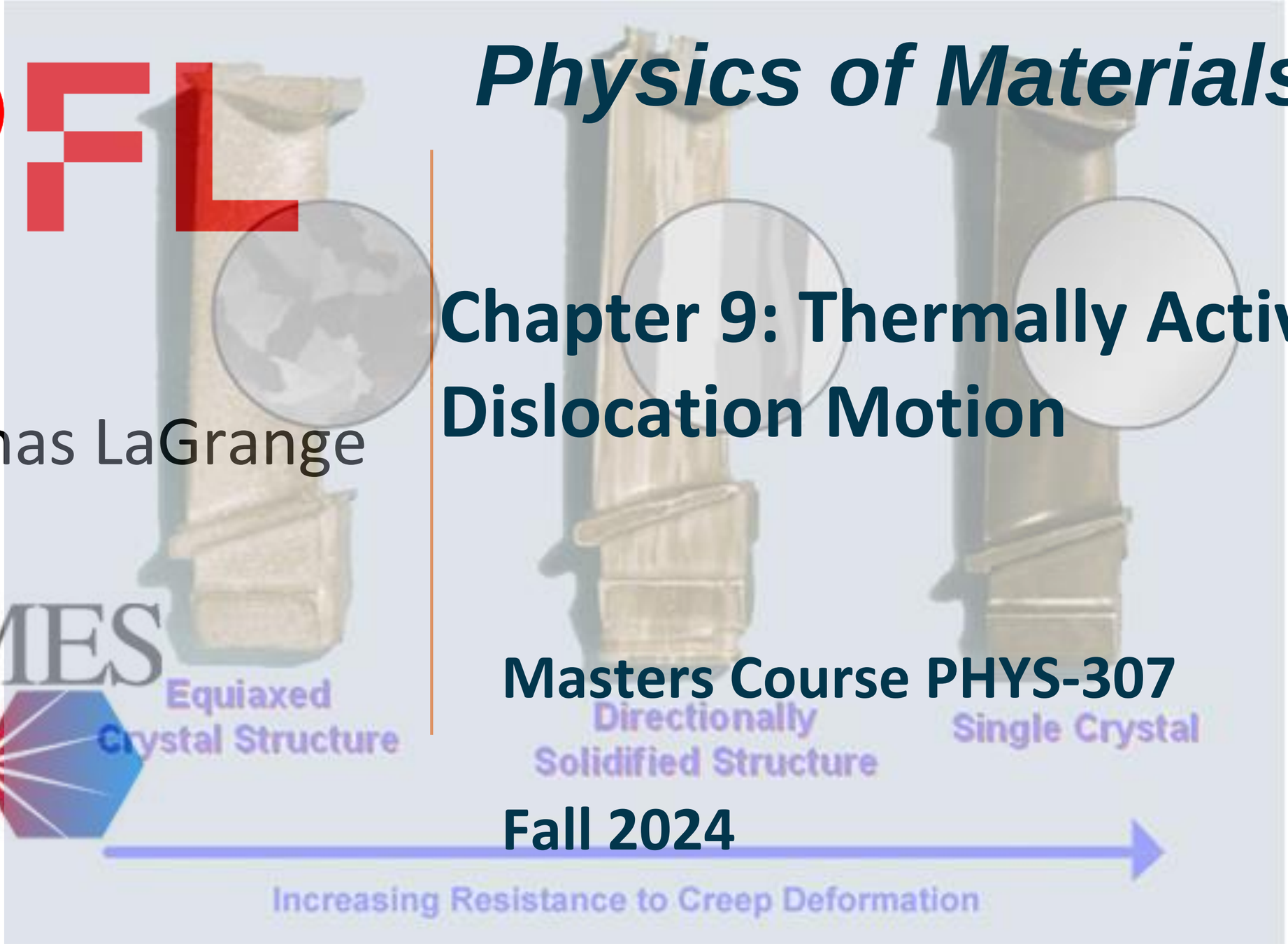
Physics of Materials

Chapter 9: Thermally Activated Dislocation Motion

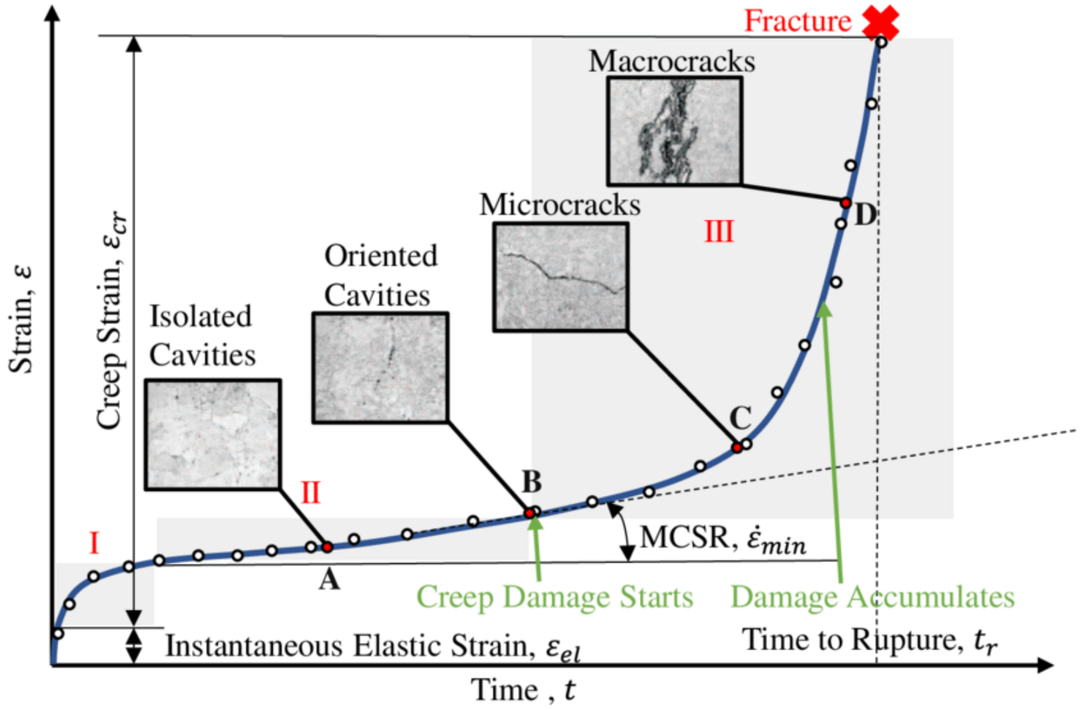
Dr. Thomas LaGrange

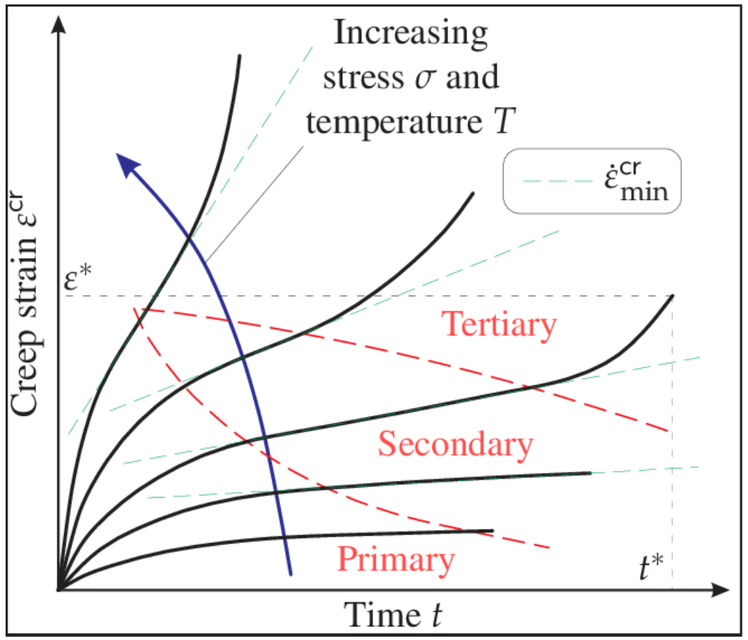


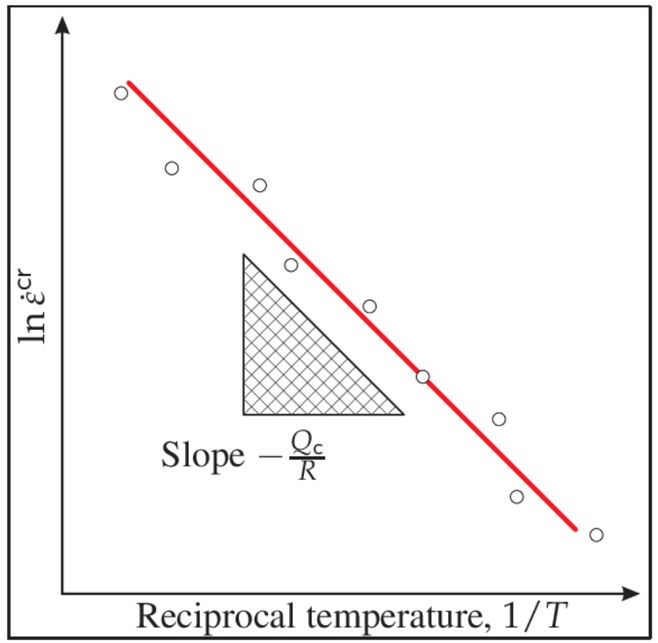
Masters Course PHYS-307

Fall 2024

Thermal activation under stress: Creep damage







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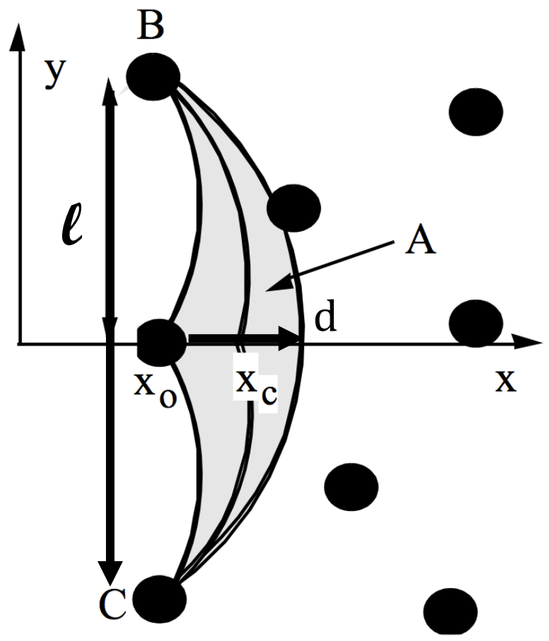
Orowan equation

$$\boxed{\dot{\varepsilon} = \Lambda b v}$$



$$v \simeq \frac{d}{t_i + t_g} \approx \frac{d}{t_i} = \frac{A}{\ell}\frac{1}{t_i}$$

$$\bar{v} = \frac{A}{\ell} P \qquad P = \nu_0 \exp\left(-\frac{\Delta G_a}{kT}\right) \qquad \nu_0 = \nu_D \frac{b}{\ell}$$

$$\dot{\varepsilon} \simeq \Lambda A \nu_D \left(\frac{b}{\ell}\right)^2 \exp\left(-\frac{\Delta G_a}{kT}\right) = \dot{\varepsilon}_0 \exp\left(-\frac{\Delta G_a}{kT}\right)$$

$$\Delta G_a = kT \ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right) \qquad \Delta G_a = \alpha kT \qquad \alpha \approx 25$$

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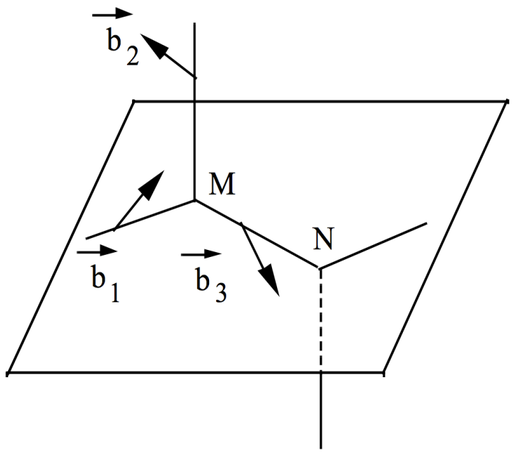
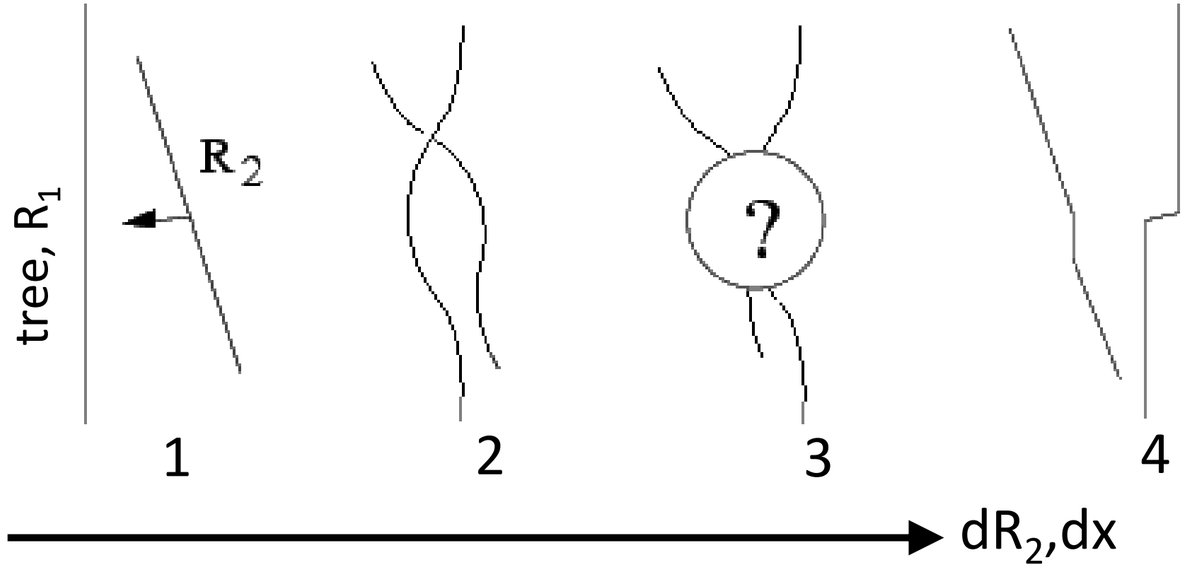
Thermal activation under stress: phenomenology





Work : variation of the internal energy

$$dW = f_0(T, R_2\sigma_a)dR_2 + f_i(R_1, R_2)dR_2 - \sigma_a(T, R_2)b\ell dR_2 + F_a(T)dx - PdV$$

if the friction force is zero and
no internal energy variation

$$F_a(T)dx - \sigma_a(t, R_2)b\ell dR_2 = 0$$

$$dE = TdS + dW = TdS + f_0 dR_2 + f_i dR_2 - PdV$$

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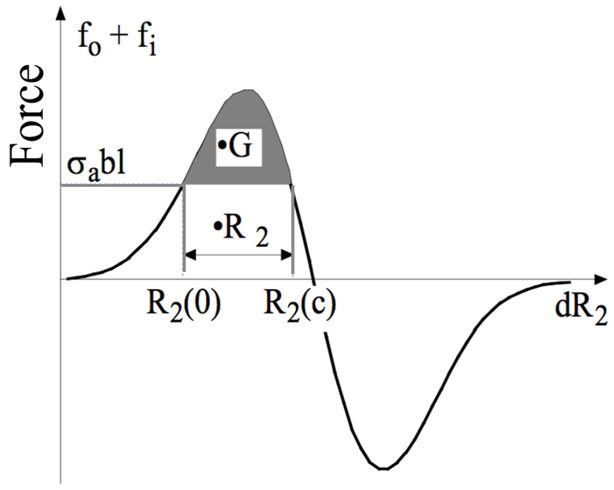
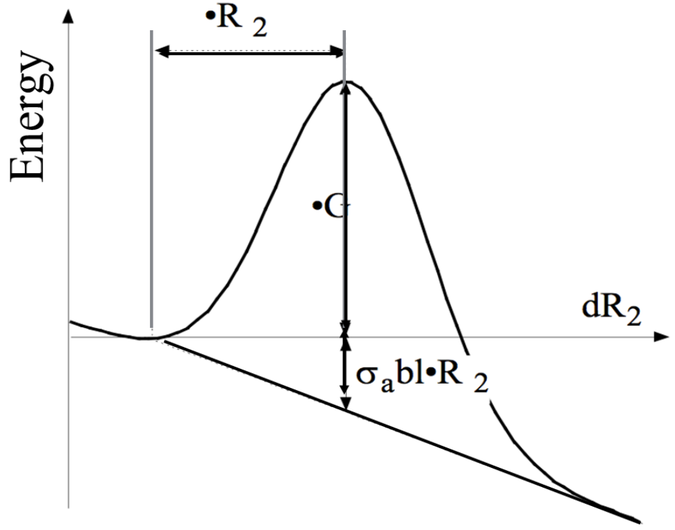
Calculation of Gibbs free energy

$$dE = TdS + dW = TdS + f_0 dR_2 + f_i dR_2 - PdV$$



(a)



(b)

$$G_a = E + PV - TS - F_a x$$

$$F_a = const \quad P = const$$

$$T = const \quad R_1 = const$$

$$dG_a = f_0 dR_2 + f_i dR_2 - \sigma_a b\ell dR_2$$

$$\Delta G_a = \int_{R_2(0)}^{R_2(c)} \left(\frac{\partial G_a}{\partial R_2} \right) dR_2 = \int_{R_2(0)}^{R_2(c)} \left[f_0 + f_i - \sigma_a b\ell \right] dR_2$$

$$\Delta G_a = \int_{R_2(0)}^{R_2(c)} \left(f_0 + f_i \right) dR_2 - \sigma_a b\ell \Delta R_2$$

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Activation volume

$$d(\Delta G_a) = \left.\frac{\partial \Delta G_a}{\partial \sigma_a}\right)_{T,P,R_1} d\sigma_a + \left.\frac{\partial \Delta G_a}{\partial T}\right)_{\sigma_a,P,R_1} dT$$

Definition

$$\boxed{V_a = -\left.\frac{\partial \Delta G_a}{\partial \sigma_a}\right)_{T,P,R_1}}$$

$$V_a = -\frac{\partial}{\partial \sigma_a}\left(\int_{R_2(0)}^{R_2(c)} \left[f_0 + f_i - \sigma_a b\ell\right] dR_2\right)$$

$$\boxed{\Delta G_a = \int_{R_2(0)}^{R_2(c)} \left(f_0 + f_i\right) dR_2 - \sigma_a b\ell \Delta R_2}$$

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Activation volume

Definition

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$$\boxed{\Delta G_a = \int_{R_2(0)}^{R_2(c)} \left(f_0 + f_i\right) dR_2 - \sigma_a b \ell \Delta R_2}$$

$$V_a = -\frac{\partial}{\partial \sigma_a}\left(\int_{R_2(0)}^{R_2(c)} \left[f_0 + f_i - \sigma_a b \ell\right] dR_2\right)$$

Leibniz Integral Rule

$$\frac{\partial}{\partial y}\left(\int_{a_0(y)}^{a_1(y)} g(x,y)\,dx\right) = g(a_1,y)\frac{\partial a_1}{\partial y} - g(a_0,y)\frac{\partial a_0}{\partial y} + \int_{a_0}^{a_1} \frac{\partial g(x,y)}{\partial y}\,dx$$

$$V_a = -\left.\frac{\partial \Delta G_a}{\partial R_2}\right)_{R_2(c)} \frac{\partial R_2(c)}{\partial \sigma_a} + \left.\frac{\partial \Delta G_a}{\partial R_2}\right)_{R_2(0)} \frac{dR_2(0)}{d\sigma_a} - \int_0^c \frac{\partial}{\partial \sigma_a}\left[f_0 + f_i - \sigma_a b \ell\right] dR_2$$

$$V_a = b\ell \Delta R_2 - \int_{R_2(0)}^{R_2(c)} \cancel{\frac{\partial f_0}{\partial \sigma_a}}\, dR_2$$

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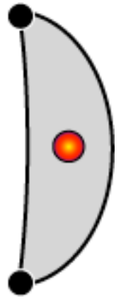
Activation volume



$$V_a = b\ell\Delta R_2$$

area swept by the dislocation
for overcoming the obstacle

$$\Delta G_a = \Delta G_0 + \sigma_a \left(\frac{\partial \Delta G_a}{\partial \sigma_a} \right) = \Delta G_0 - \sigma_a V_a$$

$$\boxed{\Delta G_0 = \sigma_a V_a + kT \ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \right)}$$

$$25\ kT \sim 0.5\ eV \rightarrow T \sim 230\ K \qquad \sigma_a V_a = 0.5\ eV \sim 0.1\ \mu b^3$$

$$\sigma_a \sim 10^{-2}\ \mu \text{ for } V_a = 10\ b^3 \text{ to } \sigma_a \sim 10^{-4}\ \mu \text{ for } V_a = 1000\ b^3$$

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Activation volume: thermodynamics

Classically $$\Delta V = -\left.\frac{\partial \Delta G_a}{\partial P}\right)_{T,F_a}$$

$$\boxed{\Delta G_a = \int_{R_2(0)}^{R_2(c)} \left(f_0 + f_i\right) dR_2 - \sigma_a b \ell \Delta R_2}$$

For dislocations $$\boxed{A_a = -\frac{1}{b}\left.\frac{\partial \Delta G_a}{\partial \sigma_a}\right)_{T,P,R_1}}$$

Enthalpy $$\Delta H_a = \Delta G_a + T\Delta S_a = \Delta G_a - T\left.\frac{\partial \Delta G_a}{\partial T}\right)_{\sigma_a, P, R_1} = \left.\frac{\partial\left(\Delta G_a / T\right)}{\partial\left(1/T\right)}\right)_{\sigma_a, P, R_1}$$

Entropy at σ_a constant $$\Delta S_a = -\int_{R_2(0)}^{R_2(c)} \frac{\partial}{\partial T}\left(f_0 + f_i\right) dR_2$$

In most cases f_0 and f_i depend on the shear-stress and modulus μ which allows us to calculate the variation ΔG_a with the temperature

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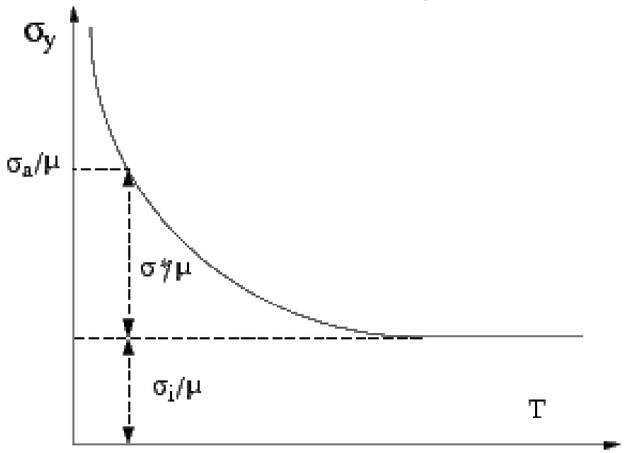
Effective stress σ^*

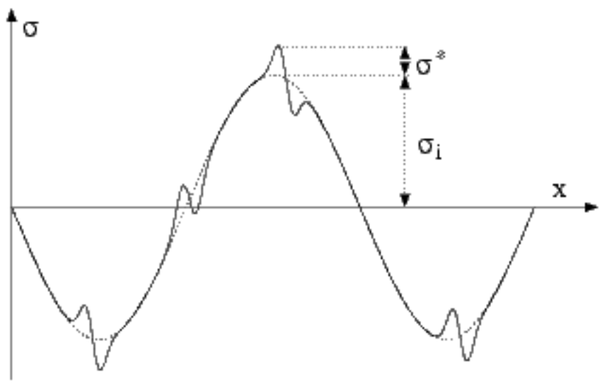
$$\Delta G_0 = \sigma_a V_a + kT \ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right) \qquad \sigma_a = \frac{\Delta G_0}{V_a} - \frac{kT}{V_a}\ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)$$

There exists $T_c = \dfrac{\Delta G_0}{k \ln\left(\dfrac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)}$ so that $\sigma_a \to 0$

$$\sigma_i \approx \alpha \frac{\mu b}{l}$$

in reality





effective stress $\sigma^* = \sigma_a - \sigma_i$

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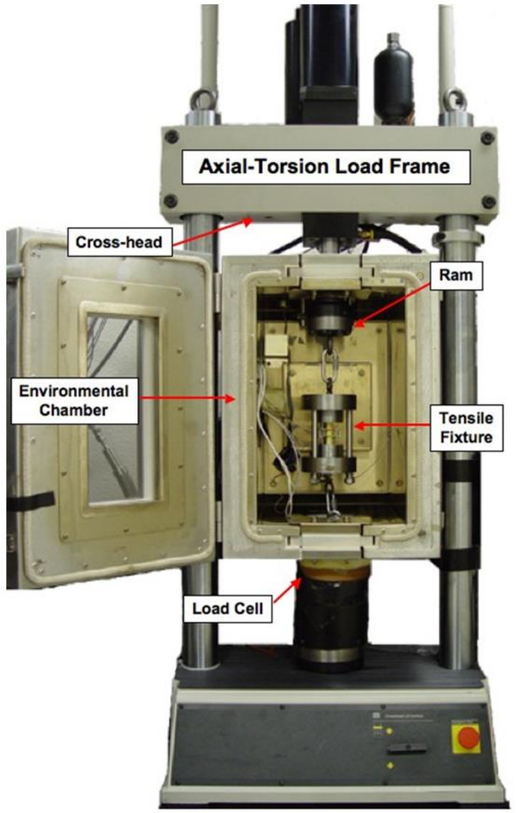
Experimental measurements of thermodynamic magnitudes

Creep Test



$$\left.\frac{\partial ln\dot{\varepsilon}}{\partial \sigma_a}\right|_T, \left.\frac{\partial ln\dot{\varepsilon}}{\partial T}\right|_{\sigma_a}, \left.\frac{\partial \sigma_a}{\partial T}\right|_{\dot{\varepsilon}}$$

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp\left(-\frac{\Delta G_a}{kT}\right) \Rightarrow \ln\dot{\varepsilon} = \ln\dot{\varepsilon}_0 - \frac{\Delta G_a}{kT}$$

Measurement of the activation volume

$$\boxed{V_a = -\left.\frac{\partial \Delta G_a}{\partial \sigma_a}\right)_{T,P,R_1}}$$

$$V_{\exp} = kT\left.\frac{\partial \ln\dot{\varepsilon}}{\partial \sigma_a}\right)_T = V_a + kT\left.\frac{\partial \ln\dot{\varepsilon}_0}{\partial \sigma_a}\right)_T$$

If for instance $\dot{\varepsilon}_0 = B\sigma_a^m$

$$V_{\exp} = V_a + kT\left(\frac{m}{\sigma_a}\right)$$

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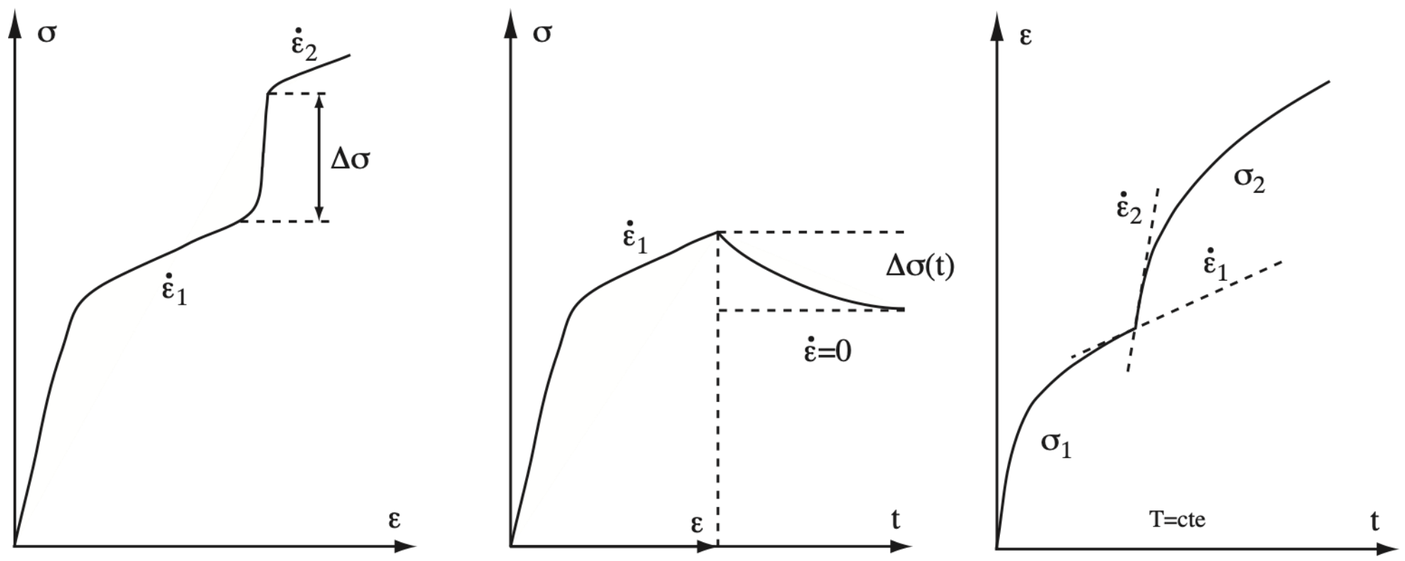
Experimental measurements of thermodynamic magnitudes

Measurement of the activation volume

$$V_{\exp} = kT \left.\frac{\partial \ln \dot{\varepsilon}}{\partial \sigma_a}\right)_T = V_a + kT \left.\frac{\partial \ln \dot{\varepsilon}_0}{\partial \sigma_a}\right)_T$$



jump in strain rate relaxation of the stress stress jump

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Experimental measurements of thermodynamic magnitudes

Measurement of the activation energy ΔG_a

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp\left(-\frac{\Delta G_a}{kT}\right) \Rightarrow \ln\dot{\varepsilon} = \ln\dot{\varepsilon}_0 - \frac{\Delta G_a}{kT}$$

$$\left.\frac{\partial \ln\dot{\varepsilon}}{\partial T}\right)_{\sigma_a} = -\frac{1}{k}\left.\frac{\partial(\Delta G_a/T)}{\partial T}\right)_{\sigma_a} + \left.\frac{\partial \ln\dot{\varepsilon}_0}{\partial T}\right)_{\sigma_a}$$

$$\Delta G_a = \Delta H_a - T\Delta S$$

$$-\frac{1}{k}\left.\frac{\partial(\Delta G_a/T)}{\partial T}\right)_{\sigma_a} = \frac{1}{kT^2}\left.\frac{\partial(\Delta G_a/T)}{\partial(1/T)}\right)_{\sigma_a} = \frac{\Delta H_a}{kT^2}$$

$$\left.\frac{\partial \ln\dot{\varepsilon}}{\partial T}\right)_{\sigma_a} = \frac{\Delta H_a}{kT^2} + \left.\frac{\partial \ln\dot{\varepsilon}_0}{\partial T}\right)_{\sigma_a}$$

thus $$\Delta H_{\exp} = kT^2 \left.\frac{\partial \ln\dot{\varepsilon}}{\partial T}\right)_{\sigma_a} = \Delta H_a + kT^2 \left.\frac{\partial \ln\dot{\varepsilon}_0}{\partial T}\right)_{\sigma_a}$$

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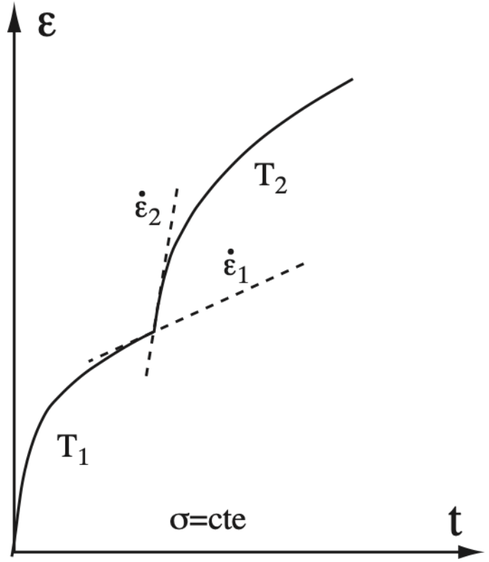
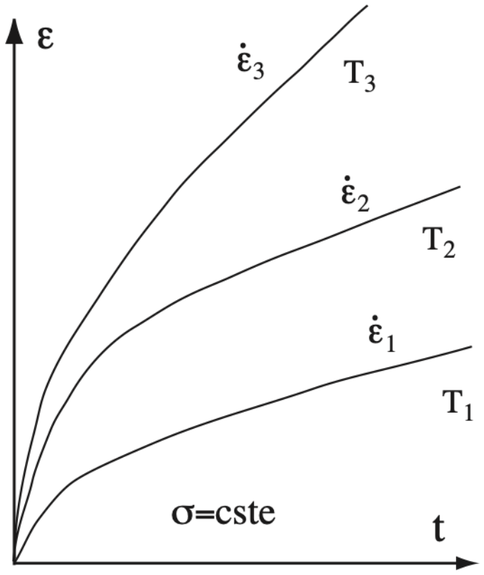
Experimental measurements of thermodynamic magnitudes

Measurement of the activation energy



Jump in temperature in creep



Measurement of the creep rate at different temperatures

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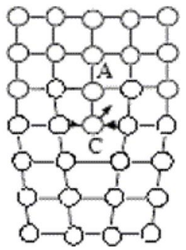
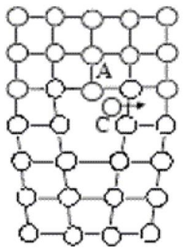
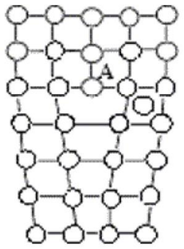
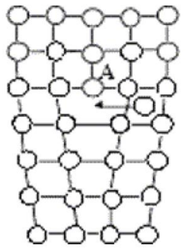
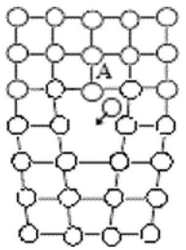
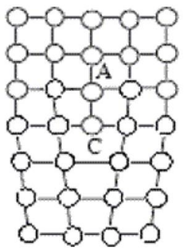
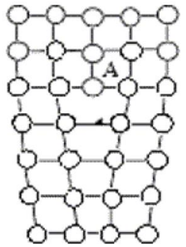
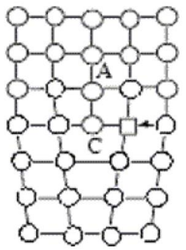
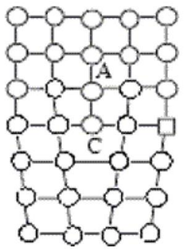
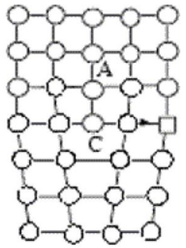
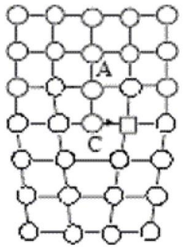
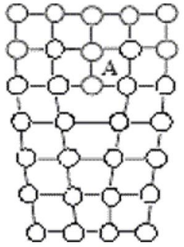
Dislocations climb

	Initial position	Unstable position	Final position
- creation of an interstitial			
- absorbtion of an interstitial			

	Initial position	Unstable position	Final position
- creation of a vacancy			
- absoption of a vacancy			

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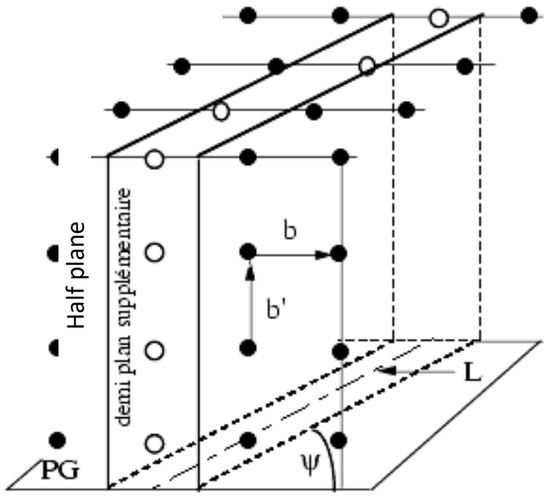
Geometrical aspects of the climb

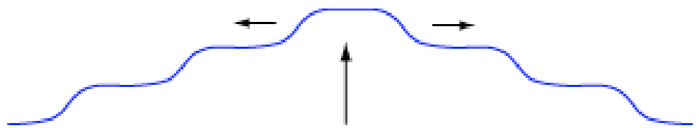


Mixed dislocation $\vec{\xi} \cdot \vec{b} = \cos\psi$

Displaced volume $V_a = \ell \vec{\xi} \wedge \vec{b} \cdot \vec{b}'$

$$b = b' \rightarrow V_a = \ell b^2 \sin\psi \qquad \Omega = b^3, N = \frac{l}{b}\sin\psi$$

the climb is generally obtained by the movement of jogs



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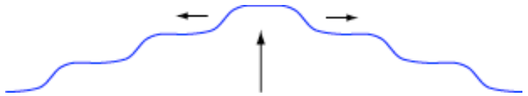
Concentration of jogs



$$\psi = \frac{\pi}{2} \qquad C_j = \frac{n_j}{\ell / b} = \frac{n_j b}{\ell} \qquad \ell / b = N$$

number of atoms of a volume of b^3

Energy variation of a vacancy

$$dG = \mu_{Vc} - \mu_{Vd}$$

Energy variations linked to the climb forces

concentration of vacancies	external stresses	line tension
$kT \ln\left(\frac{C}{C_V}\right)$	σb^3	$\frac{\tau b^2}{R}$

$$R = \frac{\tau}{\sigma b}$$

$$\mu_{Vc} - \mu_{Vd} = kT \ln\left(\frac{C}{C_V}\right) - \sigma b^3 - \frac{\tau b^2}{R}$$

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Climb needs thermal activation

$$dG = \mu_{Vc} - \mu_{Vd} = kT \ln\left(\frac{C}{C_V}\right) - \sigma b^3 - \frac{\tau b^2}{R}$$

$$dG = \mu_{Vc} - \mu_{Vd} = kT \ln\left(\frac{C}{C_V}\right) - \sigma b^3$$

For a straight dislocation

$dG = 0 \Rightarrow$ force equilibrium

$$C = C_V \exp\left(\frac{\sigma b^3}{kT}\right)$$

athermal plateau

$$\sigma b^3 = \Delta G_V^F \rightarrow \sigma \approx \frac{\mu}{5}$$

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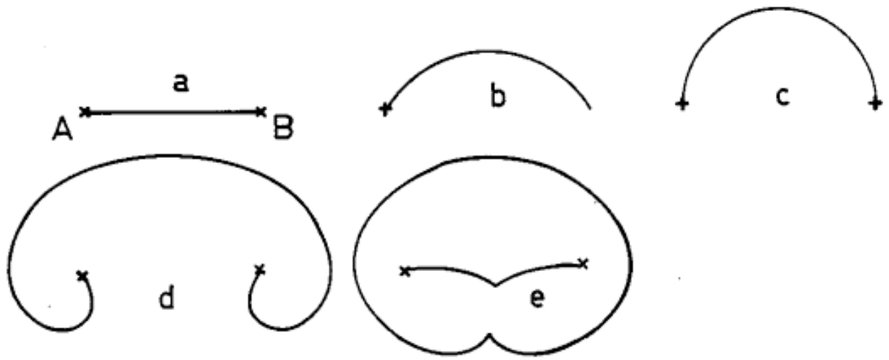
Bardeen-Herring sources



$$dG = \mu_{Vc} - \mu_{Vd} = kT \ln\left(\frac{C}{C_V}\right) - \frac{\tau b^2}{R} \qquad \frac{\tau}{R} \le \frac{kT}{b^2} \ln\left(\frac{C}{C_V}\right)$$

$$\tau = \frac{1}{2}\mu b^2 \quad R \le \frac{\ell}{2}$$

propagation of the source $\ln\left(\frac{C}{C_V}\right) \ge \frac{\mu b^4}{\ell kT}$

Aluminum: $\mu = 25\,[GPa], b = 2.3\,[\text{Å}],$

$$\ell = 10^{-6}\,[m], T = 500\,[K] \qquad \frac{C}{C_V} \approx 1.02$$

2% oversaturation activates 1 µm source

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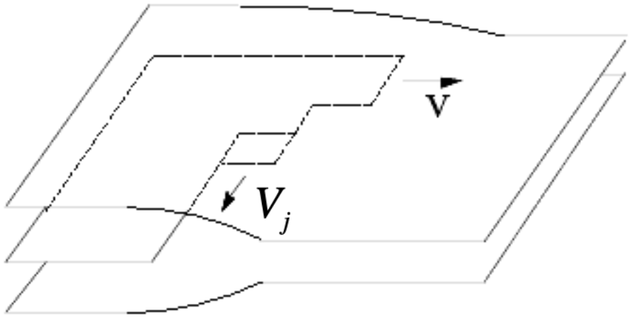
Climb velocity of a dislocation



$$V = \frac{b}{\ell / V_j} = \frac{bV_j}{\ell}$$

$$V = \frac{bV_j n_j}{\ell} = C_J V_j$$ for n_j jogs

$$V = bC_j \Delta\nu$$

$$\Delta\nu = \Delta\nu_e - \Delta\nu_a$$ difference in frequency of emission and absorption of vacancies

Thermally activated $\Delta\nu \sim D_{sd} \exp\left(\frac{\sigma b^3}{kT}\right) = D_0 \exp\left(\frac{-Q + \sigma b^3}{kT}\right)$

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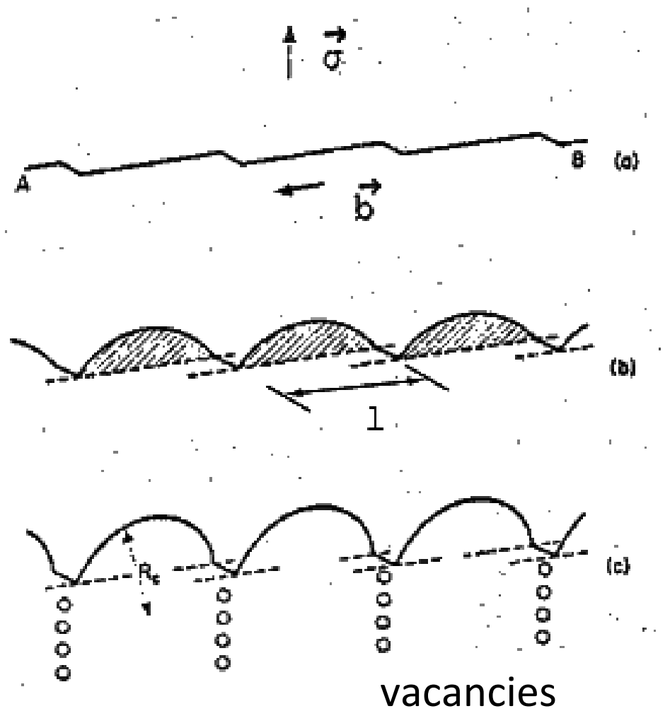
Particular case: jogs on a screw dislocation



Screw with edge jogs

Screw segments cross-slip

Screw dragging edge jogs

$$\Delta\nu = \frac{D_{SD}}{b^2}\left\{\exp\left[\frac{\sigma\ell\, b^2}{kT}\right] - \exp\left[\frac{b^2 F_s/(d\ell)}{kT}\right]\right\}$$

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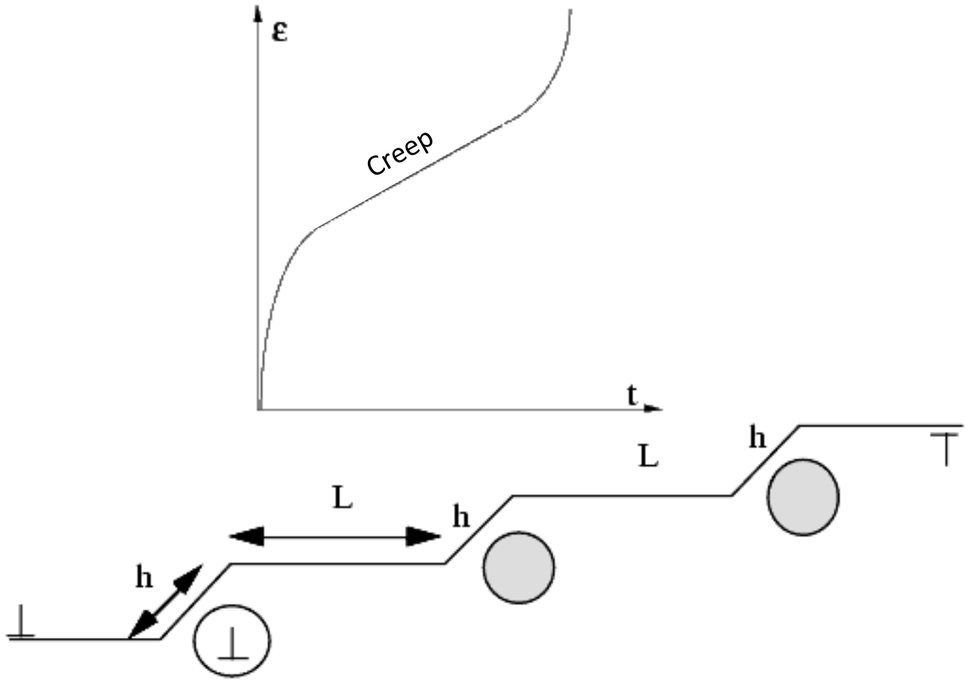
Steady-state creep



slip

$$v \simeq \frac{d}{t_i + t_g} \approx \frac{d}{t_i} = \frac{A}{\ell}\frac{1}{t_i}$$

$$\dot{\varepsilon} = \Lambda b v$$

climb

$$v \simeq \frac{L}{t_{cl} + t_g} \approx \frac{L}{t_{cl}} = L\frac{v_e}{h}$$

$$\dot{\varepsilon} = \Lambda b L \frac{v_e}{h}$$

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Steady-state creep

$$\dot{\varepsilon} = \Lambda b L \frac{v_e}{h}$$

Frank lattice

$$\Lambda \approx \frac{1}{L^2}$$

Steady-state regime

$$\sigma = \sigma_i \approx \frac{\mu b}{L} \propto \sqrt{\Lambda} \Rightarrow \Lambda \propto \left(\frac{\sigma}{\mu}\right)^2$$

$$\dot{\varepsilon} \propto \left(\frac{\sigma}{\mu}\right)^2 bL\frac{v_e}{h} \propto \left(\frac{\sigma}{\mu}\right)^2 Lv_e$$

$$\mathrm{v}_e = \frac{2\pi D_{SD}}{bkT}\frac{\sigma_n b^3}{\ln\left(\frac{R}{b}\right)}$$

climb controlled by diffusion

$$\dot{\varepsilon} = A\frac{\sigma^3}{kT}\exp\left(-\frac{H_{sd}}{kT}\right)$$

In general we use the Dorn law

$$\dot{\varepsilon} = A\sigma^n \exp\left(-\frac{H}{kT}\right)$$

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