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.

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

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

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

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

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

Figure 13.11

$$\frac{\text{Gas bubbles destroyed}}{\text{cm}^3\text{-sec}} = b'C_m$$

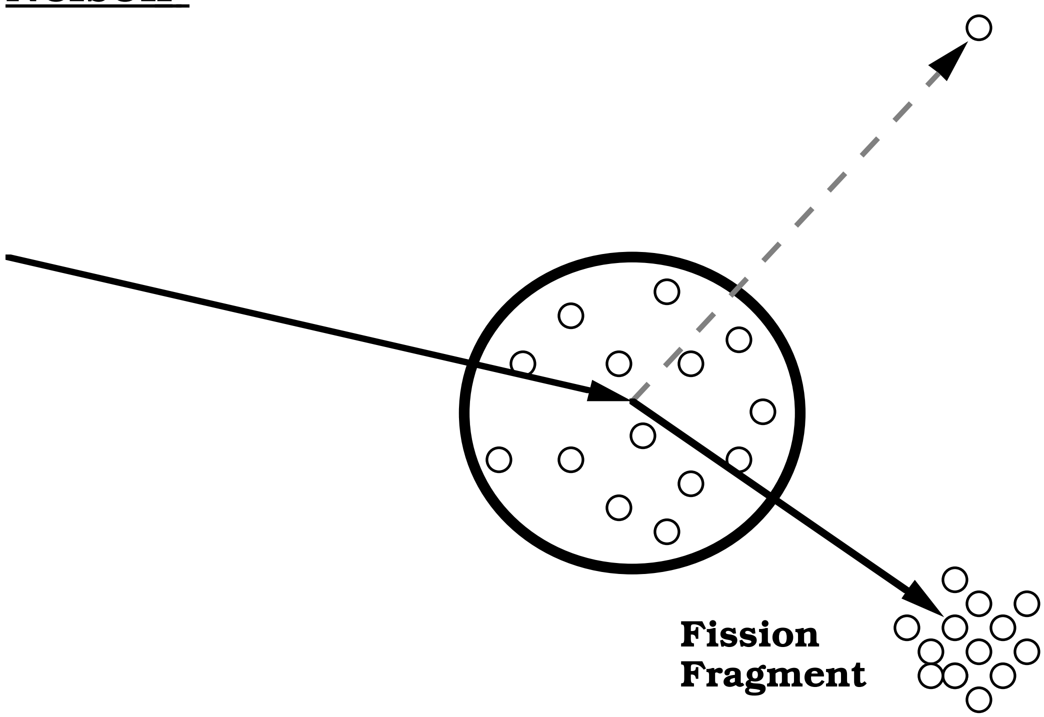
b' = prob./s that a bubble in fuel is destroyed.

$$= 2\pi R^2 \mu_{ff} \overset{\Sigma}{F}$$

gas atoms returned to the matrix from bubble per cm^3 and per second. = b'm N

bubbles/cm^3 which contain m gas atoms

Nelson



Need several things;

1.) Flux of FF's
2.) Energy of FF's
3.) Cross section for interaction (usually Coulomb)
4.) Energy of gas atom that can make it out of the bubble

$$\frac{\textit{gas atoms returned to matrix from bubbles}}{cm^3 \ sec}$$

$$= bmN$$

Where

$$b = \frac{2\pi Z^4 e^4}{E_{ff} T_{min}} \left[\ln\left(\frac{E_{ff}^{max}}{T_{min}} \right) \right] \mu_{ff} \overset{\Sigma}{F}$$

----
in fact, even this is too small and Nelson includes the interaction between the PKA's and gas atoms in the bubble to get results which are closer to experiment.

Nelson found that the efficiency of pushing gas atoms back into the matrix varies from 44% for very large bubbles to 100 % when diameters are ≈ 30 Å

13.8 Nucleation of Fission Gas Bubbles

First distinction is between nucleation.

- ***Homogeneous***
- ***Heterogeneous***

13.8.1 Homogeneous Nucleation

Assume stable nuclei are diatomic cluster of gas atoms, see figure 13.12

Define 1.) Nucleation time $\left(\frac{\partial C_2}{\partial t} = 0\right)_{t_c}$

2.) Nucleation density, C_2 at t_c

3.) Note; assume constant concentration of bubbles after t_c

Sequence

$$\frac{dC}{dt} = Y_{Xe}\overset{\Sigma}{F} - 2k_{11}C^2 - k_{12}CC_2$$

Fission--> g

Conc.of single gas atoms — **2 consumed per diatomic** — **Triatomic**

g +g <==> g_2

g + g_2 <=> g_3

$$-k_{1m}CC_m + 2(2C_2)b + \ldots + mC_mb$$

....

g + g_m <=> g_{m+1}

Assumes whole bubble dissolved

note; only simple gas atoms added, not clusters.
For diatomic clusters

$$\frac{dC_2}{dt} = k_{11}C^2 - k_{12}CC_2 - (2C_2)b + (3C_3)b + \ldots.$$

in general,

$$\frac{dC_m}{dt} = k_{1,m-1}CC_{m-1} - k_{1m}CC_m - (bmC_m) + (m+1)C_{m+1}b$$

Balence on gas atoms;

$$Y_{Xe}\overset{\Sigma}{F} = \frac{dC}{dt} + 2\frac{dC_2}{dt} + \ldots\ldots + m\frac{dC_m}{dt}$$

Use the above analysis to determine the concentration of single and diatomic gas atom clusters at the at the end of the nucleation period, t_c.

$$Y_{Xe}\overset{\Sigma}{F} = \frac{\left(3k_{11}k_{12}C_c^3\right)}{\left[k_{12}C_c + 2b\right]}$$

Growth by addition **Resolution**

and $C_{2c} = \dfrac{k_{11}C_c^2}{\left(k_{12}C_c + 2b\right)}$

Figure 13.13

at high temperatures and low fission rates;

$$C_c = \sqrt{\frac{Y_{Xe}\overset{\Sigma}{F}}{3k_{11}}}$$

$$C_{2c} = \sqrt{\frac{Y_{Xe}\overset{\Sigma}{F}k_{11}}{3k_{12}^2}}$$

at low temperatures and high fission rates;

$$C_c = \left(\frac{2bY_{Xe}\overset{\Sigma}{F}}{3k_{11}k_{12}}\right)^{\frac{1}{3}}$$

$$C_{2c} = \left(\frac{Y_{Xe}\overset{\Sigma}{F}\sqrt{k_{11}}}{3\sqrt{2b}k_{11}k_{12}}\right)^{\frac{2}{3}}$$

Problem 13.3

13.8.2 Heterogeneous Nucleation

Speculation about the effect of fission fragment path length and nucleation on dislocations.

13.9 Growth of Stationary Bubbles

Assumptions

1.) *After t_C, the bubble density is constant, they only change in size.*

2.) *Neglect directed motion.*

3.) *Use growth only by single vacancies or gas atoms.*

4.) *Assume all bubbles the same radius at the start.*

*5.) *No gas in the matrix, all in bubbles.*

*6.) *Resolution neglected.*

*7.) *Bubbles are in mechanical equilibrium.*

8.) *Either perfect or Van der Waal's gas law is applicable.*

13.9.1 Simplest growth model

Condition 5 yields;

$$Y_{Xe}\overset{\Sigma}{F}t = mN$$

show;

$$R = \sqrt{\frac{3kTY_{Xe}\overset{\Sigma}{F}t}{4\pi 2\gamma N}}$$

and;

$$\frac{\Delta V}{V} = \sqrt{\frac{3}{4\pi N}}\,\Sigma\left(\frac{kT}{2\gamma}\right)^{\frac{3}{2}} \Sigma\left(Y_{Xe}\,\overset{\Sigma}{F}\,t\right)^{\frac{3}{2}}$$

13.9.2 Allowance for Gas Remaining in the Matrix

Finds that allowance for some gas to remain in the matrix can reduce swelling by a factor of 10 at low temperatures, but there is very little effect at T > 1000 - 1500 °K

13.9.3 Bubble Growth with Resolution

Starting with;

$$\frac{dC}{dt} = Y_{Xe}\,\overset{\Sigma}{F} - 2k_{11}C^2 - \left(\sum_{m=2}^{\infty} k_{lm}C_m\right)C + 2C_2 b + \left(\sum_{m=2}^{\infty} mC_m\right)b$$

can neglect in growth stage

After much manipulation;

$$\frac{(1-f_b)}{f_b^{\frac{2}{3}}} = \frac{b}{(4\pi N)^{\frac{2}{3}} D_{Xe}\left(3BY_{Xe}\,\overset{\Sigma}{F}\,t\right)^{\frac{2}{3}}}$$

Where f_b = fraction of gas in bubbles

Figure 13.15

Resolutioning important at high fission rates and low temperature.

Figure 13.16

==

13.9.4 Growth of non Equilibrium Bubbles

We normally assume the bubble can attract all the vacancies it needs to retrain mechanical equilibrium. But as the bubble gets bigger, it needs more vacancies ;

$$\frac{(m_v)_{eq}}{m_{gas}} = \left(\frac{kT}{2\gamma}\right)\frac{R}{\Omega} + \frac{B}{\Omega}$$

R Å	$\frac{(m_v)_{eq}}{m_{gas}}$
10	2
100	6
1000	27

Orlander next sets up vacancy and interstitial equations to get growth.

(solves for C_v and C_i)

Figures 13.17 a & b

Olander finds that growth rate is;

$$\frac{dR}{dt} = \frac{\Omega}{R}\left[D_v\left(1-\frac{Z_v}{Z_i}\right)\left(C_v - C_v^{eq}\right) + \frac{\Omega}{kT}\left(p - \frac{2\gamma}{r}\right)\left(D_v C_V^{eq} + D_i C_i^{eq}\right)\right]$$

effect of supersaturation **Effect of pressure on growth imbalance .. $p > 2\gamma/r$**

Chemical stress term

13.9.5 Bubble Size Distribution During Growth

Read for general information
(Problem 13.9)