

13.4.5 Interactions of Migrating Point Defects With Dislocations

Two things to consider here;

1.) Capture of intrinsic defects (vacancies, interstitials). This causes dislocations to move.

2.) Capture of gas atoms (this may cause dislocations to be pinned).

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Capture radius ---- Figure 13.6

Since the number of capture sites per cm³
= $Z_{gt} C_t$

Sites per trap Trapping centers

$$= \frac{Z_{vd}}{a_0} d$$

Per unit length of dislocation

and, $L^2 = \frac{1}{Z_{vd} d}$

Rate of vacancy capture by dislocations/cm³ = $D_V Z_{vd} d C_V$

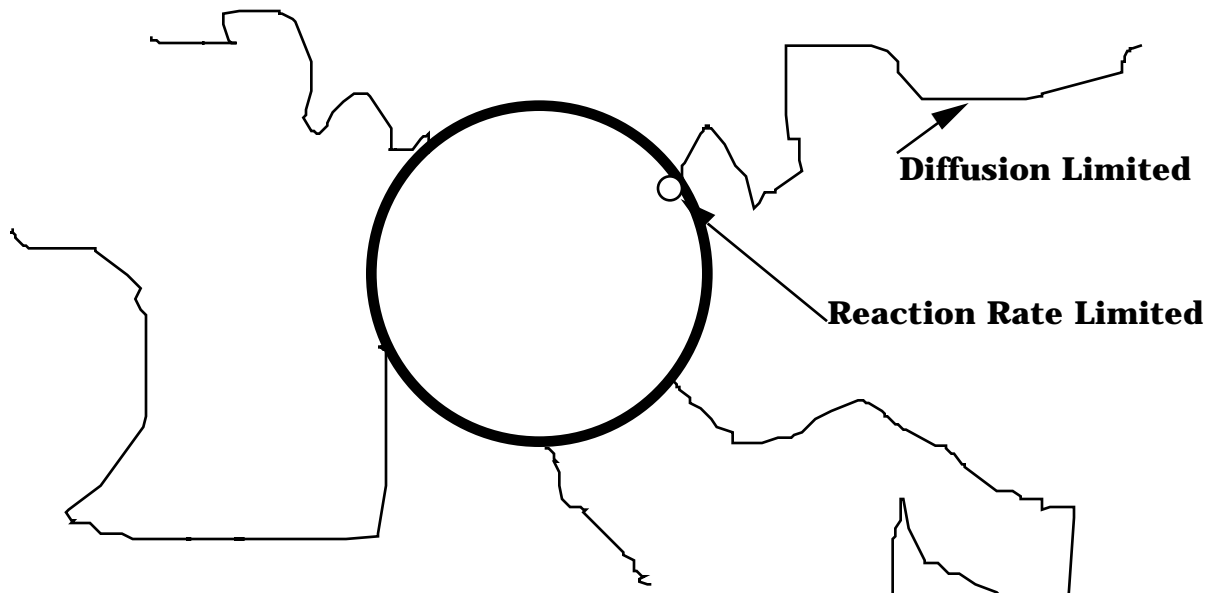
Rate of interstitial capture by dislocations/cm³ = $D_I Z_{id} d C_i$

Capture rate of gas atoms by dislocations/cm³ = $D_{Xe} Z_{gd} d C$

13.5 Diffusion Limited Reactions

Interaction rates have two components

- 1.) Diffusion in the bulk to the defect**
- 2.) Reaction rate at the surface of the defect**



13.5.1 Diffusion to Spherical Sinks

Set up unit cell - Figure 13.7

$$\frac{C}{t} = \frac{D}{r^2} \frac{r^2 C}{r} + Y \dot{F}$$

**Time
Variation**

**Spatial
Variation**

**Uniform
Production**

Note : Neglecting Recombination

at equilibrium,

$$\frac{d}{dr} \frac{r^2 dC}{dr} = -Y \dot{F}$$

Noting ;

$$\frac{C}{r} = 0$$

and

$$C(R, t) = C_R$$

Then;

$$C(r) = C_R + \frac{Y \dot{F}}{6D} \frac{2r^2(r - R)}{rR} - (r^2 - R^2)$$

Assume $r \gg R$, Figure 13.8

Region 1 (neglect production rate)

$$\frac{1}{r^2} \frac{d}{dr} \frac{r^2 dC}{dr} = 0$$

$$\text{and } C(\infty) = C(0)$$

Solving;

$$C(r) = C_R + [C(\infty) - C_R] \cdot \left(1 - \frac{R}{r}\right)$$

Since

$$J = -D \frac{dC}{dr} \bigg|_R$$

$$J = -D \frac{[C(\infty) - C_R]}{R}$$

Two parameters of Importance

1.) Absorption by a sphere

$$= - (4\pi R^2) J$$

$$= 4 \pi R [C(\infty) - C_R] D$$

What is this?

$$\frac{4}{3} \pi (R^3 - r^3) Y \dot{F} = 4 \pi R D [C(\infty) - C_R]$$

$$C(r) = C_R + \frac{Y \dot{F} r^3}{3 D R}$$

2.) Absorption by all spheres

$$\text{if } C(\) \gg C_R \\ = 4pRDCC_t$$

$$\text{rate constant} \\ k = 4pRD$$

see page 213 for derivation of bubble radius during post Irradiation annealing

$$\ln \frac{[R_f + R]}{[R_f - R]} = \frac{3D_{Xe}R_f t}{3}$$

Note : only good for ideal gas

13.5.2 Diffusion to Dislocations

1.) Switch to cylindrical co - ordinates

$$(p^2) r_d = 1$$

2.) At equilibrium;

$$\frac{D_v}{r} \frac{d}{dr} \frac{rdC_v}{dr} = -Y_{vi} \dot{F} + k_{vi} C_v C_i$$

recombination

approximate this by

$$Y \dot{F}_{eff} = Y_{vi} \dot{F} - k_{vi} C_v C_i$$

3.) Exact Solution

$$C_v(r) = C_{R_d} + \frac{Y \dot{F}}{2 D_v} \ln \frac{r}{R_d} - \frac{1}{2} \frac{r^2 - R_d^2}{2}$$

4.) Approximate Solution

$$C_v(\) = C_{R_d} + \frac{Y \dot{F}}{2 D_v} \ln \frac{r}{R_d} - \frac{1}{2}$$

5.) Rate of Vac. Capture by Dislocations/cm³

$$= \frac{2 D_v}{\ln \frac{r}{R_d}} \frac{dC_v}{dr} \quad \text{This is all diffusion controlled}$$

13.5.3 Mixed Rate Control

For a reaction rate control to dislocations, the vacancy capture/cm³

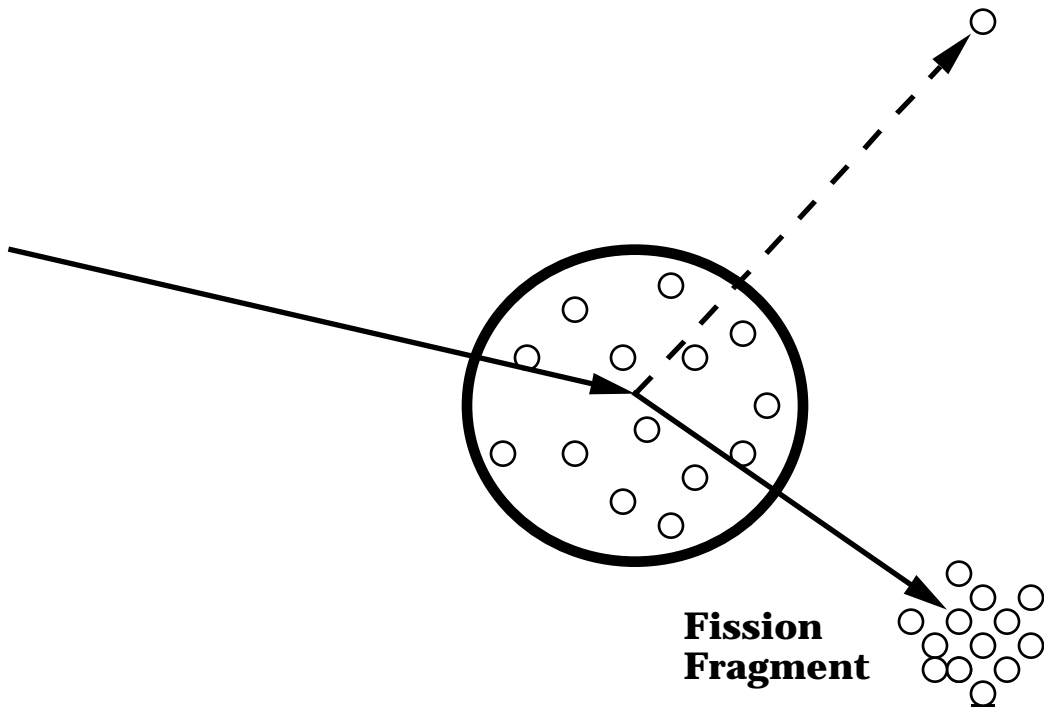
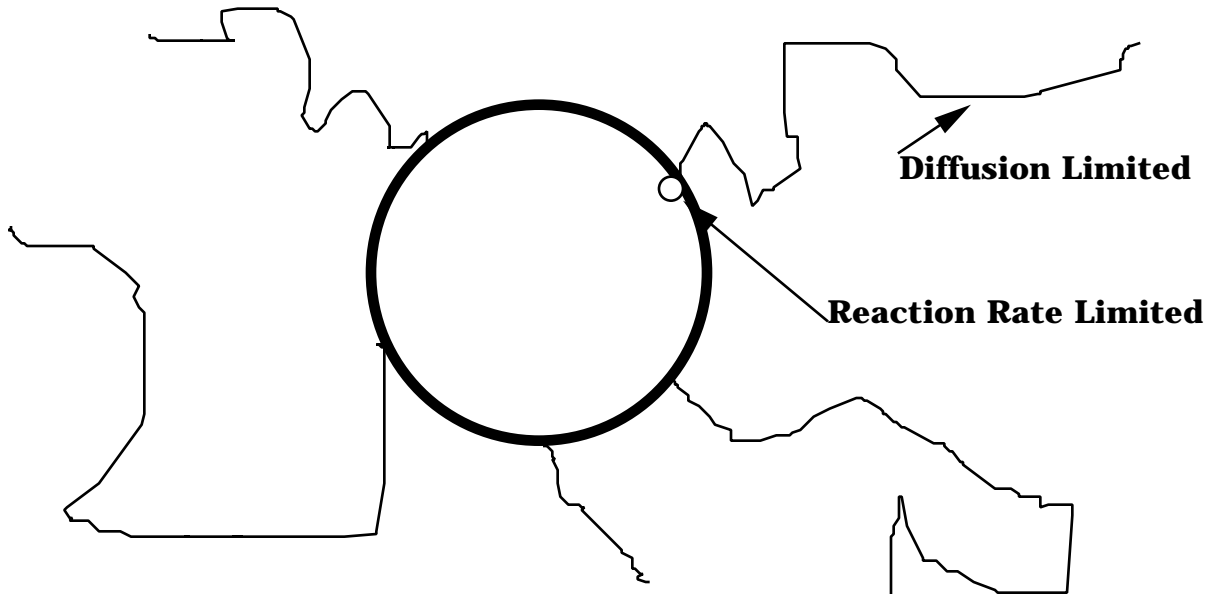
$$= D_v Z_{vd} r_d C_v$$

Analogous to heat conduction, use vacancy capture/cm³ to be, (in the intermediate regime)

$$= \frac{D_v dC_v}{\frac{1}{Z_{vd}} + \frac{\ln \frac{r_d}{R_d}}{2}}$$

Reaction Rate	Diffusion (for $r_d = 10^{10}$)
0.04	0.7

Hence, the vacancy absorption is almost entirely diffusion controlled



Problem 13.6

- In a fuel pellet we have N bubbles/cm³ of radius R plus one bubble of radius R^*
- Both bubble sizes are in equilibrium and large enough to use perfect gas laws.
- When R^* exceeds R_C^* , the large bubble can gobble up small bubbles and grow spontaneously.
- Determine R_C^* (critical radius)
- If $R_C^* = 10R$, what is swelling at breakaway?

Condition of mechanical equilibrium means

$$p = \frac{2}{r} \quad \text{and} \quad p \frac{4}{3} r^3 = mkT$$

$$\text{or,} \quad m = \frac{8}{3kT} r^2 = Cr^2 \quad 1)$$

If the large bubble expands by dR^* , it sweeps out a volume $4 R^{*2} dR^*$.

This volume contains N bubbles of radius R per cc and each bubble contains

$$m = CR^2 \quad \text{atoms}$$

Therefore, the number of additional gas atoms acquired by the large bubble as a result of expansion by dR^* is;

$$dm^* = 4 R^{*2} \cdot dR^* \cdot N \cdot C \cdot R^2 \quad 2)$$

However, to maintain mechanical equilibrium according to eq. 1), the number of additional gas atoms required is given by;

$$\begin{aligned} dm^{*'} &= \frac{d(CR^{*2})}{dR^*} dR^* \\ &= 2CR^* dR^* \quad 3) \end{aligned}$$

The bubble will grow spontaneously if

$$dm^* > dm^{*'}$$

or if $4 R^{*2} \cdot N \cdot C \cdot R^2 > 2CR^*$

or, $R^* \frac{1}{2 NR^2}$ 4)

Now if $\frac{R^*}{R} = 10$, then from eq. 4

$$N = \frac{1}{2 \cdot 10 \cdot R^3}$$

But

$$V_{\text{bubble}} = \frac{4 R^3}{3}$$

$$NV_{\text{bub}} = V = \frac{\frac{4 R^3}{3}}{2 \cdot 10 \cdot R^3} = \frac{2}{30} = 0.0667$$

$$\text{Swelling} \frac{V}{V} = \frac{0.0667}{1 - 0.0667} = \frac{0.0667}{0.9333} = 7.2\%$$