Continuum Mechanics

Lecture 3

Elastic waves and dislocations

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Outline

- Elastic waves
- Seismic applications
- Waves in beams
- Dislocations as topological defects
- Structure and dynamics of dislocations

The elastic wave equation

In 3-dimensional space, the acceleration is given by

$$\rho \frac{d\vec{v}}{dt} = \rho \overrightarrow{g} + \overrightarrow{\nabla} \cdot \overline{\overline{\sigma}}$$

In solid mechanics, we considered only equilibrium states. Now we want to study time dependent solutions.

We still consider a reference equilibrium state, for which $\overline{\overline{\sigma}} = 0$.

We then consider the time-dependent displacement field from this reference state $\vec{u}(x,t)$. The velocity field is defined as $\vec{v}(x,t) = \frac{d\vec{u}}{dt}$.

Neglecting gravity, we obtain the following dynamical equation.

$$\rho \frac{d^2\vec{u}}{dt^2} = (\lambda + \mu)\mathrm{grad}\,(\mathrm{div}\vec{u}) + \mu\Delta\vec{u}$$

For any scalar quantity $\alpha(t,\vec{x})$, the Lagrangian time derivative writes

$$\frac{d\alpha}{dt} = \frac{d}{dt}\left[\alpha(t,\vec{x}(t))\right] = \frac{\partial\alpha}{\partial t} + \frac{\partial\alpha}{\partial\vec{x}} \cdot \vec{v} \quad \text{(chain rule)}$$

Dropping the non-linear, high order terms in the displacement field, we get:

$$\boxed{\rho \frac{\partial^2\vec{u}}{\partial t^2} = (\lambda + \mu)\mathrm{grad}\,(\mathrm{div}\vec{u}) + \mu\Delta\vec{u}}$$

Planar wave solutions

We are looking for plane waves of the form $\vec{u}(t,\vec{x}) = \vec{f}(\vec{e}\cdot\vec{x} - ct)$

where the unit vector $\vec{e}$ marks the direction of propagation of the wave.

$$\rho c^2 \vec{f}'' = (\lambda + \mu)(\vec{f}'' \cdot \vec{e})\vec{e} + \mu \vec{f}''$$

where we used $\dfrac{\partial \vec{u}}{\partial x_i} = \vec{f}'(s)\dfrac{\partial s}{\partial x_i} = \vec{f}'(s)e_i$ with $s = \vec{e}\cdot\vec{x} - ct$

and $\dfrac{\partial \vec{u}}{\partial t} = \vec{f}'(s)\dfrac{\partial s}{\partial t} = -\vec{f}'(s)c$

We have two types of solutions:

1- Transversal waves for which $\vec{f}\cdot\vec{e} = 0$ and $\rho c^2 \vec{f}'' = \mu \vec{f}''$

2- Longitudinal waves for which $\vec{f} = f\vec{e}$ and $\rho c^2 \vec{f}'' = (\lambda + 2\mu)\vec{f}''$

Non-trivial solutions have wave speeds $\boxed{c_T = \sqrt{\dfrac{\mu}{\rho}}}$ and $\boxed{c_L = \sqrt{\dfrac{2\mu + \lambda}{\rho}}}$

$$\frac{c_T}{c_L} = \sqrt{\frac{1 - 2\nu}{2(1-\nu)}} \leq \sqrt{2}/2 \simeq 0.7$$

Transversal waves are always slower than longitudinal waves.

Analogy with electromagnetic waves

We use the Helmholtz decomposition $\vec{u} = \vec{\nabla}\phi + \vec{\nabla} \times \vec{A}$

which reads in components form $u_i = \frac{\partial \phi}{\partial x_i} + \frac{\partial A_k}{\partial x_j} - \frac{\partial A_j}{\partial x_k}$

with the Gauge condition $\vec{\nabla} \cdot \vec{A} = 0$. Using vector calculus, we have

$$\Delta\left(\vec{\nabla}\phi\right) = \vec{\nabla}\left(\Delta\phi\right) \quad \Delta\left(\vec{\nabla} \times \vec{A}\right) = \vec{\nabla} \times \left(\Delta\vec{A}\right) \quad \vec{\nabla} \cdot \left(\vec{\nabla} \times \vec{A}\right) = 0$$

$$\rho\frac{\partial^2}{\partial t^2}\left\{\vec{\nabla}\phi\right\} + \rho\frac{\partial^2}{\partial t^2}\left\{\vec{\nabla} \times \vec{A}\right\} = (\lambda + 2\mu)\vec{\nabla}\left\{\Delta\phi\right\} + \mu\vec{\nabla} \times \left\{\Delta\vec{A}\right\}$$

This is equivalent to the following 2 equations:

$$\rho\frac{\partial^2\phi}{\partial t^2} = (\lambda + 2\mu)\Delta\phi \qquad \rho\frac{\partial^2\vec{A}}{\partial t^2} = \mu\Delta\vec{A}$$

We can put these equation in the d'Alembert form

$$\boxed{\left(\Delta - \frac{1}{c_L^2}\frac{\partial^2}{\partial t^2}\right)\phi = 0} \qquad \boxed{\left(\Delta - \frac{1}{c_T^2}\frac{\partial^2}{\partial t^2}\right)\vec{A} = 0}$$

Although different, these are analogous to the electromagnetic waves equations.

Monochromatic plane waves

The most general harmonic solution for the previous equations are

$$\phi = \phi_0 \exp^{i(\omega t - \vec{k}_L \cdot \vec{r})} \qquad \overrightarrow{A} = \overrightarrow{A}_0 \exp^{i(\omega t - \vec{k}_T \cdot \vec{r})} \qquad \overrightarrow{A}_0 \cdot \vec{k}_T = 0$$

where k_L and k_R are *vectors of complex numbers*.

If any of the 3 components is imaginary, we have surface or evanescent waves.

If the 3 components are real, we have volume waves.

In the latter case, we can write $\vec{k}_T = k_T \vec{e} \longrightarrow k_T^2 - \frac{\omega^2}{c_T^2} = 0$

$$\vec{k}_L = k_L \vec{e} \longrightarrow k_L^2 - \frac{\omega^2}{c_L^2} = 0$$

We have 2 types of volume waves:

1- Longitudinal waves: P waves, Pressure waves or Primary waves:

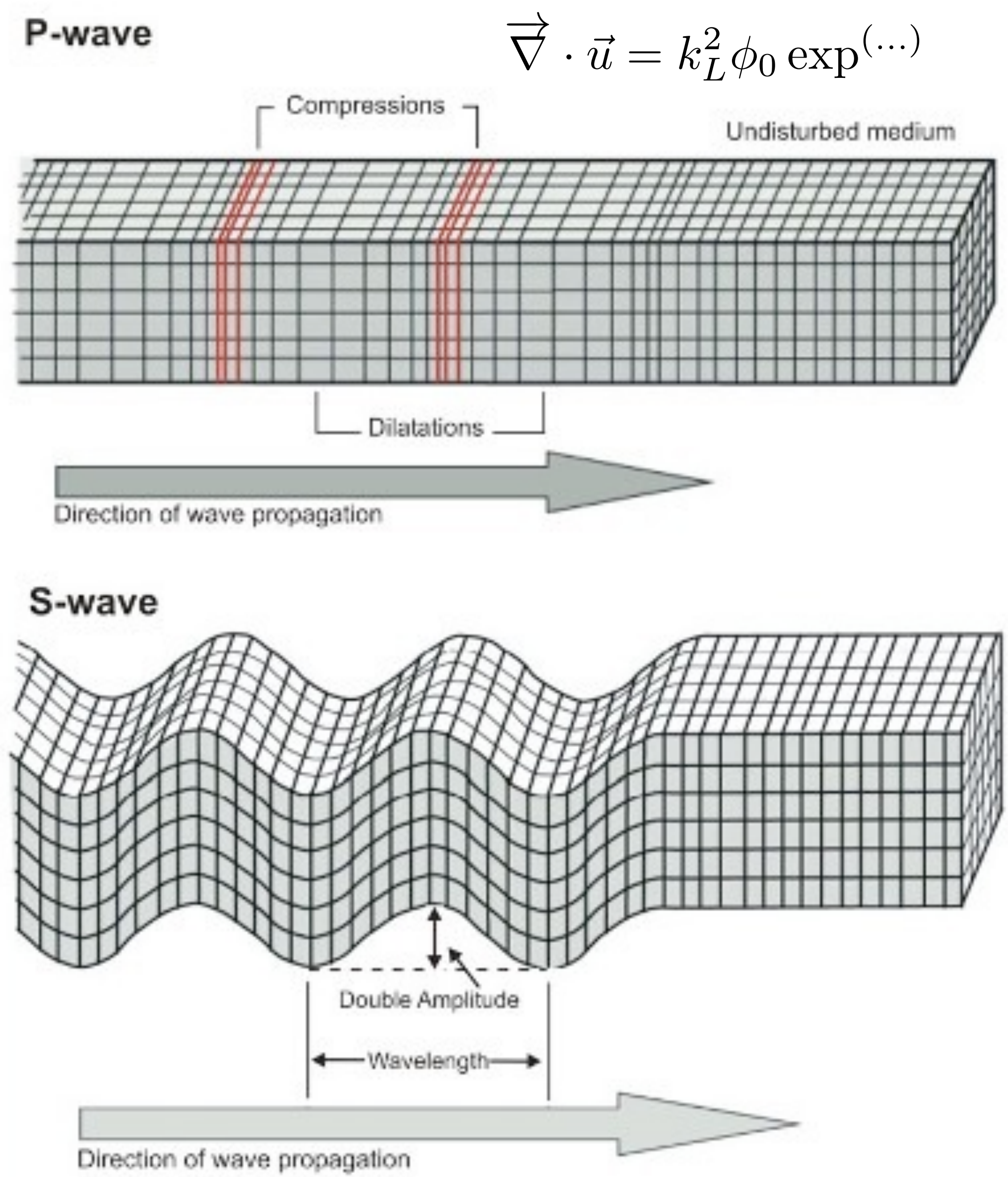
$$\vec{u} = \overrightarrow{\nabla} \phi = \mathrm{Re}\left(-i k_L \vec{e} \phi_0 \exp^{i(\omega t - k_L \vec{e} \cdot \vec{r})}\right)$$

2- Transversal waves: S waves, Shear waves or Secondary waves:

$$\vec{u} = \overrightarrow{\nabla} \times \overrightarrow{A} = \mathrm{Re}\left(-i k_T \vec{e} \times \overrightarrow{A}_0 \exp^{i(\omega t - k_T \vec{e} \cdot \vec{r})}\right)$$

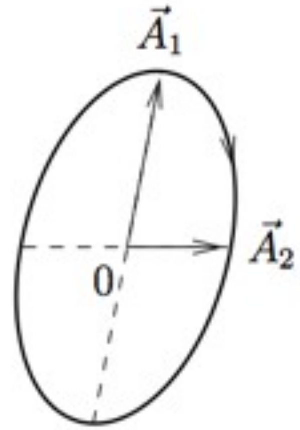
Valid for an infinite medium: boundary conditions don't play any role !

Volume waves



$$\vec{\nabla} \cdot \vec{u} = k_L^2 \phi_0 \exp^{(\dots)}$$

S waves are polarized



$$\vec{u}(t, \vec{r} = 0) = \mathrm{Re}(\vec{A}_0 \exp^{-i\omega t})$$

$$= \vec{A}_1 \cos(\omega t) + \vec{A}_2 \sin(\omega t)$$

where $\vec{A}_0 = \vec{A}_1 + i\vec{A}_2$

Linear polarization

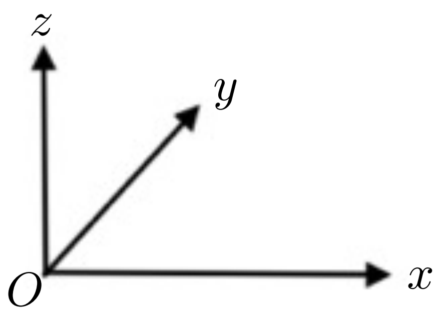
$$\vec{A}_1 \parallel \vec{A}_2$$

Circular polarization

$$\vec{A}_1 \perp \vec{A}_2 \quad \|\vec{A}_1\| = \|\vec{A}_2\|$$

Surface waves

We are looking for wave solutions propagating along the x direction, with a boundary surface at plane z=0.



These waves must be trapped near the surface.

We consider $\vec{k}_T = k_{T,x}\vec{e}_x + ik_{T,z}\vec{e}_z \quad \vec{k}_L = k_{L,x}\vec{e}_x + ik_{L,z}\vec{e}_z$

We restrict ourselves to waves with $k_{T,x} = k_{L,x} = \frac{\omega}{c}$

Injecting the general solution in the wave equations, we have 2 dispersion relations

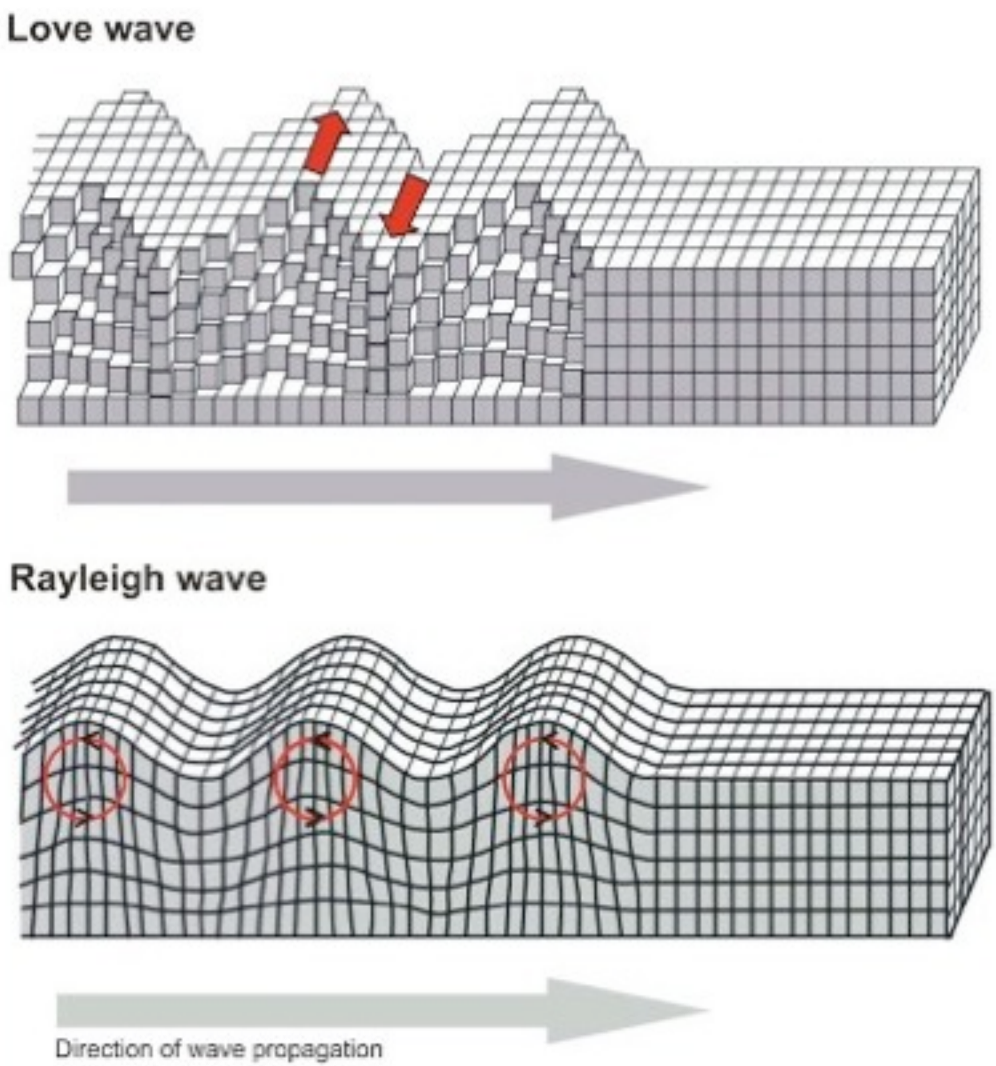
$$k_{L,z}^2 = k_L^2 = \omega^2\left(\frac{1}{c^2} - \frac{1}{c_L^2}\right) \quad k_{T,z}^2 = k_T^2 = \omega^2\left(\frac{1}{c^2} - \frac{1}{c_T^2}\right) \quad c < c_T < c_L$$

The two potentials write now $\phi = \phi_0 \exp^{k_L z} \exp^{i\omega(t-x/c)} \quad \overrightarrow{A} = \overrightarrow{A}_0 \exp^{k_T z} \exp^{i\omega(t-x/c)}$

These waves are evanescent in the z-direction, they propagate only along x. They are localized within a thin layer $\Delta z_{L,T} \simeq 1/k_{L,T}$

The wave velocity *c* is however still unknown. It will be determined using specific surface boundary conditions on the plane z=0.

Surface waves



The displacement field is given by

$$u_x = \frac{\partial \phi}{\partial x} - \frac{\partial A_y}{\partial z} = -i\frac{\omega}{c}\phi - k_T A_y$$

$$u_y = -\frac{\partial A_z}{\partial x} = +i\frac{\omega}{c}A_z$$

$$u_z = \frac{\partial \phi}{\partial z} + \frac{\partial A_y}{\partial x} = k_L \phi - i\frac{\omega}{c}A_y$$

Displacements along y are called «Love waves» while the vertical-longitudinal waves are called «Rayleigh» waves.

Planar waves travel without attenuation (no dissipative effects).

Love waves on a free surface

The displacement field is $u_x = 0 \quad u_y = i\dfrac{\omega}{c}A_z \quad u_z = 0$

$$\overline{\overline{\epsilon}} = \left| \begin{array}{ccc} 0 & \frac{1}{2}\frac{\omega^2}{c^2}A_z & 0 \\ \frac{1}{2}\frac{\omega^2}{c^2}A_z & 0 & \frac{i}{2}\frac{\omega}{c}k_T A_z \\ 0 & \frac{i}{2}\frac{\omega}{c}k_T A_z & 0 \end{array} \right| \qquad \overline{\overline{\sigma}} = \mu \left| \begin{array}{ccc} 0 & \frac{\omega^2}{c^2}A_z & 0 \\ \frac{\omega^2}{c^2}A_z & 0 & i\frac{\omega}{c}k_T A_z \\ 0 & i\frac{\omega}{c}k_T A_z & 0 \end{array} \right|$$

We have $\mathrm{Tr}(\overline{\overline{\epsilon}}) = 0$. Love waves are pure shear waves.

On the free surface at z=0, we have $\overrightarrow{T} = \overline{\overline{\sigma}} \left(\begin{array}{c} 0 \\ 0 \\ 1 \end{array} \right) = \mu \left(\begin{array}{c} 0 \\ i\frac{\omega}{c}k_T A_z \\ 0 \end{array} \right)$

Imposing T=0 means that the amplitude is zero.

Love waves don’t propagate on a free surface with an homogeneous half-space.

They propagate however in a stratified medium (see later).

Rayleigh waves on a free surface

The displacement field is $u_x = -i\frac{\omega}{c}\phi - k_T A_y \quad u_y = 0 \quad u_z = k_L\phi - i\frac{\omega}{c}A_y$

The strain tensor has the following components:

$$\epsilon_{xx} = -\frac{\omega^2}{c^2}\phi + i\frac{\omega}{c}k_T A_y \qquad \epsilon_{xy} = 0 \qquad \epsilon_{xz} = -i\frac{\omega}{c}k_L\phi - \frac{1}{2}\left(k_T^2 + \frac{\omega^2}{c^2}\right)A_y$$

$$\epsilon_{yy} = 0 \qquad \epsilon_{yz} = 0$$

$$\epsilon_{zz} = k_L^2\phi - i\frac{\omega}{c}k_T A_y$$

Volume changes are due to the longitudinal component $\mathrm{Tr}(\overline{\overline{\epsilon}}) = \left(k_L^2 - \frac{\omega^2}{c^2}\right)\Phi$

We then use the elastic law $\overline{\overline{\sigma}} = \lambda \mathrm{Tr}(\overline{\overline{\epsilon}})\overline{\overline{1}} + 2\mu\overline{\overline{\epsilon}}$ and the surface boundary condition

$$-i\frac{\omega}{c}k_L\phi - \frac{1}{2}\left(k_T^2 + \frac{\omega^2}{c^2}\right)A_y = 0$$

$$\left((\lambda+2\mu)k_L^2 - \lambda\frac{\omega^2}{c^2}\right)\phi - 2\mu i\frac{\omega}{c}k_T A_y = 0$$

We require the determinant to be zero (non trivial solution), so we have:

$$\frac{1}{2}\left(k_T^2 + k^2\right)\left\{(\lambda+2\mu)k_L^2 - \lambda k^2\right\} - 2\mu k_L k_T k^2 = 0$$

The solution of this equation (together with the dispersion relations) will give $k = \omega/c$

Rayleigh wave speed

If we define $s = \frac{c}{c_T}$ and $q^2 = \frac{c_T^2}{c_L^2} = \frac{1-2\nu}{2(1-\nu)}$, the solution is obtained by solving

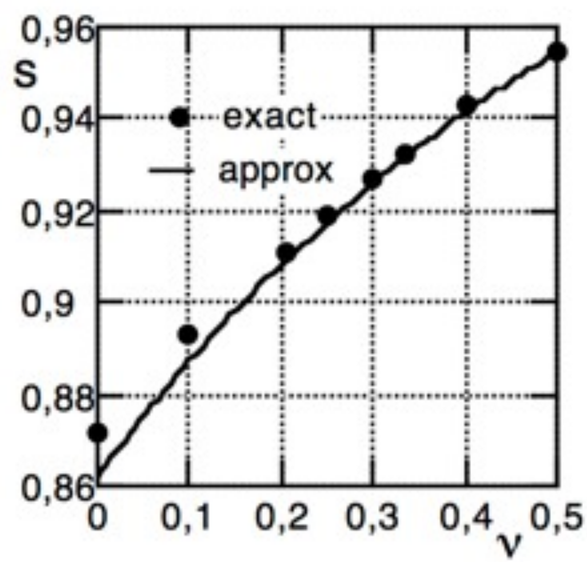
$$s^6 - 8s^4 - 8(2q^2-3)s^2 + 16(q^2-1) = 0$$

The only physically relevant root is

$$s \simeq \frac{0.862 + 1.14\nu}{1+\nu}$$

For the Earth, we have $\nu \simeq 0.25$

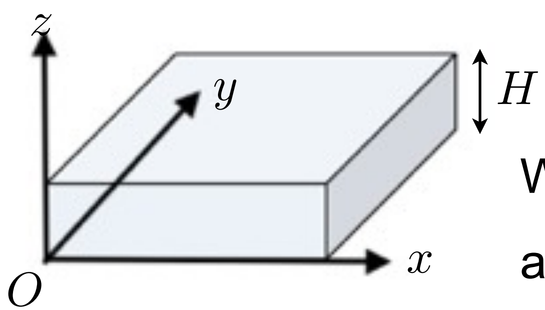
The Rayleigh waves speed is $\boxed{c_R \simeq 0.918 c_T}$



Rayleigh waves are slower than S-waves: they are the slowest seismic waves.

Love waves in a layer on top of a free surface

We are looking for wave solutions propagating along the x direction, with a boundary surface at z=0 separating a layer of finite thickness H from an infinite half-plane.



The planar layer has density ρ_1 and S speed c_1

while the infinite half space below has ρ_2 and c_2

Waves are evanescent in the half-space. We must choose a complex z-component: $\vec{k}_2 = k_{2,x}\vec{e}_x + ik_{2,z}\vec{e}_z$

In the planar layer, however, we consider fully harmonic waves $\vec{k}_1 = k_{1,x}\vec{e}_x + k_{1,z}\vec{e}_z$

We are looking for propagating solutions of the form $k_{1,x} = k_{2,x} = k = \dfrac{\omega}{c}$

where the z-component of the potential vector write:

for z>0: $A_{z,1} = \left(A_1^+ \exp(ik_1 z) + A_1^- \exp(-ik_1 z)\right)\exp(i(\omega t - kx))$ $\quad k_1 = k_{1,z}$

for z<0: $A_{z,2} = A_2 \exp(k_2 z)\exp(i(\omega t - kx))$ $\quad k_2 = k_{2,z}$

Boundary conditions are:

- free surface at z=H: $\overline{\overline{\sigma}}_1 \vec{n} = 0$
- contact discontinuity at z=0: $\overline{\overline{\sigma}}_1 \vec{n} = \overline{\overline{\sigma}}_2 \vec{n}$

$$\vec{u}_1 = \vec{u}_2$$

Dispersion relations are:

$$k^2 + k_1^2 = \frac{\omega^2}{c_1^2} \qquad k^2 - k_2^2 = \frac{\omega^2}{c_2^2}$$

$$\boxed{c_1 < c < c_2}$$

Love waves in a layer on top of a free surface

Free surface boundary condition at z=H writes: $A_1^+ \exp(ik_1 H) = A_1^- \exp(-ik_1 H)$

Contact boundary condition at z=0 writes: $\mu_1 i k_1 \left(A_1^+ - A_1^-\right) = \mu_2 k_2 A_2$

Continuity of the displacement at z=0 is: $A_1^+ + A_1^- = A_2$

Looking for non-trivial solutions gives the dispersion relation: $\boxed{\tan(k_1 H) = \frac{\mu_2 k_2}{\mu_1 k_1}}$

$$\boxed{k_1^2 = \omega^2 \left(\frac{1}{c_1^2} - \frac{1}{c^2}\right)} \quad \boxed{k_2^2 = \omega^2 \left(\frac{1}{c^2} - \frac{1}{c_2^2}\right)}$$

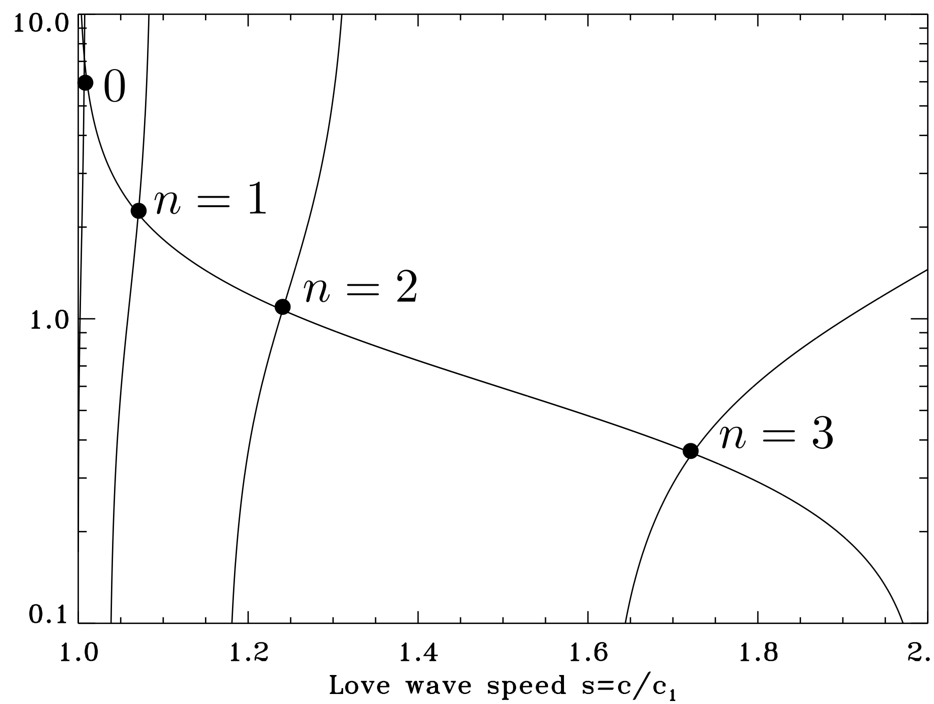
We use a dimensionless speed $s = c/c_1$

For each frequency ω, there is a finite number of modes $c_n(\omega)$ with $n = 0, 1, 2...$

n=0 is the fundamental mode. It has the lowest velocity and the highest energy.

Love's wave are dispersive waves for which the group velocity is

$$v_g = \frac{\partial \omega}{\partial k} \neq c$$



Seismic waves

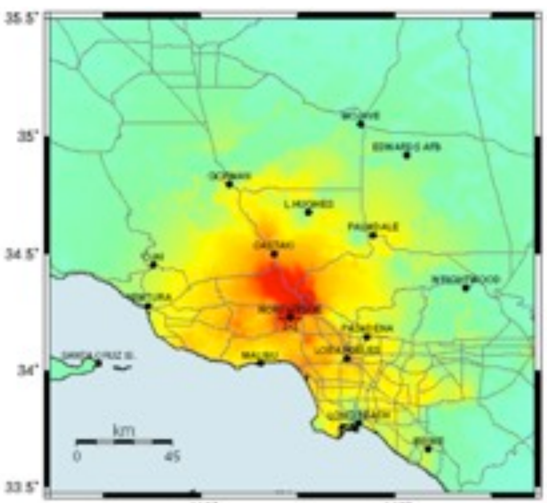
In nature, waves originate from a single point, an earthquake. They propagate around this point in a spherical (volume waves) or cylindrical (surface waves) pattern.

The elastic energy of a spherical wave decays as $1/r^2$ because $4\pi r^2 \mu \phi^2 = \text{constant}$.

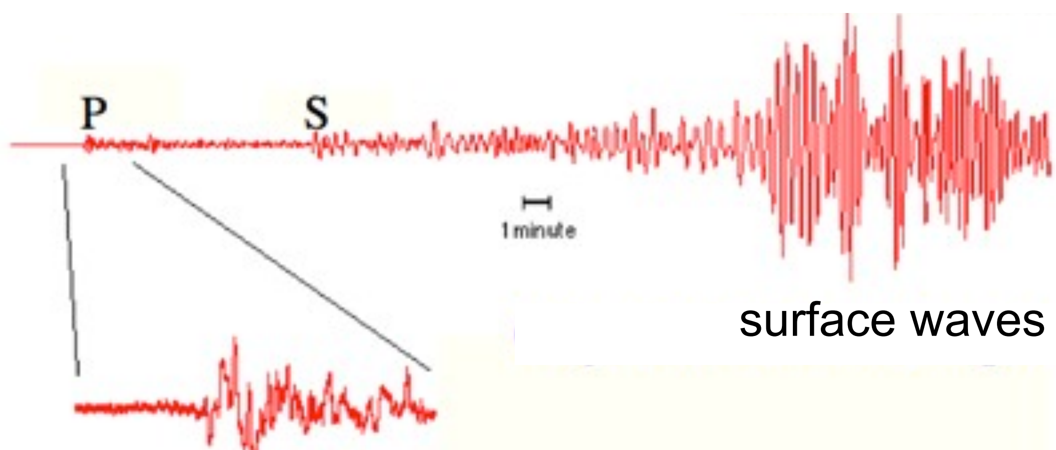
In cylindrical geometry, it decays as $1/r$ and the amplitude decays as $1/\sqrt{r}$.

P-waves are the fastest, followed by S-waves. The amplitude decreases quickly as the inverse of the distance.

Rayleigh and Love waves are the slowest, but they are surface waves, so their amplitude decreases slowly. They are the most dangerous waves.



Northridge earthquake (1994)



Izmit earthquake (1999), recorded in Boston.

Elastic waves in elongated structures

We consider the curvilinear *dynamical* equilibrium equations. We consider only vertical displacements and vertical velocities.

$$\mu\frac{dv_x}{dt} = \frac{dT_x}{dx} = 0 \qquad u_x = 0$$

$$\mu\frac{dv_y}{dt} = \frac{dT_y}{dx} + \mu g_y \qquad v_y = \frac{du_y}{dt}$$

$$0 = \frac{dM}{dx} + T_y \qquad \frac{d\omega}{dx} = \frac{M}{EI} \qquad \omega = \frac{du_y}{dx}$$

We linearize the velocity terms, and dropping the y index we get:

$$\frac{\partial^2 u}{\partial t^2} + \frac{EI}{\mu}\frac{\partial^4 u}{\partial x^4} = g$$

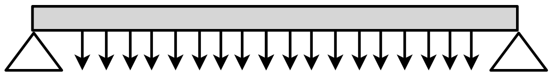
Without external forces, we are looking for solutions of the form

$$u(x,t) = \mathrm{Re}\left(u_0 \exp^{i(wt-kx)}\right)$$

We find the dispersion relation $\omega^2 = \frac{EI}{\mu}k^4$ with group velocity $v_g(k) = \frac{d\omega}{dk} = 2\sqrt{\frac{EI}{\mu}}k$

The final solution is found by applying boundary conditions at the beam extremities.

Elastic waves in elongated structures



We consider a beam with 2 supporting points and an external force.

Boundary conditions write $u(0) = u(L) = 0$ and $u''(0) = u''(L) = 0$ (no torque).

Allowed solutions are $u^n(t,x) = u_0^n \exp^{i\omega^n t} \sin\left(\frac{2\pi n}{L} x\right)$ $\quad \omega^n = \sqrt{\frac{EI}{\mu}} \left(\frac{2\pi n}{L}\right)^2$

General solutions write $u(t,x) = \sum_0^{+\infty} u^n(t) \sin\left(\frac{2\pi n}{L} x\right)$

These are called the normal modes of the beam.

If we apply now a time-dependent external force, we have in the normal mode basis

$$\frac{\partial^2 u^n}{\partial t^2} + (\omega^n)^2 u^n = g^n(t)$$

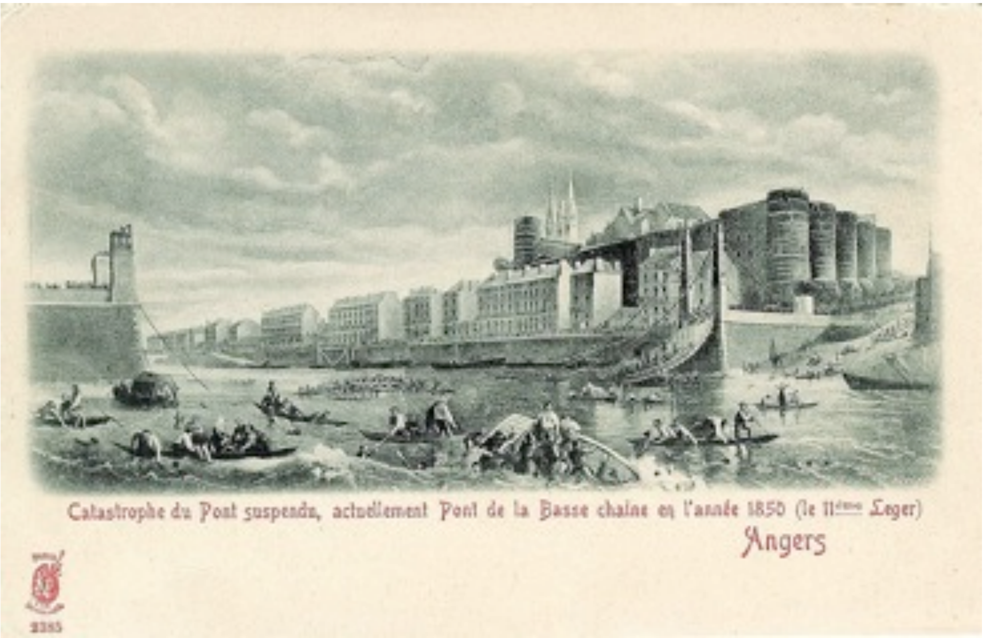
If the forcing is monochromatic, $g^n(t) \propto \exp^{i\omega t}$, the solution is $u_0^n = \frac{g_0^n}{(\omega^n)^2 - \omega^2}$

If the external forcing frequency is close to a normal mode frequency, we have a resonant response and the amplitude of the wave can be arbitrarily large.

Resonant elastic response

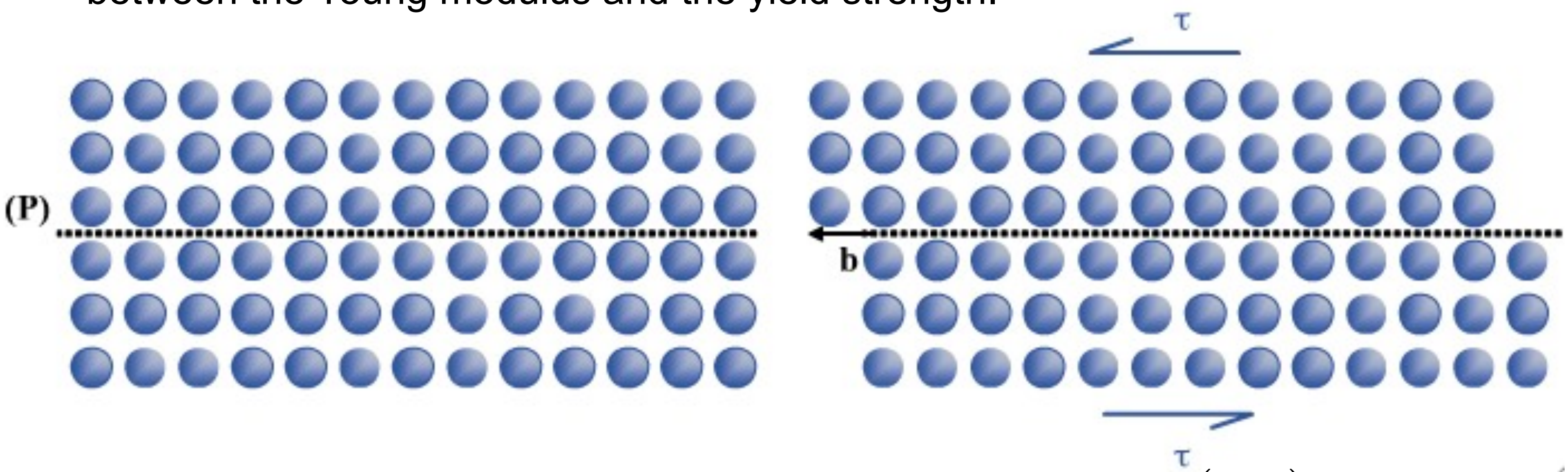
Millennium bridge in London (2000)

Basse-Chaine bridge in Angers (1850)



Theory of dislocations

The idea of dislocations in crystal structures originates from the large difference between the Young modulus and the yield strength.



We model the shear stress as a periodic function $\tau = \tau_0 \sin\left(\frac{2\pi x}{b}\right)$

Parameter τ_0 is the yield strength required to get an irreversible evolution.

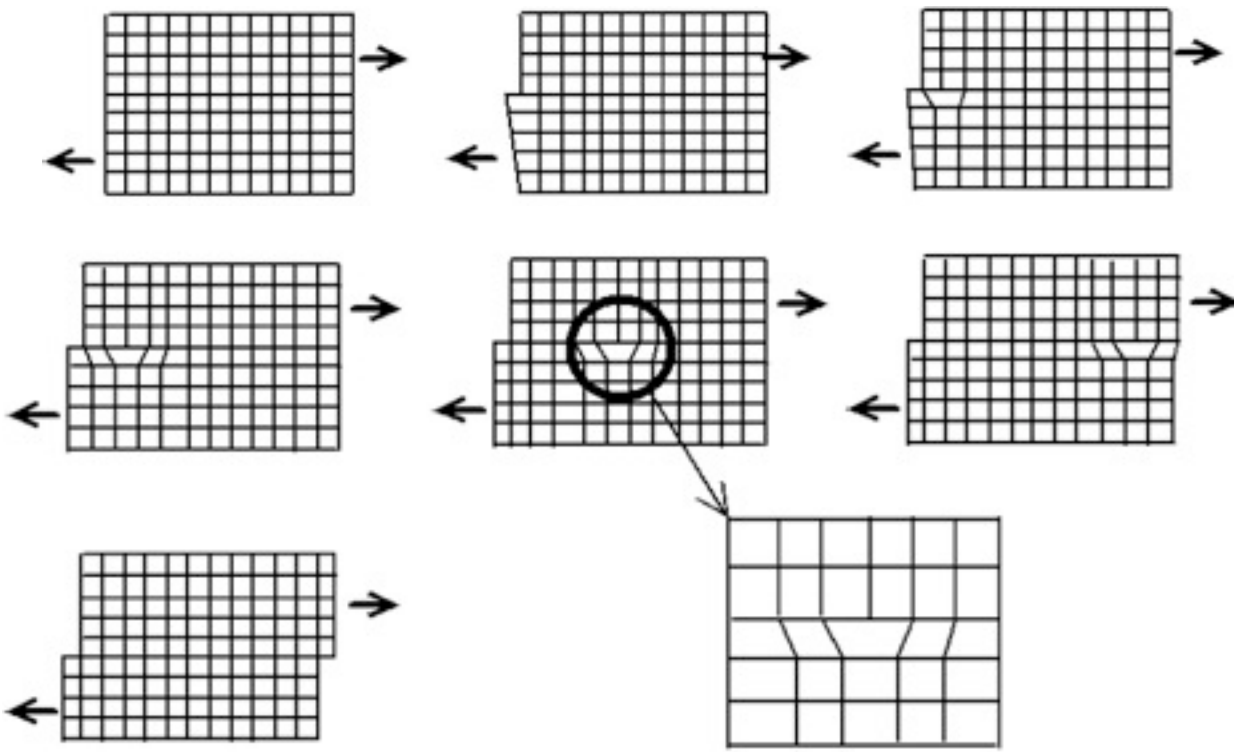
We match our non-linear model to the linear regime $\tau \simeq \tau_0 \left(\frac{2\pi}{b}\right) x = \mu \frac{x}{b}$

We obtain $\boxed{\sigma_y = \frac{\mu}{2\pi}}$, although experimentally $\sigma_y \sim 10^{-4} \text{ to } 10^{-3} E$

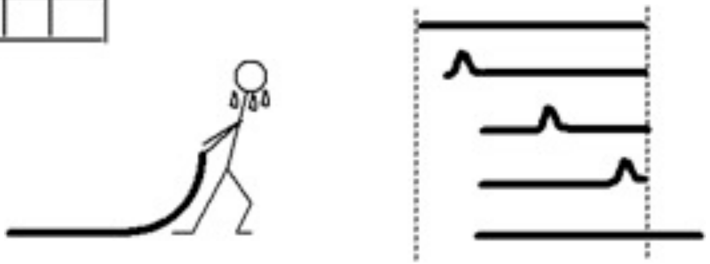
This remained a mystery for centuries !

Theory of dislocations

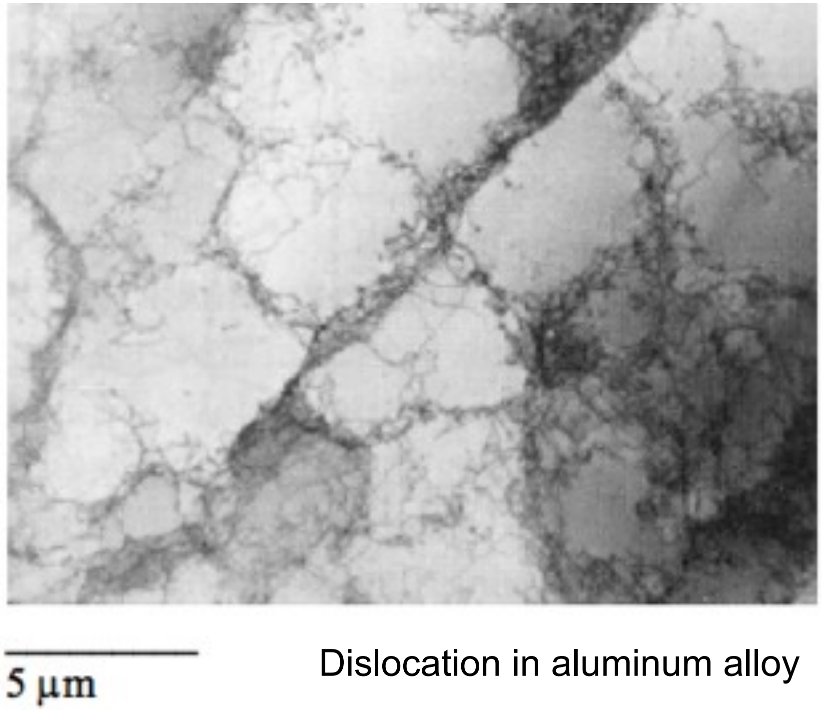
In 1934, Taylor, Orowan and Polanyi proposed independently that defects in the crystal structure might explain this puzzle. These little imperfections, mostly linear in shape, move through the crystal and trigger plastic deformations.



These topological defects are called *dislocations*.
It is possible to shift a whole plane by one atomic unit with much less energy: the «carpet analogy».

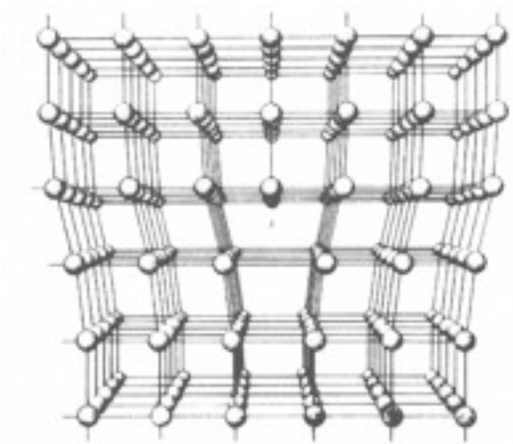


Geometry of dislocations

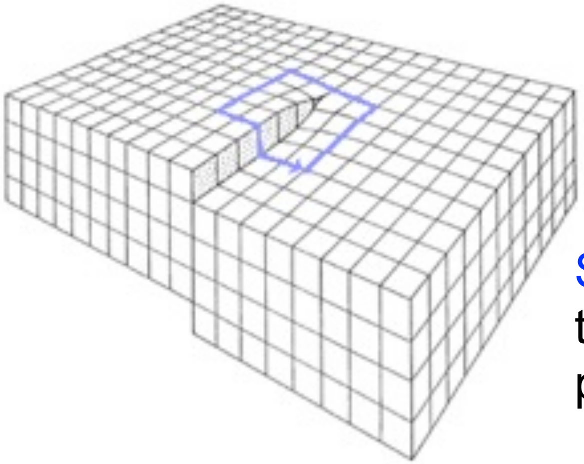


Dislocation in aluminum alloy

Although dislocations are in general of arbitrary shapes, they are usually the superposition of 2 basics geometries that form a basis for dislocations.



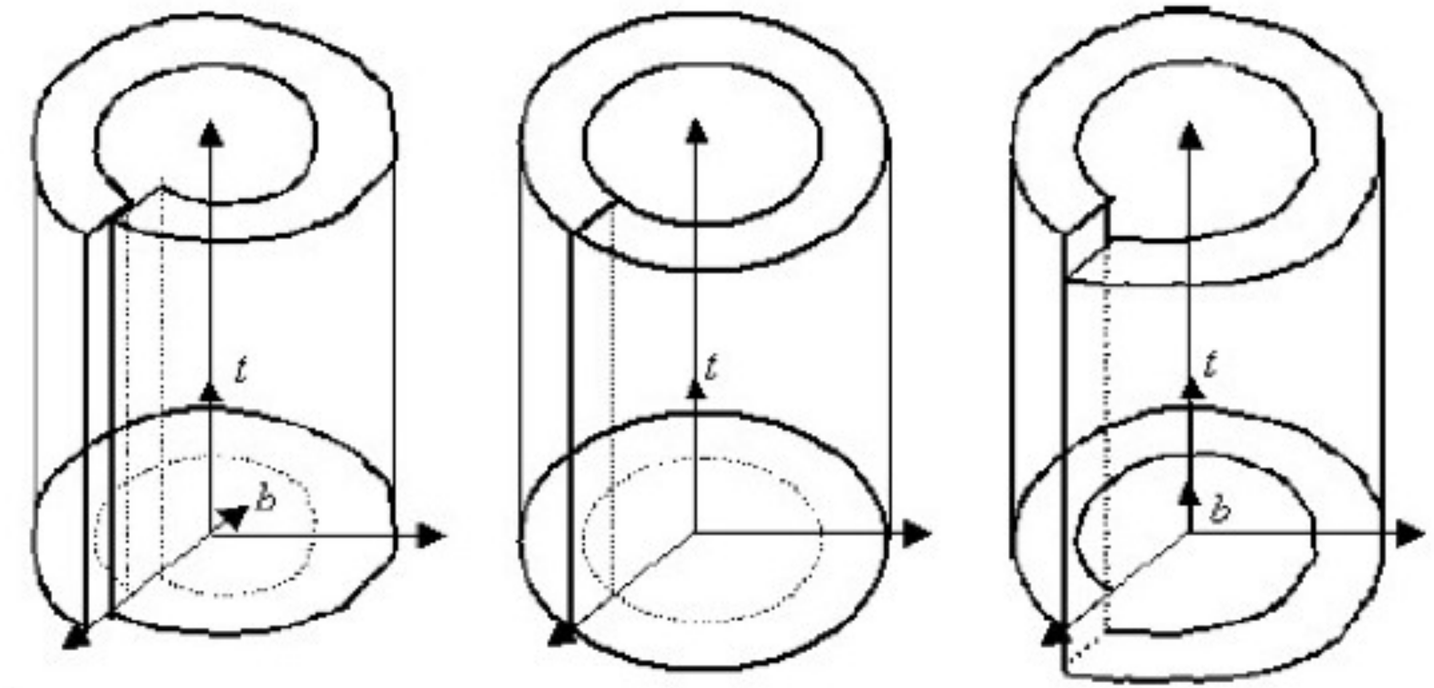
Edge dislocations, for which the displacement field is perpendicular to the defect line.



Screw dislocations, for which the displacement field is parallel to the defect line.

The Volterra construction

We consider a linear defect of infinite length, described by its tangent vector $\vec{t}$. We cut the cylinder vertically and displace the two ridges by a constant vector $\vec{b}$.



Edge dislocation

$$\vec{b} \perp \vec{t}$$

Screw dislocation

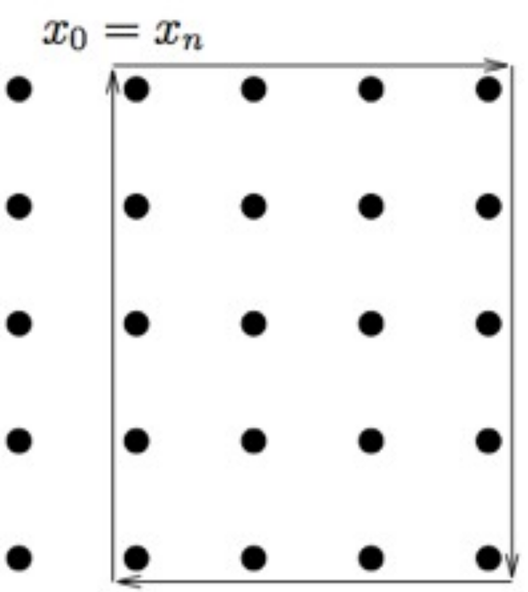
$$\vec{b} \parallel \vec{t}$$

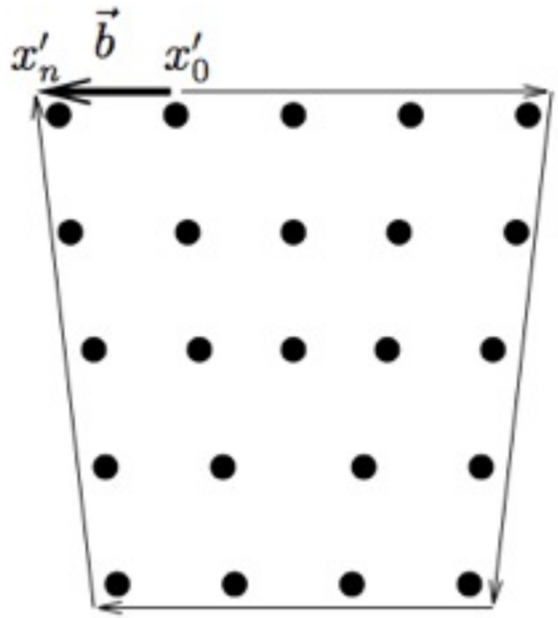
$\vec{b}$ is called the Burgers vector of the dislocation.

Its length is usually one atomic separation.

$$\oint_C \mathrm{d}\vec{u} = \oint_C \frac{d\vec{u}}{ds}\mathrm{d}s = \vec{b}$$

The Volterra construction





In a perfect crystal, we have:

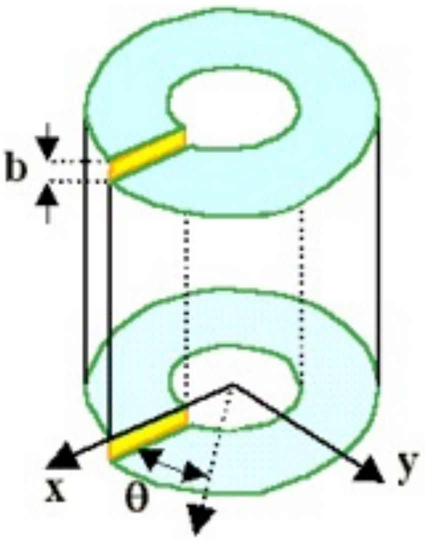
$$\sum_{i=0}^{n-1} (\vec{x}_{i+1} - \vec{x}_i) = \vec{x}_n - \vec{x}_0 = \vec{0}$$

A dislocation creates a topological defect, independent of the path used.

$$\sum_{i=0}^{n-1} (\vec{x}_{i+1} - \vec{x}_i) = \vec{x}_n - \vec{x}_0 = \vec{b}$$

Screw dislocation

We find the equilibrium displacement field around a screw dislocation (elastic theory).



We have no displacement in the x and y directions $u_x = u_y = 0$

The unknown is here $u_z(x,y)$. We have $\vec{\nabla} \cdot \vec{u} = 0$.

The Navier equation reads $\Delta u_z = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_z}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u_z}{\partial \theta^2} = 0$

Boundary condition: $\oint_C \mathrm{d}u_z = \oint_C \frac{\partial u_z}{\partial \theta}\mathrm{d}\theta = b$

The solution is: $u_z(r,\theta) = \frac{b\theta}{2\pi}$ with $\overline{\overline{\epsilon}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{b}{4\pi r} \\ 0 & \frac{b}{4\pi r} & 0 \end{pmatrix}$

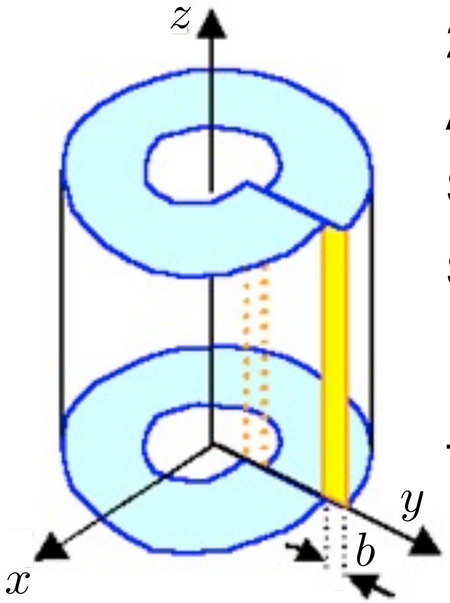
The stress tensor is purely deviatoric (pure shear). The elastic energy per unit length is

$$\frac{dE}{dl} = \frac{1}{2}\int_S \mathrm{Tr}(\overline{\overline{\sigma}}\ \overline{\overline{\epsilon}})\mathrm{d}S = \mu\frac{b^2}{4\pi}\int\frac{\mathrm{d}r}{r} = \mu\frac{b^2}{4\pi}\ln\left(\frac{r_{max}}{r_{min}}\right)$$

The minimum radius corresponds to the core of the dislocation $r_{min} \simeq b \simeq 0.2\ \mathrm{nm}$ for which the continuum approach breaks down and $r_{max} \simeq 10^{-4}\ \mathrm{cm}$ to the average distance between 2 dislocations in the crystal.

Standard approximation for the dislocation energy: $\boxed{E \simeq \frac{1}{2}\mu b^2 L}$

Edge dislocation



2D plain strain problem $\vec{u} = (u_x(x,y), u_y(x,y), 0)$

Airy's bi-harmonic function satisfying $\Delta\Delta\phi = 0$

Symmetry along the z axis, with a discontinuity at *x*=0

Simplest harmonic function antisymmetric wrt the x axis

$$\Delta\phi = a\frac{\partial}{\partial x}\ln r = a\frac{x}{r^2} \quad \text{where} \quad r = \sqrt{x^2+y^2}$$

Trick: find *v* such as $\Delta v = \ln r$ and then $\phi = a\frac{\partial}{\partial x}v$

Solution: $v = \frac{r^2}{4}\ln r - \frac{r^2}{4}$ so that $\boxed{\phi = \frac{a}{2}\left(x\ln r - \frac{x}{2}\right)}$

The stress tensor writes $\sigma_{xx} = \frac{\partial^2\phi}{\partial y^2} = \frac{a}{2}\frac{x}{r^4}\left(x^2-y^2\right)$

$$\sigma_{xy} = -\frac{\partial^2\phi}{\partial x\partial y} = \frac{a}{2}\frac{y}{r^4}\left(x^2-y^2\right)$$

$$\sigma_{yy} = \frac{\partial^2\phi}{\partial x^2} = \frac{a}{2}\frac{x}{r^4}\left(x^2+3y^2\right)$$

Hooke's law in 2D gives $\epsilon_{xx} = \frac{a}{4\mu}\frac{x}{r^4}\left[(1-2\nu)x^2-(1+2\nu)y^2\right]$

(plane strain)

$$\epsilon_{yy} = \frac{a}{4\mu}\frac{x}{r^4}\left[(1-2\nu)x^2+(3-2\nu)y^2\right]$$

$$\epsilon_{xy} = \frac{a}{4\mu}\frac{y}{r^4}\left[x^2-y^2\right]$$

Edge dislocation

We have $$\frac{\partial u_x}{\partial x} = \epsilon_{xx} = \frac{a}{4\mu}\left[(1-2\nu)\frac{x}{r^2} - 2\frac{y^2 x}{r^4}\right]$$

which integrates easily into: $$\boxed{u_x = \frac{a}{4\mu}(1-2\nu)\ln r + \frac{a}{4\mu}\frac{y^2}{r^2}}$$

For the other component, we pose $\theta = \arctan\frac{y}{x}$ to get $\frac{\partial u_y}{\partial \theta} = \frac{a}{4\mu}\left[2(1-\nu) - \cos 2\theta\right]$

Integrating with respect to θ gives $$\boxed{u_y = \frac{a}{2\mu}(1-\nu)\theta - \frac{a}{4\mu}\frac{xy}{r^2}}$$

We now use the boundary conditions: $$\boxed{a = \frac{\mu}{(1-\nu)\pi}b}$$

$$\oint_C \mathrm{d}u_x = \oint_C \frac{\partial u_x}{\partial \theta}\mathrm{d}\theta = 0 \qquad \oint_C \mathrm{d}u_y = \oint_C \frac{\partial u_y}{\partial \theta}\mathrm{d}\theta = \frac{a}{\mu}\pi(1-\nu) = b$$

The stress tensor in cylindrical coordinates reads $\overline{\overline{\sigma}} = \frac{a}{2r}\begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$

The eigenvalues are $\sigma_{1,2} = \frac{a}{2r}\left(\cos\theta \pm \sin\theta\right)$, $\sigma_3 = \nu\left(\sigma_1 + \sigma_2\right) = \frac{a}{2r}2\nu\cos\theta$

Using Hooke's law $\overline{\overline{\epsilon}} = \frac{1}{2\mu}\left(\overline{\overline{\sigma}} - \frac{\nu}{1+\nu}(\mathrm{Tr}\overline{\overline{\sigma}})\overline{\overline{I}}\right)$, we get $\epsilon_{1,2} = \frac{a}{4\mu r}\left(\cos\theta(1-2\nu) \pm \sin\theta\right)$

$$\boxed{E_{\mathrm{edge}} = \frac{1}{1-\nu}E_{\mathrm{screw}}}$$

The elastic energy density is just $\frac{1}{2}\left(\sigma_1\epsilon_1 + \sigma_2\epsilon_2\right)$

The elastic energy per unit length is $$\frac{dE}{dl} = \frac{a^2}{4\mu}(1-\nu)\pi\int\frac{\mathrm{d}r}{r} = \frac{\mu}{1-\nu}\frac{b^2}{4\pi}\ln\left(\frac{r_{max}}{r_{min}}\right)$$

Non-singular dislocation model

In the two previous models, the stress tensor diverges as x, y all tend to zero.

The elastic energy is also infinite, unless one introduces a cut-off radius.

For an edge dislocation, along y=0, we have $\sigma_{xx} = \dfrac{\mu}{1-\nu}\dfrac{b}{2\pi x}$

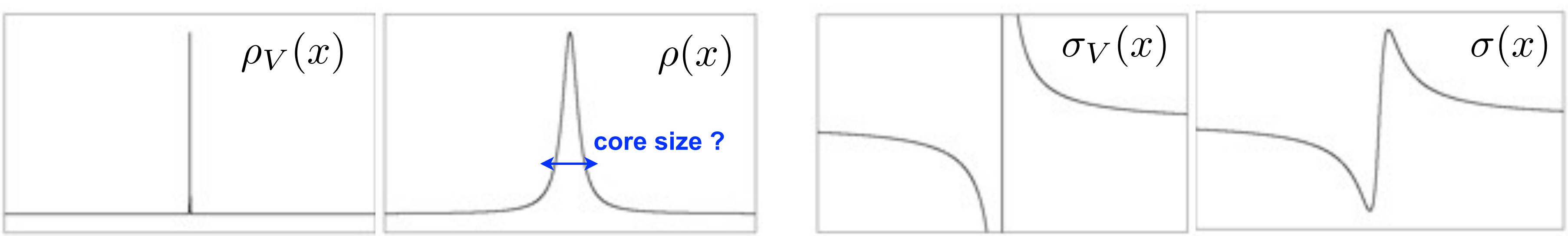
and for a screw dislocation, $\sigma_{yz} = \mu\dfrac{b}{2\pi x}$. The singularity at x=0 is due to the continuous approach, neglecting the effect of the underlying crystal structure.

To remove the core singularity, one idea is to replace the Burgers vector by a continuous distribution of Burgers «charge» density $\rho(x)$ such that $\int_{-\infty}^{+\infty}\rho(x)\mathrm{d}x = b$

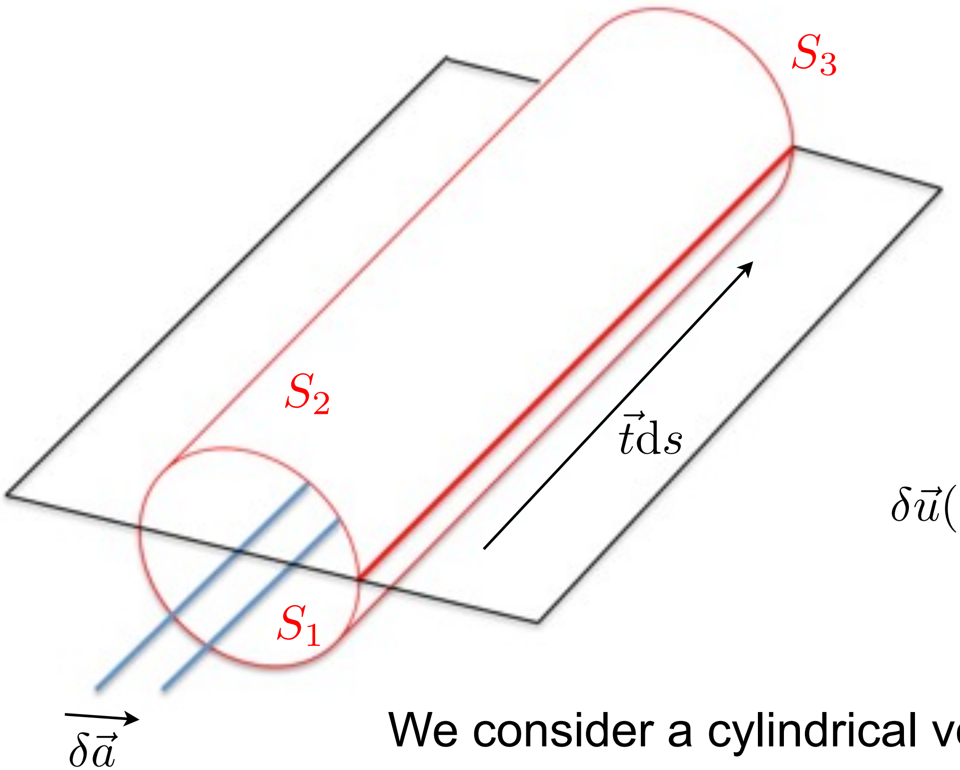
The singular case from the Volterra construction is just $\rho_V(x) = b\delta(x)$.

We then construct a non-singular stress field using a convolution

$$\boxed{\sigma_{xx}(x) = \sigma_V(x) \star \rho(x) = \frac{\mu}{2\pi(1-\nu)}\int_{-\infty}^{+\infty}\frac{\rho(x')}{x-x'}\mathrm{d}x'}$$



Work required to move a dislocation line



We consider a infinitesimal dislocation line a length d*s.* We displace it by a fixed perpendicular vector $\delta\vec{a}$.

We know from before the displacement field u around the dislocation line (edge or screw). The difference between the initial and the final displacement field is:

$$\delta\vec{u}(\vec{x}) = \vec{u}(\vec{x}-\delta\vec{a}) - \vec{u}(\vec{x}) \simeq -\frac{\partial\vec{u}}{\partial\vec{x}}\delta\vec{a} = -\overline{\overline{G}}\delta\vec{a}$$

We consider a cylindrical volume along the dislocation line.

This cylinder is cut by the plane containing the initial and final dislocation. Its surface is decomposed into 3 main surfaces.

$$S = S_1 + S_2 + S_3$$

We now consider a *constant external stress field* applied to move the line.

The work required is just $\delta W = \int_S \overrightarrow{T}\cdot\delta\vec{u}\mathrm{d}S = -\int_S \overline{\overline{\sigma}}\vec{n}\cdot\overline{\overline{G}}\delta\vec{a}\mathrm{d}S$

Work required to move a dislocation line

We now compute the work, using these various steps.

We have first from the dot product and the symmetry of the stress tensor:

$$\left(\overline{\overline{G}}\delta\vec{a}\right)\cdot\left(\overline{\overline{\sigma}}\vec{n}\right)=\left(\overline{\overline{\sigma}}\overline{\overline{G}}\delta\vec{a}\right)\cdot\vec{n}$$

Using the component form, $\sigma_{ki}G_{ij}\delta a_j=\delta a_j\dfrac{\partial}{\partial x_j}\left(\sigma_{ki}u_i\right)=\delta a_j\dfrac{\partial v_k}{\partial x_j}$

we can therefore simplify the expression into this:

$$\left(\overline{\overline{G}}\delta\vec{a}\right)\cdot\left(\overline{\overline{\sigma}}\vec{n}\right)=\left(\delta\vec{a}\cdot\vec{\nabla}\right)\vec{v}$$

We used the fact that the stress tensor is uniform and we introduced $\vec{v}=\overline{\overline{\sigma}}\vec{u}$.

We now used the famous vector identity

$$\vec{\nabla}\times\left(\vec{A}\times\vec{B}\right)=\vec{A}\left(\vec{\nabla}\cdot\vec{B}\right)-\vec{B}\left(\vec{\nabla}\cdot\vec{A}\right)+\left(\vec{B}\cdot\vec{\nabla}\right)\vec{A}-\left(\vec{A}\cdot\vec{\nabla}\right)\vec{B}$$

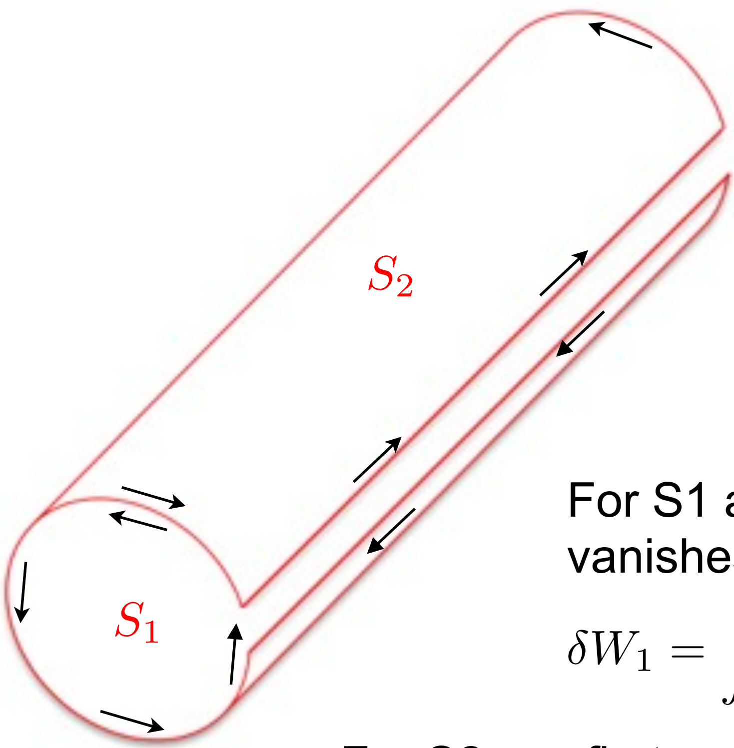
to get

$$\vec{\nabla}\times\left(\delta\vec{a}\times\vec{v}\right)=\delta\vec{a}\left(\vec{\nabla}\cdot\vec{v}\right)-\left(\delta\vec{a}\cdot\vec{\nabla}\right)\vec{v}$$

Using Stoke's theorem, we finally obtain (introducing the line contour *C* bounding the cylindrical surface *S*)

$$\boxed{\delta W=\int_C\left(\delta\vec{a}\times\vec{v}\right)\cdot\mathrm{d}\vec{l}-\int_S\left(\vec{\nabla}\cdot\vec{v}\right)\delta\vec{a}\cdot\vec{n}\mathrm{d}S}$$

Work required to move a dislocation line



We will now compute these 2 terms (a surface term and a contour term) for each of the 3 main surface elements defining our cylinder.

Note that since the dislocation is a topological singularity, we need to cut S2 in the mid plane to account for the Burgers vector.

For S1 and S3, since $\vec{n} = \vec{t}$ and $\delta\vec{a} \perp \vec{t}$, the surface term vanishes and we have (care with the right-handedness)

$$\delta W_1 = \int_{C_1} (\delta\vec{a} \times \vec{v}) \cdot \mathrm{d}\vec{l} \qquad \delta W_3 = \int_{C_3} (\delta\vec{a} \times \vec{v}) \cdot \mathrm{d}\vec{l}$$

For S2, we first compute the contribution from the contour term.

We see from the diagram that S2 shares a fraction of contour with S1 and S3.

$$\delta W_{2,C} = -\delta W_1 - \delta W_3 + \int_{C_2} (\delta\vec{a} \times \vec{v}) \cdot \mathrm{d}\vec{l}$$

On each side of the mid plane cut, we have

$$\vec{v}\left(0^+\right) - \vec{v}\left(0^-\right) = \overline{\overline{\sigma}}\vec{b}\,,\ \mathrm{d}\vec{l}^+ = \vec{t}\mathrm{d}s\,,\ \mathrm{d}\vec{l}^- = -\vec{t}\mathrm{d}s$$

$$\boxed{\int_{C_2} (\delta\vec{a} \times \vec{v}) \cdot \mathrm{d}\vec{l} = \left(\delta\vec{a} \times \overline{\overline{\sigma}}\vec{b}\right) \cdot \vec{t}\mathrm{d}s}$$

Work required to move a dislocation line

We now compute the surface term: $\delta W_{2,S} = -\int_{S_2} \left(\vec{\nabla} \cdot \vec{v} \right) \delta \vec{a} \cdot \vec{n} \mathrm{d}S$

For a screw dislocation with a *non-singular* core, we have $\left| \vec{\nabla} \cdot \vec{v} \right| < \sigma_{\max} \frac{b}{4\pi r}$

so that $|\delta W_{2,S}| < \left| \vec{\nabla} \cdot \vec{v} \right| \delta a 2\pi r \mathrm{d}s \longrightarrow 0$ as $r \longrightarrow 0$.

Collecting all the contributions, we finally have the work required to move the line as

$$\delta W = \delta W_1 + \delta W_{2,C} + \delta W_{2,S} + \delta W_3 = \left(\delta \vec{a} \times \overline{\overline{\sigma}} \vec{b} \right) \cdot \vec{t} \mathrm{d}s$$

$$\delta W = \delta \vec{a} \cdot \left(\overline{\overline{\sigma}} \vec{b} \times \vec{t} \right) \mathrm{d}s = \vec{F} \mathrm{d}s \cdot \delta \vec{a}$$

where we defined the *Peach-Koehler configuration force* (per unit length)

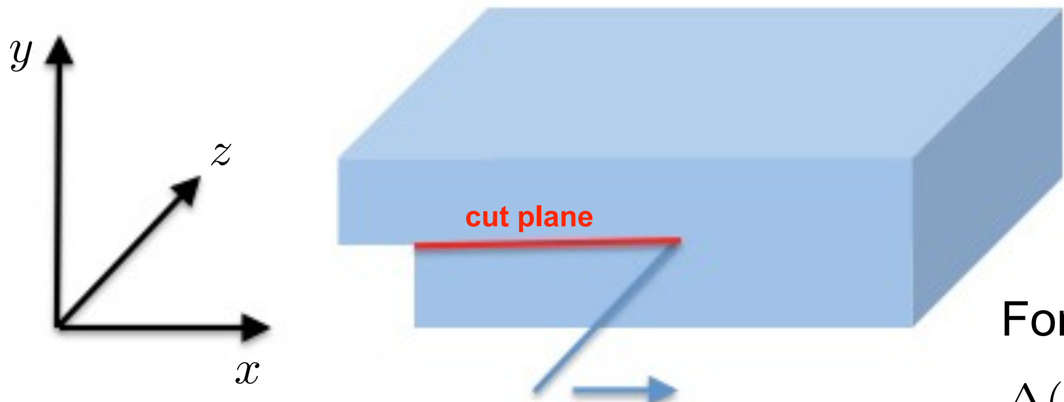
$$\boxed{\vec{F} = \overline{\overline{\sigma}} \vec{b} \times \vec{t}}$$

This force is not a true force associated to some interaction. It is just related to the energy that is required to move a dislocation over some distance.

This energy comes from a topological rearrangement of the crystal structure.

There is a strong analogy with the Biot-Savart force and magnetic field induced from a current loop.

Peierls-Nabarro model



The displacement field above and below the cut plane is discontinuous. We define

$$\Delta(x) = u_x(x, 0^+) - u_x(x, 0^-)$$

For a Volterra edge dislocation, we have

$\Delta(x) = b$ for $x < 0$ and $\Delta(x) = 0$ for $x > 0$

Using the same regularization technique, for a non-singular dislocation we can define a smoothed displacement jump as $\Delta(x) = \int_x^{+\infty} \rho(x')\mathrm{d}x'$

We now compute the elastic energy in a cubic volume containing the cut plane.

Clapeyron's theorem states that $F = \frac{1}{2}\int_V \mathrm{Tr}\left(\overline{\overline{\sigma}}\,\overline{\overline{\epsilon}}\right)\mathrm{d}V = \frac{1}{2}\int_S \overrightarrow{T}\cdot\vec{u}\mathrm{d}S$

The normal vectors are just $\vec{n} = \pm\vec{e}_y$ so that when the cube vanishes in its vertical dimension we have $F = \frac{1}{2}\int_{-\infty}^{+\infty} \sigma_{xy}(x,0)\left(u_x(x,0^+) - u_x(x,0^-)\right)\mathrm{d}x$

$$\boxed{F = \frac{1}{2}\int_{-\infty}^{+\infty} \sigma_{xy}(x)\Delta(x)\mathrm{d}x}$$

Peierls-Nabarro model

For a Volterra edge dislocation with $\vec{b} = b\vec{e}_x$, we have $\sigma_{xy} = \frac{\mu}{1-\nu}\frac{b}{2\pi x}$

and the elastic energy $F = \frac{\mu}{1-\nu}\frac{b^2}{4\pi}\int_{-\infty}^{0}\frac{\mathrm{d}x}{x}$ is infinite.

Including now the core regularization mechanism, $\sigma_{xy}(x) = \frac{\mu}{2\pi(1-\nu)}\int_{-\infty}^{+\infty}\frac{\rho(x')}{x-x'}\mathrm{d}x'$

so that $F = \frac{1}{2}\int_{-\infty}^{+\infty}\sigma_{xy}(x)\Delta(x)\mathrm{d}x = \frac{\mu}{4\pi(1-\nu)}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{\rho(x')\Delta(x)}{x-x'}\mathrm{d}x\mathrm{d}x'$

Integrating by parts, we get $\boxed{F = \frac{\mu}{4\pi(1-\nu)}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\rho(x)\rho(x')\log|x-x'|\mathrm{d}x\mathrm{d}x'}$

The elastic energy is now finite, but it depends directly on the core density $\rho(x)$ under the normalization constraint $\int_{-\infty}^{+\infty}\rho(x)\mathrm{d}x = b$. The energy decreases as the dislocation density becomes wider and wider. Ultimately, the dislocation dissipates.

In fact, the core density is stabilized by the *misfit energy* between the upper and lower atomic layer wrt to the cut plane. It is modeled using a periodic function of the displacement to ensure the confinement of the core.

$$\boxed{\phi(\Delta) = \phi_0\left(1-\cos\frac{2\pi\Delta}{b}\right)}$$

Peierls-Nabarro model

The total energy of the cut plane is therefore the sum of 2 components:

$$E_{\rm tot} = \int_{-\infty}^{+\infty} \phi(\Delta(x)){\rm d}x + \frac{\mu}{4\pi(1-\nu)} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho(x)\rho(x') \log|x-x'|{\rm d}x{\rm d}x'$$

where the unknown core density satisfies $\rho(x) = -\frac{\partial \Delta(x)}{\partial x}$

We use the Variational Principle to find the core density that minimizes the energy.

We write $\Delta(x) = \Delta_0(x) + \delta\Delta(x)$ and compute $\delta E_{\rm tot}$ as

$$\delta E_{\rm tot} = \int_{-\infty}^{+\infty} \delta\Delta(x) \left[\frac{\partial \phi}{\partial \Delta}(\Delta_0) + \frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{+\infty} \frac{\rho_0(x')}{x-x'}{\rm d}x' \right]$$

The energy is minimized if the integrand is uniformly zero. Our misfit energy model gives us an integro-differential equation found by Peierls and Nabarro

$$\frac{\mu}{2\pi(1-\nu)} \int_{-\infty}^{+\infty} \frac{\Delta_0'(x')}{x-x'}{\rm d}x' = \phi_0 \frac{2\pi}{b} \sin \frac{2\pi\Delta_0}{b}$$

The solution was found by Peierls to be $\boxed{\Delta_0(x) = \frac{b}{2} - \frac{b}{\pi} \arctan \frac{x}{\xi}}$

Peierls-Nabarro potential

We have now an explicit form for the core density $\rho(x) = \frac{b}{\pi} \frac{\xi}{\xi^2 + x^2}$

The core size $\xi = \frac{\mu b^2}{8\pi^2(1-\nu)\phi_0}$ is set by the competition between the elastic Lamé coefficient that tends to spread the dislocation and the misfit potential that tends to localize the core. The stress field along the x-axis follows the non-singular solution

$$\sigma_{xy}(x) = \frac{\mu b}{2\pi(1-\nu)} \frac{x}{\xi^2 + x^2}$$

In order to account for the crystal structure, we introduce explicitly the atomic lattice as well as the time-dependent coordinate of the dislocation. We are trying to get a dynamical description of the dislocation, beyond the static non-singular core model.

$$E_{\mathrm{misfit}} = \int_{-\infty}^{+\infty} \phi(\Delta(x))\mathrm{d}x \simeq \sum_{n \in \mathbf{Z}} \phi(\Delta(nb - x_d))b$$

Using various trigonometric identities, we get $E_{\mathrm{misfit}} = 2\phi_0 \xi^2 b \sum_{n \in \mathbf{Z}} \frac{1}{\xi^2 + (nb - x_d)^2}$

Peierls-Nabarro potential

We now use the Poisson summation method $\sum_{n\in\mathbf{Z}} f(n) = \sum_{k\in\mathbf{Z}} \int_{-\infty}^{+\infty} f(x)\mathrm{e}^{i2\pi kx}\mathrm{d}x$

to write the following expansion $E_{\mathrm{misfit}} = 2\phi_0\xi \sum_{k\in\mathbf{Z}} \mathrm{e}^{i2\pi k\frac{x_d}{b}}\mathrm{e}^{-2\pi\left|k\frac{\xi}{b}\right|}$

We consider only the leading order terms (*k*=-1,0,+1) to get finally

$$\boxed{E_{\mathrm{misfit}} = 2\phi_0\xi\left(1+2\mathrm{e}^{-2\pi\xi/b}\cos\left(2\pi\frac{x_d}{b}\right)\right)}$$

We can get the force required to move the dislocation using $F_d = -\frac{\partial}{\partial x_d}E_{\mathrm{misfit}}$

This force per unit length is another configuration force. It reads

$$\boxed{F_d = \frac{\mu b}{\pi(1-\nu)}\mathrm{e}^{-2\pi\xi/b}\sin\left(2\pi\frac{x_d}{b}\right)}$$

We now determine the yield strength by requiring that a dislocation of length L moves along the entire crystal dimension L to generate a plastic displacement of size b. This translates into the relation $\sigma_y Sb = \max(F_d)L^2$.

Assuming S=L^2, we finally get $\boxed{\sigma_y = \frac{\mu}{\pi(1-\nu)}\mathrm{e}^{-2\pi\xi/b} \ll \frac{\mu}{2\pi}}$