

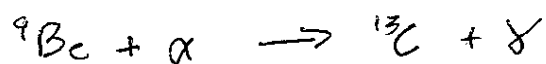
1/20/04

QE studying M11s

Alex Hagen

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Given Be w/ incident  $\alpha$  of energy, what's the recoil?



Energy conservation

$$T_\alpha + m_\alpha c^2 + m_0 c_{\text{Be}}^2 = T_\gamma + m_0 c_{13}^2 + T_{\text{C-13}}$$

Momentum conservation

$$p_\alpha = p_\gamma + p_{\text{C-13}}$$

Solve

$$T_\alpha + [m_\alpha c^2 + m_0 c_{\text{Be}}^2 - m_0 c_{\text{C-13}}^2] = T_\gamma + T_{\text{C-13}}$$

$$5.3 \text{ MeV} + 931.5 \frac{\text{MeV}}{924} [9 + 4 - 13] = T_\gamma + T_{\text{C-13}}$$

$$\frac{1}{2} \sqrt{(T_\alpha + 2m_\alpha c^2) T_\alpha} = \frac{E_\gamma}{c} + \frac{1}{2} \sqrt{(T_{\text{C}} + 2m_0 c^2) T_{\text{C}}}$$

$$\sqrt{(T_\alpha + 2m_\alpha c^2) T_\alpha} = E_\gamma + \sqrt{(T_{\text{C}} + 2m_0 c^2) T_{\text{C}}}$$

$$T_\gamma = 15.55 \text{ MeV} - T_{\text{C}}$$

$$\sqrt{(T_\alpha + 2m_\alpha c^2) T_\alpha} = 15.55 \text{ MeV} - T_{\text{C}} + \sqrt{(T_{\text{C}} + 2m_0 c^2) T_{\text{C}}}$$

$$198.85 \text{ MeV} - 15.55 \text{ MeV} = \sqrt{(T_{\text{C}} + 2m_0 c^2) T_{\text{C}}} - T_{\text{C}}$$

$$(T_{\text{C}} + 183.3 \text{ MeV})^2 = (T_{\text{C}}^2 + T_{\text{C}} 2m_0 c^2)$$

$$T_{\text{C}}^2 + 2 \cdot 183.3 \text{ MeV} T_{\text{C}} + (183.3 \text{ MeV})^2 = T_{\text{C}}^2 + T_{\text{C}} 2m_0 c^2$$

$$T_{\text{C}} = - \frac{(183.3 \text{ MeV})^2}{2 \cdot 183.3 \text{ MeV} - 2m_0 c^2}$$

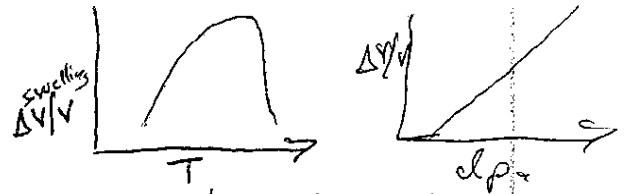
$$T_{\text{C}} = 1.408 \text{ MeV}$$

## Swelling and Creep

Creep — Time-dependent deformation of a metal under constant load at high temperature

irradiation increases creep over thermal creep, or induces creep in temperatures where it wasn't before.

Swelling — volumetric expansion



Swelling is the isotropic volume expansion of a solid without an external stress. Creep is the volume conservative distortion of a solid under applied stress.

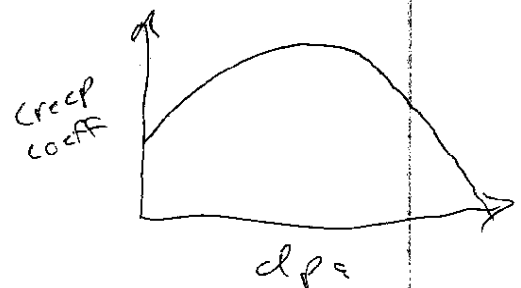
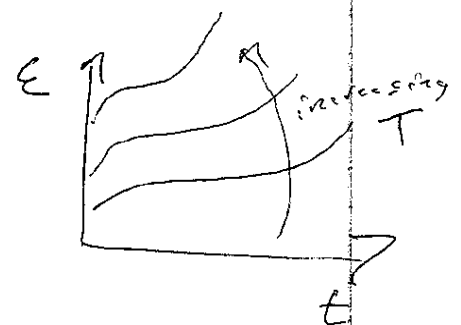
Swelling concern

- dis. dimensional increase
- particle transport
- $t_h$
- failure path on voids
- depends on dose dose rate, comp. temp
- freely migrating defects, long range migration — steel

$$C_V = \frac{1}{N} \exp\left(\frac{-S_f}{k}\right) \exp\left(\frac{-H_f}{kT}\right)$$

Creep Concern

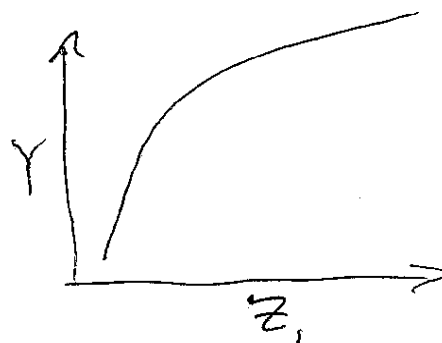
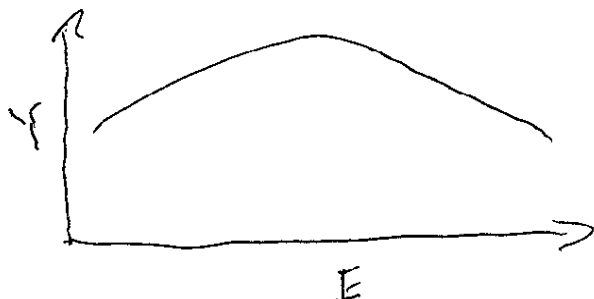
- reduced failure time
- deformation
- embrittlement
- cracking
- lowered fracture resistance



Sputtering

$$Y = \text{sputtering yield} = \frac{\text{emitted atoms}}{\text{incident particle}}$$

Sputtering yield depends on  
structure and comp of target  
parameters of beam  
geometry



Matsunami:

$$Y_E(E) = 0.47 \frac{\alpha_s Q_s S_n(E)}{U_0 [1 + 0.35 U_0 S_2(E)]} \left[ 1 - (E_{th}/E)^{0.5} \right]^{2.8}$$

Steady state concentration

at  $t=0$

← flux ratio

$$\frac{J_B}{J_A} = r \left( \frac{N_B}{N_A} \right) \quad 0.8 < r < 2 \Rightarrow (J_A + J_B) = Y J_i$$

at steady state

$$J_A = J_i \Rightarrow \frac{N_A}{N_B} = r(Y-1)^{-1}$$

Also → Preferential sputtering  
at  $t=0$

$$\frac{Y_A(0)}{Y_B(0)} = r \frac{N_A^s(0)}{N_B^s(0)} = r \frac{N_A^b}{N_B^b}$$

at  $t=\infty$

$$\frac{N_A^s(\infty)}{N_B^s(\infty)} = \frac{1}{r} \frac{N_A^b}{N_B^b}$$

$$\frac{Y_A(\infty)}{Y_B(\infty)} = \frac{N_A^b}{N_B^b}$$

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S/E

Range Integration

$$R = \int_{E_i}^0 \frac{dE}{dE/dx}$$

for nuclear

$$\left. \frac{dE}{dx} \right|_n = N_{\pi} \frac{Z_1^2 Z_2^2 e^4 M_1}{E_1 M_2} \ln \frac{\Delta E_i}{E_u}$$

$$R = \int_{E_i}^0 \frac{dE}{dE/dx} = \int_{E_i}^0 \frac{dE}{kE^{1/2}}$$

for nuclear

$$\left. \frac{dE}{dx} \right|_e = kE^{1/2}$$

$$R = \int_{E_i}^0 \frac{dE}{kE^{1/2}}$$

Maximum Energy Transfer / Weighted Average Recoil Spectrum

$$T_{max} = \Delta E = \frac{4M_1 M_2}{(M_1 + M_2)^2}$$

Weighted Average Recoil Spectrum

$$\bar{T} = \frac{1}{2} \Delta E_i = \frac{\int_0^{\Delta E_i} T \sigma(E, T) dT}{\int_0^{\Delta E_i} \sigma(E, T) dT} \quad \nearrow \text{isotropic scattering w/ } \sigma_s$$

for Coulomb potential

$$\sigma = \frac{\pi}{4} \frac{(Z_1 Z_2 e^2)^2}{E^2} \left( \frac{T_m}{E_d} - 1 \right)$$

$$\bar{T} = E_d \ln \frac{\Delta E_i}{E_d} \quad E_d \ll \Delta E_i$$

Weighted average recoil spectrum

$$W(T) = \frac{\int_{E_d}^T T \sigma(E, T) dT}{\int_{E_d}^{\Delta E} T \sigma(E, T) dT}$$

harder spectrum for higher mass

More displacements at higher recoil energy for higher primary atom energy!

Potential Forms

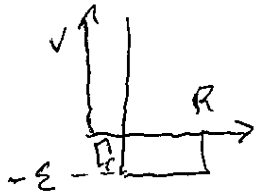
Hard sphere -

$$V(r) = \begin{cases} \infty, & r < r_0 \\ 0, & r > r_0 \end{cases}$$



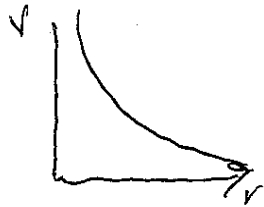
Square Well -

$$V(r) = \begin{cases} \infty, & r < r_0 \\ -\epsilon, & r_0 < r < R \\ 0, & r > R \end{cases}$$



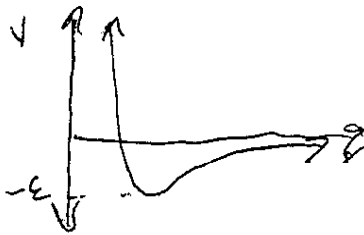
Inverse Power -

$$V(r) = \epsilon \left( \frac{r_0}{r} \right)^n$$



Lennard-Jones

$$V(r) = \epsilon \left[ \left( \frac{r_0}{r} \right)^{12} - \left( \frac{r_0}{r} \right)^6 \right]$$



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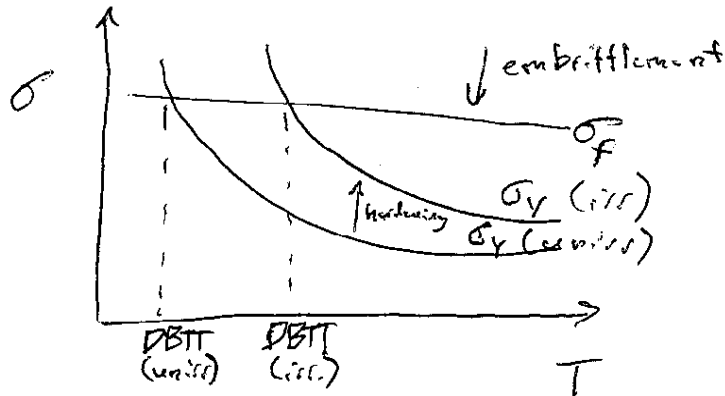
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Ductile to Brittle Transition Temperature

DBTT defined as the point ~~at~~ in temperature where the yield and fracture stresses are equal! Means it fractures immediately after the elastic deformation section.

Increased by irradiation as shown below



→ neutron environment effect on DBTT is approx

$$\Delta T_{db} = A \Phi^{(0.28-1.0, \Phi)}$$

so increases change in DBTT w/ increasing fluence

Reversal

→ thermal annealing - depends on (re)irradiation

almost full recovery after 70-150 hr at 450°C

[1] Was - p.

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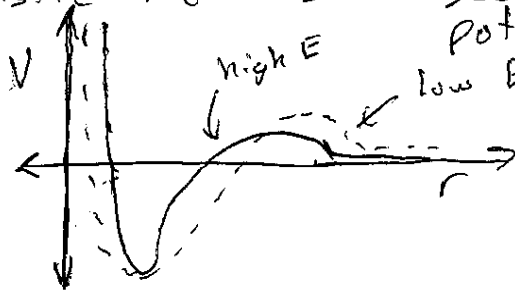
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Macroscopic parameters to Potential Well shapes

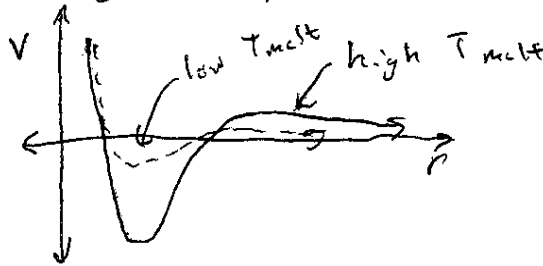
Binding Energy - Depth of well

$$E_b \equiv \Delta H_s \equiv \frac{1}{2} n_c N_A E_b$$

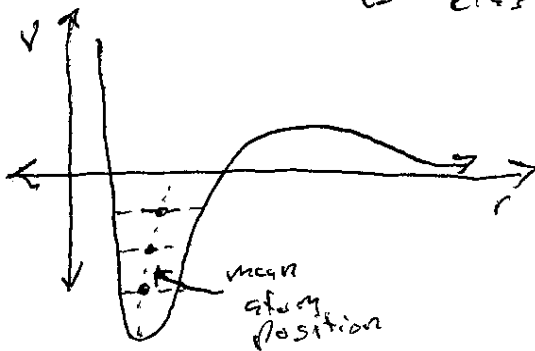
Elastic Modulus - second derivative of potential at its minimum



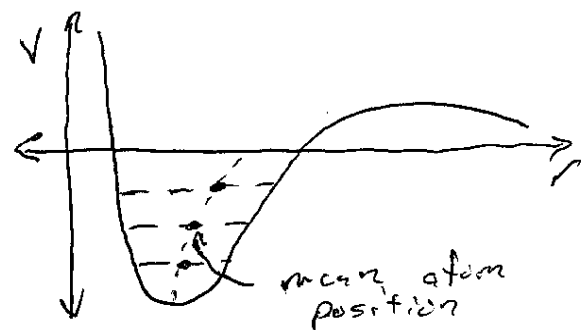
Melting Temperature - proportional to Binding Energy



Coefficient of Thermal Expansion - <sup>inversely</sup> proportional to elastic modulus



High E, low thermal expansion



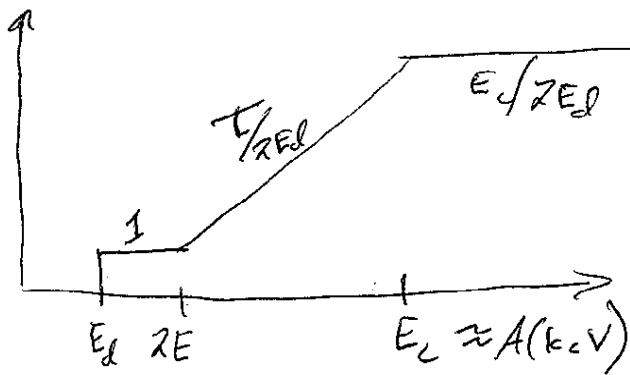
Low E, high thermal expansion

[1] Nestesi p. 19-24



DPA Calculations

we have  $v(T) = \#$  of displacements



$$\Delta = \frac{4M_1 M_2}{M_1 + M_2}$$

Hard sphere

$$\sigma(E, T) = \frac{\sigma_P}{\Delta E} = \frac{C}{E}$$

displacement rate

$$R_d = \int_{E_d}^{\infty} \phi(E) \sigma_d(E, T) E$$

$$\sigma_d = \int_{E_d}^{E = T_{max}} v(T) \sigma(E, T) dT$$

$$\begin{aligned} \sigma_d &= \int_{E_d}^{E_d} \left[ (0) \frac{\sigma_P}{\Delta E} + (1) \frac{\sigma_P}{\Delta E} + \frac{T}{2E_d} \frac{\sigma_P}{\Delta E} \right] dT \\ &= \left( \frac{\sigma_P}{\Delta E} \right) (E_d - E_d) + \left( \frac{\sigma_P}{2\Delta E_d} \right) \left( \frac{(E_d)^2}{2} - \frac{E_d^2}{2} \right) \end{aligned}$$

$R_d$  is dpa/sec

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Stopping Power / Cross Section

$$S \equiv \frac{dE/dx}{N} = \cancel{\frac{1}{N}} \cancel{\frac{dE}{dx}} \cancel{dE}$$