TD defects (recap)

Min $G = H - TS$

$$c_v = e^{-G_v^f/k_BT} = e^{S_v^f/k_B}\, e^{-H_v^f/k_BT}$$

For Fe, $H_v^f \sim 2eV$; $k_B = 8{,}62 \cdot 10^{-5}\, eV/K$

$S_v^f \sim 2k_B$

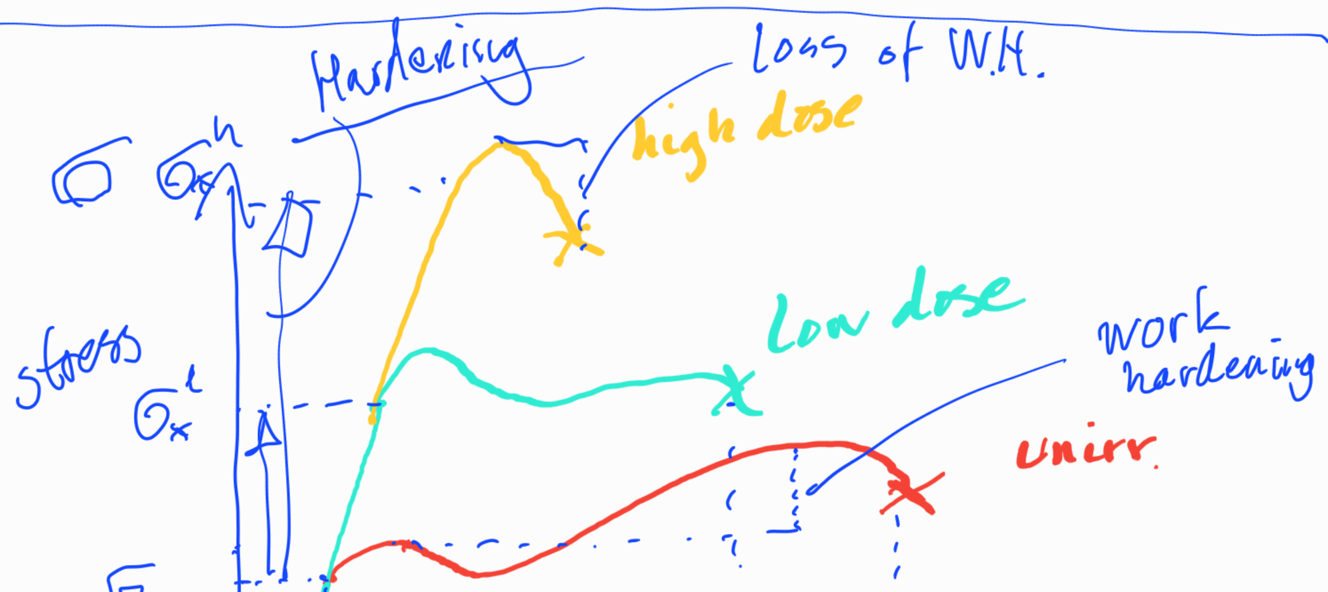
$$\text{For } T = \begin{cases} 300K \\ 600K \\ 900K \\ 1200K \end{cases} \Rightarrow \boxed{c_v = \begin{cases} 10^{-33} \\ 10^{-17} \\ 10^{-11} \\ 10^{-8} \end{cases}}$$

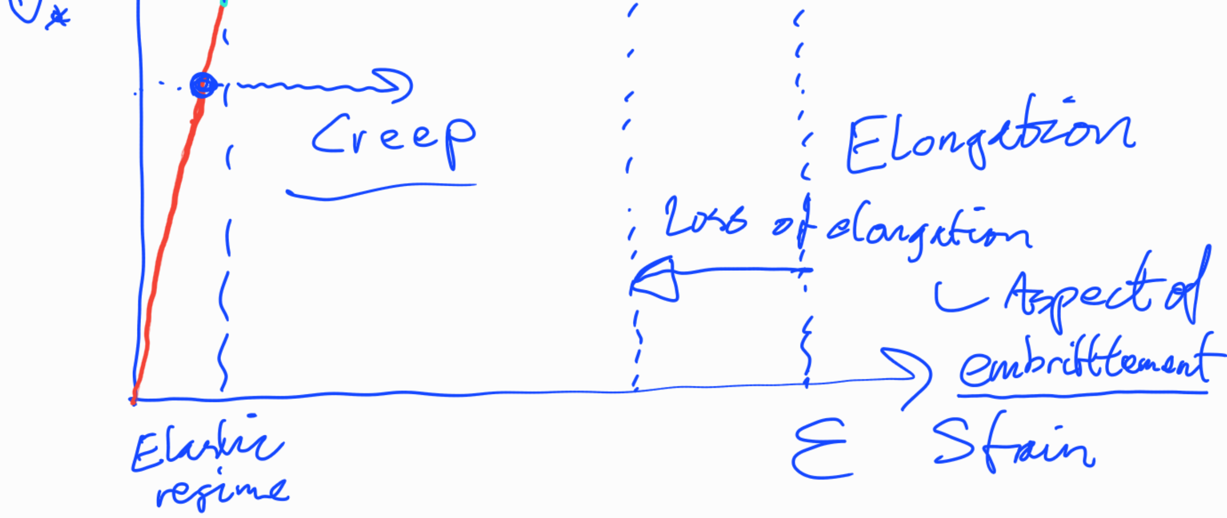
(Fe) $H^f_{SIA} \sim 4eV$

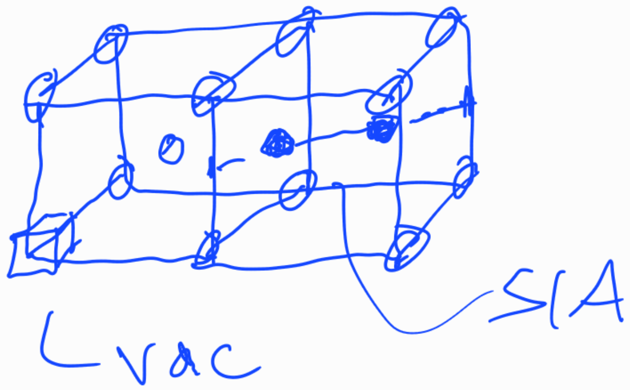
$S^f_{SIA} \sim 7k_B$

$$C_{SIA} = \begin{cases} 10^{-65} \\ 10^{-33} \\ 10^{-17} \\ 10^{-14} \end{cases}$$

Never any thermal SIA! (in metals)







bcc

The damage event (chapter 1)

Particle with high energy E_i

$\sigma_s(E_i, E_f, \Omega)$ ← solid angle

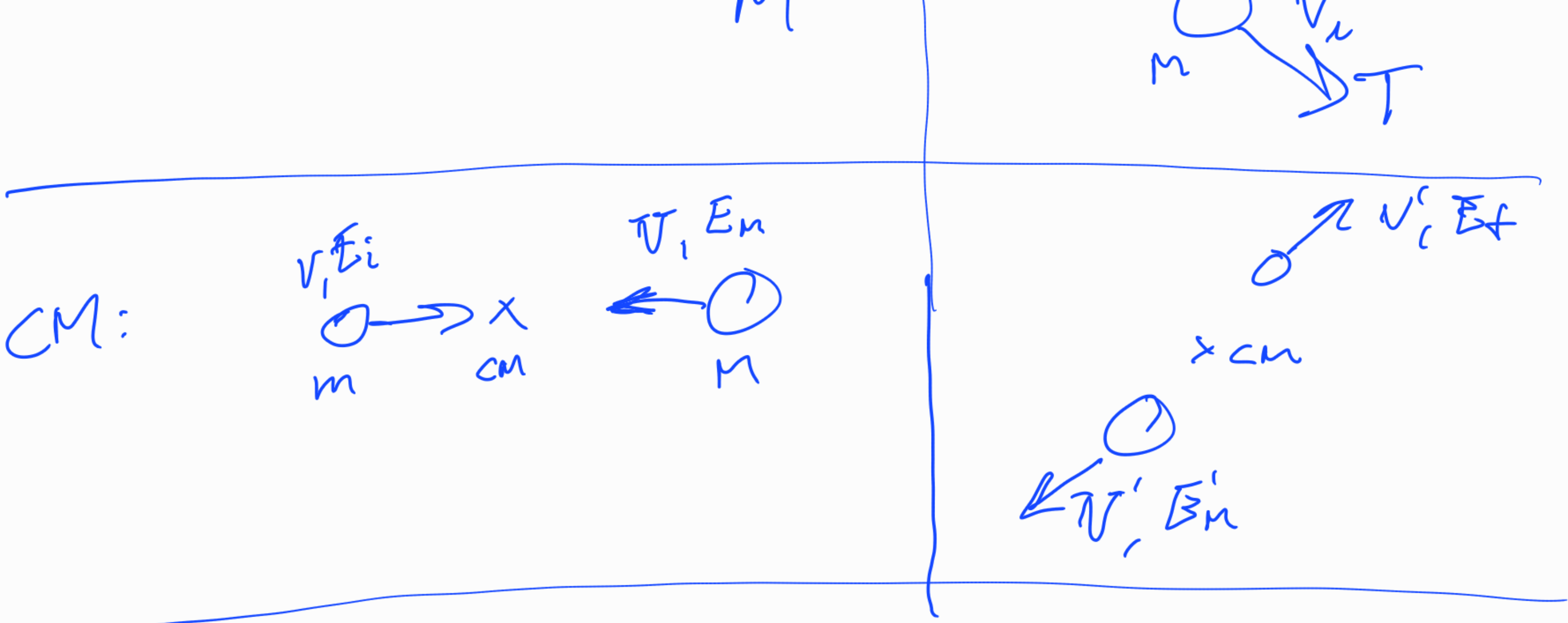
We want $\sigma_s(E_i, T)$ ← transmitted energy

$$\sigma_s(E_i, \Omega) = \int \sigma_s(E_i, E_f, \Omega)\, dE_f$$

Total XS $\sigma_s(E_i) = \int \sigma_s(E_i, \Omega)\, d\Omega$

Relation btw (E_i, T) :

Before	After



Head-on collision

* Cons. of momentum
* — " — energy

$$\left.\begin{array}{l}P_{before} = P_{after} \\ E^k_{before} = E^k_{after}\end{array}\right\}$$

$$\Rightarrow T(m, M, E_i) = \underbrace{\frac{4mM}{(m+M)^2}}_{\gamma} E_i \qquad (\underline{ex})$$

$$\Rightarrow \boxed{\hat{T} = \gamma E_i}$$

$(\hat{T} = \text{maximal } T)$

For a neutron:
$m = 1$; $M = A$

$$\Rightarrow \boxed{\gamma = \frac{4A}{(1+A)^2}}$$

<u>Ex</u>: What is γ for a neutron $\to$ <u>Fe</u> ?

- Assume 1 MeV n: How much energy is transferred to an Fe-atom maximally?
$(A = 55{,}85)$

$\gamma = 0{,}069$

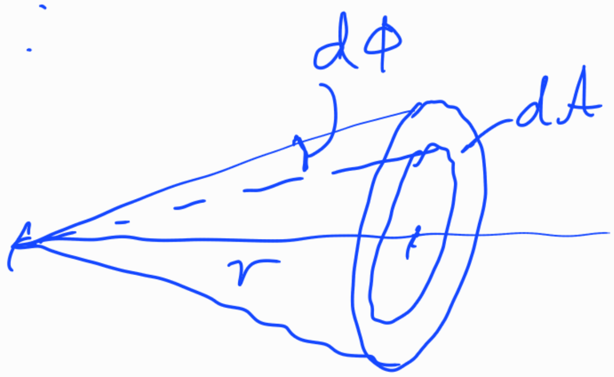
$\hat{T}(Fe) \simeq 69\ keV$

General: $\boxed{T = \frac{\gamma}{2}(1-\cos\phi) E_i}$

Max $\hat{T} = \gamma E_i$

Min $\check{T} = E_d$ (threshold for displacement)

Probability to impart T:



$\sigma_s(E_i, T)\, dT =$

$= 2\pi\, \sigma_s(E_i, \phi) \sin\phi\, d\phi$

Given $T = \frac{\gamma}{2}(1-\cos\phi) E_i \Rightarrow$

$dT = \frac{\gamma}{2} E_i \sin\phi\, d\phi$

$\Rightarrow \sigma_s(E_i, T) = \frac{4\pi}{\gamma E_i} \sigma_s(E_i, \phi)$

Isotropic scattering then

$\sigma_s(E_i) = \int \sigma_s(E_i, \phi)\, d\Omega = 4\pi\, \sigma_s(E_i \phi)$

$\Rightarrow \sigma_s(E_i, T) = \frac{\sigma_s(E_i)}{\gamma E_i}$ (indep of T)

Average T: $$\bar{T} = \frac{\int_{\check{T}}^{\hat{T}} T\,\sigma_s(E_i,T)\,dT}{\int_{\check{T}}^{\hat{T}} \sigma_s(E_i,T)\,dT} = \frac{\check{T}+\hat{T}}{2} \approx \frac{\hat{T}}{2} = \frac{\gamma E_i}{2}$$

(PKA) Primary knock-on atom

Atom-atom interactions