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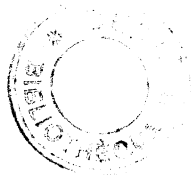

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Higher-Order Recombination Effects in Radiation Damage

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by

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ABSTRACT

Radiation damage processes in structural materials are important for the determination of fission and fusion reactor performance. To model the evolving microstructure during particle bombardment of metals using the rate theory of void swelling, irradiation creep and growth, it is necessary to evaluate the strengths of the various sinks for migrating point defects. Conventionally, because of the complexity of the problem, bulk recombination of such defects has been neglected in sink strength derivations.

In this paper we calculate, by means of an original mathematical formulation, void sink strengths which include the higher-order bulk recombination effects. Detailed comparison of computed void swellings obtained with our new void sink strength expressions and those derived previously disregarding bulk recombination show rigorously, for the first time, the effect of neglecting the higher-order corrections to the void sink strengths arising from bulk recombination.

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1. Introduction

The phenomena of void swelling, irradiation creep and growth observed in structural materials have important consequences for fission and fusion reactor performance. The fundamental microstructural processes manifesting themselves in these physical observables are now fairly well understood, and may be described mathematically using a chemical rate theory formulation. Crucial to the employment of this model is the evaluation of the strengths attributed to the various sinks for migrating point defects in the rate theory continuum. Brailsford and Bullough (1980) have discussed the philosophy and present state-of-the-art for the sink strength determination in a recent comprehensive work, and have noted that (apart from empirical modifications or perturbation and iterative treatments) bulk recombination of point defects is conventionally ignored in such derivations. More recently, however, Wood, Jones and Pierce (1980) have calculated, for the first time, sink strength expressions including bulk recombination effects directly; in their case for the thin foil surface sink, as used in high voltage electron microscopy (HVEM) studies.

Here, we extend the Wood, Jones and Pierce analysis tackling the generally more important void sink for which strengths in the presence of bulk recombination are rigorously derived. Numerical sink strength values are given for expressions derived both without and with bulk recombination, and the results compared. To examine the sensitivity of the different formulae appropriate void swelling calculations have been performed, and it is concluded that the sink strengths obtained previously by neglecting bulk recombination introduce only small errors in the regime of physical interest. Using results for the void case, the derivation of grain boundary sink strengths with bulk recombination is presented for completeness in an appendix to this paper.

2. Void Sink Strengths

We consider the diffusive flow of irradiation produced point defects to a spherical void of radius r_c embedded in an infinite and homogeneous lossy continuum. Point defect loss in the medium is to fixed extended sinks, such as dislocations, grain boundaries and cavities, and through bulk recombination of interstitials and vacancies. The steady state continuity equations for the interstitial (i) and vacancy (v) fractional concentrations outside the void (i.e. for $r_c \leq r < \infty$) are;

$$\frac{D_i}{r^2}\frac{d}{dr}\left(r^2\frac{dc_i}{dr}\right) + K - D_i k_i^2 c_i - \alpha c_i c_v = 0, \qquad (1)$$

and

$$\frac{D_v}{r^2}\frac{d}{dr}\left(r^2\frac{dc_v}{dr}\right) + K - D_v k_v^2 c_v - \alpha c_i c_v = 0, \qquad (2)$$

where spherical coordinates with their origin at the centre of the cavity have been adopted. Here D_i and D_v are the interstitial and vacancy diffusivities respectively, K is the point defect production rate, α is the bulk recombination coefficient, and k_i^2 and k_v^2 denote sums of the strengths of all sinks in the lossy continuum for migrating interstitials and vacancies respectively. Conceiving the void as an ideal sink, the solution of the coupled differential equations (1) and (2) is subject to the boundary condition;

$$c_i = c_v = 0 \quad \text{at} \quad r = r_c, \qquad (3)$$

and to the requirement that;

$$c_i = c_i^\infty, \quad c_v = c_v^\infty \quad \text{when } r \to \infty \qquad (4)$$

be finite.

Brailsford and Bullough (1980) have shown how void sink strengths may be calculated by equating the respective loss rates of point defects to the central void with the corresponding loss rates in the lossy continuum: the

resulting expressions for the sink strengths are, in terms of the solution of equations (1) and (2):

$$k_{iC}^2 = 4\pi r_C^2 C_C \left.\frac{dc_i}{dr}\right]_{r=r_C} \Big/ c_i^\infty \tag{5}$$

and

$$k_{vC}^2 = 4\pi r_C^2 C_C \left.\frac{dc_v}{dr}\right]_{r=r_C} \Big/ c_v^\infty, \tag{6}$$

respectively, where C_C denotes the volume concentration of voids in the medium. Assuming $\alpha c_i c_v = 0$ (nonlinear bulk recombination has been ignored in most previous derivations of void sink strengths) the uncoupled equations resulting from (1) and (2) are readily solved yielding the *interstitial sink strength*;

$$k_{iC}^2 = 4\pi r_C C_C (1+k_i r_C), \tag{7}$$

and the *vacancy sink strength*;

$$k_{vC}^2 = 4\pi r_C C_C (1+k_v r_C). \tag{8}$$

To allow for recombination, (1) and (2) may be written in terms of the variables $y_i = D_i c_i$ and $y_v = D_v c_v$, to yield;

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dy_i}{dr}\right) + K - k_i^2 y_i - \frac{\alpha}{D_i D_v} y_i y_v = 0, \tag{9}$$

and

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dy_v}{dr}\right) + K - k_v^2 y_v - \frac{\alpha}{D_i D_v} y_i y_v = 0. \tag{10}$$

Defining,

$$\left.\begin{aligned} y &= (y_i + y_v)/2 \\ z &= (y_i - y_v)/2 \\ k_i^2 &= k^2 + \beta \\ k_v^2 &= k^2 - \beta \\ A &= \alpha/D_i D_v, \end{aligned}\right\} \tag{11}$$

equations (9) and (10) become;

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dy}{dr}\right) + K - k^2y - Ay^2 = \beta z - Az^2, \tag{12}$$

and

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dz}{dr}\right) - k^2z = \beta y. \tag{13}$$

Also, the condition (3) becomes;

$$y = z = 0 \quad \text{at } r = r_c, \tag{14}$$

and the requirement (4) is replaced by;

$$y = y^\infty,\ z = z^\infty \quad \text{when } r \to \infty \tag{15}$$

be bounded.

In their paper treating foil surface sink strengths with bulk recombination, Wood, Jones and Pierce (1980) have justified introducing the approximate relation;

$$\beta z - Az^2 = 0, \tag{16}$$

to solve an equation similar to (12) above. Here, we also adopt this relation* and consider henceforth, instead of (12), the equation;

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dy}{dr}\right) + K - k^2y - Ay^2 = 0 \tag{17}$$

together with (13). Employing the asymptotic solution of (17) for $r \to \infty$;

$$y^\infty = k^2Q/2A, \tag{18}$$

where

$$Q = (1 + 4AK/k^4)^{\frac{1}{2}} - 1, \tag{19}$$

together with the quantities;

$$\left.\begin{aligned} f &= k^2r_c^2Q/2 \\ S &= 1/Q, \end{aligned}\right\} \tag{20}$$

and the normalized variables;

---

*The errors incurred in adopting this relation for the present analysis are discussed at the end of this section.

$$\left.\begin{aligned} r' &= r/r_C \\ y' &= y/y^{\infty} \\ z' &= z/y^{\infty} \end{aligned}\right\} \tag{21}$$

equations (17) and (13) can be reformulated to give;

$$\frac{1}{r'^2}\frac{d}{dr'}\left(r'^2\frac{dy'}{dr'}\right) + f\left\{(1+S)^2 - (y'+S)^2\right\} = 0, \tag{22}$$

and

$$\frac{1}{r'^2}\frac{d}{dr'}\left(r'^2\frac{dz'}{dr'}\right) - k^2r_C^2z' = \beta r_C^2 y', \tag{23}$$

respectively. The condition (14) then becomes;

$$y' = z' = 0 \quad \text{at } r' = 1, \tag{24}$$

and the requirement (15) is written;

$$y' = 1,\ z' = z'^{\infty} \quad \text{when} \quad r' \to \infty \tag{25}$$

with z'^{∞} bounded. The nonlinear differential equation (22) is of the Emden type (Davis, 1962) and apparently does not have an exact solution in closed form. To establish a convenient and accurate approximate solution, we use the limit of vanishing recombination, $A \to 0$, when (22) degenerates to the linear differential equation*;

$$\frac{1}{r'^2}\frac{d}{dr'}\left(r'^2\frac{dy'}{dr'}\right) + k^2r_C^2\,(1-y') = 0. \tag{26}$$

The solution of (26), subject to (24) and (25), is;

$$y' = 1 - \frac{1}{r'}\exp[-kr_C(r'-1)]. \tag{27}$$

The form of (27) suggests the ansatz;

$$y' = 1 - \frac{1}{r'}\exp[-G(r'-1)], \tag{28}$$

with a (positive) constant G to be determined, as an approximate solution of equation (22) when recombination is present.

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*Notice that $y^{\infty} = K/k^2$ in (21) for $A \to 0$ according to (18) and (19).

Inserting the expression for y' from equation (28), into equation (22) leads to the implicit relationship;

$$G^2 = f\left\{2(1+S) - \frac{1}{r'}\exp[-G(r'-1)]\right\}, \tag{29}$$

which gives G as a function of r' rather than a constant, as assumed in the derivation of (29) from (22). An approach to remove this contradiction is indicated by expanding y' as a series in powers of G;

$$y' = 1 - \frac{1}{r'}\left\{1 + \sum_{n=1}^{\infty}(-1)^n \frac{1}{n!} G^n (r'-1)^n\right\}. \tag{30}$$

Hence, we consider replacing the function G(r') from equation (29) by its moments;

$$\langle G^n\rangle = \lim_{R'\to\infty} \frac{3}{R'^3-1} f^{n/2} \int_1^{R'} r'^2\{2(1+S)- \frac{1}{r'}\exp[-G(r')(r'-1)]\}^{n/2}\, dr', \quad n = 1,2,3,\ldots . \tag{31}$$

Because of the inequalities;

$$S > 0, \tag{32}$$

and

$$\frac{1}{r'}\exp[-G(r')(r'-1)] < 1, \tag{33}$$

(the latter holding in the entire range $1 < r' < \infty$ since, due to (29), G(r') is positive definite) we may expand the integrand in equation (31) in a binomial series to obtain;

$$\langle G^n\rangle = [2f(1+S)]^{n/2}\left\{1 + \sum_{\nu=1}^{\infty}(-1)^{\nu}\binom{n/2}{\nu}[2(1+S)]^{-\nu} \times \lim_{R'\to\infty} \frac{3}{R'^3-1}\int_1^{R'} (r')^{2-\nu}\exp[-\nu G(r')(r'-1)]dr'\right\}, \quad n = 1,2,3,\ldots \tag{34}$$

The following outcome is easily verified;

$$\lim_{R'\to\infty} \frac{3}{R'^3-1}\int_1^{R'} (r')^{2-\nu}\exp[-\nu G(r')(r'-1)]dr' = 0, \quad \nu = 1,2,3,\ldots . \tag{35}$$

Hence,

$$\langle G^n \rangle = [2f(1+S)]^{n/2}, \quad n = 1,2,3,... \tag{36}$$

revealing the identity,

$$\langle G \rangle^n \equiv \langle G^n \rangle , \quad n = 1,2,3, \ldots . \tag{37}$$

If we choose in equation (28),

$$G = \langle G \rangle = [2f(1+S)]^{\frac{1}{2}}, \tag{38}$$

or, by the definitions (20),

$$G = kr_c(1 + Q)^{\frac{1}{2}}, \tag{39}$$

we obtain an approximation to the solution of equation (22) which reproduces all moments of $G(r')$ exactly and, since

$$G = kr_c \quad \text{if} \quad A \to 0, \tag{40}$$

tends to the exact solution (27) in the zero recombination limit.

We are now able to solve equation (23) for z' subject to (24) and (25). Substitution of y' given by equation (28) yields*;

$$z' = \left\{ \begin{array}{l} \beta\left\{\left(\frac{1}{k^2} + \gamma\right)\frac{1}{r'} \exp[-kr_c(r'-1)] - \frac{1}{k^2} - \frac{\gamma}{r'} \exp[-G(r'-1)]\right\} , \; G > kr_c \\ \beta\left\{\left(\frac{1}{k^2} - \delta\right)\frac{1}{r'} \exp[-kr_c(r'-1)] - \frac{1}{k^2} + \delta \exp[-kr_c(r'-1)]\right\} , \; G = kr_c \end{array} \right\} \tag{41}$$

*By following an analogous procedure to that outlined above for the void sink taking bulk recombination effects into account, it can be shown that the theoretical results for point defect concentration profiles across irradiated thin foils given by Lam, Rothman and Sizmann (1974), and successfully employed by Wood, Jones and Pierce (1980) to derive related sink strengths, are obtained identically. In this case detailed comparison between the exact numerical solution of the corresponding steady state continuity equations and the approximate solution, equivalent to (28) and (41) with (39), displayed good agreement for computed defect concentrations, and led to accurate sink strengths and computed irradiation growth strains within a wide range of values for the parameters involved. From a physical viewpoint, it is clear that an extremely high accuracy in the solution of (17) is not necessary since, of the coupled equations (12) and (13), it is (13) that generates the important interstitial - vacancy differential effect in the sink strengths.

where

$$\gamma = r_C^2/(G^2 - k^2 r_C^2), \quad \delta = r_C/2k \tag{42}$$

The required void sink strengths from (5) and (6) are given in terms of the primed variables introduced by (21) and (25) by;

$$k_{iC}^2 = 4\pi r_C C_C \left[\frac{dy'}{dr'} + \frac{dz'}{dr'}\right]_{r'=1} \Big/ \left[1 + z'^{\infty}\right] \tag{43}$$

and

$$k_{vC}^2 = 4\pi r_C C_C \left[\frac{dy'}{dr'} - \frac{dz'}{dr'}\right]_{r'=1} \Big/ \left[1 - z'^{\infty}\right]. \tag{44}$$

Application of the expressions (28) and (41) finally yields the results for $G \geq kr_C$:

interstitial sink strength;

$$k_{iC}^2 = 4\pi r_C C_C \{\beta_i(1+G) + (1-\beta_i)[1 + Gkr_C/(G+kr_C)]\}, \tag{45}$$

vacancy sink strength;

$$k_{vC}^2 = 4\pi r_C C_C \{\beta_v(1+G) + (1-\beta_v)[1 + Gkr_C/(G+kr_C)]\}, \tag{46}$$

where;

$$\beta_i = k^2/(k^2 - \beta), \quad \beta_v = k^2/(k^2 + \beta). \tag{47}$$

Since $G \geq kr_C$ according to (39) and (40), the expressions (45) and (46) indicate that both interstitial and vacancy sink strengths are enhanced in the presence of bulk recombination. Furthermore, we note the limiting case of a neutral lossy continuum (where void growth cannot occur) whence $\beta = 0$, $\beta_i = \beta_v$ and thus $k_{iC}^2 \equiv k_{vC}^2$.

Having achieved our objective of determining void sink strengths with bulk recombination, we consider the error involved in the approximation (16). For dislocations the only biased sinks in the rate theory continuum (i.e. the only sinks admitting a strength for interstitials different to that for vacancies) we may write by use of (11)

$$\beta/k^2 \leq (Z_i - Z_v)/(Z_i + Z_v), \qquad (48)$$

where the parameters Z_i and Z_v define the preference of dislocations relative to vacancies. With typical values of Z_i and Z_v we find $\beta/k^2 \leq 0.1$, and more neutral sinks present in k^2 could imply $\beta/k^2 << 0.1$. We realise from (28) and (41) that

$$z'/y' = -\beta/k^2 \quad \text{when} \quad r' \to \infty; \qquad (49)$$

hence, it seems appropriate to neglect the terms on the right hand side of equation (12), the approximation (16). A more rigorous analysis on the sink strength expressions (45) and (46) for the zero recombination limit (40) in comparison to the exact formulae (7) and (8) reveals errors due to the adoption of (16) to be of order $(\beta/k^2)^2$ and are therefore at most 1% and often, substantially smaller.

3. Results and Discussion

The physical and irradiation data used in this section and purporting to relate to 316 stainless steel under HVEM conditions are given in table 1.

We have calculated values of void sink strengths for interstitials and vacancies derived both without, equations (7) and (8), and with, equations (45) and (46), the inclusion of bulk recombination effects. The results, presented in tables 2 to 5 for different temperatures covering the void swelling regime and a range of dislocation densities, exhibit the same features as previously found for the thin foil surface sink strengths (Wood et al. 1980), that is:

(1) The zero recombination results are independent of temperature and point defect production rate, behaviour which may be contrasted with that obtained when recombination is included. This feature is obvious since the expressions (45) and (46) include the recombination and diffusion coefficients and the defect production rate explicitly, while equations (7) and (8) do not.

(2) Rather large errors can originate in the zero recombination sink strength values at low temperatures and dislocation densities.

(3) The agreement between corresponding pairs of results is best at high temperatures and dislocation densities, i.e. when point defect loss due to bulk recombination becomes small.

However, simply comparing numerical steady state sink strength values may indicate little about the performance of such sink strengths in actual void swelling calculations. We have, therefore, alternatively incorporated the respective sink strength formulae, equations (45) and (46) on the one hand and equations (7) and (8) on the other hand, in the full rate theory void swelling VS2 computer program (Windsor, Bullough and Wood, 1980) which numerically integrates the rate equations with the recombination and thermal emission terms present. Figure 1 illustrates the predicted swelling as a function of temperature. The full curves have been calculated with the void sink strengths including bulk recombination, equations (45) and (46), whereas the dots refer to neglecting recombination in the sink strength derivation, equations (7) and (8). Figure 2 displays errors in swelling* which arise from the use of the sink strengths without recombination, for the results of figure 1: errors are revealed to be either positive or negative, and are always less than 4% in magnitude. For the identical set of results, figure 3 shows the evolution of the error in swelling with dose up to 100 dpa at 550^{o}C; this temperature being chosen because it gives the maximum error at 100 dpa (c.f. figure 2). The sign of the error changes from negative to positive between 10 and 20 dpa, and the error then increases to 100 dpa. At the same temperature, the calculated swelling against dislocation density behaviour

*Error in swelling is defined as the difference in swelling obtained using the void sink strengths without and with recombination relative to the swelling for the void sink strengths with recombination.

is presented in figure 4. Again, the curve and dots have been obtained, for 100 dpa dose, using the sink strengths with and without recombination, respectively. For this series of computations we have plotted, in figure 5, the error in swelling due to the employment of the sink strengths without recombination: as expected the error becomes very small at high dislocation densities. The maximum error, less than 4%, is found for a dislocation density of $\sim 10^{14}$ m^{-2}.

All the calculations described above have been repeated at a constant void concentration of 1×10^{21} m^{-3} for temperatures below 550°C to account for possible heterogeneous void nucleation at low temperatures*. Within this series of calculations the maximum error occurred at 400°C, the lowest temperature of computation. Hence, in figures 6 and 7 we show the computed error in swelling as a function of dose and dislocation density, respectively, for this temperature. Comparison of figures 3 and 6 indicates a qualitatively different behaviour with dose at these two temperatures: in the latter the error decreases monotonically from $\sim$ +6% to $\sim$ -10% between 0.1 dpa and 100 dpa. Figure 7 reveals larger errors than figure 5, the maximum error with the lower void concentration being $\sim$ -14% at a dislocation density of about 10^{15} m^{-2}.

4. Conclusion

By means of an original mathematical formulation we have derived, rigorously and for the first time, void sink strength expressions which take the higher-order bulk recombination effects into account, for use in the rate theory of void swelling.

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*This value for the void concentration is two orders of magnitude smaller than that following from the corresponding Arrhenius law in table 1 at a temperature of 400°C.

We have performed detailed swelling calculations employing both the new, with recombination, void sink strengths and formulae previously obtained by disregarding the recombination. The computations exhibit that the derived sink strength expressions without recombination yield generally acceptable results in the physical void swelling regime. Larger errors are found at low temperatures and moderately high dislocation densities when heterogeneous nucleation of voids is considered.

Acknowledgement

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Table 1

Data used in Calculations

Interstitial diffusion coefficient $D_i = D_i^o \exp(-E_i^m/k_BT)$;

$$D_i^o = 1\times10^{-7}\ m^2s^{-1},\quad E_i^m = 0.2\ eV.$$

Vacancy diffusion coefficient $D_v = D_v^o \exp(-E_v^m/k_BT)$;

$$D_v^o = 6\times10^{-5}\ m^2s^{-1},\quad E_v^m = 1.3\ eV.$$

Bulk recombination coefficient α given by $\alpha/D_i = 1\times10^{20}\ m^{-2}$.

Interstitial bias parameter $Z_i = 1.025$.

Vacancy bias parameter $Z_v = 1.0$.

Void radius (for sink strength calculations only) $r_c = 1\times10^{-8}m$.

Void concentration (for swelling calculations only) $C_c=C_c^o \exp(E_c/k_BT)$;

$$C_c^o = 2.73\times10^{12}\ m^{-3},\ E_c = 1.42\ eV.$$

Defect production rate $K = 5\times10^{-3}$ dpa s^{-1}.

Table 2

Void Sink Strengths Calculated at 300°C*

k^{2**},m^{-2}	Without Recombination		With Recombination	
	k^2_{iC}	k^2_{vC}	k^2_{iC}	k^2_{vC}
10^{12}	1.269	1.269	5.183	5.086
10^{13}	1.297	1.296	5.183	5.087
10^{14}	1.383	1.381	5.182	5.088
10^{15}	1.656	1.651	5.179	5.091
10^{16}	2.521	2.505	5.182	5.108
10^{17}	5.255	5.206	5.958	5.895

*Void sink strength values given per volume concentration of voids in units of 10^{-7} m.

**$k_i^2 = k^2 + \beta$

with $\beta/k^2 = (Z_i - Z_v)/(Z_i + Z_v)$

$k_v^2 = k^2 - \beta$

Table 3

Void Sink Strengths Calculated at 450°C*

k^{2**},m^{-2}	Without Recombination		With Recombination	
	k^2_{iC}	k^2_{vC}	k^2_{iC}	k^2_{vC}
10^{12}	1.269	1.269	2.259	2.234
10^{13}	1.297	1.296	2.258	2.235
10^{14}	1.383	1.381	2.257	2.236
10^{15}	1.656	1.651	2.262	2.244
10^{16}	2.521	2.505	2.629	2.611
10^{17}	5.255	5.206	5.259	5.210

*Void sink strength values given per volume concentration of voids in units of 10^{-7}m.

**$k_i^2 = k^2 + \beta$

with $\beta/k^2 = (Z_i - Z_v)/(Z_i + Z_v)$

$k_v^2 = k^2 - \beta$

Table 4

Void Sink Strengths Calculated at 600°C*

k^2**,m^{-2}	Without Recombination		With Recombination	
	k^2_{iC}	k^2_{vC}	k^2_{iC}	k^2_{vC}
10^{12}	1.269	1.269	1.665	1.656
10^{13}	1.297	1.296	1.665	1.656
10^{14}	1.383	1.381	1.665	1.657
10^{15}	1.656	1.651	1.736	1.730
10^{16}	2.521	2.505	2.525	2.509
10^{17}	5.255	5.206	5.256	5.206

*Void sink strength values given per volume concentration of voids in units of 10^{-7}m.

**$k_i^2 = k^2 + \beta$

with $\beta/k^2 = (Z_i - Z_v)/(Z_i + Z_v)$

$k_v^2 = k^2 - \beta$

Table 5

Void Sink Strengths Calculated at 750°C*

k^{2**},m^{-2}	Without Recombination		With Recombination	
	k^2_{iC}	k^2_{vC}	k^2_{iC}	k^2_{vC}
10^{12}	1.269	1.269	1.474	1.468
10^{13}	1.297	1.296	1.473	1.469
10^{14}	1.383	1.381	1.479	1.475
10^{15}	1.656	1.651	1.665	1.660
10^{16}	2.521	2.505	2.522	2.506
10^{17}	5.255	5.206	5.256	5.206

*Void sink strength values given per volume concentration of voids in units of 10^{-7} m.

**$k_i^2 = k^2 + \beta$

with $\beta/k^2 = (Z_i - Z_v)/(Z_i + Z_v)$

$k_v^2 = k^2 - \beta$

Appendix

Grain Boundary Sink Strengths

In this appendix we present a derivation of grain boundary sink strengths including bulk recombination, which closely parallels the presentation given for the void case in section 2.

Considering a spherical grain of radius R_G embedded in an infinite and homogeneous lossy continuum, the steady state continuity equations for the fractional concentrations of irradiation produced interstitials and vacancies *outside* the grain (i.e. for $R_G \leq r < \infty$) are;

$$\frac{D_i}{r^2}\frac{d}{dr}\left(r^2\frac{dc_i}{dr}\right) + K - D_i k_i^2 c_i - \alpha c_i c_v = 0, \qquad (A1)$$

and

$$\frac{D_v}{r^2}\frac{d}{dr}\left(r^2\frac{dc_v}{dr}\right) + K - D_v k_v^2 c_v - \alpha c_i c_v = 0, \qquad (A2)$$

whereas *inside* the grain (i.e. for $0 \leq r \leq R_G$) they are given by;

$$\frac{D_i}{r^2}\frac{d}{dr}\left(r^2\frac{d\bar{c}_i}{dr}\right) + K - D_i k_{iSC}^2 \bar{c}_i - \alpha \bar{c}_i \bar{c}_v = 0 \qquad (A3)$$

and

$$\frac{D_v}{r^2}\frac{d}{dr}\left(r^2\frac{d\bar{c}_v}{dr}\right) + K - D_v k_{vSC}^2 \bar{c}_v - \alpha \bar{c}_i \bar{c}_v = 0, \qquad (A4)$$

respectively. Here, spherical coordinates with their origin at the centre of the grain have been adopted and the quantities D_i, D_v, K, α, k_i^2 and k_v^2 are defined as in section 2. In addition, k_{iSC}^2 and k_{vSC}^2 denote sums of the strengths of all sinks within the (single crystal) grain for migrating interstitials and vacancies, respectively. We employ the ideal sink boundary condition;

$$c_i = c_v = 0, \quad \bar{c}_i = \bar{c}_v = 0 \quad \text{at} \quad r = R_G \qquad (A5)$$

in the two sets of coupled differential equations (A1) to (A4) together with the requirement that both

$$c_i = c_i^{\infty}, \quad c_v = c_v^{\infty} \quad \text{when } r \to \infty, \tag{A6}$$

and

$$\bar{c}_i = \bar{c}_i^{o}, \quad \bar{c}_v = \bar{c}_v^{o} \quad \text{when } r \to 0 \tag{A7}$$

be finite. The mathematical problem established for the range $R_G \leq r < \infty$ is formally the same as that of the void in section 2, and the problem for $0 \leq r \leq R_G$ is similar to that of the thin foil discussed previously (Wood et al., 1980, Lam et al., 1974).

Following Brailsford and Bullough (1980) grain boundary sink strengths may be obtained by equating the average point defect loss rates to the surface of the central grain with the respective loss rates in the lossy continuum. Use of the solutions of equations (A1) to (A4) therefore yields

$$k_{iGB}^2 = 2\pi R_G^2 C_G \left[\frac{dc_i}{dr} - \frac{d\bar{c}_i}{dr}\right]_{r=R_G} \Big/ c_i^{\infty} \tag{A8}$$

and

$$k_{vGB}^2 = 2\pi R_G^2 C_G \left[\frac{dc_v}{dr} - \frac{d\bar{c}_v}{dr}\right]_{r=R_G} \Big/ c_v^{\infty}, \tag{A9}$$

respectively, where C_G is the volume concentration of grains in the medium. We note that disregarding bulk recombination in (A1) to (A4) yields the *interstitial sink strength:*

$$k_{iGB}^2 = 2\pi R_G C_G \left\{1 + k_i R_G + (k_i^2/k_{iSC}^2)(k_{iSC} R_G \coth k_{iSC} R_G - 1)\right\} \tag{A10}$$

and the *vacancy sink strength:*

$$k_{vGB}^2 = 2\pi R_G C_G \left\{1 + k_v R_G + (k_v^2/k_{vSC}^2)(k_{vSC} R_G \coth k_{vSC} R_G - 1)\right\}. \tag{A11}$$

Including the effects of bulk recombination, (A3) and (A4) may be reformulated in terms of $\bar{y}_i = D_i \bar{c}_i$ and $\bar{y}_v = D_v \bar{c}_v$, thus;

$$\frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{d\bar{y}_i}{dr}\right) + K - k_{iSC}^2 \bar{y}_i - \frac{\alpha}{D_i D_v} \bar{y}_i \bar{y}_v = 0, \tag{A12}$$

and

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\bar{y}_v}{dr}\right) + K - k_{vSC}^2\bar{y}_v - \frac{\alpha}{D_iD_v}\bar{y}_i\bar{y}_v = 0. \tag{A13}$$

Through the definitions;

$$\left.\begin{aligned} \bar{y} &= (\bar{y}_i + \bar{y}_v)/2 \\ \bar{z} &= (\bar{y}_i - \bar{y}_v)/2 \\ k_{iSC}^2 &= \bar{k}^2 + \bar{\beta} \\ k_{vSC}^2 &= \bar{k}^2 - \bar{\beta} \\ A &= \alpha/D_iD_v \end{aligned}\right\} \tag{A14}$$

equations (A12) and (A13) become;

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\bar{y}}{dr}\right) + K - \bar{k}^2\bar{y} - A\bar{y}^2 = \bar{\beta}\bar{z} - A\bar{z}^2, \tag{A15}$$

and

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\bar{z}}{dr}\right) - \bar{k}^2\bar{z} = \bar{\beta}\bar{y}, \tag{A16}$$

the condition (A5) is written;

$$\bar{y} = \bar{z} = 0 \quad \text{at} \quad r = R_G \tag{A17}$$

and the requirement (A7) becomes;

$$\bar{y} = \bar{y}^o\ , \quad \bar{z} = \bar{z}^o \quad \text{when} \quad r \to 0 \tag{A18}$$

be bounded.

We adopt the approximation;

$$\bar{\beta}\bar{z} - A\bar{z}^2 = 0, \tag{A19}$$

which has been justified by Wood, Jones and Pierce (1980) for an equation similar to (A15) above, and consider henceforth, instead of (A15);

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\bar{y}}{dr}\right) + K - \bar{k}^2\bar{y} - A\bar{y}^2 = 0. \tag{A20}$$

Introducing the solution of (A20) when the Laplace term vanishes;

$$\bar{y}_o = \bar{k}^2\bar{Q}/2A, \tag{A21}$$

with

$$\bar{Q} = (1 + 4AK/\bar{k}^4)^{\frac{1}{2}} - 1, \tag{A22}$$

and the quantities;

$$\left.\begin{aligned} \bar{f} &= \bar{k}^2 R_G^2 \bar{Q}/2 \\ \bar{S} &= 1/\bar{Q} \end{aligned}\right\} \tag{A23}$$

as well as the normalized variables;

$$\left.\begin{aligned} r' &= r/R_G \\ \bar{y}' &= \bar{y}/\bar{y}_o \\ \bar{z}' &= \bar{z}/\bar{y}_o, \end{aligned}\right\} \tag{A24}$$

equations (A20) and (A16) may be cast into the form;

$$\frac{1}{r'^2}\frac{d}{dr'}\left(r'^2\frac{d\bar{y}'}{dr'}\right) + \bar{f}\left\{(1+\bar{S})^2 - (\bar{y}'+\bar{S})^2\right\} = 0 \tag{A25}$$

and

$$\frac{1}{r'^2}\frac{d}{dr'}\left(r'^2\frac{d\bar{z}'}{dr'}\right) - \bar{k}^2 R_G^2 \bar{z}' = \bar{\beta} R_G^2 \bar{y}', \tag{A26}$$

respectively. The condition (A17) is then;

$$\bar{y}' = \bar{z}' = 0 \quad \text{at} \quad r' = 1 \tag{A27}$$

and the stipulation (A18) becomes;

$$\bar{y}' = \bar{y}'^o, \quad \bar{z}' = \bar{z}'^o \quad \text{when } r' \to 0 \tag{A28}$$

be finite. In the limit of vanishing recombination, $A \to 0$, equation (A25) reduces to*;

$$\frac{1}{r'^2}\frac{d}{dr'}\left(r'^2\frac{d\bar{y}'}{dr'}\right) + \bar{k}^2 R_G^2 (1-\bar{y}') = 0, \tag{A29}$$

the solution of which is;

$$\bar{y}' = 1 - \frac{1}{r'}\frac{\sinh \bar{k} R_G r'}{\sinh \bar{k} R_G} \tag{A30}$$

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*Notice that $\bar{y}_o = K/\bar{k}^2$ in (A24) for $A \to 0$ according to (A21) and (A22).

for the conditions (A27) and (A28). From the form of the solution (A30) we make the ansatz;

$$\bar{y}' = 1 - \frac{1}{r'} \frac{\sinh \bar{G} r'}{\sinh \bar{G}} , \tag{A31}$$

as an approximate solution of equation (A25) when recombination is present, with a (positive) constant $\bar{G}$ to be deliberately fixed.

Substitution of $\bar{y}'$, equation (A31), into equation (A25) gives the implicit relationship;

$$\bar{G}^2 = \bar{f} \left\{ 2(1+\bar{S}) - \frac{1}{r'} \frac{\sinh \bar{G} r'}{\sinh \bar{G}} \right\} , \tag{A32}$$

which indicates $\bar{G}$ is a function of r' rather than a constant, as assumed for the derivation of (A32) from (A25). As in section 2, an approach to proceed is by considering the series representation of $\bar{y}'$ in powers of $\bar{G}$;

$$\bar{y}' = 1 - \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{(2n+1)!} \bar{G}^{2n} (r')^{2n} \right\} \Big/ \left\{ 1 + \sum_{n=1}^{\infty} \frac{1}{(2n+1)!} \bar{G}^{2n} \right\} . \tag{A33}$$

Hence, it seems appropriate to replace the function $\bar{G}(r')$ from equation (A32) by its moments;

$$\langle \bar{G}^{2n} \rangle = 3\bar{f}^n \int_0^1 r'^2 \left\{ 2(1+\bar{S}) - \frac{1}{r'} \frac{\sinh \bar{G}(r') r'}{\sinh \bar{G}(r')} \right\}^n dr' , \quad n=1,2,3,... \tag{A34}$$

Expanding the power beneath the integral in (A34) into a binomial series yields the form;

$$\langle \bar{G}^{2n} \rangle = [2\bar{f}(1+\bar{S})]^n \left\{ 1 + \sum_{\nu=1}^{n} (-1)^{\nu} \binom{n}{\nu} [2(1+\bar{S})]^{-\nu} \times \right.$$

$$\left. \times\ 3 \int_0^1 (r')^{2-\nu} \frac{\sinh^{\nu} \bar{G}(r') r'}{\sinh^{\nu} \bar{G}(r')} dr' \right\} , \quad n=1,2,3... , \tag{A35}$$

which may be evaluated by means of an iteration technique. As a first step, the following limits are considered: for $|\bar{G}(r')| \ll 1$ in the range $0 \leq r' \leq 1$, we approximate to the lowest order;

$$3\int_0^1 (r')^{2-\nu}\,\frac{\sinh^{\nu}\bar{G}(r')r'}{\sinh^{\nu}\bar{G}(r')}\,dr' = 1, \quad \nu = 1,2,3,\ldots,n \tag{A36}$$

and get from equation (A35);

$$\langle\bar{G}^{2n}\rangle_{(1)} = [\bar{f}(1+2\bar{S})]^n, \quad n = 1,2,3,\ldots \tag{A37}$$

revealing the identity

$$\langle\bar{G}^{2}\rangle^n_{(1)} \equiv \langle\bar{G}^{2n}\rangle_{(1)}, \quad n = 1,2,3,\ldots . \tag{A38}$$

Therefore, to a first approximation, all moments of $\bar{G}(r')$ are obtained from one constant;

$$\bar{G}_a = [\bar{f}(1+2\bar{S})]^{\frac{1}{2}}. \tag{A39}$$

Similarly, for $|\bar{G}(r')| \gg 1$ in the range $0 \leq r' \leq 1$, it can be shown that, to a first approximation, all moments of $\bar{G}(r')$ originate from the constant;

$$\bar{G}_b = [2\bar{f}(1+\bar{S})]^{\frac{1}{2}}. \tag{A40}$$

To proceed to a second order of approximation would require $\bar{G}_a$ and $\bar{G}_b$, respectively, to be inserted in the integrand in equation (A35). Since, however, replacing $\bar{G}_b$ by $\bar{G}_a$ yields only a small error if $|\bar{G}(r')| \gg 1$, we use for both limits, $|\bar{G}(r')| \ll 1$ and $|\bar{G}(r')| \gg 1$, the constant $\bar{G}_a$ from equation (A39) in (A35) obtaining;

$$\langle\bar{G}^{2n}\rangle_{(2)} = [2\bar{f}(1+\bar{S})]^n \left\{1 + \sum_{\nu=1}^{n} (-1)^{\nu}\binom{n}{\nu}[2(1+\bar{S})]^{-\nu} \times \right.$$

$$\left. \times\, 3\int_0^1 (r')^{2-\nu}\,\frac{\sinh^{\nu}\bar{G}_a r'}{\sinh^{\nu}\bar{G}_a}\,dr'\right\}, \quad n = 1,2,3,\ldots . \tag{A41}$$

Obviously, the expression within the curly brackets in equation (A41) in general does not constitute a power of some other expression, thus precluding a simultaneous reduction of all moments as for the first approximation. But, with regard to (A33), we try a refined evaluation of the leading second moment of $\bar{G}(r')$ taking equation (A41) for n = 1 to give;

$$\langle \bar{G}^2 \rangle_{(2)} = \bar{f} \left\{ 2(1 + \bar{S}) - (3/\bar{G}_a^2)(\bar{G}_a \coth \bar{G}_a - 1) \right\} . \qquad (A42)$$

By further consideration of the limits $\bar{G}_a \ll 1$ and $\bar{G}_a \gg 1$, we conclude that the form;

$$\langle \bar{G}^2 \rangle = (\bar{f}/5) \left\{ 7 + 10\bar{S} - 2\bar{f}^{\frac{1}{2}}/\sinh \bar{f}^{\frac{1}{2}} \right\} \qquad (A43)$$

approximates the moment under consideration with a sufficient accuracy. Substituting into equation (A31) the constant;

$$\bar{G} = \langle \bar{G}^2 \rangle^{\frac{1}{2}} = (\bar{f}/5)^{\frac{1}{2}} \left\{ 7 + 10\bar{S} - 2\bar{f}^{\frac{1}{2}}/\sinh \bar{f}^{\frac{1}{2}} \right\}^{\frac{1}{2}} \qquad (A44)$$

or, by the definitions (A23),

$$\bar{G} = \bar{k}R_G \left\{ 1 + (\bar{Q}/5)[7/2 - \bar{k}R_G(\bar{Q}/2)^{\frac{1}{2}}/\sinh \bar{k}\, R_G(\bar{Q}/2)^{\frac{1}{2}}] \right\}^{\frac{1}{2}} \qquad (A45)$$

therefore provides a good approximation to the solution of equation (A25) for $\bar{G}$ both small and large which, because of

$$\bar{G} = \bar{k}R_G \quad \text{if} \quad A \to 0, \qquad (A46)$$

tends to the exact solution (A30) in the without recombination limit.

We turn now to solve equation (A26) for $\bar{z}'$ subject to (A27) and (A28). Inserting $\bar{y}'$ from equation (A31) yields

$$\bar{z}' = \bar{\beta} \left\{ \left(\frac{1}{\bar{k}^2} + \bar{\gamma} \right) \frac{1}{r'} \frac{\sinh \bar{k}R_G r'}{\sinh \bar{k}R_G} - \frac{1}{\bar{k}^2} - \frac{\bar{\gamma}}{r'} \frac{\sinh \bar{G}r'}{\sinh \bar{G}} \right\} , \quad \bar{G} > \bar{k}R_G \qquad (A47)$$

with

$$\bar{\gamma} = R_G^2/(\bar{G}^2 - \bar{k}^2 R_G^2). \qquad (A48)$$

To calculate the grain boundary sink strengths including bulk recombination, we refer to the basic formulae (A8) and (A9), which in terms of the primed variables defined by equations (21) and (25) in section 2* and by (A24) are written;

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*Understanding in these and in related equations R_G instead of r_C

$$k^2_{iGB} = 2\pi R_G C_G \left\{ \frac{dy'}{dr'} + \frac{dz'}{dr'} - \frac{\bar{y}_o}{y^\infty}\left[\frac{d\bar{y}'}{dr'} + \frac{d\bar{z}'}{dr'}\right]\right\}_{r'=1} \Big/ [1 + z'^\infty] \qquad (A49)$$

and

$$k^2_{vGB} = 2\pi R_G C_G \left\{ \frac{dy'}{dr'} - \frac{dz'}{dr'} - \frac{\bar{y}_o}{y^\infty}\left[\frac{d\bar{y}'}{dr'} - \frac{d\bar{z}'}{dr'}\right]\right\}_{r'=1} \Big/ [1 - z'^\infty] \qquad (A50)$$

respectively. With the expressions (28) and (41) from section 2 as well as (A31) and (A47) the following results hold for $G > kR_G$, $\bar{G} > \bar{k}R_G$:

interstitial sink strength;

$$k^2_{iGB} = 2\pi R_G C_G \{\beta_i(1+G) + (1-\beta_i)[1 + GkR_G/(G+kR_G)] +$$

$$+ \beta_i(\bar{k}^2\bar{Q}/k^2Q)[\bar{\varepsilon}_i(\bar{G}\coth\bar{G} - 1) + \bar{\zeta}_i(\bar{k}R_G \coth \bar{k}R_G - 1)]\}, \qquad (A51)$$

vacancy sink strength;

$$k^2_{vGB} = 2\pi R_G C_G \{\beta_v(1+G) + (1-\beta_v)[1 + GkR_G/(G+\bar{k}R_G)] +$$

$$+ \beta_v(\bar{k}^2\bar{Q}/k^2Q)[\bar{\varepsilon}_v(\bar{G}\coth\bar{G} - 1) + \bar{\zeta}_v(\bar{k}R_G \coth \bar{k}R_G - 1)]\}, \qquad (A52)$$

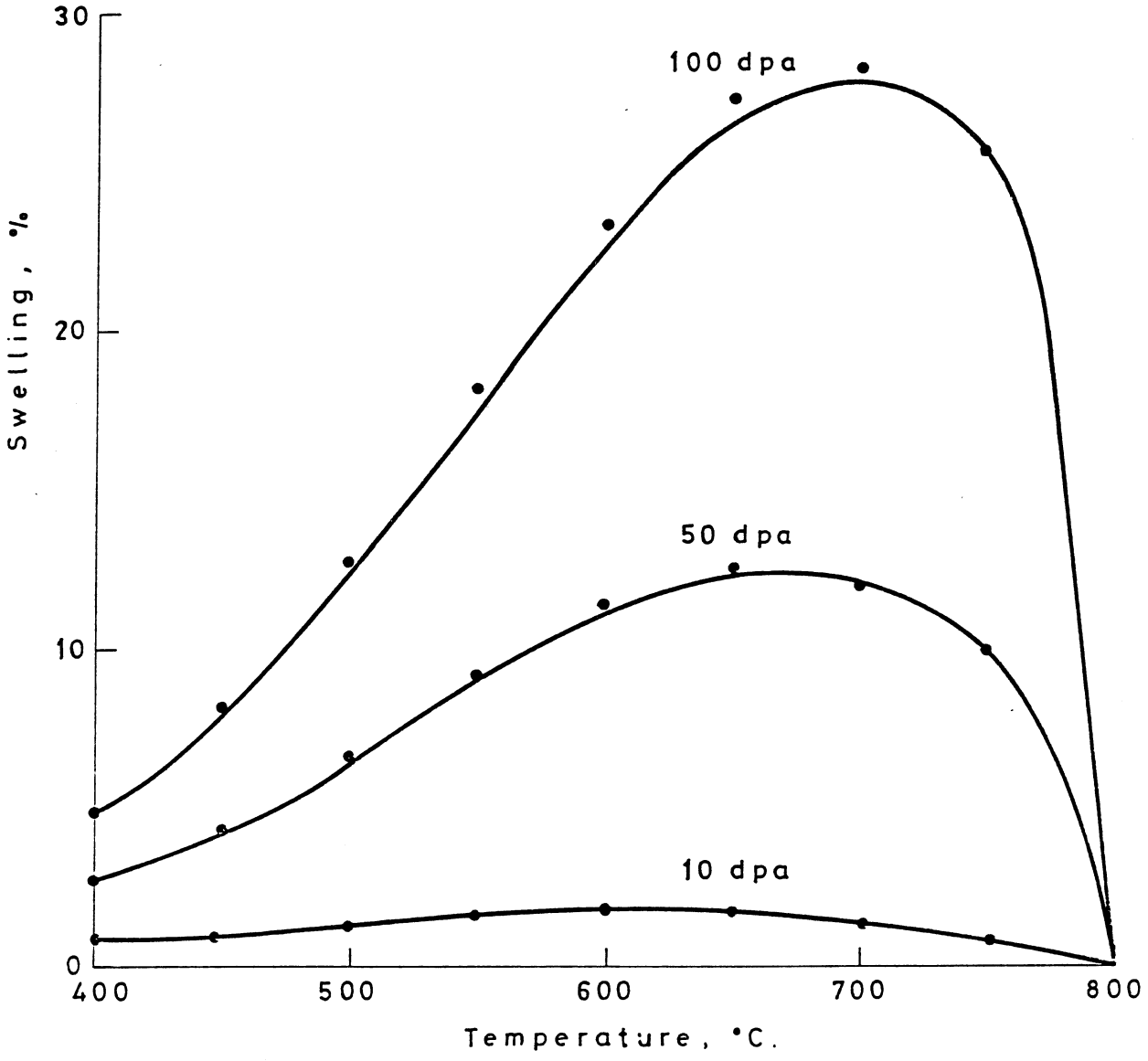
where the abbreviations;

$$\bar{\varepsilon}_i = 1 + \bar{\beta}\bar{\gamma}, \quad \bar{\varepsilon}_v = 1 - \bar{\beta}\bar{\gamma} \qquad (A53)$$

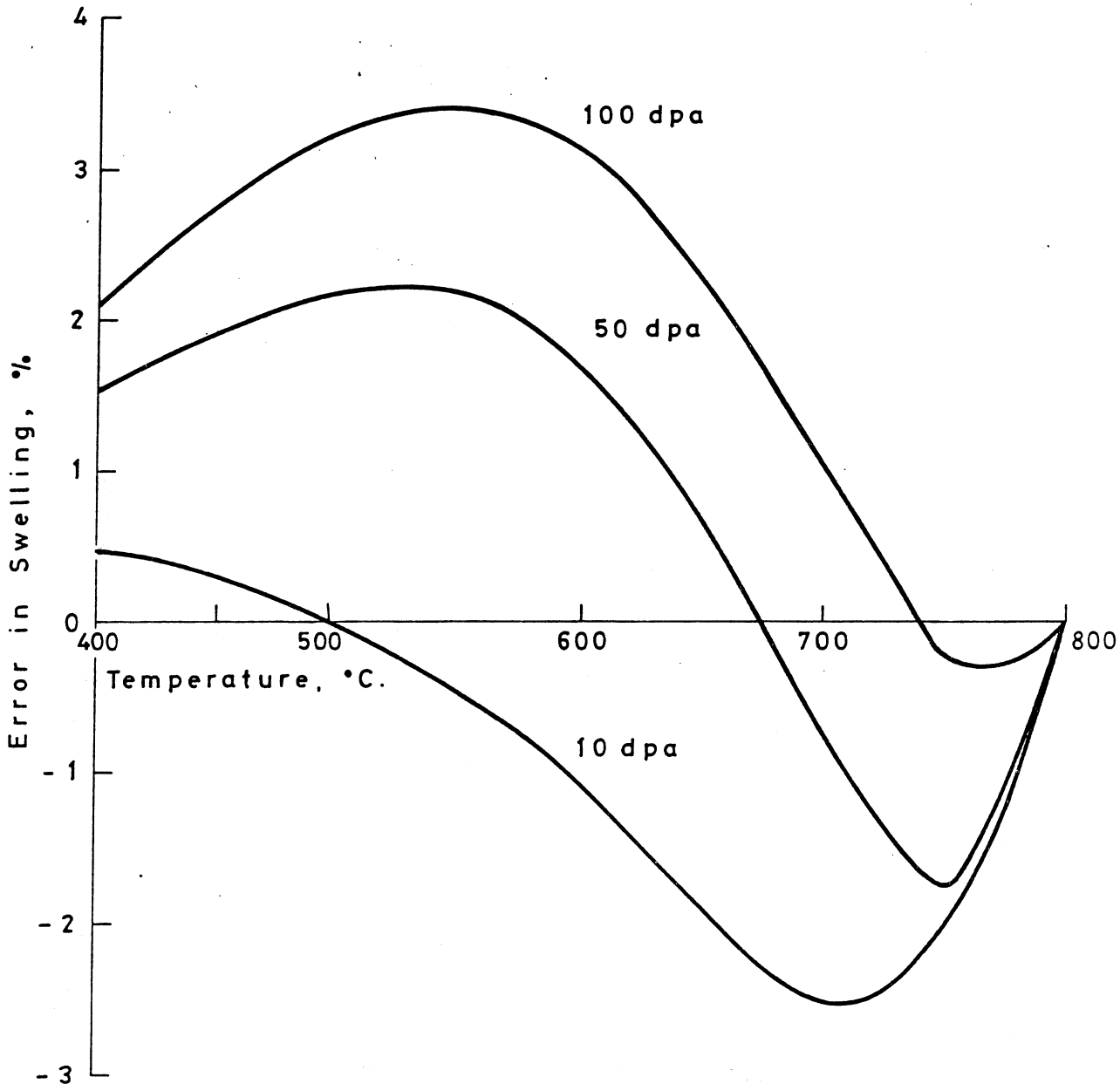
and

$$\bar{\zeta}_i = -\bar{\beta}(1/\bar{k}^2 + \bar{\gamma}), \quad \bar{\zeta}_v = \bar{\beta}(1/\bar{k}^2 + \bar{\gamma}) \qquad (A54)$$

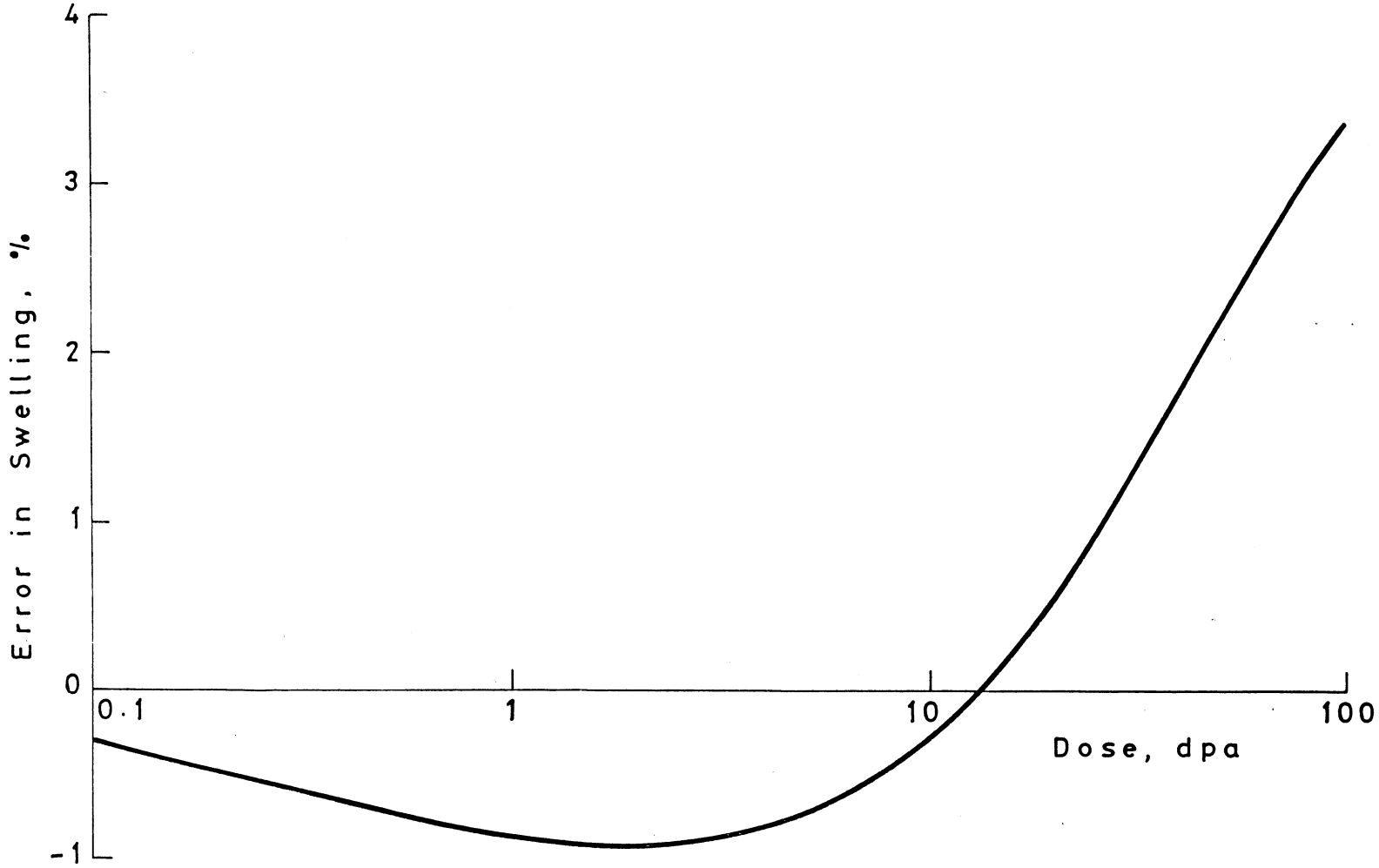
have been introduced.



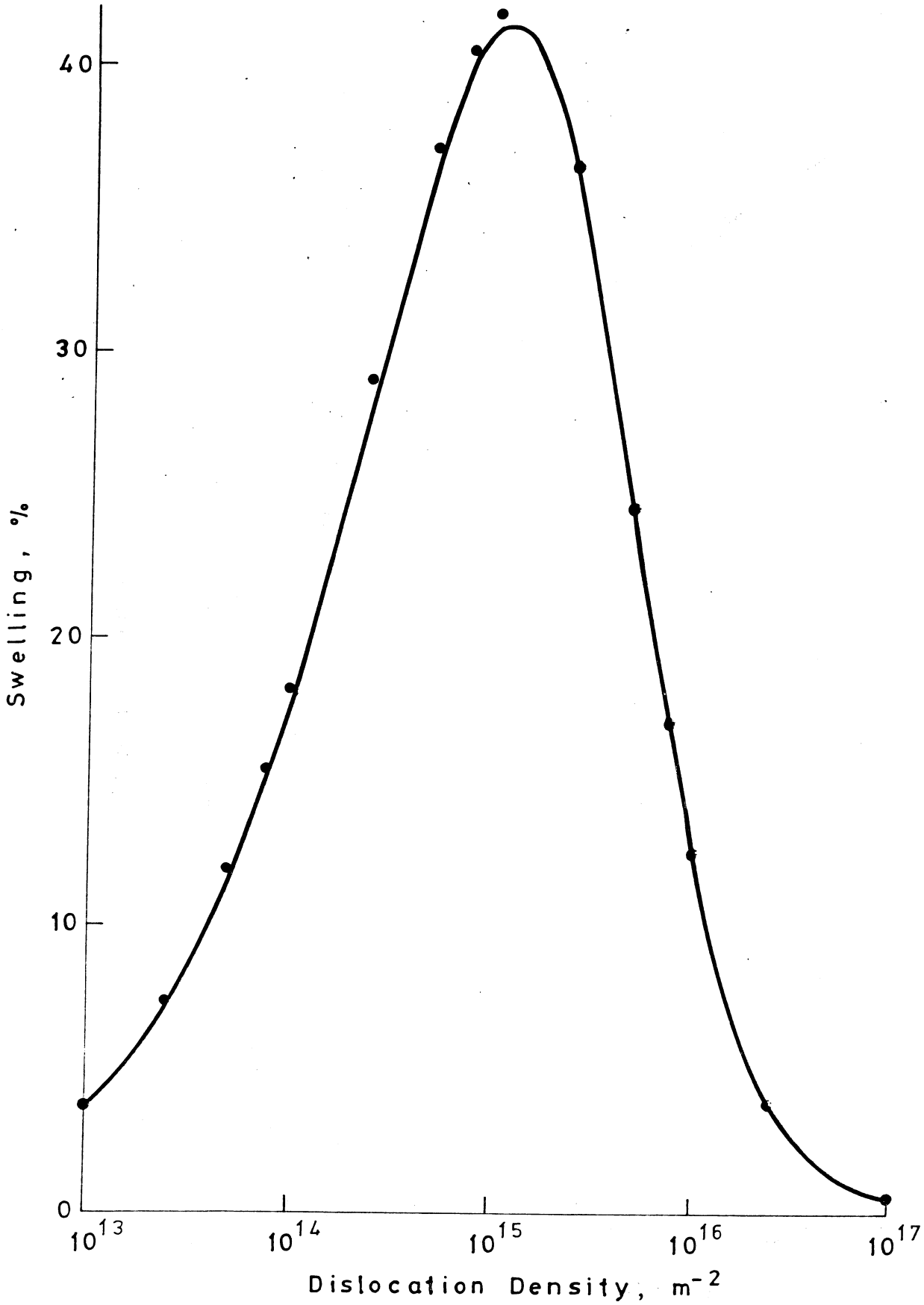
AERE - R 9999 Fig. 1



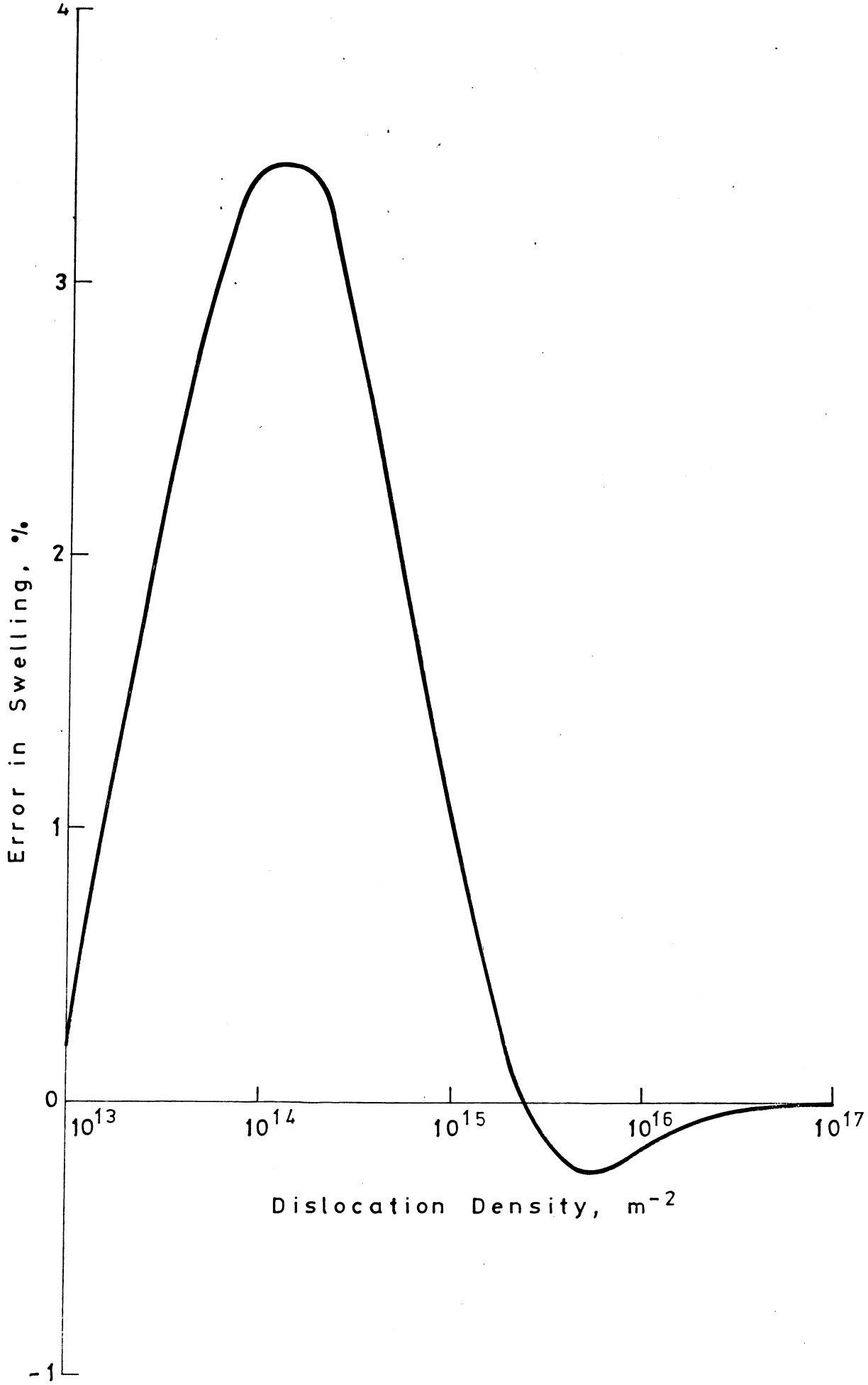
AERE - R 9999 Fig. 2



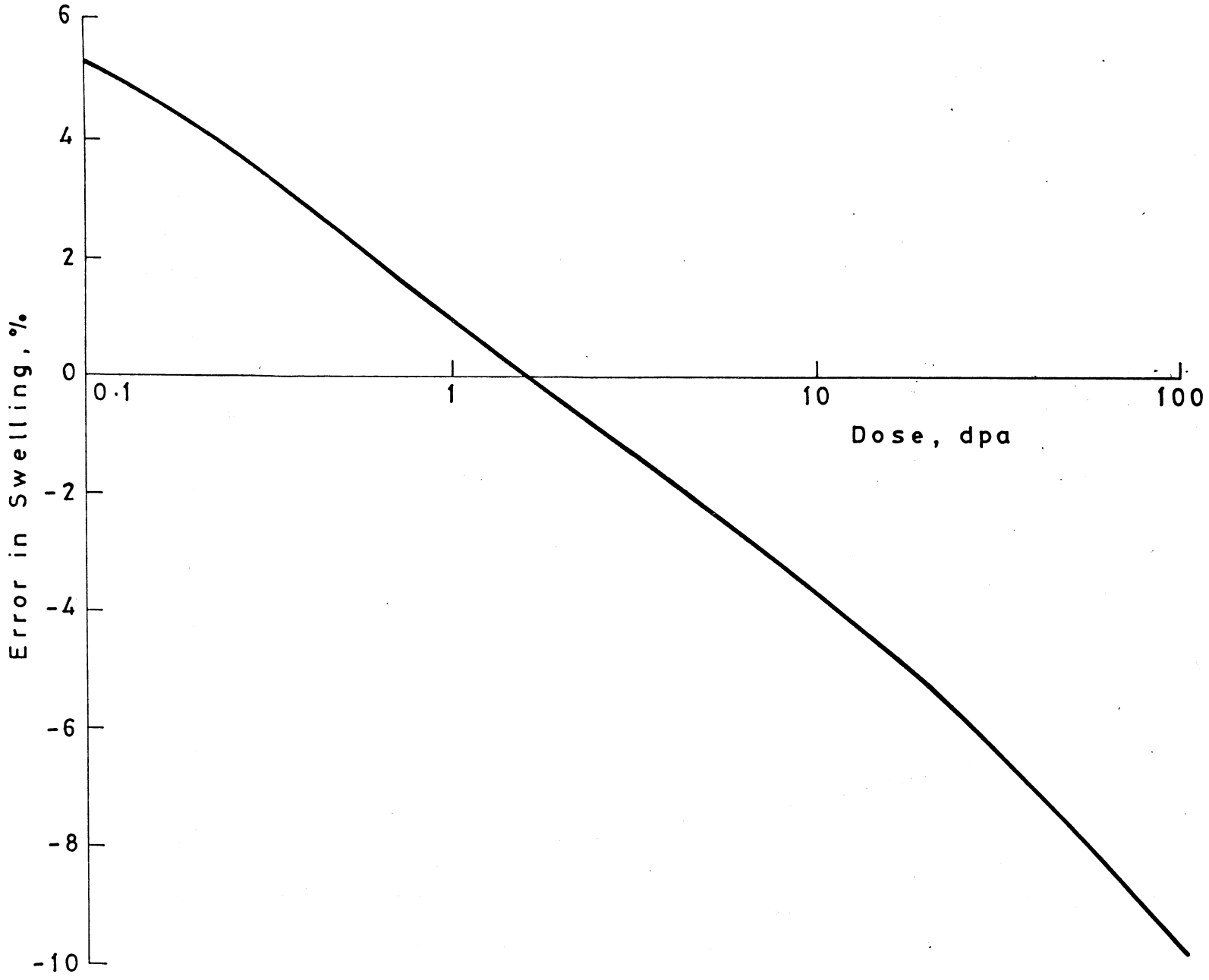
AERE - R 9999 Fig. 3



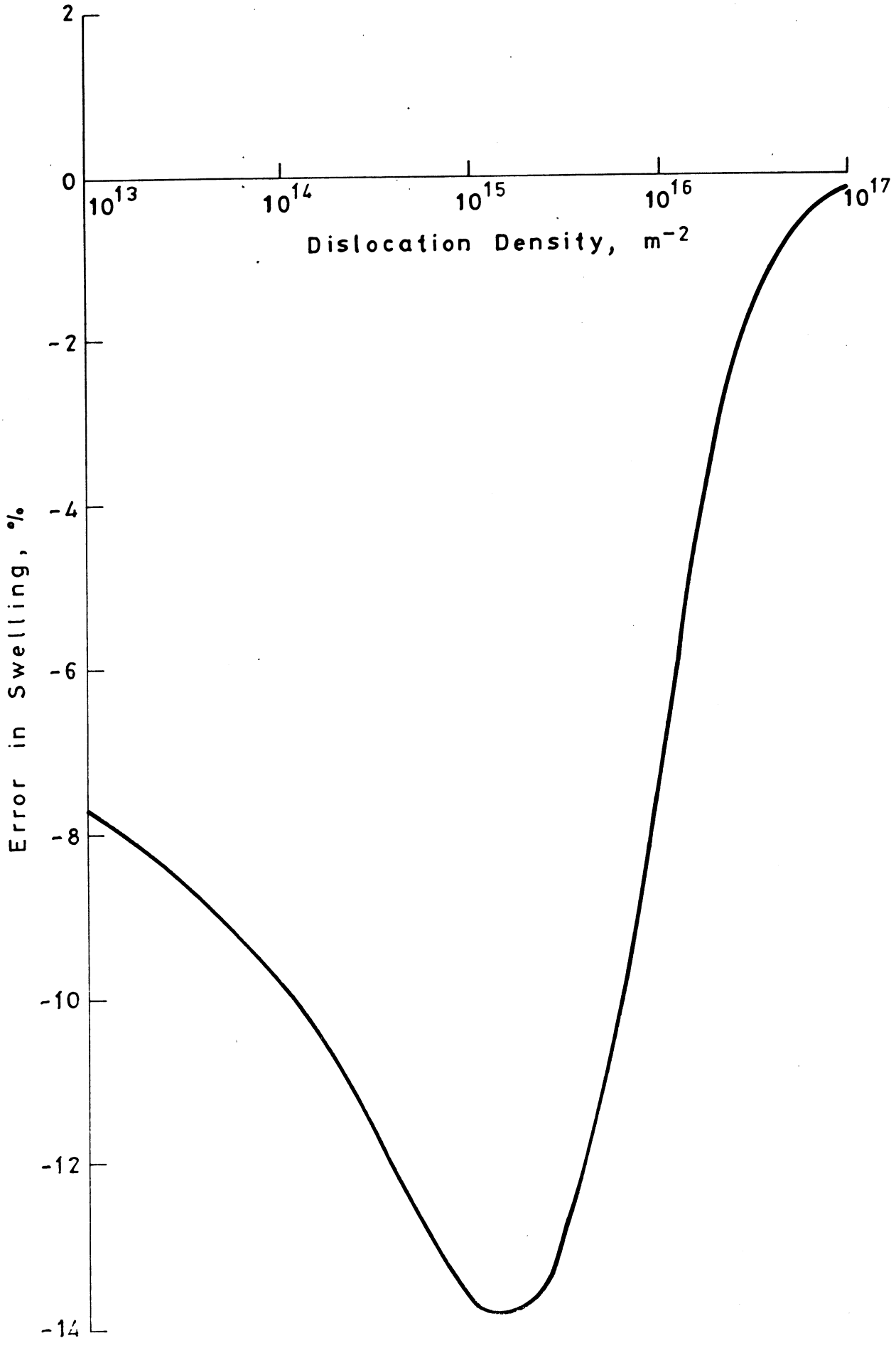
AERE - R 9999 Fig. 4



AERE - R 9999 Fig. 5



AERE - R 9999 Fig. 6



AERE - R 9999 Fig. 7