13.4.4. Interaction Between Xenon Atoms and Atomic Sized Defects

Gas atoms are not the only defects that other gas atoms can interact with, they can find point defects as well

Rate of trapping of fission gas atoms/cm^3 = $k_{gtr}\, C_t\, C$

traps gas atoms

as before,

$$k_{gtr} = \frac{Z_{gtr}\Omega D_{Xe}}{a_0^2}$$

$$\frac{\text{Rate of Gas Atom Trapping}}{\text{cm}^3} = \frac{D_{Xe}C}{L^2}$$

Trapping length

L^2	=	j	a_o^2
random walk theory		# of jumps to get to trap	lattice spacing

$$j = \frac{1}{Z_{gt}C_t\Omega}$$

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).

===

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 = $D_{Xe} Z_{gd} \rho_d C$

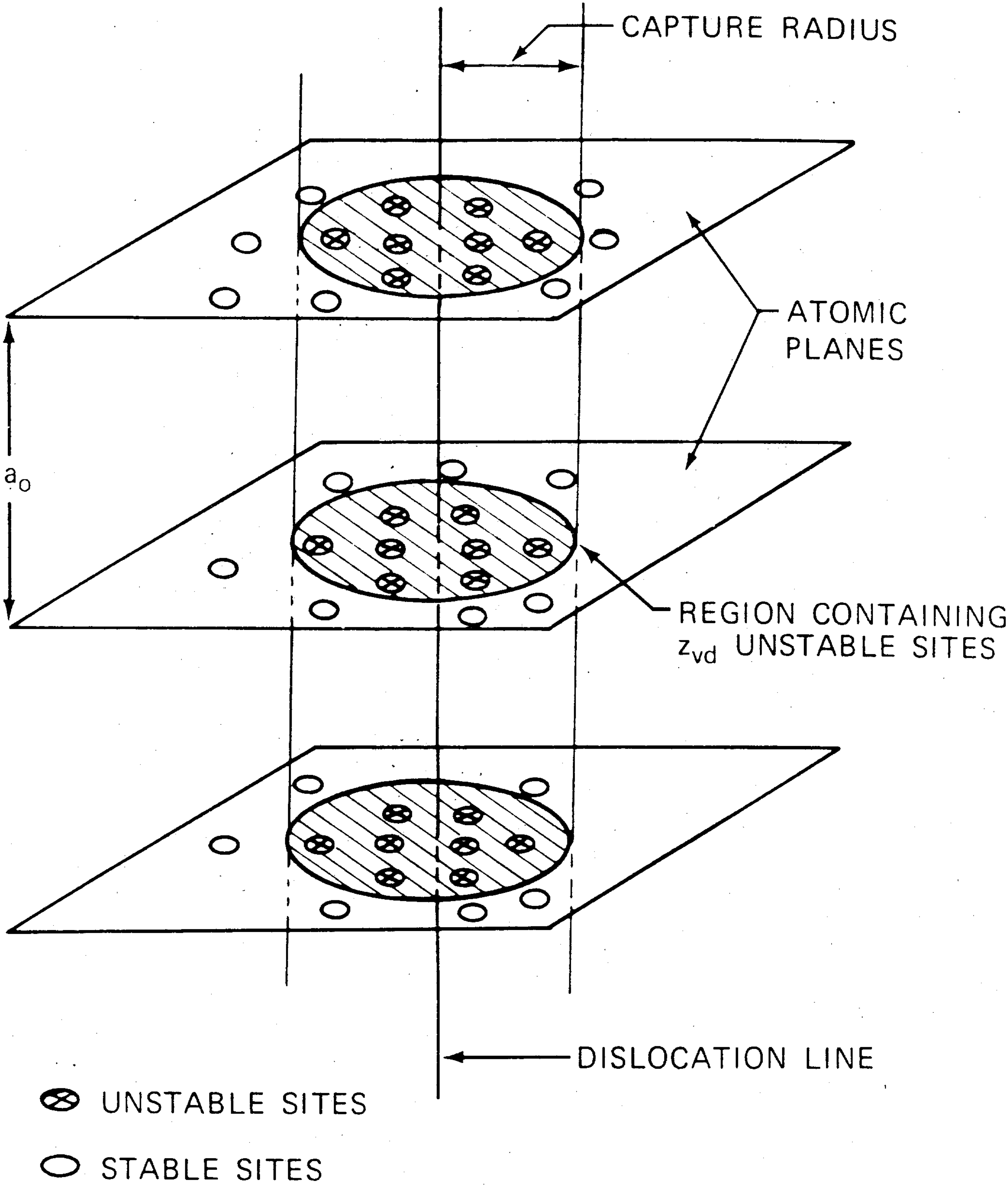


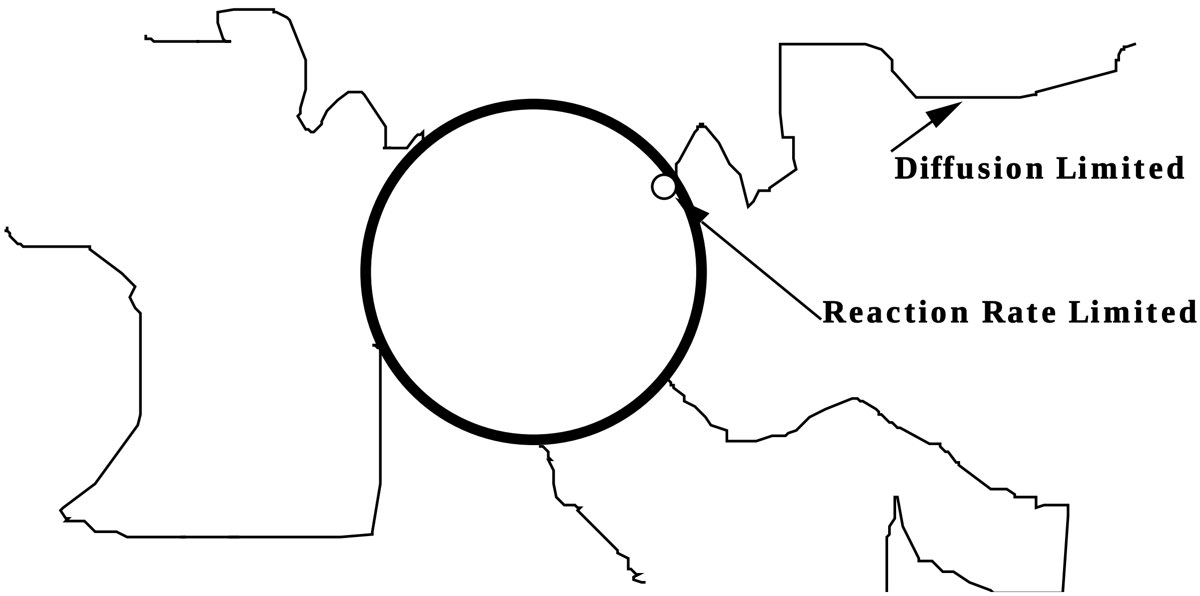
Fig. 13.6 Schematic of the capture sites around a dislocation line.

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

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

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

Note : Neglecting Recombination

at equilibrium,

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

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)

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

and C(∞) = C(   )

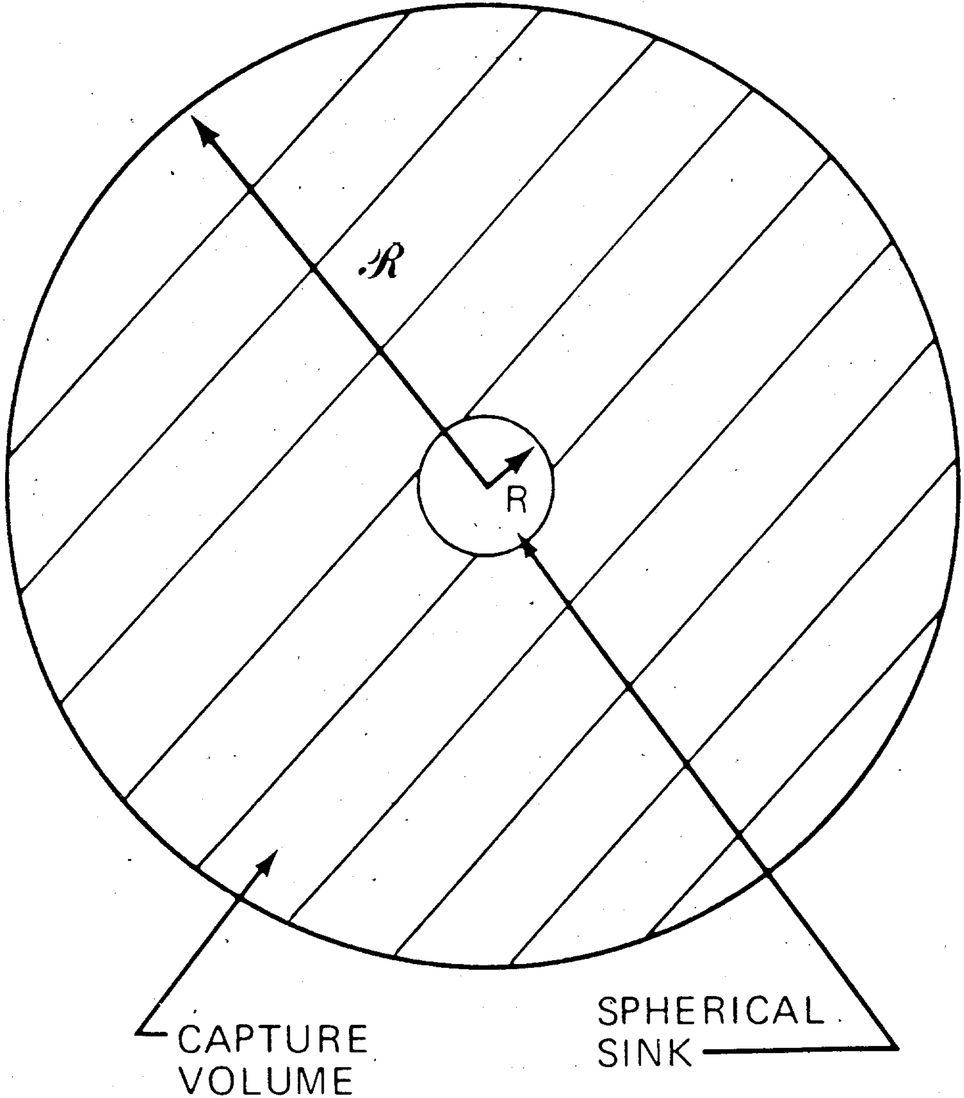


Fig. 13.7 The unit cell for computing the diffusion-controlled rate of point-defect absorption by spherical sinks.

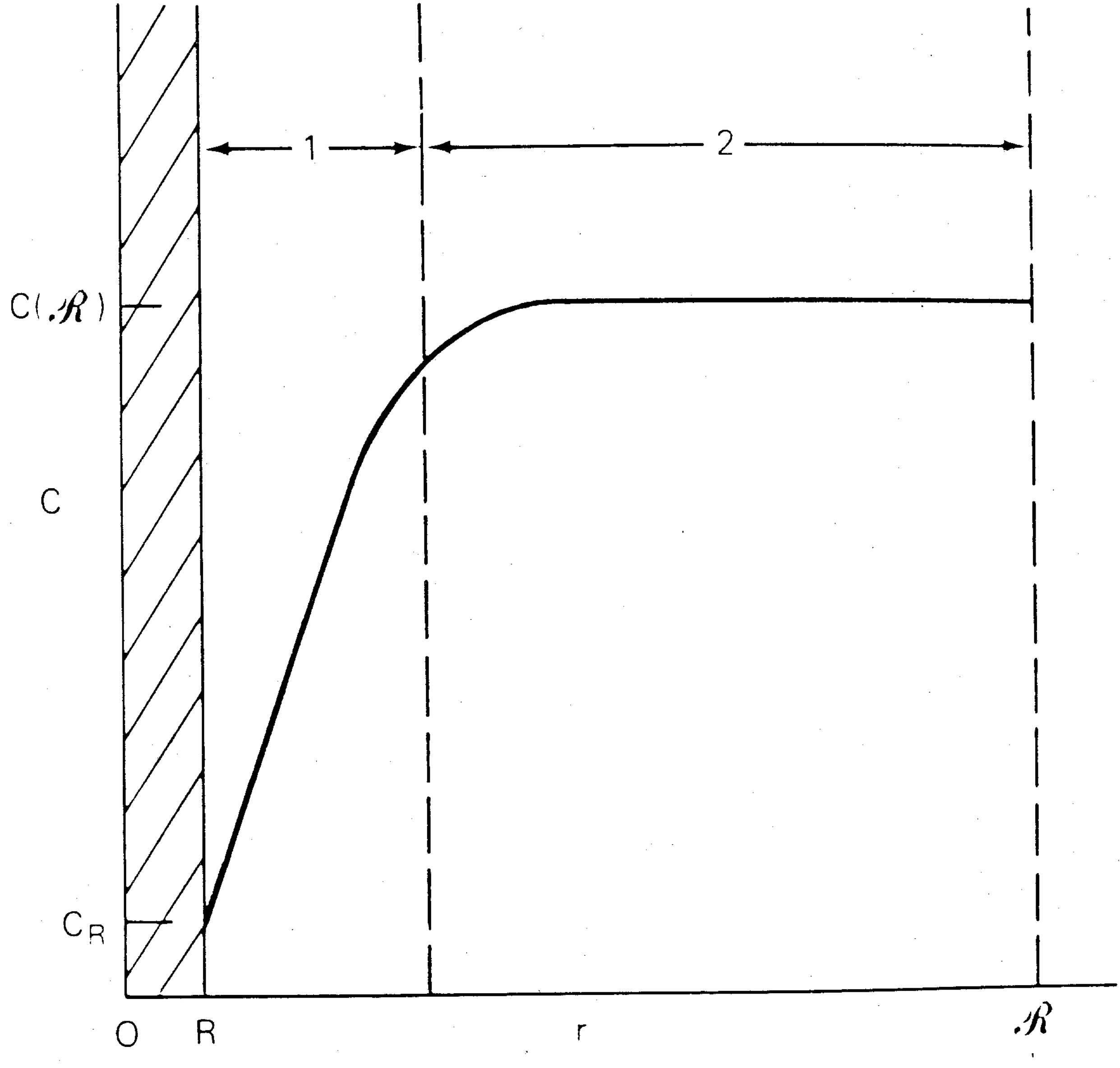


Fig. 13.8 Solution of the diffusion in a spherical shell with a uniform volumetric source.

Solving;

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

Since

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

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

Two parameters of Importance

1.) Absorption by a sphere

$$= -\left(4pR^2\right) J$$

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

What is this?

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

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

2.) Absorption by all spheres

if C( ) >> C_R
= 4pRDCC_t

rate constant
k = 4pRD

---

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

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

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;

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

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

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

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

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

This is all diffusion controlled

13.5.3 Mixed Rate Control

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

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

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

13.6 Rate Constants for Coalescence

Demonstrate that when two bubbles of equal size coalesce, the resulting equilibrium bubble volume is > twice the single bubble volume.

$$m = \left(\frac{4\pi R^3}{3}\right)\sum\left(\frac{2\gamma}{RkT}\right)$$

$$\frac{m_f}{m_o} = \frac{R_f^2}{R_0^2}$$

$$\frac{\left(\Delta V/V\right)_f}{\left(\Delta V/V\right)_0} = \frac{\left(\frac{4\pi R_f^3}{3}\right)}{\left(\frac{4\pi R_0^3}{3}\right)}\sum\left(\frac{N/2}{N}\right)$$

$$\frac{\left(\Delta V/V\right)_f}{\left(\Delta V/V\right)_0} = 2^{\frac{3}{2}} x \frac{1}{2} = \sqrt{2}$$

Analysis of bubble coalescence in the <u>Absence</u> of temperature or stress gradients

a.) First consider a fixed bubble radius R being bombarded by moving bubble of radius R. This gives;

$$Rate = 4\pi(2R)D_b\left[1 + \frac{2R}{\sqrt{\pi D_b t}}\right]C_m$$

where;

C_m**= #of bubbles containing m gas atoms**

b.) If we allow all bubbles to move;

$$Rate = 4\pi(2R)2D_b\left[1 + \frac{2R}{\sqrt{\pi 2D_b t}}\right]C_m$$

c.) Rate of collision between bubbles containing m $\frac{atoms}{cm^3}$;

$$Rate = 4\pi(2R)2D_b\left[1 + \frac{2R}{\sqrt{\pi 2D_b t}}\right]C_m^2$$

d.) More general expression for bubbles of size j and size i;

Rate Constant

$$k_{ij} = 4\pi\left(R_i + R_j\right)\sum\left(D_{bi} + D_{bj}\right)$$

$$Rate = 4\pi\left(R_i + R_j\right)\sum\left(D_{bi} + D_{bj}\right)\left\{1 + \frac{\left(R_i + R_j\right)}{\sqrt{\pi\left(D_{bi} + D_{bj}\right)t}}\right\}C_i C_j$$

Neglect when migration distance between collisions is large compared to bubble radii

5.) Include Stress or Temperature Gradients

(Biased Effects)

(see figure 13.10)

Rate at which bubbles of size i coalesce with size j in time t;

$$= \pi\left(R_i + R_j\right)^2 \left(v_{bi} - v_{bj}\right) C_i$$

But since there are $C_j \dfrac{\text{bubbles}}{\text{cm}^3}$ **;**

$$k_{ij} = \pi\left(R_i + R_j\right)^2 \left(v_{bi} - v_{bj}\right)$$

Problem 13.4

13.7 Bubble Resolution

Macroscopic Models

- ***Ross - Thermal Spike***
- ***Whapham -Chunk***
- ***Turnbull - Destroy Bubbles***

Microscopic

- ***Nelson -single atom resolution***
- ***Manley -single atom resolution***

Turnbull

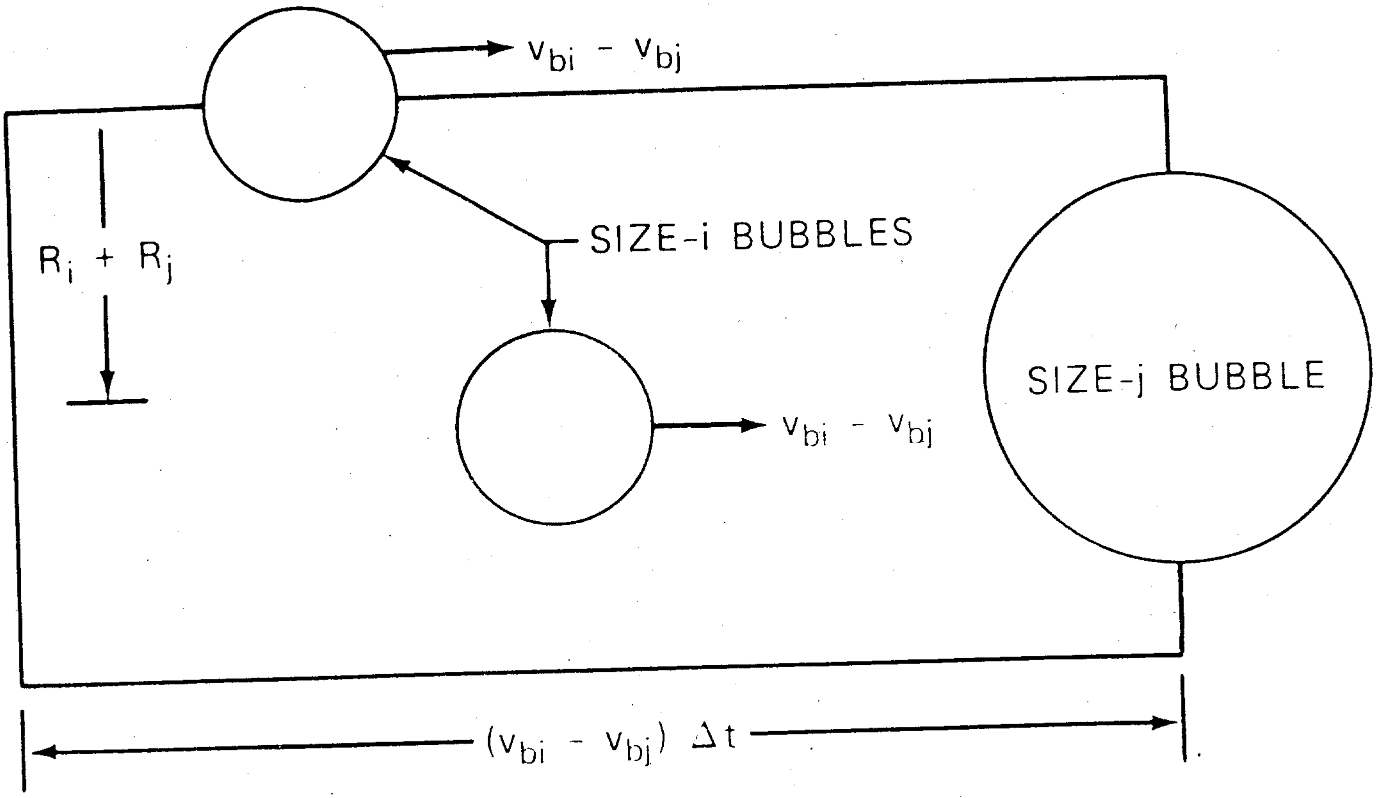


Fig. 13.10 Diagram for computing the coalescence rate for biased bubble motion.

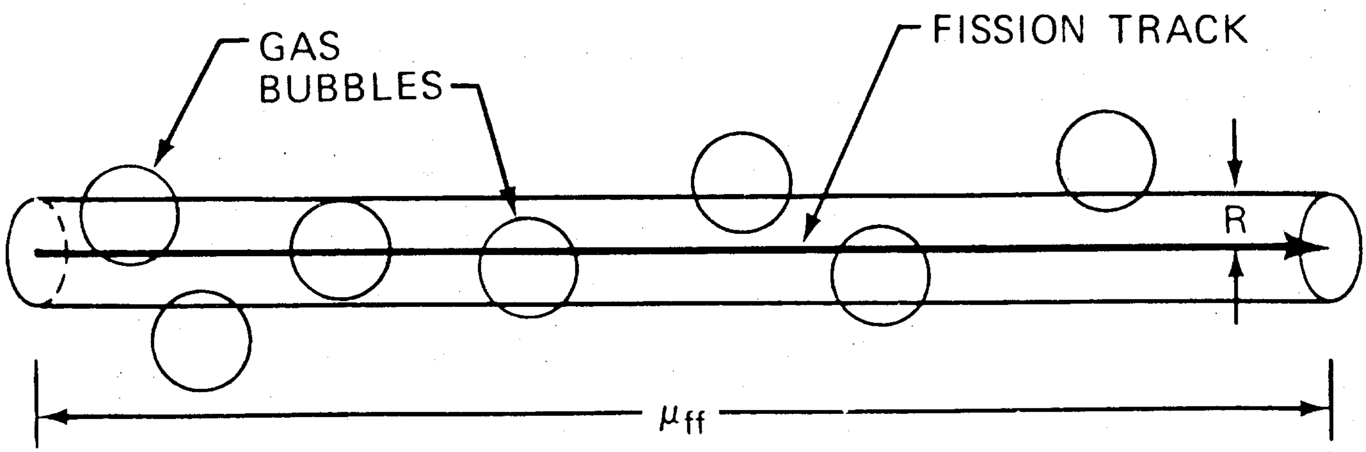


Fig. 13.11 Diagram for calculating the re-solution parameter by Turnbull's method. [After J. A. Turnbull, *J. Nucl. Mater.*, 38: 203 (1971).]