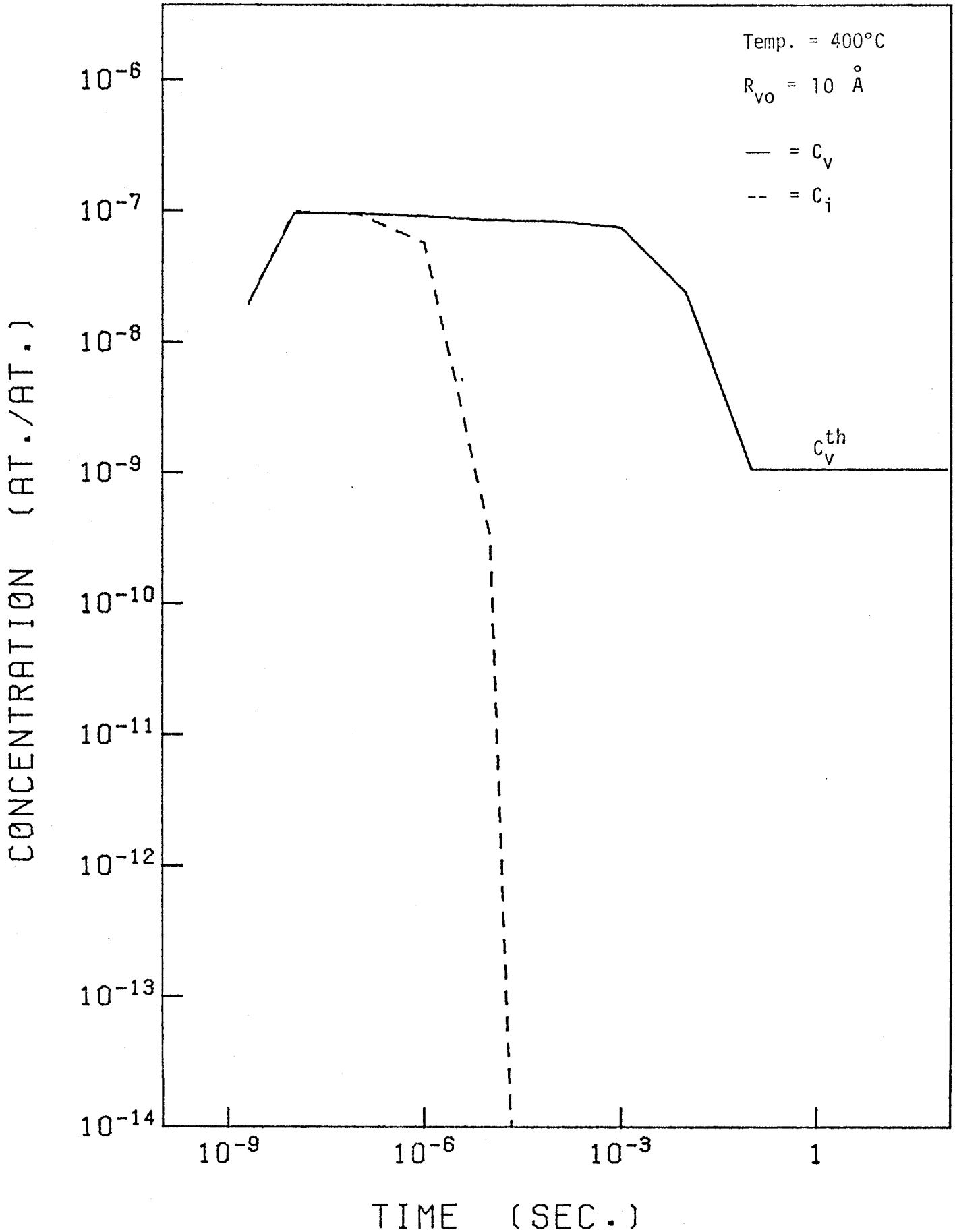


Figure 18

CHANGES IN VOID AND LOOP RADII
STEEL UNDER A PULSE OF 1.E-8 SEC WIDTH

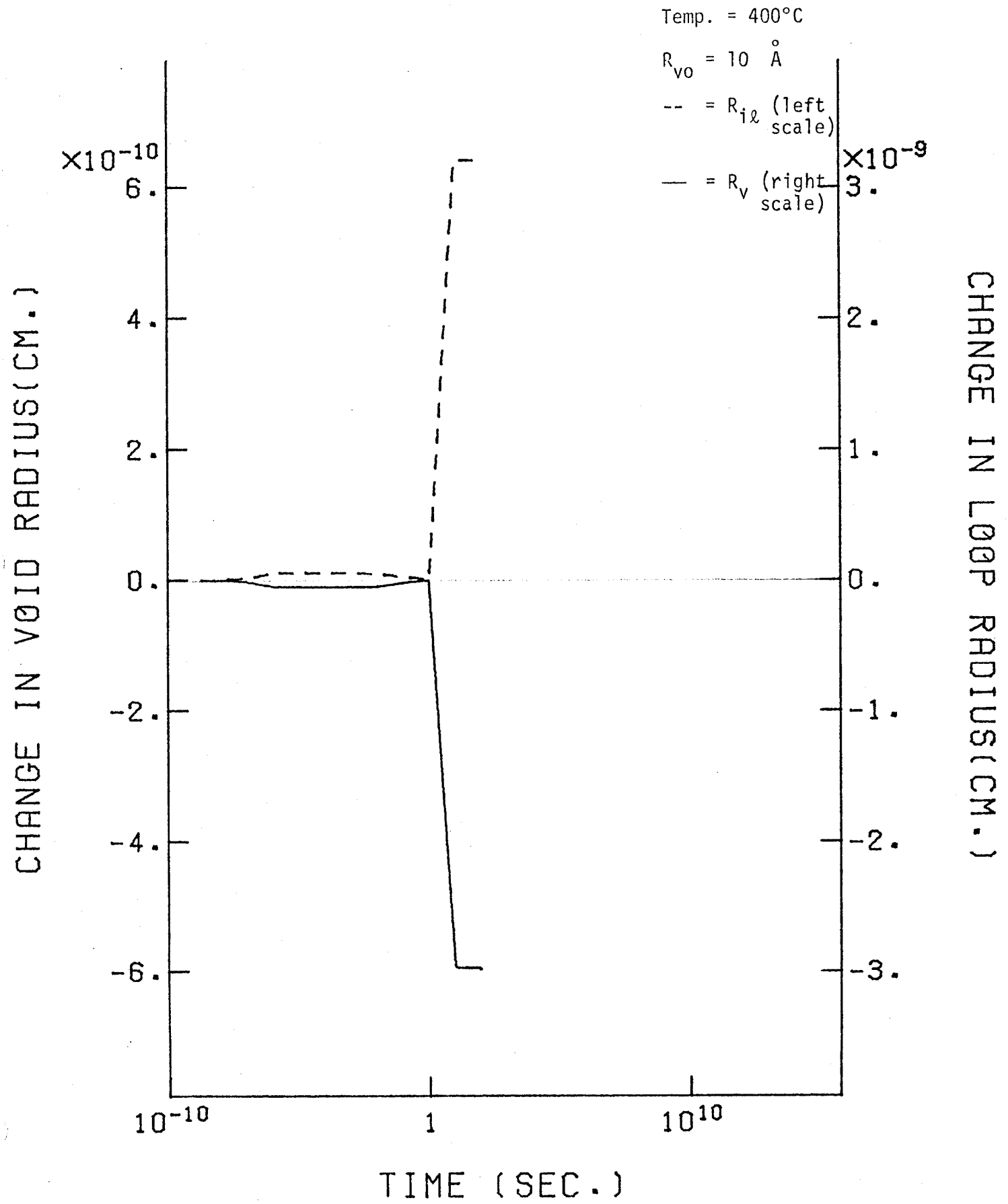


Figure 19

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width

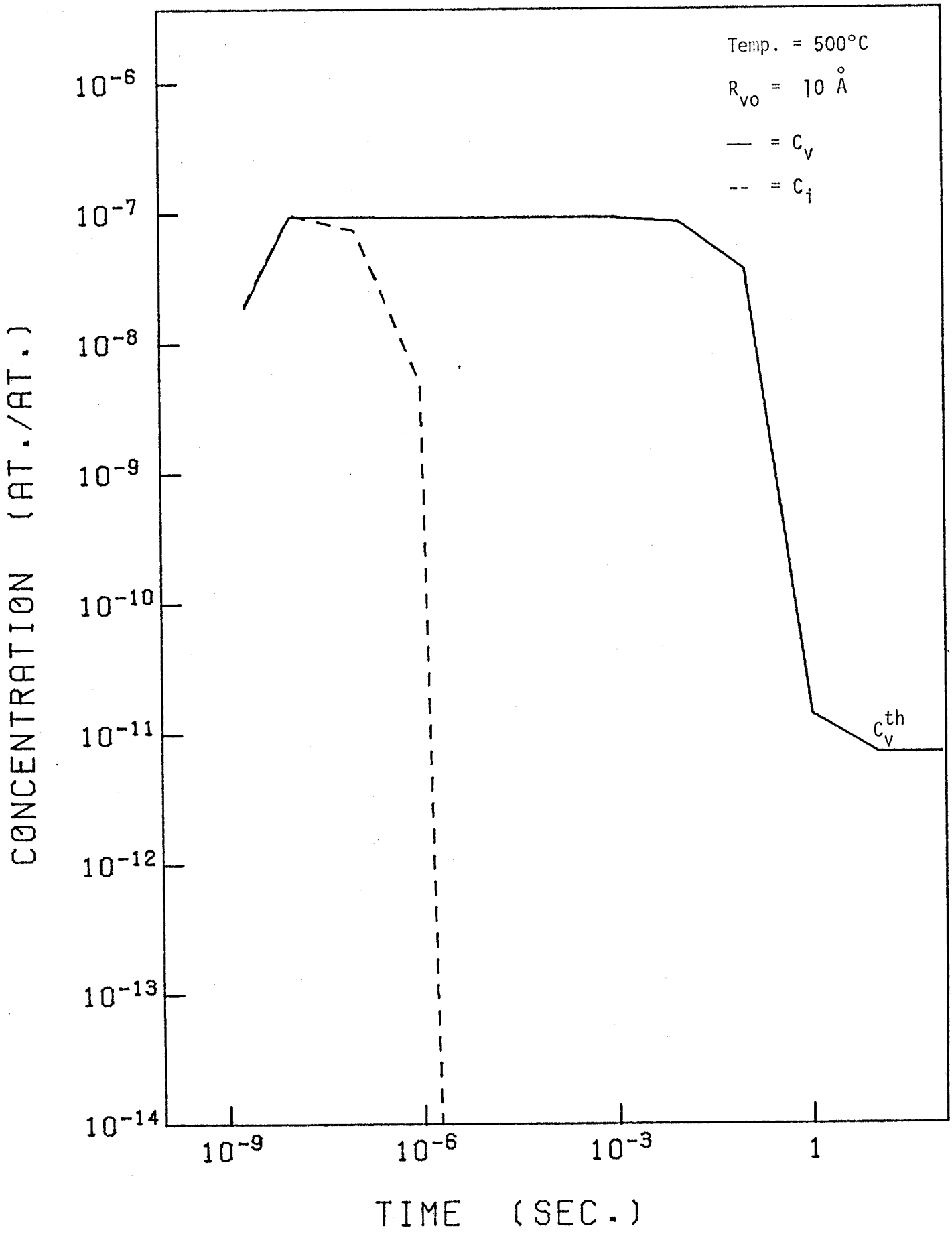


Figure 20

CHANGES IN VOID AND LOOP RADII
STEEL UNDER A PULSE OF 1.E-8 SEC WIDTH

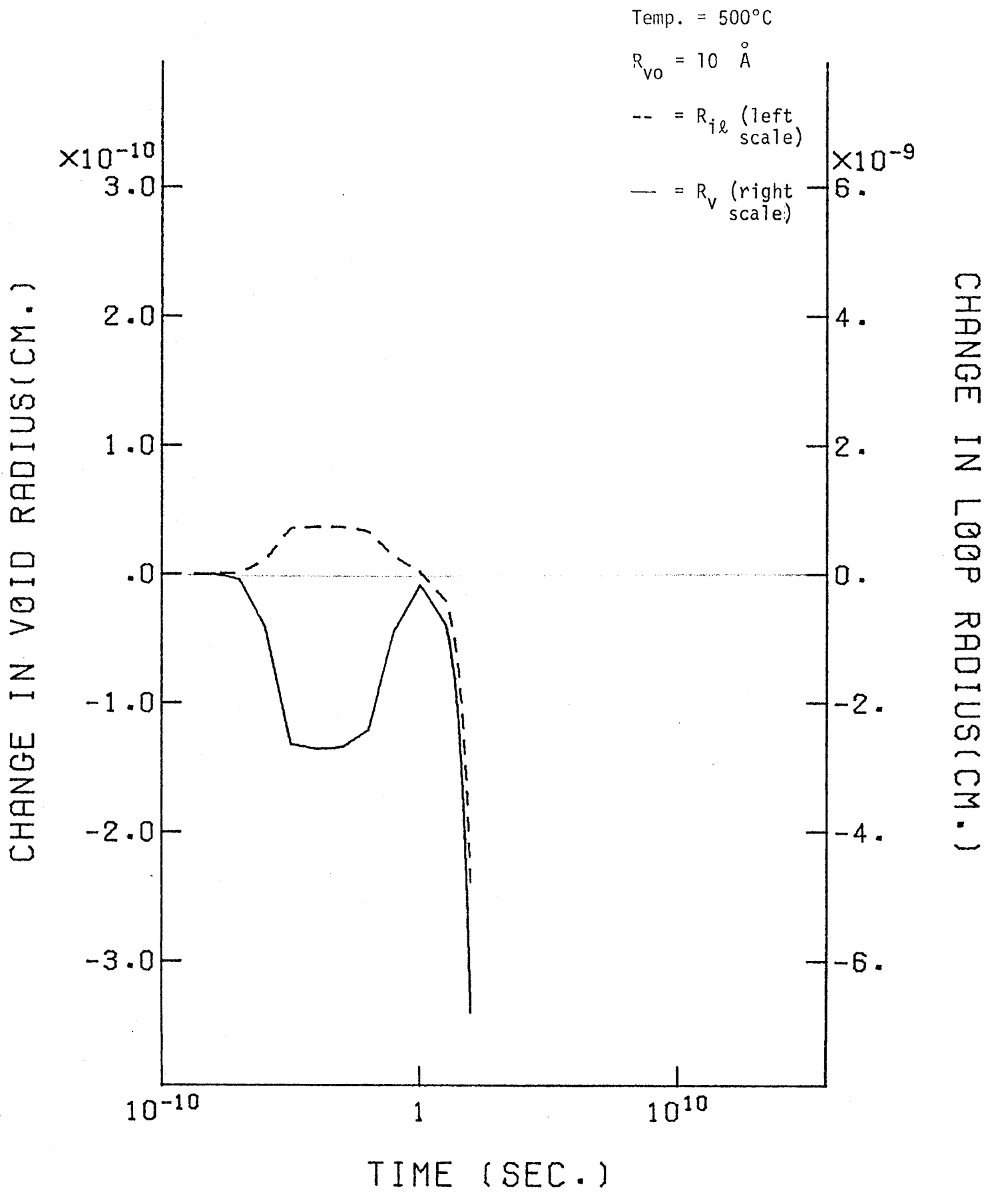


Figure 21

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width

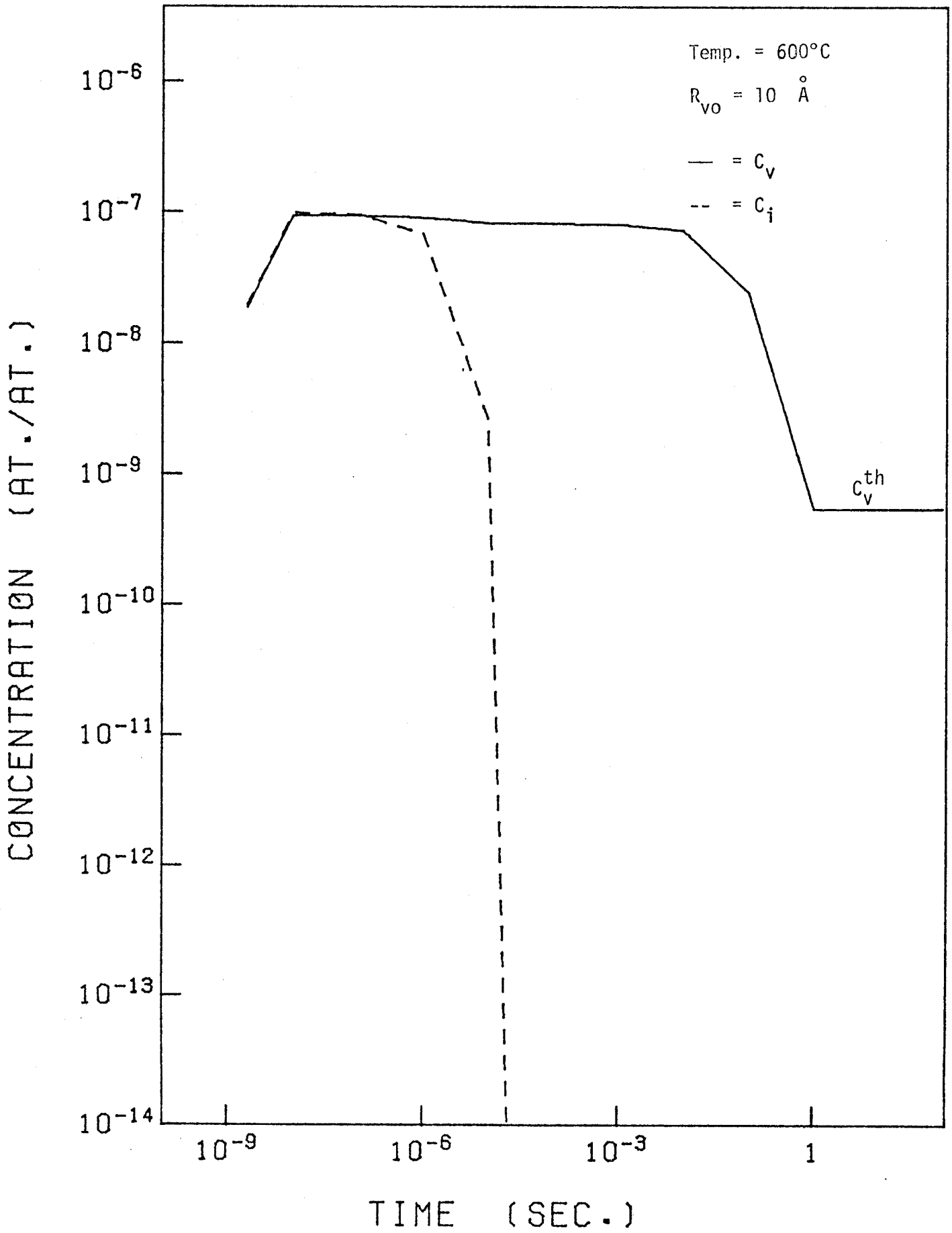


Figure 22

CHANGES IN VOID AND LOOP RADII
STEEL UNDER A PULSE OF 1.E-8 SEC WIDTH

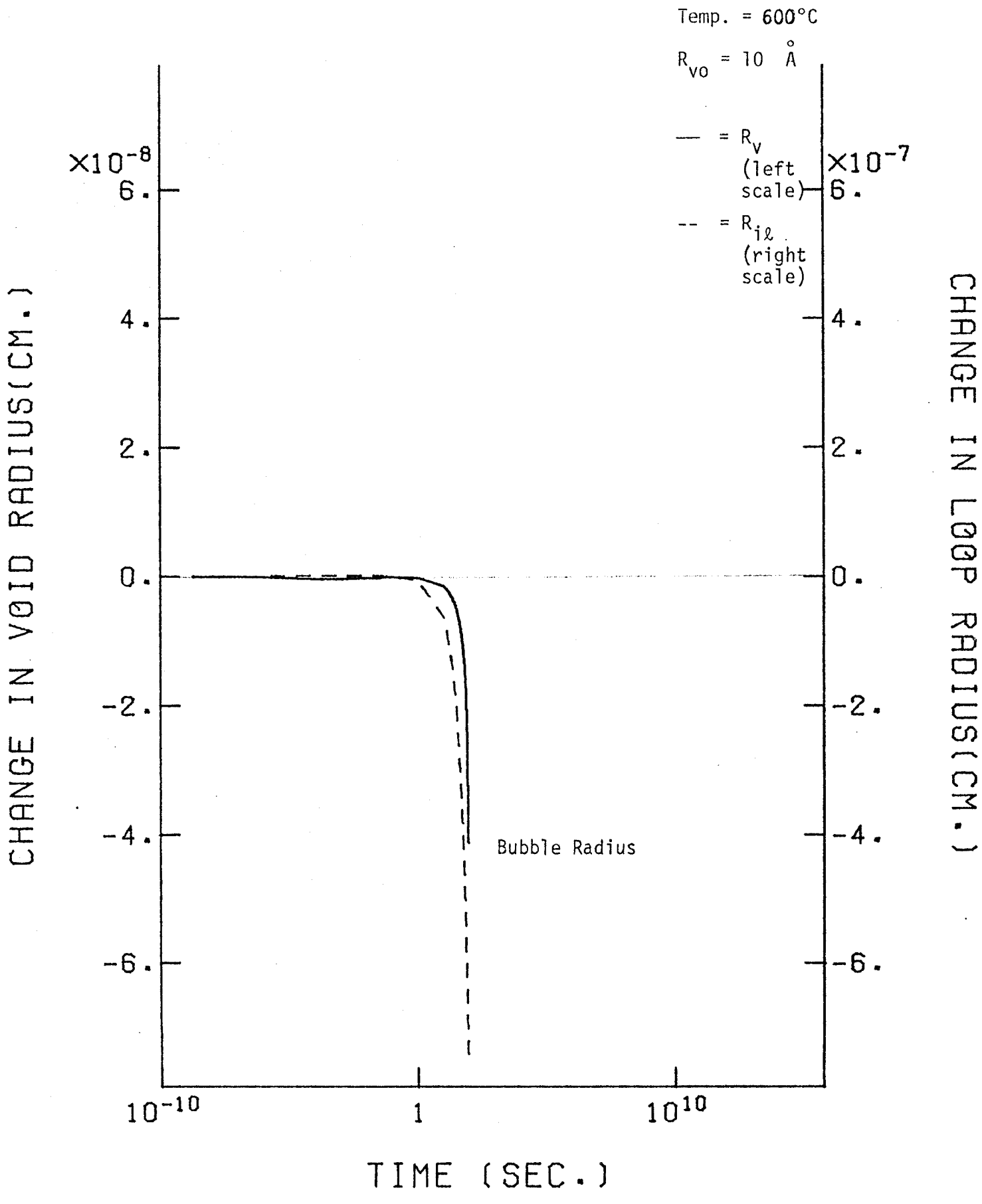
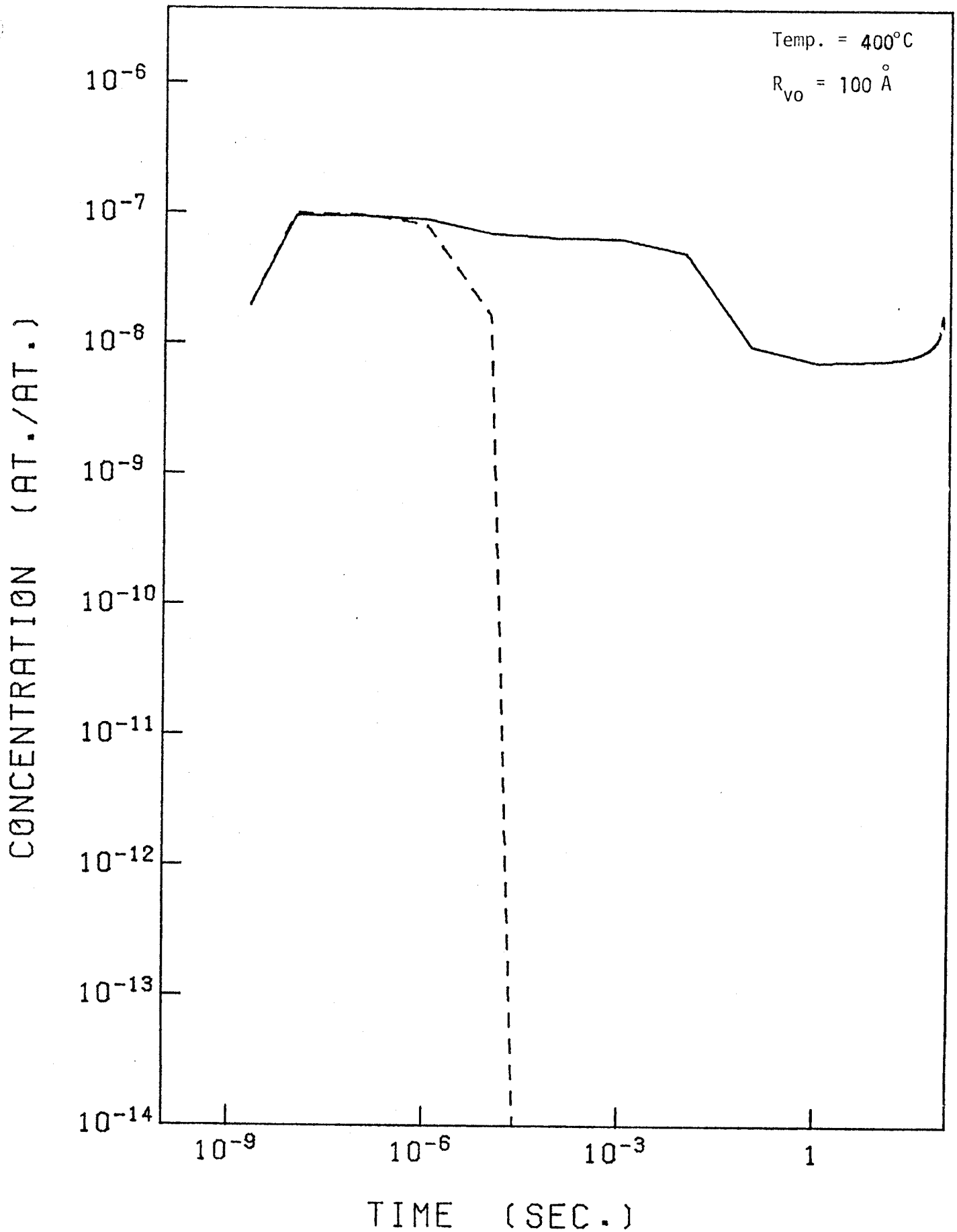


Figure 23

POINT DEFECT CONC. IN AN IRRADIATION PULSE

Steel Under A Pulse Of 1.E-8 Sec Width



Concluding Remarks

The documentation of the TRANSWELL Code has been performed in great detail so that others may find it easier to utilize the code in their work. It is expected that as we learn more about the physics of void growth, and as the data from pulsed and steady state irradiation experiments is analyzed, appropriate adjustments to the format will be made. We will update the description of the code from time to time and label each new version with a new number, e.g. VERS-II, VERS-III, etc.

Since the purpose of this document was to outline the approach taken in TRANSWELL, we did not spend much time analyzing the results of the two example cases. Previous reports[5,12] and future documents will concentrate on those aspects of the work. Finally, we would encourage comments and suggestions as to how TRANSWELL could be made even more functional for others in this field. It is only by continual upgrading that we will eventually be able to solve some of the severe problems facing us.

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(11) R. Bullough, Irradiation Creep and Effects of Stress on Swelling, Fund. Aspects of Rad. Damage in Metals Conf., Gatlinberg, Tennessee, October 1975.

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