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 cm^3

$$= Z_{gt} \, C_t$$

Sites per trap   Trapping centers

$$= \frac{Z_{vd}}{a_o} \rho_d$$

Per unit length of dislocation

and,

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

Rate of vacancy capture by dislocations/cm^3 = $D_V \, Z_{vd} \, \rho_d \, C_V$

Rate of interstitial capture by dislocations/cm^3 = $D_I \, Z_{id} \, \rho_d \, C_i$

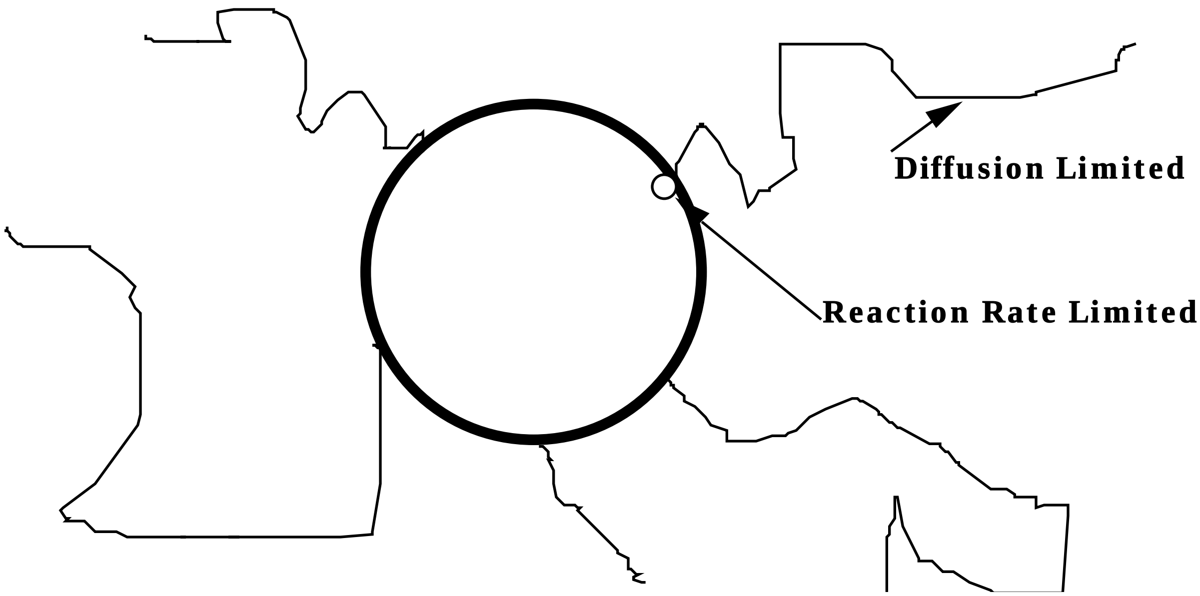
Capture rate of gas atoms by dislocations/cm^3 = $D_{Xe} \, Z_{gd} \, \rho_d C$

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

$$\frac{\partial C}{\partial t} = \left\{ \frac{D}{r^2} \right\} \frac{\partial \left(r^2 \frac{\partial C}{\partial r} \right)}{\partial r} + Y \dot{F}$$

Time Variation	**Spatial Variation**	**Uniform Production**

Note : Neglecting Recombination

at equilibrium,

$$\frac{d\left(\frac{r^{2}dC}{dr}\right)}{dr} = -Y\,\dot{F}$$

Noting ;

$$\left(\frac{\partial C}{\partial r}\right) = 0$$

and

$$C\,(R,\ t) = C_{R}$$

Then;

$$C(r) = C_{R} + \frac{Y\,\dot{F}}{6D}\left[\frac{2\quad{}^{2}(r-R)}{rR} - \left(r^{2} - R^{2}\right)\right]$$

Assume >> R, Figure 13.8

Region 1 (neglect production rate)

$$\frac{1}{r^{2}}\,\frac{d\left(\frac{r^{2}dC}{dr}\right)}{dr} = 0$$

and C(∞) = C( )

Solving;

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

Since

$$J = -D\left(\frac{dC}{dr}\right)_R$$

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

Two parameters of Importance

1.) Absorption by a sphere

$$= -\,(4pR^2)\ J$$

$$= 4\pi DR\left[C(\ \ ) - C_R\right]$$

What is this?

$$\frac{4\pi}{3}\left(\ \ ^3 - R^3\right) Y\,\dot{F} = 4\pi RD\left[C(\ \ ) - C_R\right]$$

$$C(\ \ ) = C_R + \frac{Y\,\dot{F}\ \ ^3}{3DR}$$

2.) **Absorption by all spheres**

if C( ) >> C_R
= 4pRDCC_t

rate constant
k = 4pRD

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

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

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;**

$$\frac{D_v}{r}\left[\frac{d}{dr}\left(r\frac{dC_v}{dr}\right)\right] = -Y_{vi}\dot{F} + k_{vi}C_vC_i$$

recombination

approximate this by

$$\left(Y\dot{F}\right)_{eff} = Y_{vi}\dot{F} - k_{vi}C_vC_i$$

3.) Exact Solution

$$C_v(r) = C_{R_d} + \frac{\left(Y\dot{F}\right)_{eff}\ {}^{2}}{2D_v}\left[\ln\left(\frac{r}{R_d}\right) - \frac{1}{2}\left(\frac{r^2 - R_d^2}{{}^{2}}\right)\right]$$

4.) Approximate Solution

$$C_v(\quad) = C_{R_d} + \frac{\left(Y\dot{F}\right)_{eff}\ {}^{2}}{2D_v}\left[\ln\left(\frac{\quad}{R_d}\right) - \frac{1}{2}\right]$$

5.)Rate of Vac. Capture by Dislocations/cm^3

$$= \left[\frac{2\pi D_v \rho_d C_v}{\ln\left(\frac{\quad}{R_d}\right)}\right]$$

This is all diffusion controlled

13.5.3 Mixed Rate Control

For a reaction rate control to dislocations, the vacancy capture/cm^3

$$= D_v\, Z_{vd}\, \rho_d\, C_v$$

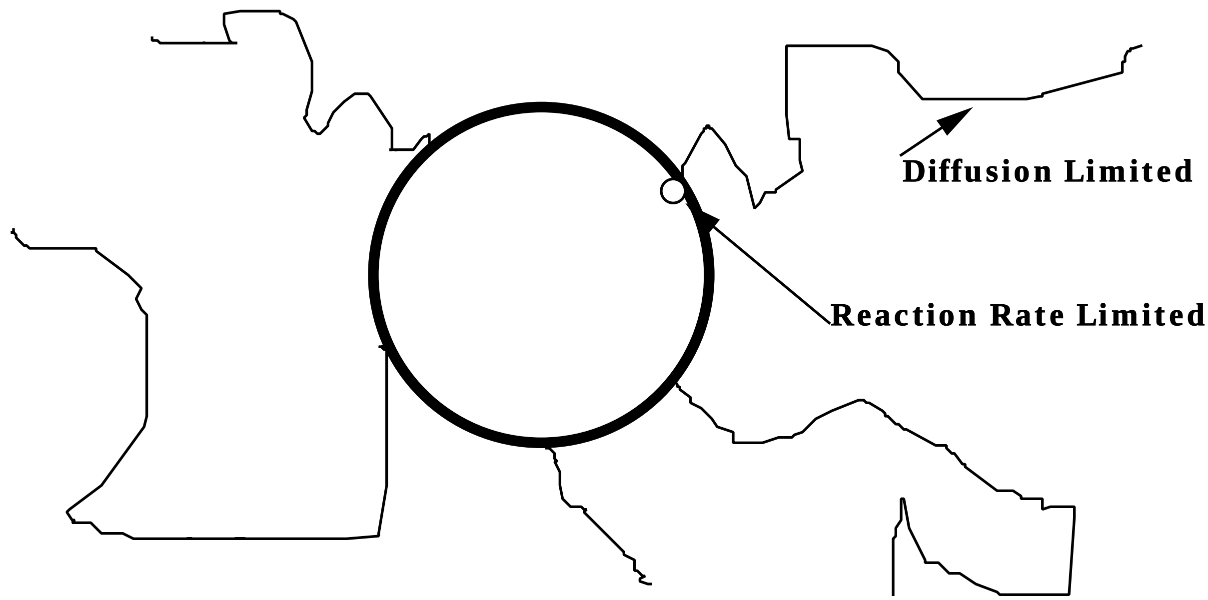
Analogous to heat conduction, use vacancy capture/cm^3 to be,(in the intermediate regime)

$$= \frac{D_v \rho_d C_v}{\left(\frac{1}{Z_{vd}}\right) + \left(\frac{\ln\left(\frac{\ }{R_d}\right)}{2\pi}\right)}$$

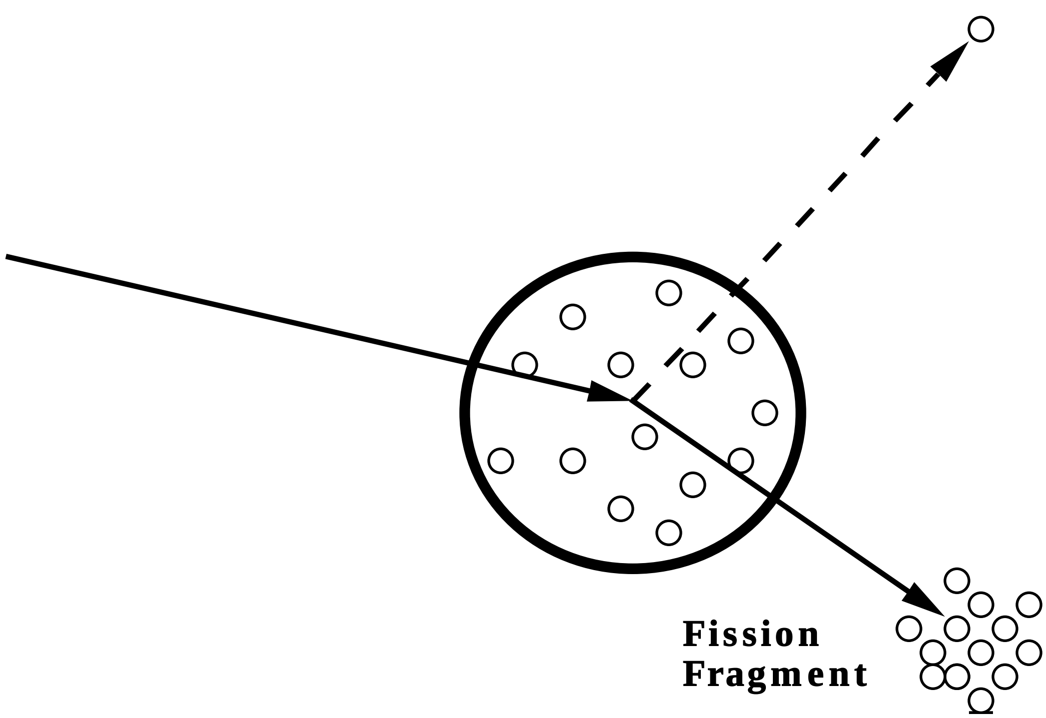
Reaction Rate **Diffusion (for $r_d \approx 10^{10}$)**

≈ 0.04 **≈ 0.7**

Hence, the vacancy absorption is almost entirely diffusion controlled



Diffusion Limited
Reaction Rate Limited



Fission
Fragment

Problem 13.6

- In a fuel pellet we have N bubbles/cm^3 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

$$p = \frac{2\gamma}{r} \quad \text{and} \quad p\left(\frac{4\pi r^3}{3}\right) = mkT$$

or, $$m = \left[\frac{8\pi\gamma}{3kT}\right] r^2 = Cr^2 \qquad 1)$$

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

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

$$dm^{*} = 4\pi R^{*^2} \bullet dR^{*} \bullet N \bullet C \bullet R^{2} \qquad 2)$$

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

$$dm^{*'} = \frac{d\left(CR^{*^2}\right)}{dR^{*}} dR^{*}$$

$$= 2CR^{*} dR^{*} \qquad 3)$$

The bubble will grow spontaneously if

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

or if $\quad 4\pi R^{*^2} \bullet N \bullet C \bullet R^{2} > 2CR^{*}$

or, $\quad R^{*} \geq \dfrac{1}{2\pi N R^{2}} \qquad 4)$

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

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

But

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

$$NV_{bub} = \Delta V = \frac{\frac{4\pi R^3}{3}}{2\pi \bullet 10 \bullet R^3} = \frac{2}{30} = 0.0667$$

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