Example calculation for BCC Fe

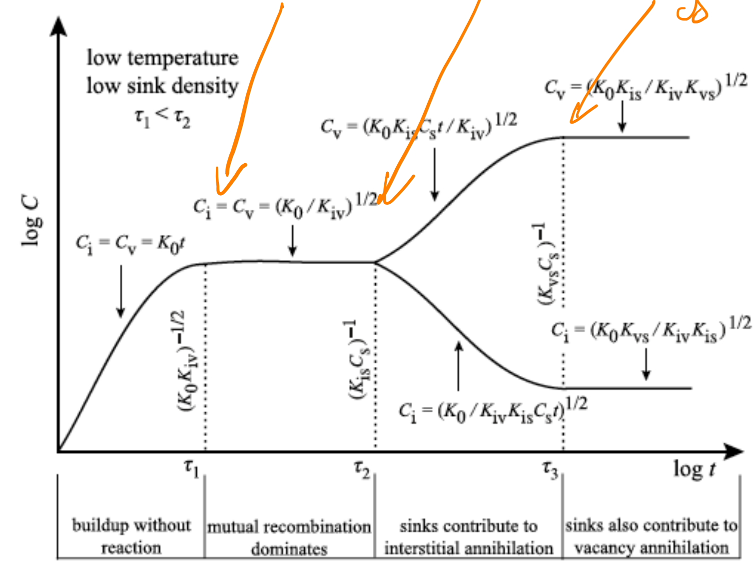
- Problem: Calculate the typical times of the different stages of C_v and C_i for BCC Fe using the following parameters:

13 days

2.5E12 years

60s

293K neutron irradiation
Lattice parameter ($\boldsymbol{a_0}$) of 2.82 Å
Dislocation density ($\boldsymbol{p_d}$) of 10^8 cm^{-2}
Interstitial migration energy ($\boldsymbol{E_m^i}$) of 0.65 eV
Vacancy migration energy ($\boldsymbol{E_m^v}$) of 1.5 eV
Capture radius($\boldsymbol{r_{iv}}$) of 10$\mathbf{a_0}$
Displacement rate ($\boldsymbol{K_0}$) of 10^{-7} dpa/s
Vibration frequency ($\boldsymbol{v}$) of 10^{13} Hz



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Example calculation for BCC Fe

- Problem: Calculate the typical times of the different stages of C_v and C_i for BCC Fe using the following parameters:
  - Step 1: Calculate the recombination constant:

And the recombination rate constant is:

$$K_{\mathrm{iv}} = P_{\mathrm{iv}} \nu e^{-\frac{E_{\mathrm{m}}^{\mathrm{i}}}{kT}} = 200 \times 10^{13} \times e^{-\frac{0.65}{(293 \times 8.62 \times 10^{-5})}}$$
$$= 1.33 \times 10^{4} \mathrm{s}^{-1}$$

  - Now calculate the time for recombination to become significant

Thus the time for recombination to become significant is:

$$\tau_1 = \sqrt{\frac{1}{K_{iv} k}} = \tau_1 = \sqrt{\frac{1}{1.33 \times 10^{4} \times 10^{-7}}} = 27.4s$$

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Example calculation for BCC Fe

- Problem: Calculate the typical times of the different stages of C_v and C_i for BCC Fe using the following parameters:

For bcc Fe, Z=8 and the elemental jump distance is equal to:

$$\frac{a_0}{2}\sqrt{3} = 2.44\text{Å}$$

This means that the diffusion coefficient for interstitial is:

$$D_i = \frac{1}{6}a^2 \nu Z e^{-\frac{E_m^i}{kT}} = \frac{8}{6} \times \left(2.44 \times 10^{-8}\right)^2 \times 10^{13} \times e^{-\frac{0.65}{(293 \times 8.62 \times 10^{-5})}} = 5.3 \times 10^{-14}\text{cm}^2/\text{s}$$

And the diffusion coefficient for vacancies is:

$$D_v = \frac{1}{6}a^2 \nu Z e^{-\frac{E_m^i}{kT}} = \frac{8}{6} \times \left(2.44 \times 10^{-8}\right)^2 \times 10^{13} \times e^{-\frac{1.5}{(293 \times 8.62 \times 10^{-5})}} = 1.27 \times 10^{-28}\text{cm}^2/\text{s}$$

The time for interstitials to arrive at sinks is:

$$\tau_2 = \frac{1}{\rho_d Z_i D_i} = \frac{1}{10^8 \times 1.02 \times 5.3 \times 10^{-14}} = 1.86 \times 10^5 s = 51\text{hrs}$$

The final steady state is reached when vacancies arrive at sinks:

$$\tau_3 = \frac{1}{\rho_d Z_v D_v} = \frac{1}{10^8 \times 1 \ \times 1.27 \times 10^{-28}} = 7.8 \times 10^{19} s = 2.48 \times 10^{12}\text{years!!!}$$