Journal of Nuclear Materials 69 & 70 (1978) 816–820


# SWELLING OF METALS DURING PULSED IRRADIATION

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## 1. Introduction

There has been a great deal of interest recently in fusion power reactors based on the internal confinement approach [1,2]. One of the unique problems associated with this concept is the very high instantaneous neutron displacement rates (~1–10 dpa/s) that may exist in the first wall for times on the order ~10 ns. Previous experimental data on, and theoretical treatments of, neutron irradiated metals have all been associated with low ($\sim 10^{-7}$–$10^{-6}$ dpa/s) displacement rates which are constant in time. It has been shown by high energy heavy ion bombardment [3–5] and theoretical analysis [6] that such information is not directly applicable to pulsed irradiation conditions and therefore both new experimental data and theoretical models must be developed before one can realistically assess the potential of inertially confined fusion reactors. It is the objective of this paper to present a model which can treat the growth of voids under pulsed irradiation conditions.

## 2. Fully dynamic rate theory of metal swelling

Previous treatments of void growth in neutron irradiated metals at high temperature have used rate theory to calculate the vacancy and interstitial concentrations, $C_v$ and $C_i$, respectively, based on the work of Brailsford and Bullough [7]. The present work has allowed most of the parameters in the rate theory to vary with time and the present fully dynamic rate theory (FDRT) takes the following form (a more detailed treatment can be found in ref. [8]):

$$\frac{dC_I(t)}{dt} = P(t) - \lambda_I(t)\, C_I(t) - \alpha C_I(t)\, C_V(t)\,, \qquad (1)$$

$$\frac{dC_V(t)}{dt} = P_e(t) + (1-\epsilon)\, P(t) - \lambda_V(t)\, C_V(t) - \alpha C_I(t)\, C_V(t)\,. \qquad (2)$$

The different rate processes are given by

$P_R(t)$ = rate of recombination (at.at.$^{-1}$s$^{-1}$),
$P_{SI}(t)$ = rate of interstitial leakage to all sinks (at.at.$^{-1}$s$^{-1}$),
$P_{SV}(t)$ = rate of vacancy leakage to all sinks (at.at.$^{-1}$s$^{-1}$),
$P_e(t)$ = rate of vacancy emission from all sinks (at.at.$^{-1}$s$^{-1}$),

and

$$P_e(t) = P_e^V(t) + P_e^d(t) + P_e^{il}(t) + P_e^{Vl}(t)\,, \qquad (3)$$

where

$P_e^V(t)$ = rate of thermal vacancy emission from voids,
$P_e^d(t)$ = rate of thermal vacancy emission from edge dislocations,
$P_e^{il}(t)$ = rate of thermal vacancy emission from interstitial loops,
$P_e^{vl}(t)$ = rate of thermal vacancy emission from vacancy loops.

The previous rates of emission are now expressed explicitly as

$$P_e^V(t) = 4\pi r_V(t)\, N_V C_V^0 \exp\{[2\gamma/r_V(t) - p_g]\, b^3/kT\} \qquad (4)$$

$$P_e^d(t) = Z_V \rho_d^0 D_V C_V^0\,, \qquad (5)$$

$$P_e^{il}(t) = Z_V^{il} \rho_d^{il}(t)\, D_V C_V^0\,, \qquad (6)$$

$$P_e^{Vl}(t) = Z_V^{vl} \rho_d^{vl}(t)\, D_V C_V^0\,. \qquad (7)$$

The interstitial and vacancy loop dislocation densities are given respectively by

$$\rho_d^{il}(t) = 2\pi r_{il}(t)\, N_{il}\,, \qquad (8)$$

$$\rho_d^{vl}(t) = 2\pi r_{vl}(t)\, N_{vl}(t)\,. \qquad (9)$$

Here $N_{vl}(t)$ and $N_{il}$ are the vacancy and interstitial loop concentrations/cm$^3$, while $r_{vl}(t)$ and $r_{il}(t)$ are the vacancy and interstitial loop average radii, respectively. Also

$$P_R(t) = \alpha C_I(t)\, C_V(t)\,, \tag{10}$$

where $\alpha$ is the recombination coefficient and

$$P_{SI,SV}(t) = \lambda_{I,V}(t)\, C_{I,V}(t)\,, \tag{11}$$

in which

$$\lambda_{I,V}(t) = \lambda^{V}_{I,V}(t) + \lambda^{d}_{I,V}(t)\,. \tag{12}$$

$\lambda_{I,V}(t)$ is a time dependent total point defect leakage strength while

$$\lambda^{V}_{I,V}(t) = 4\pi r_V(t)\, N_V D_{I,V} \tag{13}$$

is a time dependent point defect leakage strength to voids and

$$\lambda^{d}_{I,V}(t) = Z_{I,V} D_{I,V}\,[\rho^0_d + \rho^{Vl}_d(t) + \rho^{Il}_d(t)] \tag{14}$$

is a time dependent point defect leakage strength to different dislocations. The leakage strength is defined as the leakage rate per unit concentration of the particular point defect.

According to the previous definitions, eqs. (1) and (2) for the time rate of change of Frenkel pairs could be written as

$$\frac{dC_I(t)}{dt} = P(t) - P_{SI}(t) - P_R(t)\,, \tag{15}$$

and

$$\frac{dC_V(t)}{dt} = P^e_v(t) + (1-\epsilon)\,P(t) - P_{SV}(t) - P_R(t)\,, \tag{16}$$

where $\epsilon$ is the fraction of vacancies produced in the form of vacancy loops. The equations for point defect concentrations together with other four coupled nonlinear rate equations are solved using TRANSWEL code [9]. The four coupled rate equations [8,10] are for the average void radius, the average interstitial loop radius, the fraction of vacancies retained in vacancy loops and the number of vacancy loops per unit volume.

## 3. Calibration of FDRT against steady state irradiation data

FDRT is particularly suitable for time dependent irradiations. However, it can be easily applied to

Table 1
M316 stainless steel parameters used for these calculations

| Parameter | Symbol | Value | Dimensions |
|---|---|---|---|
| Surface energy | $\gamma$ | $1.25 \times 10^{15}$ | eV cm$^{-2}$ |
| Vacancy formation energy | $E^v_f$ | 1.6 | eV |
| Vacancy migration energy | $E^v_m$ | 1.3 | eV |
| Interstitial formation energy | $E^f_i$ | 4.0 | eV |
| Interstitial migration energy | $E^m_i$ | 0.2 | eV |
| Vacancy diffusion preexponential | $D^0_v$ | 0.6 | cm$^2$s$^{-1}$ |
| Recombination coefficient / Interstitial diffusion coefficient | $\frac{\alpha}{D_i}$ | $10^{16}$ | cm$^{-2}$ |
| Stacking fault energy | $\gamma_{sf}$ | $9.4 \times 10^{12}$ | eV cm$^{-2}$ |
| Deformation produced dislocation density | $\rho^0_d$ | $10^8$ | cm$^{-2}$ |
| Burgers vector | $b$ | $2 \times 10^{-8}$ | cm |
| Dislocations bias for vacancies | $Z_v$ | 1.00 | |
| Dislocation bias for interstitials | $Z_i$ | 1.08 | |
| Effective modulus | $\mu' = \frac{\mu}{1-\nu}$ | $4 \times 10^{11}$ | dyne cm$^{-2}$ |

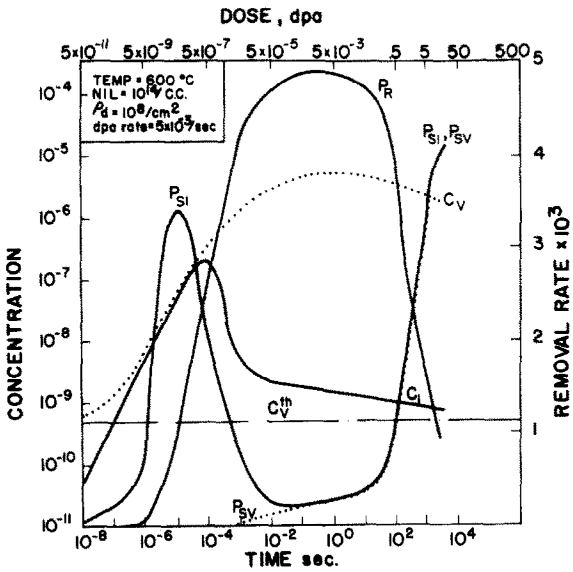

Fig. 1. Point defect concentrations $C_V$, $C_I$ and removal rates $P_R$, $P_{SI}$, $P_{sv}$ in electron irradiated M316 SS using the fully dynamic rate theory (FDRT).

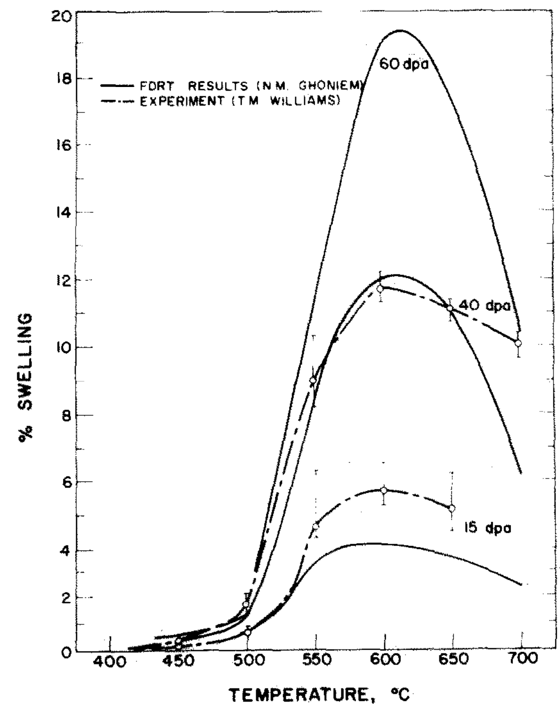

Fig. 2. Comparison between the FDRT and experimental results from T.M. Williams (AERE, Harwell). The temperature dependence of void swelling in M316 SS irradiated with 22 MeV $C^{2+}$ ions.

simulate steady state irradiations (constant rate of Frenkel pair production). For example, we have compared the theoretically predicted swelling to that experimentally measured from 1 MeV electron irradiated and 22 MeV $C^{2+}$ ion irradiated [12,13] stainless steel. The parameters used in the calculations are given in table 1. The following complete nucleation conditions are used [10].

(1) 1 MeV electron irradiation: $\epsilon = 0, N_V = 6.5 \times 10^8 \exp(1.0\ \text{eV}/kT), N_{il} = 6.7 \times 10^{-3} \exp(2.8\ \text{eV}/kT)$.

(2) 22 MeV $C^{2+}$ irradiation: $\epsilon = 0.044$, $N_V = 3.15 \times 10^{11} \exp(0.625\ \text{eV}/kT)$, $N_{il} = 1.34 \times 10^{-4} \exp(2.8\ \text{eV}/kT)$.

Fig. 1 illustrates the dynamic behavior of the total interstitial sink removal rate ($P_{SI}$), the total vacancy sink removal rate ($P_{SV}$), the recombination rate ($P_R$) and the point defects concentrations for the heavy ion irradiation case. Results for electrons are quoted elsewhere [8]. It is clear that the magnitude and relative importance of these parameters are heavily time dependent, especially at the start of irradiation. Fig. (2) shows the good agreement between the FDRT theory and experiment [12,13] in steady state applications for heavy ion irradiated in 316 SS. The initial conditions used are: $C_v(0) = C_V^{th}$, $C_I(0) = C_I^{th}$,

$$r_v(0) = 10\ \text{Å}; \qquad r_{il}(0) = [4 r_V^3(0) N_V / 3 b N_{il}]^{1/2} ,$$

$$N_{vl}(0) = 0; \qquad \rho_d^{Vl}(0) = 0; \quad P_g(0) < [2\gamma / r_V(0)] .$$

## 4. Application of FDRT to pulsed irradiations

The example studied here corresponds to an approximate damage pulse represented by [8]

$$\text{dpa rate} \begin{cases} = 10\ \text{dpa/s}, & 0 \leq t \leq 10^{-8}\ \text{s}, \\ = \ 0\ \text{dpa/s}, & 10^{-8} < t < \infty\ \text{s}. \end{cases}$$

Figs. 3 and 4 show the temperature and time dependence of the point defect concentrations and their effect on an initial 40 Å radius void. It can be seen that irradiation at 400°C causes the void to shrink initially due to the interstitial flux and then to grow to $r > 40$ Å after the vacancies migrate to the void. Annealing thereafter is a result of thermal vacancy

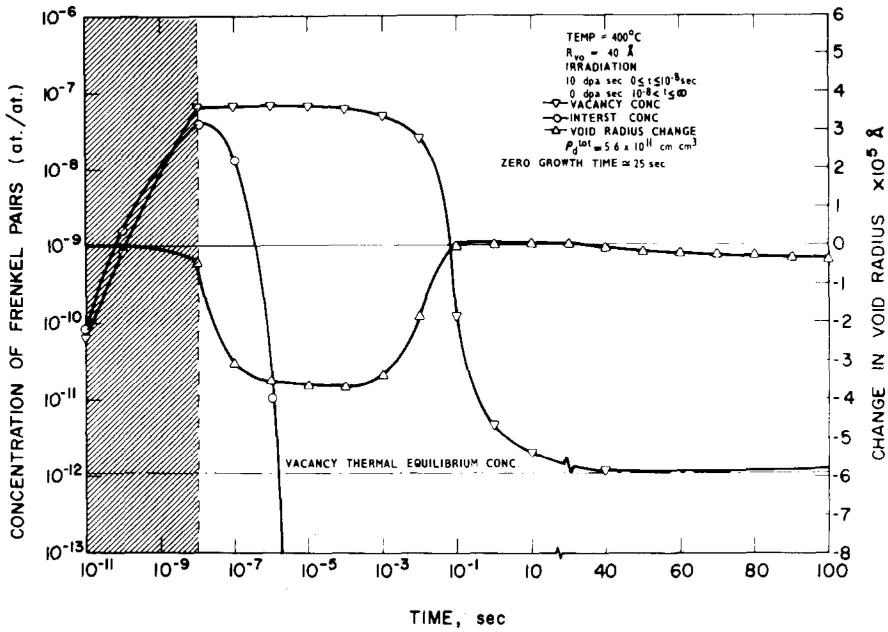


Fig. 3. Point defect concentrations and change in void radius as a function of time during and after an irradiation pulse at 400°C for S.T. 316 SS.

emission from the void surface. The significance of the 25 s recovery time is that if another damage pulse occurs in that time period, the void will grow. If the pulse occurs at times larger than 25 s, the void will shrink. Fig. 4 shows that the behavior at 600°C is generally the same except that the void never regains its ini-

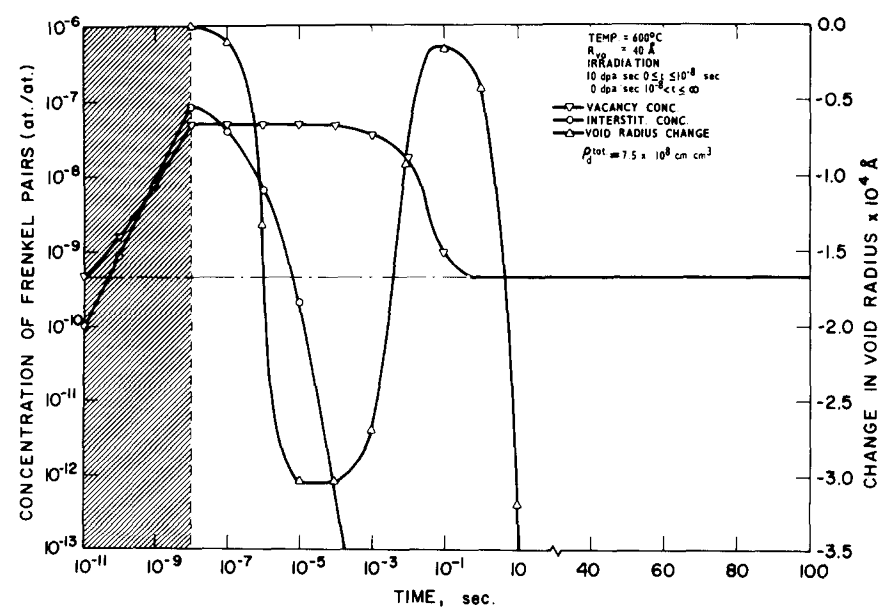


Fig. 4. Point defect concentration and change in void radius as a function of time during and after an irradiation pulse at 600°C for S.T. 316 SS.

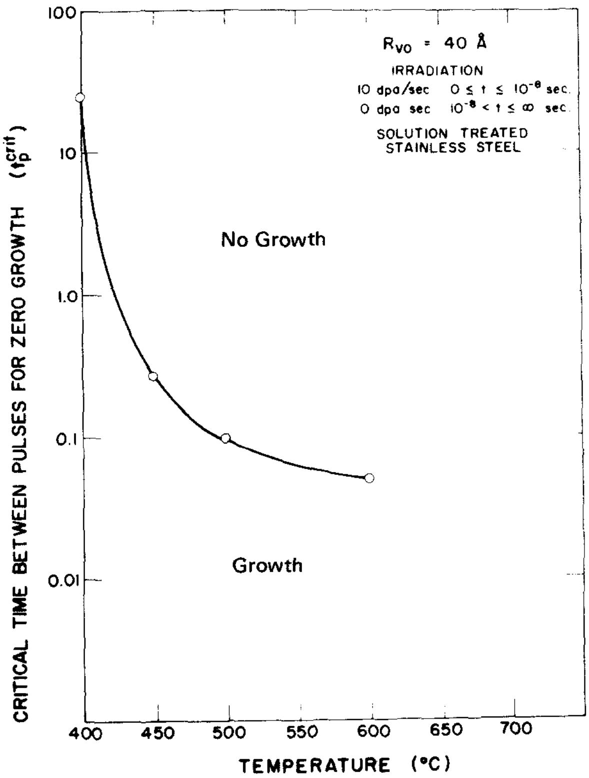


Fig. 5.

tial radius of 40 Å. The increased thermal emission at 600°C causes the void to shrink faster than the rate at which vacancies can be added. Therefore, under these conditions one would not expect swelling to increase with dose. This situation is summarized in fig. 5 where the regions of void growth and shrinkage are related to temperature and time between pulses for the given conditions.

## 5. Discussion and conclusion

A principle aim of the present work has been to develop a calculational method, based on the rate theory approach, to describe the behavior of voids and dislocation loops in metals under pulsed irradiation. The method has been shown to be applicable to irradiations under constant rate of point defect production (figs. 1 and 2). Application of FDRT to simulate pulsed irradiation (figs. 3–5) has shown that there is a critical time between pulses for zero growth of the void ($t_p^{crit}$) as a function of temperature (fig. 5). For times less than $t_p^{crit}$ voids grow and for times greater than $t_p^{crit}$ voids will shrink.

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