MASTER

PREDICTION OF THE BEHAVIOR OF STRUCTURAL MATERIALS UNDER
IRRADIATION THROUGH MODELING OF THE MICROSTRUCTURE

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Abstract

The development of the radiation-induced microstructure occurs in several stages: formation of small defect clusters, formation of dislocation loops, nucleation and growth of voids, and regeneration of the dislocation network. With the exception of the latter, these processes can be modeled with rate equations of similar form. However, instead of using one rate equation for each defect cluster of a given size, the discrete formulation is transformed in a continuous one leading to Fokker-Planck equations. It is shown by comparing the steady-state nucleation rates of both formulations that the Fokker-Planck equation derived is the correct continuous description.

A path-integral solution for the Fokker-Planck equation was derived to provide the basis for a numerical solution procedure, capable of dealing with the vastly different time scales involved in cluster formation, nucleation, and growth.

Void nucleation depends in a crucial way on the void bias factors. Therefore, a comprehensive evaluation was carried out for the bias factors of coated voids. It is shown that a segregation layer around a void with slightly different elastic properties has a significant effect on the void bias. If the elastic shear modulus is enhanced in the layer, an activation barrier for point defect diffusion is created. The barrier height depends mainly on the relaxation energy of the point defect, the difference in lattice parameters between shell and matrix, and on the stress. Due to the large relaxation volume of interstitials, a void coating mainly influences the interstitial diffusion. As a result, voids with hard surface layers are biased against interstitials.

A critical assessment of irradiation creep mechanisms was carried out with the major conclusion that a glide process is dominant at low doses of radiation damage, whereas SIPA-creep dominates at high doses. To establish more firmly these mechanisms it is proposed that decisive experiments be conducted with single crystal specimens. Accordingly, constitutive laws for irradiation creep of fcc single crystal were derived for three mechanisms: stress-induced preferential absorption on faulted loops (SIPAL), on dislocations (SIPAD), and climb-controlled glide (CCG).

I. Introduction

The formation of voids and dislocation loops in irradiated metals has been the subject of intensive research in the past [1,2] because of its technological implications in the design of nuclear reactors. Whereas the formation of voids is the result of vacancy cluster formation, interstitial-type dislocation loops originate from the clustering of interstitial atoms. Both processes can be treated theoretically within one framework, the stochastic theory of cluster formation.

In the past, the theoretical description of this cluster formation has been divided into a nucleation phase and a growth phase. Whereas the nucleation theory has been developed [3,4,5] in accordance with the stochastic nature of a clustering process, the growth models for both voids and dislocation loops [6,7] were mostly treated as a deterministic process. The disjoint treatment appears to be justified by the experimental observation on swelling as a function of the dose. During the initial incubation dose little swelling is measured, and this is followed by a growth phase of rapid swelling. Although this division is convenient for a phenomenological and qualitative description of swelling, it has hampered a unified quantitative treatment of both nucleation and growth of voids.

A somewhat different misconception has been prevailing with regard to interstitial loop formation that can be traced back to the disjoint treatment of nucleation and growth. The view that an activation barrier exists for interstitial loop nucleation is inappropriate upon closer examination as the dissociation of an interstitial cluster by thermal emission of interstitials is negligibly small. However, the lack of a nucleation process in the traditional sense does not imply that the interstitial loop growth can be described by a deterministic theory.

These reasons, among others, are the major motivation behind a stochastic formulation of the clustering process, described in Section II.

Although a unified formulation of nucleation and growth can be accomplished and cast into a concise form in terms of Fokker-Planck equations, their solution presents a great challenge. The major reason is that a numerical treatment along conventional lines leads to an extremely stiff system of ordinary differential equation with characteristic response times covering several orders of magnitude. In a numerical integration of these equations, the time step has to be chosen so small that only short-time clustering can be studied. For this reason, a formulation in terms of path integrals is presented in Section III. The path integrals allow a physical interpretation of the evolution of the cluster size-distribution, and the insights gained thereby can be useful in a numerical solution.

Many materials parameter enter into the clustering theory. In order to study their importance, the steady-state void nucleation theory is used in Section IV to demonstrate the importance of bias factors and impurity segregation on void formation.

A similar study is carried out in Section V for the formation and growth of interstitial loops. The application of the stochastic formulation to interstitial loop formation brings out a new feature. Under irradiation, a stationary loop size distribution is eventually reached with the average loop size changing only in response to a slowly varying dislocation network density. Nevertheless, the individual loop growth rate changes rapidly. Therefore, the dislocation loop population is continuously replaced in spite of a stationary appearance of the loop size distribution.

This fact enables us to construct a dynamic model in Section V for the evolution of the network dislocation structure. According to this model, the network is continuously regenerated by the unfauling of the dislocation loops. A dynamic balance is again reached when the regeneration rate is equal to the recovery rate.

II. Stochastic Theory of Defect Cluster Formation and Growth

II.1 Sources for the Stochastic Nature

Before embarking on the details of the theoretical formulation some of the major causes of the stochastic nature of cluster formation and growth will be discussed. To avoid speaking in the abstract, the discussions will concentrate on the case of void formation. However, they apply equally well to loop formation or precipitate formation.

Let us consider a void of a given size. It can change its size by three reactions: capture of a vacancy, capture of an interstitial, and thermal emission of a vacancy. The individual events of capture and emission occur at random and, it is assumed, also independent of each other.

The rate of capture of vacancies and interstitials depends on the concentrations of these point defects in the vicinity of the void. These concentrations are subject to fluctuations themselves because the displacement events occur at random in time as well as space. Finally, the flow of point defects to a given void also depends on the proximity of other sinks, on random internal stress fields, and on local variations in chemical compositions in the case of alloys. Hence, one can identify the following sources contributing to the fluctuations in the capture and emission of point defects:

- 1) Individual capture and emission events are random.
- 2) Displacement events and cascade formation occur at random both in time and space.
- 3) The distance and the effect of adjacent sinks on the point defect concentration is subject to variations..

- 4) Fluctuating internal stresses affect local point defect diffusion and formation energies.
- 5) Fluctuations in the composition of the crystal lattice in alloys affect local point defect diffusion and formation energies.

These stochastic sources affect the growth or shrinkage of a void by the capture or emissions of monomers only. If, however, larger point defect clusters exist abundantly and if they are mobile, an additional contribution to the random growth arises from coagulation of mobile clusters and from capture of these clusters. We associate this additional stochastic source with

- 6) The coagulation processes.

In the following, we shall neglect all stochastic sources 2 to 6 by assuming that the capture events at a given void are entirely determined by an appropriate average concentration of point defects. In addition, we consider only mono-vacancies and mono-interstitials as the dominant mobile point defects. Furthermore, the equations that determine their concentrations are assumed to be deterministic equations.

The theory so obtained for the cluster size distribution is known as the birth-and-death formulation in the stochastic literature. Because of the omission of the stochastic sources 2 to 6, the birth-and-death formulation has its limitations. In a more general context, this has been pointed out by Nicolis and Prigogine (8), and it is known that such a formulation for stochastic processes is incapable of describing critical phenomena. Applying this to the case of radiation damage, we conjecture that the inclusion of the stochastic sources 3 and 4 is necessary to explain and derive the transition temperature for the formation of void and loop lattices. However, this phenomenon will not be investigated here.

II.2 The Rate Equations

Let us consider the birth-and-death formulation for void formation in greater detail. We denote the concentration of clusters containing x vacancies by $f(x,t)$. This function is a continuous function with regard to the time t , but depends discretely on the integer x .

The three reaction rates for capture and emission are denoted as

$\alpha(x,t)$, the capture rate of interstitials,

$\beta(x,t)$, the capture rate of vacancies, and

$\theta(x,t)$, the thermal emission rate of vacancies by a x -vacancy cluster.

We note that these reaction rates are volume-averaged rates as discussed in Ref. 9. Without further specification of these rates one can immediately give the following equation for the rate of change of the cluster density $f(x,t)$;

$$\begin{aligned} \frac{df(x,t)}{dt} = & [\alpha(x+1,t) + \theta(x+1,t)] f(x+1,t) \\ & - [\alpha(x,t) + \beta(x,t) + \theta(x,t)] f(x,t) \\ & + \beta(x-1,t) f(x-1,t) \end{aligned} \quad (II.1)$$

This equation is valid for $x \geq 2$ if only monomers are mobile. In this case, $\beta(x,t)$ is proportional to $C_v(t) = f(1,t)$, the mono-vacancy concentration.

Equation (II.1) forms the starting point for the void nucleation theories of Burton [5], Russell [4], and Katz and Wiedersich [3]. To complete the mathematical description, additional equations are needed for the mono-vacancies and the interstitials. They are

$$\begin{aligned} \frac{dC_v}{dt} = & P - K_v(C_v - C_v^{eq}) - \alpha(1,t)C_v + \alpha(2,t)f(2,t) \\ & - \sum_{x=1}^{\infty} \beta(x,t)f(x,t) + \sum_{x=2}^{\infty} \theta(x,t)f(x,t) \end{aligned} \quad (II.2)$$

and

$$\frac{dC_i}{dt} = P - K_i C_i - \sum_{x=1}^{\infty} \alpha(x,t)f(x,t) \quad (II.3)$$

where P is the production rate of Frenkel pairs, and $K_v C_v$ and $K_i C_i$ are the loss rates of vacancies and interstitials at sinks other than the vacancy clusters. The term $\alpha(1,t) C_v$ or $\alpha(1,t) f(1,t)$ in the above equations is the recombination rate of vacancies and interstitials, $\alpha(2,t) f(2,t)$ is the reaction rate of interstitials with divacancies, $\theta(2,t) f(2,t)$ is the rate of dissociation for divacancies, and $\beta(1,t) f(1,t)$ is the rate of divacancy formation.

Strictly speaking, Eq. (II.3) should also contain terms which correspond to interstitial cluster formation. However, for reasons of simplicity, these terms are not shown explicitly but assumed to be included in the terms $K_i C_i$ and $K_v C_v$. This approach is further justified by the fact that interstitial cluster build-up occurs during a very short time in comparison to the incubation time for void nucleation. Within the time scale for void nucleation, the interstitial cluster population is in fact better represented by a quasi-stationary dislocation loop population which contributes to the sink strengths K_v and K_i .

The experimentally observed incubation time for void nucleation in a fast reactor environment ranges from 10^4 to 10^7 seconds, depending on the

material and the irradiation temperature. In contrast, the buildup time of interstitial clusters containing an average of about 30 interstitials is of the order of seconds according to recent results by Ghoniem [10].

Two other characteristic time scales are of interest in the present context, the buildup times for the interstitial and vacancy concentrations. In order to obtain an estimate for these times Eqs. (II.2) and (II.3) are written in the form

$$\frac{dC_v}{dt} = P_v - D_v C_v / L_v^2 \quad (II.4)$$

and

$$\frac{dC_i}{dt} = P - D_i C_i / L_i^2 \quad (II.5)$$

where L_i and L_v are the average migration distances for the interstitial and vacancy, respectively, to reach a sink or a reaction partner. P_v is the sum of P and the thermal vacancy emission rate from all the sinks and vacancy clusters. If we select for L_i and L_v a time independent average value, we can solve the above equations and obtain

$$C_v(t) \cong (P_v D_v / L_v^2) [1 - \exp(-D_v t / L_v^2)] \quad (II.6)$$

$$C_i(t) \cong (P D_i / L_i^2) [1 - \exp(-D_i t / L_i^2)] \quad (II.7)$$

We may now define the time constants

$$\tau_i = L_i^2 / D_i \quad (II.8)$$

and

$$\tau_v = L_v^2 / D_v \quad (II.9)$$

for the interstitial and vacancy concentration buildup. These time constants can also be interpreted as average lifetimes of the point defects. With a dislocation density of 10^{10} cm^{-2} , L_i and L_v are at most of the order of 10^{-5} cm or smaller. Therefore, τ_i ranges from 10^{-6} to 10^{-5} sec within a temperature range of 300°C to 700°C , assuming that the interstitial migration energy is 0.2 eV . The lifetime for vacancies ranges from 10^{-3} sec to 10^3 sec in the case of Ni irradiated in a fast-reactor flux within the above temperature range. It should be noted that the relatively long time of 10^3 sec at 300°C will in fact be substantially shorter, since at this irradiation temperature the sink and cluster density will reach higher values corresponding to a migration distance of $L_v = 10^{-6} \text{ cm}$.

The drastic differences in the time scales, i.e., between the interstitial lifetime τ_i , the vacancy lifetime τ_v , the interstitial loop lifetime τ_ℓ , and finally the incubation time for void nucleation τ_0 , make it impossible to simply integrate the set of rate equations (II.1), (II.2), (II.3) plus those for the interstitial clusters, since each process requires a different time-step.

For the initial time period τ_i during which C_i changes rapidly, C_v changes little. In turn, over the time period τ_v , where C_v increases, no voids are nucleated. Hence, for time periods much larger than both τ_v and τ_i one can make what has been called by Haken [11] the adiabatic approximation. In our case, this approximation amounts to the assumption that $dC_i/dt \approx dC_v/dt \approx 0$, and it implies that the production rate $P(t)$ as well as the reaction rates $\alpha(x,t)$, $\beta(x,t)$, and $\theta(x,t)$ are averaged values over time periods of the order of or larger than τ_v . The reaction rates

become then "time independent" and they can be computed with a diffusion-controlled reaction model. Assuming a spherical void shape one obtains:

$$\bar{\alpha}(x) = (4\pi)^{2/3} (3\Omega x)^{1/3} D_i C_i Z_i^0(x) \quad (II.10)$$

$$\bar{\beta}(x) = (4\pi)^{2/3} (3\Omega x)^{1/3} D_v C_v Z_v^0(x) \quad (II.11)$$

$$\bar{\theta}(x) = (4\pi)^{2/3} (3\Omega x)^{1/3} D_v C_v^0(x) Z_v^0(x) \quad (II.12)$$

Here, D_i and D_v are the migration coefficients for interstitial and vacancy diffusion, respectively, and Ω is the atomic volume. The void bias factors for interstitials and vacancies, $Z_i^0(x)$ and $Z_v^0(x)$, will be given below. The local vacancy concentration in thermodynamical equilibrium with the void containing x vacancies is given by

$$C_v^0(x) = C_v^{eq} \exp\{[(4\pi)^{1/3} (3\Omega)^{2/3} \gamma [x^{2/3} - (x-1)^{2/3}] / kT - p\Omega / kT\} \quad (II.13)$$

where θ is the surface energy and p the gas pressure in the void. C_v^{eq} is the thermal equilibrium concentration of vacancies in a perfect crystal.

In summary, the equations that describe the time-dependent void nucleation problem are

$$\begin{aligned} P(t) - K_v (C_v - C_v^{eq}) - \bar{\alpha}(1) C_v + \bar{\alpha}(2) f(2,t) \\ - \sum_{x=1}^{\infty} \bar{\beta}(x) f(x,t) + \sum_{x=2}^{\infty} \bar{\theta}(x) f(x,t) = 0 \end{aligned} \quad (II.13)$$

$$P(t) - K_i C_i - \sum_{x=1}^{\infty} \bar{\alpha}(x) f(x,t) = 0 \quad (II.14)$$

$$\begin{aligned} \frac{d}{dt} f(x,t) = [\bar{\alpha}(x+1) + \bar{\theta}(x+1)] f(x+1,t) + \bar{\beta}(x-1) f(x-1,t) \\ - [\bar{\alpha}(x) + \bar{\beta}(x) + \bar{\theta}(x)] f(x,t) \end{aligned} \quad (II.15)$$

provided that mono-vacancies and mono-interstitials are the only mobile point defects of sufficient abundance. Using the rate coefficients, as expressed in the form of Eqs. (II.10) to (II.12), implies the adoption of the "quasi-steady-state" rate equations (II.13) and (II.14). Time-variations in the production rates occurring with frequencies greater than $1/\tau_v$ have no effect on the void nucleation or growth kinetics. Pulsed irradiations with frequencies greater than $1/\tau_v$ are in fact like steady-state irradiations.

Conversely, pulsing frequencies with frequencies smaller than $1/\tau_v$ are better termed interrupted irradiations. The point defect concentrations $C_v(t)$ and $C_i(t)$, and hence the capture rates $\bar{\alpha}$ and $\bar{\beta}$, are in synchrony with $P(t)$. Therefore, these pulsed irradiations differ from steady-state irradiations only because of intermittent annealing of the voids.

Theoretical studies, in which the time derivations dC_v/dt and dC_i/dt are retained while still using the rate coefficients of Eqs. (II.10) and (II.11) are superfluous.

II.3 The Fokker-Planck Formulation

The equation (II.15), the so-called master equation for void nucleation, actually represents an extremely large set of coupled ordinary differential equations. The range that x must cover to include voids of all sizes extends from $x_{\min}=2$ to $x_{\max} \approx 10^7$. Clearly, this system must be condensed into something more tractable. To this end, we consider now x as a continuous variable, and $f(x,t)$ as well as the reaction rates $\bar{\alpha}(x)$, $\bar{\beta}(x)$, and $\bar{\theta}(x)$ as analytic functions of x . Next, we expand all functions of $(x-1)$ and $(x+1)$ into Taylor series, and we replace the master equation (II.15) by

$$\frac{\partial f}{\partial t} = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n}{\partial x^n} A_n(x) f(x,t), \quad (\text{II.16})$$

where $A_n(x) = \bar{\alpha}(x) + \bar{\theta}(x) + (-1)^n \bar{\beta}(x)$. Eq. (II.16) is known as the Kramers-Moyal expansion. To be useful, the expansion in Eq. (II.16) must be truncated after a finite number of terms. This can be done consistently by invoking Pawula's theorem [12]. According to this theorem the assumption that one $A_m = 0$ for some even m implies in fact that all $A_n = 0$ for $n \geq 3$. In our case, however, it is not possible to use this theorem because all coefficients with even n are equal, i.e.,

$$A_2 = A_4 = A_6 = \dots \quad (\text{II.17})$$

In other words, there is no coefficient with even n that vanishes even approximately, and Pawula's theorem is not applicable.

Let us designate the coefficients with odd n as

$$F(x) = \bar{\beta}(x) - \bar{\alpha}(x) - \bar{\theta}(x), \quad (\text{II.18})$$

and those with even n as

$$2D(x) = \bar{\beta}(x) + \bar{\alpha}(x) + \bar{\theta}(x). \quad (\text{II.19})$$

If both of these functions as well as the function $f(x,t)$ are smooth and slowly varying, the Eq. (II.16) may be truncated after the second term, and one obtains the Fokker-Planck equation.

$$\frac{\partial f}{\partial t} = - \frac{\partial}{\partial x} \{F(x) - \frac{\partial}{\partial x} D(x)\} f(x,t)$$

(II.20)

In the next section we derive the conditions that the "drift force" $F(x)$ and the "diffusion function" $D(x)$ must satisfy in order for this truncation to be meaningful.

II.4 Comparison Between the Discrete and Continuous Formulation

One of the most important parameters to be derived from the theory is the stationary void nucleation rate. It can be obtained either from the master equation (II.15) directly or from the Fokker-Planck eq. (II.20) by assuming that $\partial f / \partial t = 0$. Although the development from the master equation is well known we summarize it here in order to facilitate the comparison.

If we write the master equation in the form

$$\frac{df(x,t)}{dt} = -I(x,t) + I(x-1,t) \quad (II.21)$$

where the cluster current is defined as

$$I(x,t) = \bar{\beta}(x) f(x,t) - [\bar{\alpha}(x+1) + \bar{\theta}(x+1)] f(x+1,t) \quad (II.22)$$

then the stationary solution must satisfy $df_s/dt = 0$ and

$$I_s(x) = I_s(x-1) = I_s,$$

i.e., equal to a constant. I_s is the stationary void nucleation rate.

To find expressions for I_s and the stationary cluster distribution function $f_s(x)$, it is customary to introduce a constrained equilibrium state and its corresponding cluster distribution $n(x)$ for which a state of detailed balance exists. In this state

$$\bar{\beta}(x)n(x) = [\bar{\alpha}(x+1) + \bar{\theta}(x+1)] n(x+1). \quad (II.23)$$

By repeated application of this recursion relation one finds

$$n(x) = n(1) \prod_{k=2}^x \frac{\bar{\beta}(k-1)}{\bar{\alpha}(k) + \bar{\epsilon}(k)} \quad (\text{II.24})$$

The assumption, that the master equation has a solution for a state of detailed balance, is necessary when the reaction rate coefficients for vacancy emission, $\bar{\epsilon}(x)$, is not known. Then, one determines $n(x)$ such that the system is in a state of global thermodynamic equilibrium subject to the constraints that the vacancy and interstitial concentrations are held at fixed values, and that $I(x,t) = 0$.

However, a simpler approach is to require that a local thermodynamic equilibrium exists in a region that contains the void cluster and its immediate surrounding consisting of a few atomic layers. The local equilibrium concentration of vacancies is then given by the condition that upon creating a vacancy in the surrounding layers and adding the atom to the x -vacancy cluster, the total change in Gibbs free energy be zero. Hence, if H_V^f is the enthalpy for vacancy formation, N_V the number of vacancies, N_O the number of atoms, p the gas pressure in the cluster, and $E(x)$ the energy of the cluster, then

$$-H_V^f + kT \Delta S + E(x) - E(x-1) - p\Omega = 0 \quad (\text{II.25})$$

where

$$\Delta S = \ln W(N_V+1) - \ln W(N_V)$$

is the change in the configurational entropy. Here,

$$W(N_V) = \frac{(N_O + N_V)!}{N_O! N_V!},$$

and assuming that $N_O \gg N_V \gg 1$ we obtain

$$\Delta S \approx \ln(N_O/N_V) = - \ln C_V^0.$$

If

$$C_V^{eq} = \exp(-H_V^f/kT) \quad (II.26)$$

is the ideal vacancy equilibrium concentration, the local equilibrium concentration can then be obtained from Eq. (II.25):

$$C_V^0(x) = C_V^{eq} \exp\{[E(x) - E(x-1) - p\Omega]/kT\} \quad (II.27)$$

This equation together with Eq. (II.12) determines the reaction rate $\bar{e}(x)$ for vacancy emission.

In summary, the assumption of a local thermodynamic equilibrium at the sink is sufficient to determine $\bar{e}(x)$, and no constrained equilibrium state need to be invoked. It becomes merely a mathematical trick to solve the stationary problem.

$$\bar{e}(x) f_s(x) - [\bar{a}(x+1) + \bar{e}(x+1)] f_s(x+1) = I_s \quad (II.28)$$

by using the constrained equilibrium distribution $n(x)$ in the following way.

One solves Eq. (II.23) for $\bar{a}(x+1) + \bar{e}(x+1)$ and obtains

$$\bar{e}(x) f_s(x) - \bar{e}(x) \frac{n(x)}{n(x+1)} f_s(x+1) = I_s$$

or

$$\frac{f_s(x+1)}{n(x+1)} - \frac{f_s(x)}{n(x)} = - \frac{I_s}{\bar{e}(x)n(x)} \quad (II.29)$$

Next, a summation is carried out giving

$$\frac{f_s(x)}{n(x)} - \frac{f_s(1)}{n(1)} = - I_s \sum_{k=1}^{x-1} \frac{1}{\bar{\beta}(k)n(k)}, \quad (II.30)$$

and one sets $f_s(1) = n(1)$ and $f_s(N)/n(N) = 0$ where N is a very large number. Hence, the stationary nucleation rate is finally given by

$$I_s = \left\{ \sum_{i=1}^{N-1} [\bar{\beta}(i)n(i)]^{-1} \right\}^{-1}, \quad (II.31)$$

and the stationary cluster distribution by

$$f_s(x) = n(x) \left\{ \sum_{i=x}^{N-1} \frac{1}{\bar{\beta}(i)n(i)} \right\} / \left\{ \sum_{i=1}^{N-1} \frac{1}{\bar{\beta}(i)n(i)} \right\}. \quad (II.32)$$

It is possible to assign a thermodynamic potential $G(x)$ to the constrained distribution function $n(x)$ by writing in place of Eq. (II.24)

$$n(x) = n(1) \exp\{-G(x)/kT\} \quad (II.33)$$

where

$$G(x) = -kT \sum_{i=2}^x \ln \left[\frac{\bar{\beta}(i-1)}{\bar{\alpha}(i) + \bar{\theta}(i)} \right] \quad \text{for } x \geq 2, \quad (II.34)$$

and $G(1) = 0$.

Then, the stationary nucleation rate can be written as

$$I_s = n(1) \left\{ \sum_{i=1}^{N-1} \frac{\exp[G(i)/kT]}{\bar{\beta}(i)} \right\}^{-1} \quad (II.35)$$

and the stationary cluster distribution as

$$f_s(x) = I_s \sum_{i=x}^{N-1} \frac{\exp[G(i) - G(x)/kT]}{\bar{\beta}(i)} \quad (II.36)$$

Eqs. (II.34), (II.35), and (II.36) are the important results of the stationary nucleation theory based on the discrete formulation with the master equation.

The derivation of the same results from the continuous formulation with the Fokker-Planck eq. (II.20) follows the same steps. First, we define the cluster current as

$$I(x,t) = [F(x) - \frac{\partial}{\partial x} D(x)]f(x,t) . \quad (II.37)$$

For the stationary solution, $\partial f_s(x,t)/\partial t = 0$, which implies that

$$I_s(x) = I_s = \text{const. or}$$

$$\frac{d}{dx} D(x)f_s(x) - F(x)f_s(x) = - I_s .$$

The solution of this equation is given by

$$D(x)f_s(x) = \exp[-G(x)/kT] \{ D(x_0)f_s(x_0) - I_s \int_{x_0}^x dx' \exp[G(x')/kT] \} \quad (II.38)$$

where

$$G(x)/kT = - \int_{x_0}^x dx' F(x')/D(x') . \quad (II.39)$$

and assuming that $f_s(x_0)$ is given. To determine I_s , we must require that for a large $x = x_1$, $f_s(x_1)\exp[G(x_1)/kT] = 0$. Then

$$I_s = D(x_0)f_s(x_0) \left\{ \int_{x_0}^{x_1} dx' \exp[G(x')/kT] \right\}^{-1} \quad (II.40)$$

Eqs. (II.38), (II.39) and (II.40) represent the solution to the stationary nucleation problem in the continuous formulation.

Let us compare now the results of both formulations. First, by inspecting Eqs. (II.34) and (II.39) we find that

$$x_n \frac{\bar{B}(x-1)}{\bar{\alpha}(x) + \bar{\gamma}(x)} \quad \text{corresponds to} \quad \frac{F(x)}{D(x)} .$$

We can assess the validity of the continuous formulation in the following manner. Write

$$\lambda_n \frac{\bar{\beta}(x-1)}{\bar{\alpha}(x) + \bar{\gamma}(x)} = \lambda_n \frac{2D(x-1) + F(x-1)}{2D(x) - F(x)}$$

by using the definitions of F and D in Eqs. (II.18) and (II.19). If we now assume that

$$\frac{F(x-1)}{D(x-1)} \approx \frac{F(x)}{D(x)} \quad (\text{II.41})$$

and that

$$\left| \frac{F(x)}{D(x)} \right| < 1 \quad (\text{II.42})$$

then we may employ the following expansion

$$\lambda_n \frac{2D + F}{2D - F} \approx \frac{F}{D} \left\{ 1 + \frac{1}{3} \frac{F}{2D} + \frac{1}{5} \left(\frac{F}{2D} \right)^2 + \dots \right\}$$

We can conclude that both formulations lead to nucleation barriers $G(x)$ which are comparable provided that $F(x)/D(x)$ satisfies the conditions (II.41) and (II.42).

It can be seen from Fig. II.1, which shows the ratio $F(x)/D(x)$ for the case of fast-neutron irradiation in a breeder reactor, that the continuous formulation is applicable for $x > 10$ when the irradiation temperature is below 600°C. If the effect of gases were included in the nucleation theory, the ratio F/D would also become small for $x > 10$ even for the high temperature case.

In order to show the equivalence of the expressions (II.35) and (II.40) we write the stationary nucleation rate for the discrete case as

$$I_s = n(1) \left\{ \int_{x_0}^x dx \frac{1}{\bar{B}(x)} \exp[G(x)/kT] \right\}^{-1}$$

where

$$\begin{aligned} G(x)/kT &= - \int_{x_0}^x dx \ln \frac{\bar{B}(x-1)}{\bar{\alpha}(x) + \bar{\gamma}(x)} \\ &\equiv - \int_{x_0}^x dx \left\{ \ln \frac{2D(x) + F(x)}{2D(x) - F(x)} - \frac{d}{dx} \ln [2D(x) + F(x)] \right\} \\ &\equiv \frac{2D(x) + F(x)}{2D(x_0) + F(x_0)} - \int_{x_0}^x dx F(x)/D(x) \end{aligned}$$

Hence, since $2D(x) + F(x) = 2\beta(x)$

$$I_s = n(1)\beta(x_0) \left\{ \int_{x_0}^x dx \exp \left[- \int_{x_0}^x dx' F(x')/D(x') \right] \right\}^{-1}$$

which is essentially the same result as Eq. (II.40) if we identify $n(1)$ with $f_s(x_0)$ and disregard the difference between $\beta(x_0)$ and $D(x_0)$.

In conclusion we can state that the Fokker-Planck equation (II.20) is a sufficiently accurate approximation to the master equation (II.15) if

$$\frac{d}{dx} \ln [2D(x) + F(x)] \ll \ln \frac{2D + F}{2D - F}$$

and if $F(x)/2D(x) \ll 1$. We may combine both of these conditions into

$$\frac{d}{dx} \ln \bar{B}(x) \ll F(x)/D(x) \ll 2 \quad (\text{II.42})$$

Using Eq. (II.11) and assuming that $Z_v^0(x) \equiv 1$ the left hand side of the inequality (II.42) is equal to $\frac{1}{3}x^{-2/3}$, and the condition (II.42) can be restated as

$$\frac{1}{3x^{2/3}} \ll F(x)/D(x) \ll 2 \quad (\text{II.43})$$

This condition is satisfied to a satisfactory degree for $x \geq 10$ in all cases of practical interest with regard to void nucleation.

III. Path Integral Formulation

The "non-linear" Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial x} \{F(x) - \frac{\partial}{\partial x} D(x)\} f(x,t) \quad (\text{III.1})$$

and its multidimensional variants have received much attention lately [8,11,13,14] as the fundamental equations from which the behavior can be derived for systems far from the thermodynamic equilibrium state.

In particular, the formal solution of the Fokker-Planck equation as a path integral has been viewed [13,14] as the stepping stone towards establishing new quantities which take the place of the thermodynamic potential and the entropy as known from equilibrium thermodynamics.

Apart from its conceptual value, the path integral, or rather its discrete version, the path sum, can be considered as an aid to solve the Fokker-Planck equation numerically. The path sum transforms, as shown below, the distribution function $f(x,t)$ into the distribution function $f(x,t+\tau)$ for small time steps τ . The implementation of a numerical procedure is our main concern in this section, and the initial steps towards it will be described below.

Before discussing this approach further, we mention the reasons why a numerical solution of the partial differential eq. (III.1) is not practical with such conventional methods as finite differences.

Let us begin by noting that the distribution function $f(x,t)$ must be evaluated for the range of x values from 10^0 to 10^6 . A further complication is that $F(x)$ and $D(x)$ vary rapidly for small values of x . Hence, the nodal points x_i of a finite difference scheme should be spaced narrowly for small x ,

but be spaced further and further apart as x increases. As an example, let us select a spacing which results in equal intervals on the log-scale. Then, the interval length $\Delta x_i \sim x_i$.

The F-P equation (III.1) can be viewed as a diffusion equation in the size space x . In order for a void to advance by "random walk" in this space by an amount Δx_i , a time

$$\tau(x_i) \cong (\Delta x_i)^2 / D(x_i)$$

is needed. Since $D(x_i) \sim x_i^{1/3}$ for large x , we find that

$$\tau(x_i) \sim x_i^{5/3}.$$

Given the x -range of interest, $\tau(x_i)$ varies over almost ten orders of magnitude, as shown in Fig. III.1.

The time-step required for a stable integration of the differential equations in a finite difference scheme should be no larger than the smallest time $\tau(x_i)$. Consequently, from a practical point of view, only short-term numerical solutions can be obtained for $f(x,t)$. These solutions are then for small clusters only. Indeed, all previous attempts to compute the time-dependent nucleation of voids or loops were restricted to point defect clusters not visible in the electron microscope.

The vastly different time constants $\tau(x_i)$ are reminiscent of the very different time scales involved in loop nucleation, loop growth, void nucleation and void growth discussed in section II.

Because of these reasons, it is necessary to develop a new approach to the short-term and long-term integration of the F-P equation. The path sum does indeed offer a new possibility.

For an unrestricted non-linear Markov process, the distribution function $f(x,t)$ is defined over the entire domain $-\infty < x < \infty$. Furthermore, it can in this case be normalized, i.e.

$$\int_{-\infty}^{+\infty} f(x,t) dx = 1. \quad (\text{III.2})$$

Several investigators [15,16,17,18] have derived for this case the path-integral solution. For our purposes, we give the path sum as stated by Dekker [17].

$$f(x,t+\tau) = \int_{-\infty}^{+\infty} dx_0 W(x,x_0;\tau) f(x_0,t) \quad (\text{III.3})$$

The transition probability is given by

$$W(x,x_0;\tau) = [4\pi\tau D(x_0)]^{-1} \exp\left\{-\frac{[(x-x_0)-\tau F(x_0)]^2}{4\tau D(x_0)}\right\} \quad (\text{III.4})$$

One can interpret Eq. (III.3) in the following manner: The clusters within the interval dx_0 around x_0 are spread after the time τ into a Gaussian distribution given by Eq. (III.4) whose standard deviation is $\sqrt{2\tau D(x_0)}$ and whose mean has shifted from x_0 to $x_0 + \tau F(x_0)$. The new distribution function at time $(t+\tau)$ is a superposition of such Gaussians weighted by the value of the previous distribution, $f(x_0,t)$. Multiple applications of small-time transformations lead to the formal solution, the path integral, when the number of applications increases beyond bounds and at the same time $\tau \rightarrow 0$. For practical computations, however, we retain a finite time step τ .

The Eq. (III.3) cannot be applied to our problem of nucleation because the size space is restricted to the domain $1 \leq x < \infty$, and the size distribution function cannot be normalized to one. Rather, in our case

$$\int_1^{\infty} f(x,t) = N(t)$$

where $N(t)$ is the total number of clusters of all sizes.

In extending the path integral approach to the restricted non-linear Markov process of void nucleation we assume for the sake of simplicity that the continuous description of the cluster size distribution can be used for the entire domain $1 \leq x < \infty$. The boundary condition at $x = 1$ is then

$$f(1,t) = C_v(t) \quad (\text{III.5})$$

where C_v is the mono-vacancy concentration.

In order to find the path sum solution for our case, we note first that the transition probability $W(x, x_0; \tau)$ for the unrestricted case has the form of Green's function for a F-P equation with constant diffusion and drift coefficients, $D(x_0)$ and $F(x_0)$, taken at the pre-point x_0 . This Green's function is in fact obtained by transforming the F-P equation with constant coefficients into a diffusion equation with no drift term. We shall make use of this procedure now to find the corresponding Green's function for the half-space $1 \leq x < \infty$. Accordingly, we seek the Green's function of the equation

$$D \frac{\partial^2 f}{\partial x^2} - F \frac{\partial f}{\partial x} - \frac{\partial f}{\partial t} = 0 \quad (\text{III.6})$$

and subsequently its solution $f(x,t)$ which satisfies the initial condition

$$f(x,0) = \phi(x) \quad (\text{III.7})$$

and the boundary condition of Eq. (III.5). As Eq. (III.6) is linear, we may write for the solution

$$f(x,t) = h(x,t) + g(x,t) , \quad (\text{III.8})$$

where $h(x,t)$ is the homogeneous solution to Eq. (III.6) with the initial and boundary conditions

$$h(x,0) = 0 \quad (\text{III.9})$$

$$h(1,t) = C_v(t) . \quad (\text{III.10})$$

$g(x,t)$ is the inhomogeneous solution which satisfies

$$g(x,0) = \phi(x) \quad (\text{III.11})$$

$$g(1,t) = 0 \quad (\text{III.12})$$

Let us introduce the transformation

$$f(x,t) = \psi(x,t) \exp\left\{\frac{F}{2D} (x-1) - \frac{F^2}{4D} t\right\} \quad (\text{III.13})$$

and insert it into Eq. (III.6). We obtain then the simple diffusion equation without drift,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{D} \frac{\partial \psi}{\partial t} \quad (\text{III.14})$$

The homogeneous and inhomogeneous solutions $\eta(x,t)$ and $\theta(x,t)$ which correspond to $h(x,t)$ and $g(x,t)$ satisfy the following initial and boundary conditions

$$\eta(x,0) = 0 \quad (\text{III.15})$$

$$\eta(1,t) = C_v(t) \exp\left[\frac{F^2}{4D} t\right] \quad (\text{III.16})$$

$$\theta(x,0) = \phi(x) \exp\left[-\frac{F}{2D}(x-1)\right] \quad (\text{III.17})$$

$$\theta(1,t) = 0 \quad (\text{III.18})$$

The Green's function for Eq. (III.14) which vanishes at the boundary $x=1$ is given by

$$G(x,t;x',t') = [4\pi D(t-t')]^{-1/2} * \quad (\text{III.19})$$

$$* \left\{ \exp\left[-\frac{(x-x')^2}{4D(t-t')}\right] - \exp\left[-\frac{(x+x'-2)^2}{4D(t-t')}\right] \right\}.$$

The homogeneous solution is then

$$\eta(x,t) = D \int_0^t \eta(1,t') \frac{\partial}{\partial x} G(x,t;1,t') dt' \quad (\text{III.20})$$

and the inhomogeneous one is

$$\theta(x,t) = \int_1^\infty \theta(x',0) G(x,t;x',0) dx' \quad (\text{III.21})$$

We transform now back to the F-P equation and obtain

$$h(x,t) = D \exp\left[\frac{F}{2D}(x-1) - \frac{F^2}{4D}t\right] * \quad (\text{III.22})$$

$$* \int_0^t C_V(t') \exp\left[\frac{F^2}{4D}t'\right] \frac{\partial}{\partial x'} G(x,t;1',t') dt'$$

and

$$g(x,t) = \exp\left[\frac{F}{2D}x - \frac{F^2}{4D}t\right] * \quad (\text{III.23})$$

$$* \int_1^\infty \exp\left[-\frac{F}{2D}x'\right] \phi(x') G(x,t;x',0) dx'$$

Since we only need the short-time expressions we may assume that C_V is constant.

Then

$$h(x,t) = \frac{1}{2}C_v \left\{ \operatorname{erfc}\left[\frac{x-1-Ft}{2\sqrt{Dt}}\right] + \exp\left[\frac{F}{D}(x-1)\right] \operatorname{erfc}\left[\frac{x-1+Ft}{2\sqrt{Dt}}\right] \right\}. \quad (\text{III.24})$$

Eq. (III.23) may be written as

$$g(x,t) = \int_1^{\infty} \phi(x_0) W(x,t;x_0,0) dx_0 \quad (\text{III.25})$$

where

$$W(x,t;x_0,0) = [4\pi Dt]^{-1/2} \left\{ \exp\left[-\frac{(x-x_0-Ft)^2}{4Dt}\right] - \exp\left[\frac{F}{D}(x-1)\right] \exp\left[-\frac{(x+x_0-2+Ft)^2}{4Dt}\right] \right\} \quad (\text{III.26})$$

As we apply these results to a path sum formulation for the solution of the F-P equation (III.1) with variable diffusion and drift coefficient, we must take F and D at the pre-point x_0 when using Eq. (III.26) as the transition probability. The homogeneous solution, however, contains then the coefficients F and D taken at $x = 1$.

The path integral solution for the restricted non-linear Markov process is then given by

$$f(x,t+\tau) = h(x,t+\tau) + \int_1^{\infty} W(x,x_0;\tau) f(x_0,t) dx_0$$

(III.27)

where

$$W(x, x_0; \tau) = [4\pi D(x_0)\tau]^{-1/2} * \left\{ \exp\left[-\frac{(x-x_0-\tau F(x_0))^2}{4\tau D(x_0)}\right] - \exp[F(x_0)(x-1)/D(x_0)] \exp\left[-\frac{(x+x_0-2+\tau F(x_0))^2}{4\tau D(x_0)}\right] \right\} \quad (\text{III.28})$$

and

$$h(x, t+\tau) = \frac{1}{2} C_v(t) \left\{ \operatorname{erfc}\left[\frac{x-1-\tau F(1)}{2\sqrt{\tau D(1)}}\right] + \exp[F(1)(x-1)/D(1)] \operatorname{erfc}\left[\frac{x-1+\tau F(1)}{2\sqrt{\tau D(1)}}\right] \right\} \quad (\text{III.29})$$

We note that Eq. (III.27) to (III.29) represent to our knowledge the first path sum formulation of a restricted non-linear Markov process. A numerical method to solve Eq. (III.27) is under investigation.

IV. Steady State Void Nucleation

IV.1. The Numerical Evaluation Procedure

Based on the discrete formulation, the nucleation rate for the steady state is given by

$$I_s = C_v \left\{ \sum_{x=1}^{N-1} \bar{\beta}^{-1}(x) \exp[G(x)/kT] \right\}^{-1} \quad (IV.1)$$

where the nucleation barrier potential is

$$G(x)/kT = - \sum_{\xi=z}^x \ln \left[\frac{\bar{\beta}(\xi-1)}{\bar{\alpha}(\xi) + \bar{\theta}(\xi)} \right] \quad (IV.2)$$

The rate coefficients $\bar{\alpha}$, $\bar{\beta}$, $\bar{\theta}$ are those of eqs. (II.10) to (II.12). The solution of the rate equation for vacancies and interstitials, eqs. (II.13) and (II.14), can be written as

$$D_v C_v = D_v (\bar{F} + \bar{C}_v) \quad (IV.3)$$

$$D_i C_i = D_v \bar{F} \bar{Z}_v / \bar{Z}_i, \quad (IV.4)$$

where

$$\bar{Z}_i = \sum_s N^s A^s Z_i^s / \bar{N} \quad (IV.5)$$

is the sink-averaged interstitial bias factor, and Z_i^s is the specific bias factor for sinks of type "s".

$$\bar{N} = \sum_s N^s A^s \quad (IV.6)$$

is the average sink density, and N^s and A^s are the density and the geometric size factor for sinks of type "s". For a void, for example, the geometric size factor is

$$A^0(x) = 4\pi r(x) = (4\pi)^{2/3} (3\Omega x)^{1/3} \quad (\text{IV.7})$$

$\bar{Z}_v$ is the sink-averaged vacancy bias factor, defined analogously to $\bar{Z}_i$.

The sink-averaged equilibrium vacancy concentration is defined as

$$\bar{C}_v^s = \sum_s N^s A^s Z_v^s C_v^s / \sum_s N^s A^s Z_v^s \quad (\text{IV.8})$$

where C_v^s is the vacancy concentration in thermal equilibrium with sinks of type "s". An example is the vacancy concentration $C_v^0(x)$, Eq. (II.27), in thermal equilibrium with a void of size x .

Finally, the radiation-induced vacancy concentration is given by

$$\bar{F} = \frac{\bar{N} \bar{Z}_i}{2\kappa D_v} \left\{ \left[\left(1 + \frac{\kappa D_v \bar{C}_v}{\bar{N} \bar{Z}_i} \right)^2 + 4P\kappa / (N Z_i Z_v) \right]^{1/2} - \left(1 + \frac{\kappa D_v \bar{C}_v}{\bar{N} \bar{Z}_i} \right) \right\} \quad (\text{IV.9})$$

where P is the production rate of Frenkel pairs surviving the in-cascade recombination, and

$$\kappa = 4\pi r_0 / D_v = n_0 b / D_v \quad (\text{IV.10})$$

is the coefficient for the recombination rate $\kappa D_v C_v D_i C_i$. We can specify κ either by a capture radius r_0 of vacancies for interstitials or by the number n_0 of lattice sites from which capture takes place.

With the above definitions we may write

$$\frac{\bar{\alpha}(x) + \bar{\theta}(x)}{\bar{\beta}(x-1)} = \left[\frac{Z_i^0(x) A^0(x)}{Z_v^0(x-1) A^0(x-1)} \frac{\bar{Z}_v}{\bar{Z}_i} F + C_v^0(x) \right] / [F + \bar{C}_v]$$

so that $G(x)$ can be written as

$$G(x)/kT = \sum_{\xi=2}^x \ln \left[1 + \frac{\Delta Z(\xi) F + C_v^0(x) - \bar{C}_v}{F + \bar{C}_v} \right] \quad (\text{IV.11})$$

with

$$\Delta Z(x) = \frac{\bar{Z}_v}{\bar{Z}_i} \frac{Z_i^0(x) A^0(x)}{Z_v^0(x-1) A^0(x-1)} - 1 \quad (\text{IV.12})$$

being the net bias of a void with size x .

The steady state nucleation rate can be expressed in the following form:

$$I_s = D_b (\bar{F} + \bar{C}_v)^2 / \left\{ \sum_{x=1}^{N-1} \exp[G(x)/kT] / [A^0(x) Z_v^0(x)] \right\} \quad (\text{IV.13})$$

For the numerical evaluation of Eqs. (IV.11) and (IV.13) a maximum cluster size of the order of $N = 10^4$ must be selected. A simple summation of all N terms is very inefficient, however, and not required for satisfactory accuracy. Therefore, only the first ten terms were summed as indicated in the above equations. The contributions of terms with $x > 10$ were computed in the following way.

Nodal points on the size axis were selected such that a logarithmic interval spacing was obtained. The nodal points can be represented by

$$x_\ell = 10^{a(\ell-1)} + 10,$$

where a is a constant determining the logarithmic spacing of the nodal points. The summation of the function $L(x)$ over the size space was then replaced by

$$\sum_{x=1}^N L(x) \rightarrow \sum_{x=1}^{10} L(x) + \frac{1}{2} \sum_{\ell=1}^{\ell_{\max}} [L(x_\ell) + L(x_{\ell-1})] \cdot (x_\ell - x_{\ell-1})$$

IV.2 The Void Bias Factor

The nucleation barrier potential as defined in Eq. (IV.11) depends critically on the ratio

$$Z_i^0(x)/Z_v^0(x-1) ,$$

where Z_i^0 and Z_v^0 are the void bias factors for interstitial and vacancy capture, respectively. It was shown earlier [9] that the void bias factor for interstitial capture at a void in a pure metal is so large for small void radii that void nucleation would not be possible. The origin of this strong void bias is to be found in the strong image interaction of an interstitial with a void. This image interaction is attractive unless the void is surrounded by an impurity shell which has a shear modulus slightly larger than the one for the matrix.

In Appendix A, a detailed analysis is given of the effect of a surface coating on the void bias factor. Included in the analysis is also the effect of the local shear modulus on the point defect energy.

Void nucleation calculations are in progress with a computer program that follows the computational procedure described in Section IV.1, and that utilizes the expressions for the void bias factors derived in Appendix A.

V. Modeling of Irradiation Creep

V.1 Assessment of Irradiation Creep Mechanisms

The experimental evidence of stress effects on the microstructure of irradiated materials provides an important confirmation of the SIPA creep mechanism. This is discussed in detail in two papers contained in Appendix B.

An important accomplishment in this context is the explanation of the size distribution for interstitial loops and the effect of stress on this size distribution.

An extensive documentation of the theoretical and numerical work for computing the size distribution is in preparation. Some results were already incorporated in the two papers of Appendix B.

V.2 Single Crystal Irradiation Creep

In order to elucidate further the mechanistic processes of irradiation creep, the most decisive experiments in the future will be on single crystal specimens.

For this reason, irradiation creep relationships were derived for face-centered-cubic single crystals. Three different mechanisms were considered:

- 1) Irradiation creep due to SIPA at faulted loops, called SIPAL creep.
- 2) Irradiation creep due to SIPA at edge dislocations and perfect loops, called SIPAD creep.
- 3) Irradiation creep due to climb-controlled glide of dislocations, called CCG creep.

For all mechanisms it was assumed that no preferred Burgers vector exists for the loop population or the dislocation network. Hence, the derived irradiation creep laws are for virgin samples with no prior deformation.

It was furthermore assumed that in the case of the CCG creep, the glide distance is proportional to the shear stress on the glide plane.

A paper describing the derivation of the irradiation creep laws is being prepared. The final result can be written in the concise form

$$\dot{\epsilon}_{ij} = \sum_{kl} \psi_{ijkl} \left(\sigma_{kl} - \frac{1}{3} \delta_{kl} \sigma_{nn} \right) \quad (V.1)$$

where $\dot{\epsilon}_{ij}$ is the creep strain rate tensor,

$\sigma_{nn} = \sigma_{11} + \sigma_{22} + \sigma_{33}$, and

$$\psi_{ijkl} = \psi_n (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \eta \sum_{n=1}^3 a_{in} a_{jn} a_{kn} a_{ln}) \quad (V.2)$$

is the irradiation creep compliance tensor.

The a_{in} are the directional cosines between the crystallographic axis of the fcc lattice and the axis of the coordinate system in which the external stresses σ_{ij} are specified.

The parameter η is given by

$$\eta = \begin{cases} 2 & \text{for the SIPAL} \\ 1 & \text{for the SIPAD} \\ -1 & \text{for the CCG} \end{cases}$$

mechanism. The three different scalar functions ψ_n depend on temperature, dose rate, and sink densities.

Assuming that only one of the three mechanisms is the dominant one, Eq. (1) was evaluated for a uniaxial tension experiment and for a torsion experiment. If we select the specimen axis as the x_3 -axis, Eq. (1) gives for the uniaxial tension case the result

$$\dot{\epsilon} = \frac{1}{3} (2\psi_{3333} - \psi_{3311} - \psi_{3322})\sigma \quad (V.3)$$

Figs. V.1 and V.3 show the quantity $3\dot{\epsilon}/\psi_{\eta}\sigma$ for different crystal orientations. The case for the SIPAL mechanism shown in Fig. V.1 is particularly notable, because a single crystal pulled along a $\{100\}$ -direction would not creep, whereas maximum creep would be obtained for tension in a $\{111\}$ -direction.

In the case of torsion we denote the twist-angle per unit length of the torsion specimen by α . It is then found by integrating Eq. (V.1) over the cross-section of the torsion specimen that

$$\dot{\alpha} = \{\psi_{2323} + \psi_{1313}\} 2\mu \alpha_{el} \quad (V.4)$$

where μ is the shear modulus and α_{el} the elastic twist angle. The quantity $\dot{\alpha}/(2\mu \alpha_{el} \psi_{\eta})$ is then only a function of the crystal orientation, and it is shown in Figs. V.4 to V.6 for the three creep mechanisms considered.

V.3 Implications of the Crystallographic Dependence of Irradiation Creep.

Irradiation creep has so far been measured only in polycrystals. An irradiation creep law for an aggregate of differently oriented grains must be derived from the creep law of single crystals. In order to preserve the compatibility of a continuous medium, different grains must develop different residual stress levels. The variation of the internal stress level from grain to grain gives rise to various effects. We have explored so far two effects. One, described in Appendix C, is the appearance of anelastic effects in a polycrystal. Under load changes these anelastic effect are easily confused with transient or primary irradiation creep occasionally observed in inreactor creep experiments.

The second effect is related to the stress-buildup in surface grains, and its significance in ion-bombardment experiments for swelling and blistering studies is discussed in Appendix D.

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