# Theory of Plasticity

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Plasticity of materials:

- Metals, Metallic compounds and alloys, Ceramics (Periodic structure)
- Polymers, Biological materials (Chain Structure)
- Complex materials (metallo –organic framework, liquid crystals, cement hydration products – lamellar structures)

Metal plasticity

Dislocation mechanisms

Twinning mechanisms

## What is Dislocation Mechanics? (as meant here)

- The study of the stress state and deformation of continua whose elastic response is mediated by the nucleation, presence, motion, and interaction of distributions of crystal defects called *dislocations*

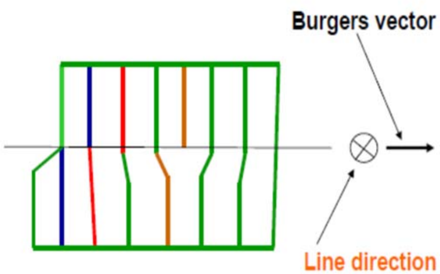
## Dislocation?

**For the moment,**

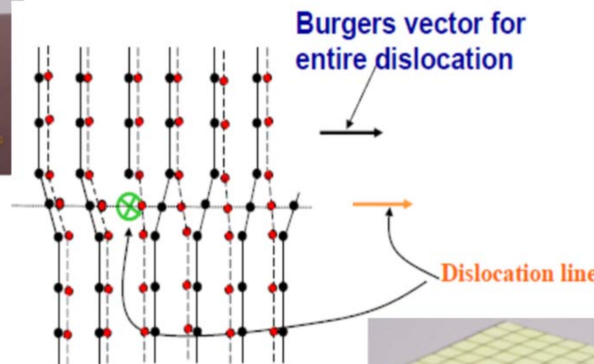
- **An imaginary curve in an elastic continuum**
  - that induces a stress field in the elastic body
  - is capable of moving and altering its shape
    —kinetics based on available elastic energy (stress)
- **Multiple dislocations interact through their stress fields**
  - The stress field of one dislocation modifies the stress acting on another thus affecting the latter's placement

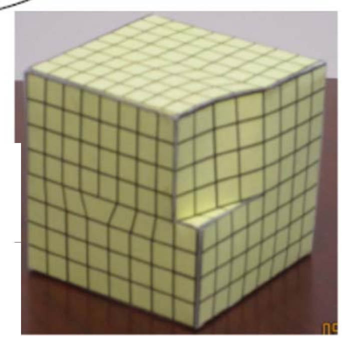
# Dislocation types

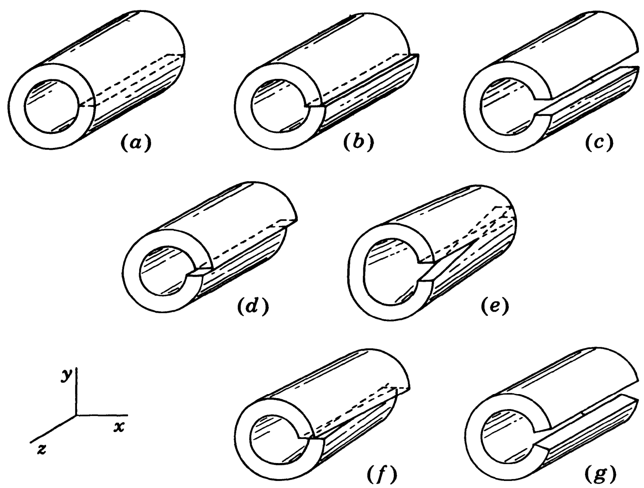
## Edge dislocation



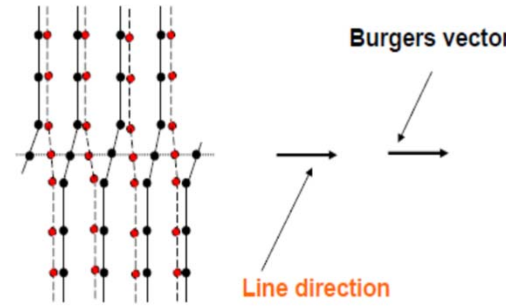

## Edge-screw dislocation

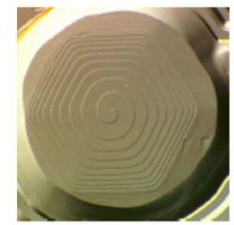


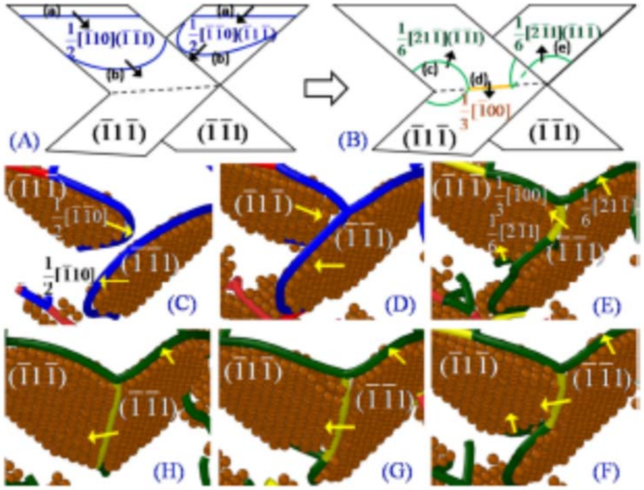



## Screw dislocation

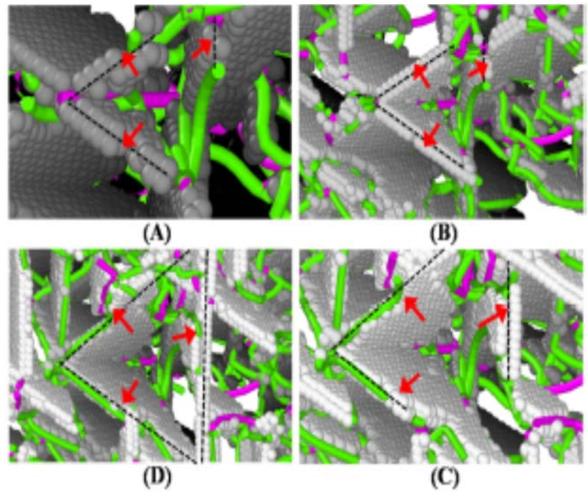


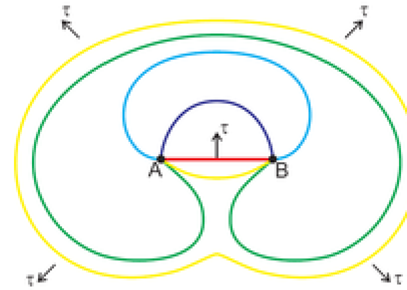
# Dislocation evolution




Hirth lock




Stacking fault tetrahedra



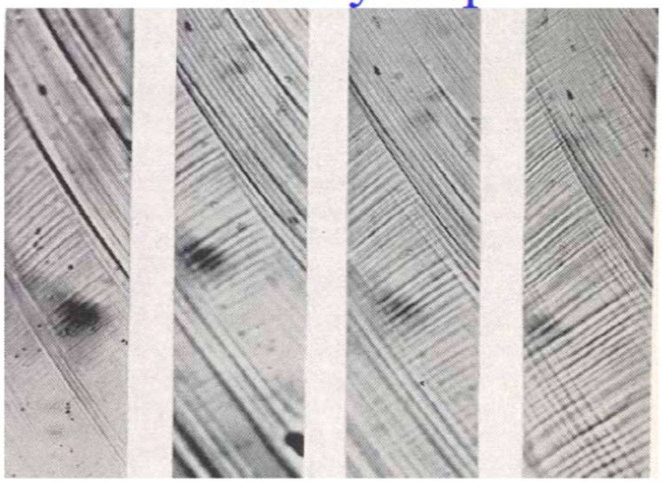

Frank Read

Mechanisms at continuum scale affected by dislocations and their reactions:

- Slip in materials leading to plasticity
- Hardening mechanisms in plasticity
- Various other time dependent behavior of materials

# Experimental observations of Dislocations in materials

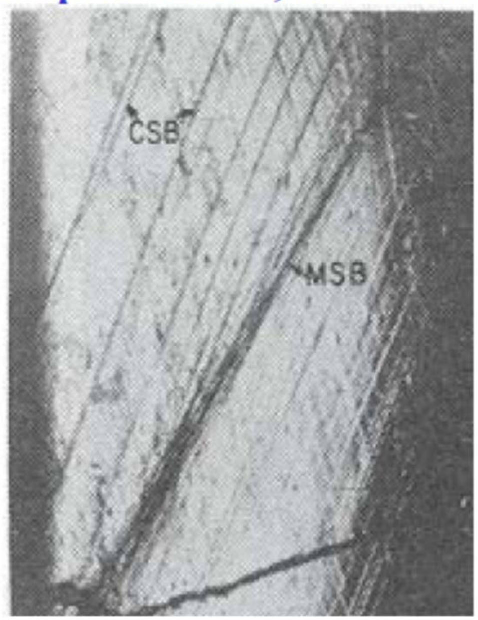
## Patchy Slip



Piercy, Cahn & Cottrell, 1955

$\alpha$ – brass

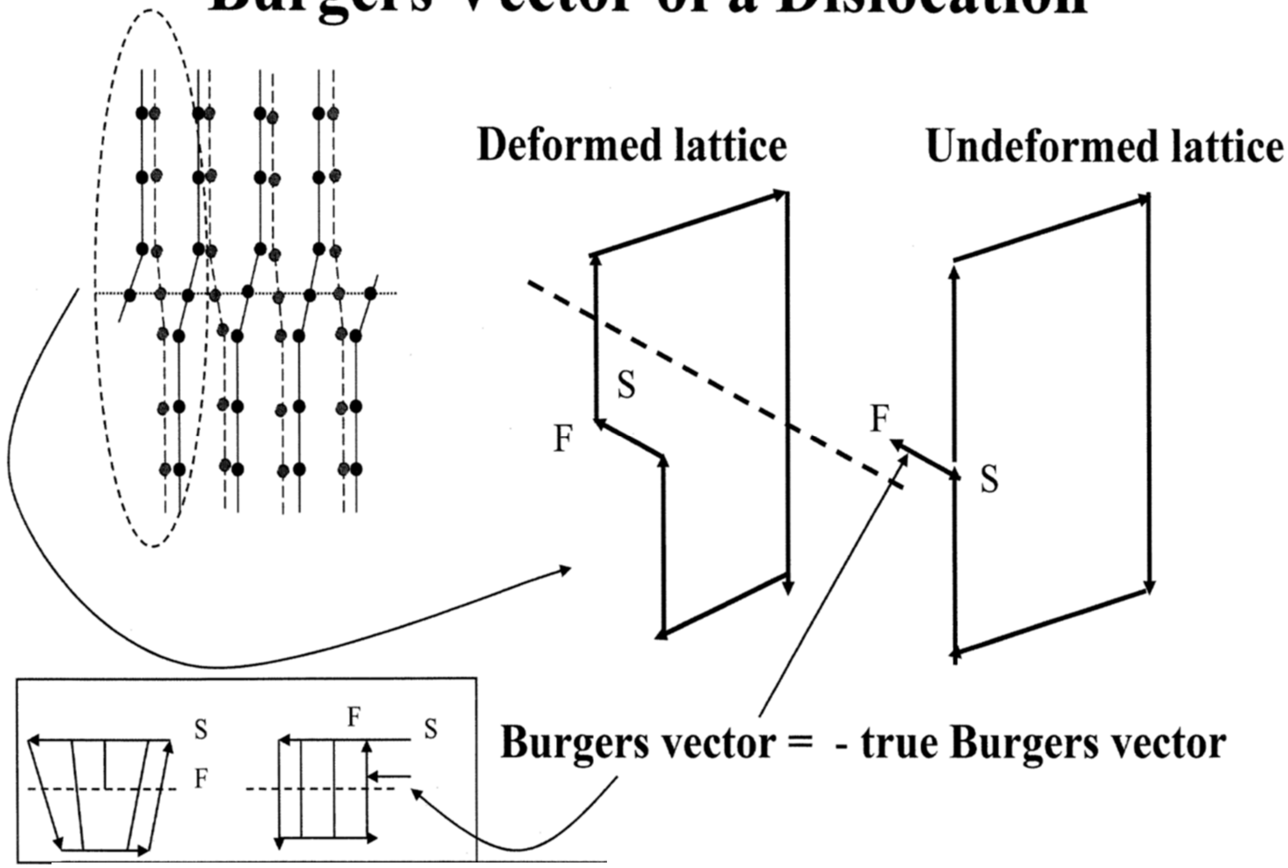
## Slip bands, localization




Chang & Asaro, 1980

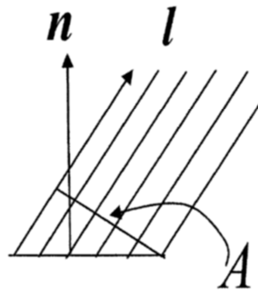
Al – Cu

# Burgers Vector of a Dislocation



# Dislocation Density

- Two-point tensor from current configuration to local unstretched lattice configuration ⟶




  - Given a direction in the current configuration
  - delivers
    - unstretched, (FS) Burgers vector/current area of dislocation lines threading unit area perpendicular to the direction

$$\alpha n = b\frac{N}{(A/\cos\theta)} = b\frac{N}{A}(l\cdot n)$$

**Construction of Dislocation density:**

$$\alpha \approx \rho b \otimes l \;;\; \rho = \frac{N}{A}$$

$N$ =# of infinitesimal dislocation lines with true Burgers vector $\boldsymbol{b}$ and line direction $\boldsymbol{l}$, threading area $A \perp$ to $\boldsymbol{l}$

Understanding Irrotational Vector fields that may not be gradients. (1)

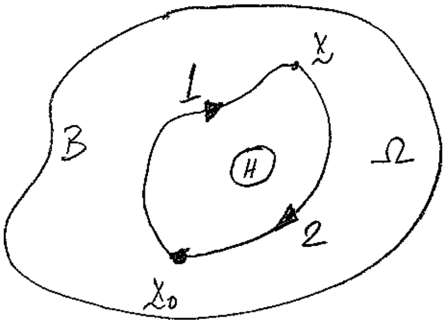
Very nice paper:

On the structure of some irrotational vector fields, I. Barza, General Mathematics, 13, 2005, 9-20.

Qn: Suppose we have a multiply-connected domain and have a 2nd-order tenser field $\underline{A}$ that is curl-free (irrotational) on it. Is it true that there exists a unique (up to a translation) displacement field $\underset{\sim}{u}$ s.t.

$$u_{i,j} \overset{?}{=} A_{ij}$$

$$\operatorname{grad} \underset{\sim}{u} = \underline{A} \quad ?$$



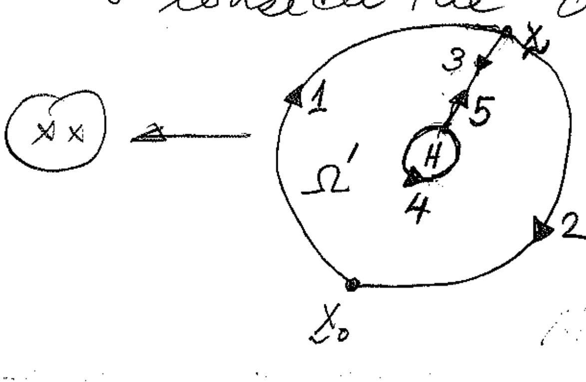

(Note that have to show that line integral is the same along all possible paths connecting $\underset{\sim}{X}_0$ to $\underset{\sim}{X}$).

So take $\underline{2}$ as shown (encircling hole H — or, H is not a hole but where $\underline{A}$ is not curl-free.)

Now $\operatorname{curl} \underline{A} = \underline{0}$ on Ω where Ω does not include the region ~~H~~. by hypothesis.

- Want to use the property that $\underline{A}$ is irrotational as in the simply connected case

So consider the circuit as shown:




$$\oint_1 \underline{A}\, d\underset{\sim}{x} + \oint_3 \underline{A}\, d\underset{\sim}{x} + \int_4 \underline{A}\, d\underset{\sim}{x} + \int_5 \underline{A}\, d\underset{\sim}{x} + \oint_2 \underline{A}\, d\underset{\sim}{x} = \int_{\Omega'} \operatorname{curl} \underline{A}\, \underset{\sim}{n}\, da = 0$$

Note, $\Omega'$ not simply-connected but making the cut with two coincident faces 3, 5 makes the region simply connected on which we apply Stokes' theorem as usual.

Additionally, $\oint_3 \underline{A}\, d\underset{\sim}{x} = -\oint_5 \underline{A}\, d\underset{\sim}{x}$.

$$\therefore \quad \oint_1 \underline{A}\, d\underset{\sim}{x} + \oint_2 \underline{A}\, d\underset{\sim}{x} = -\int_4 \underline{A}\, d\underset{\sim}{x}.$$

$$\therefore \quad \boxed{\oint_1 \underline{A}\, dx + \oint_4 \underline{A}\, d\underset{\sim}{x} = -\oint_2 \underline{A}\, d\underset{\sim}{x}}$$

So the values taken by $\underline{A}$ on the boundary of the hole matters.

Note that $H$ was not a 'hole' but part of the domain where $\underline{A}$ was specified &

$$\operatorname{curl} \underline{A} \neq 0 \quad \text{on } H$$

Then $-\int_4 \underline{A}\, d\underset{\sim}{x} = \int_H \operatorname{curl} \underline{A}\, \underset{\sim}{n}\, da$ //.

Thus, the answer to the original question is — in general NO.

There are actually <u>many</u> 'displacement' fields with discontinuities which satisfy $\operatorname{grad} \underset{\sim}{u} = \underline{A}$ !! (except on discontinuity).

Characterization:

Think of dislocations as being cylinders in the body whose 'axes' are closed space loops or they end at the boundaries of the body. Think of excavating material in the cylinders and one is left with a non-simply connected domain.

Now consider a body with one such dislocation in it. Its axis can be represented as such:

Let $f_1, f_2 : \mathcal{E}_3 \to \mathbb{R}$ be smooth scalar fields. Choose a rectangular Cartesian coordinate system for $\mathcal{E}_3$. Let $S_K = \{(x,y,z) \in \mathbb{R}^3 \mid f_K(x,y,z) = 0\}$ $K = 1,2$. be the 0-level set of $f_K$ (surfaces).
And, let the intersection of $S_1$ & $S_2$ represent the axis of the dislocation. So, $C := S_1 \cap S_2$.

- Now consider $G_K : \mathbb{R}^3 \setminus S_K \to \mathbb{R}$ scalar fields defined by

$$G_1(x,y,z) = \tan^{-1}\left(\frac{f_2(x,y,z)}{f_1(x,y,z)}\right); \quad G_2(x,y,z) = -\tan^{-1}\left(\frac{f_1(x,y,z)}{f_2(x,y,z)}\right)$$

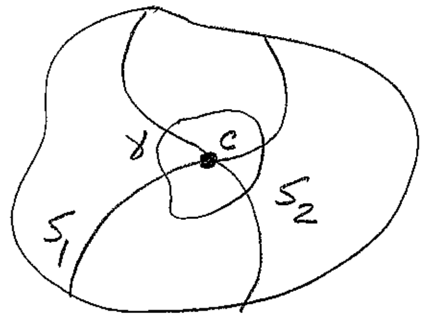
Now $\operatorname{grad} G_1$ is defined on $\mathbb{R}^3 \setminus S_1$ & $\operatorname{grad} G_2$ is defined on $\mathbb{R}^3 \setminus S_2$ by the same expressions

$$\boxed{\underset{\sim}{E} := \frac{1}{f_1^2 + f_2^2}\left(f_1 \frac{\partial f_2}{\partial x_i} - f_2 \frac{\partial f_1}{\partial x_i}\right) \underset{\sim}{e}_i}$$

elementary vector field corresponding to $C$

and note that $\underset{\sim}{E}$ is actually well-defined on $\mathbb{R}_3 \setminus C$.

On $\mathbb{R}_3 \setminus C$ $\underset{\sim}{E}$ corresponds to some gradient pointwise, hence it is irrotational.



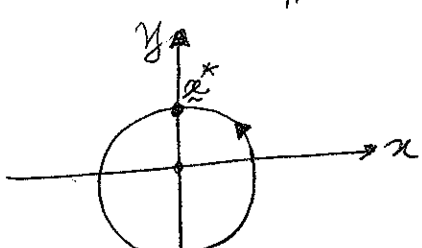

However it can be checked that $\int_\gamma \underset{\sim}{E} \, d\underset{\sim}{x} = \pm 2\pi$,

for any $\gamma$ encircling $C$, (evaluate along a convenient path, and then link any other loop to this one by procedure similar to Fig (**)).

<u>Intuition:</u> Let $C$ be $z$-axis. So let $f_1(x,y,z) = x$ i.e. $S_1 = Y$-$z$ plane ; $f_2(x,y,z) = y$ ; $S_2 = X$-$z$ plane.

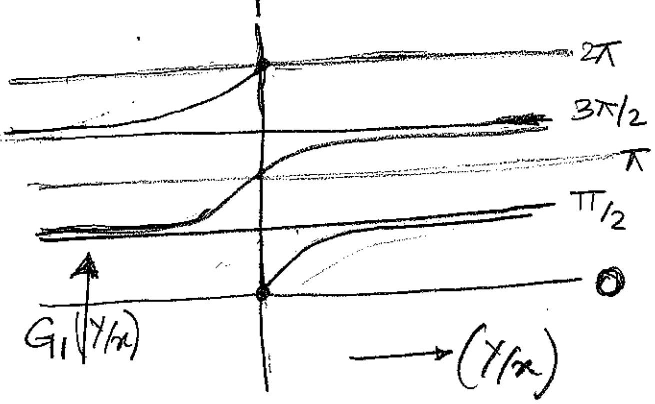
$G_1 = \tan^{-1}(Y/x)$. Let $\gamma$ be a circle.

So $\int_\gamma \underset{\sim}{E} \, d\underset{\sim}{x} = \int_\gamma \frac{\partial G_1}{\partial \underset{\sim}{x}} \, dx = ?$



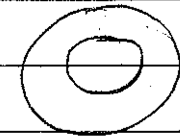

Note that on a circle $G_1 = \theta$ measured from $x$-axis

and $\therefore$ $\int_\gamma \underset{\sim}{E} \, d\underset{\sim}{x} = \int_\gamma d\theta = 2\pi$.

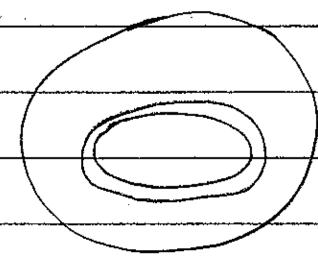


## Weingarten's Result:

* Consider multiply connected bodies of two types. Topologically same as
  - torus

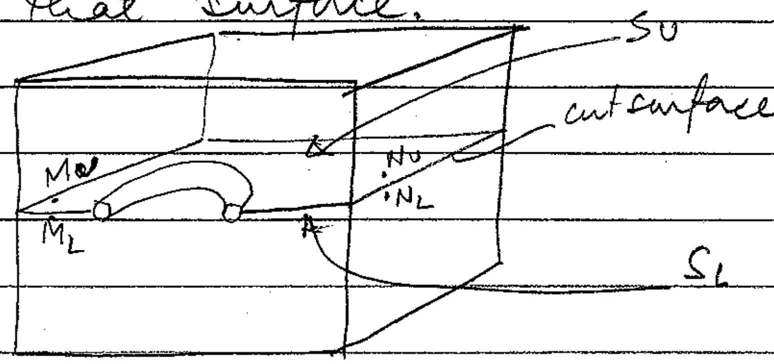


  - sphere with toroidal hole



Both doubly-connected : A closed curve can be drawn in the body that cannot be shrunk to a point while remaining in the body.

Weingarten: Let the strain in a doubly-connected body be twice-differentiable and satisfy the strain compatibility condition. Then the displacement jump field across any surface that renders the body simply connected is at most an infinitesimally rigid vector field on that surface.



Consider the cut surface shown above. Consider the simply-connected body obtained by cutting the original body along this surface.

We now have a compatible strain tensor field on a simply-connected body which is twice continuously diff across the cut. (The body has two more surfaces than the original one).

On a simply connected body we can write the displacement ~~field~~ at $N_U$ as follows.

$$u_i(N_U) - u_i(M_U) = \oint_{M_U}^{N_U} \left(e_{ik}(X') + \omega_{ik}(X')\right) dx'_k$$

(where line integral is along a path on $S_U$).

Now consider $\displaystyle\int_{M_U}^{N_U} \omega_{ik}(X')\,dx'_k$ } $\hookrightarrow$ see strain compatibility notes}.

$$= \int_{s=0}^{s=1} \omega_{ik}\,\frac{dx'_k}{ds}\,ds. \qquad \text{where } x'_j(s=0) = M_U,\quad x'_j(s=1) = N_U$$

$$= \int_{s=0}^{s=1} \frac{d}{ds}\left(\omega_{ik}\,x'_k\right) ds - \int_{s=0}^{s=1} x'_k\,\frac{d\omega_{ik}}{ds}\,ds.$$

$$= \omega_{ik}\,x'_k(s=1) - \omega_{ik}\,x'_k(s=0) - \oint_{M_U}^{N_U} x'_j\,\frac{\partial \omega_{ij}}{\partial x'_k}\,dx'_k.$$

$$= w_{ik}(N_U)\, x_k(N_U) - w_{ik}(M_U)\, x_k(M_U) - \oint_{M_U}^{N_U} x_j' \frac{\partial w_{ij}}{\partial x_k'}\, dx_k'$$

But $w_{ik}(N_U) = w_{ik}(M_U) + \oint_{M_U}^{N_U} (e_{il,k} - e_{kl,i})\, dx_l'$

$$\therefore\ \boxed{\begin{aligned} &u_i(N_U) - u_i(M_U) \\ &= w_{ik}(M_U)\, x_k(N_U) + \underbrace{x_k(N_U) \oint_{M_U}^{N_U} (e_{il,k} - e_{kl,i})\, dx_l'}_{I} \\ &- w_{ik}(M_U)\, x_k(M_U) \\ &+ \underbrace{\oint_{M_U}^{N_U} \Big[ e_{ik}(x') - x_j' \big(\overbrace{e_{ik,j}(x') - e_{jk,i}(x')}^{w_{ij,k}}\big) \Big] dx_k'}_{II} \end{aligned}}$$

Similarly

$$\begin{aligned} &u_i(N_L) - u_i(M_L) \\ &= w_{ik}(M_L)\, x_k(N_L) + \underbrace{x_k(N_L) \oint_{M_L}^{N_L} (e_{il,k}(x') - e_{kl,i}(x'))\, dx_l'}_{III} \\ &- w_{ik}(M_L)\, x_k(M_L) \\ &+ \underbrace{\oint_{M_L}^{N_L} \Big[ e_{ik}(x') - x_j' \big( e_{ik,j}(x') - e_{jk,i}(x') \big) \Big] dx_k'}_{IV} \end{aligned}$$

& since 1) $x_k(N_U) = x_k(N_L)$ & $x_k(M_U) = x_k(M_L)$

& 2) we can follow same path on $S_L$ & $S_U$ from ad 3) $\underline{c}$ is twice continuously differentiable on $S$ everywhere

$$\boxed{I = III \quad \& \quad II = IV}$$

$\therefore$ $\underset{\sim}{u}(N_U) - \underset{\sim}{u}(M_U)$

$- \underset{\sim}{u}(N_L) + \underset{\sim}{u}(M_L)$

$$= \underline{\omega}(M_U)\left[\underset{\sim}{x}(N_U) - \underset{\sim}{x}(M_U)\right]$$
$$- \underline{\omega}(M_L)\left[\underset{\sim}{x}(N_L) - \underset{\sim}{x}(M_L)\right]$$

$$\Rightarrow \boxed{\begin{aligned} &\underset{\sim}{u}(N_U) - \underset{\sim}{u}(N_L) \\ &= \left[\underset{\sim}{u}(M_U) - \underset{\sim}{u}(M_L)\right] \\ &\quad + \left[\underline{\omega}(M_U) - \underline{\omega}(M_L)\right]\left\{\underset{\sim}{x}(N) - \underset{\sim}{x}(M)\right\}. \end{aligned}}$$

Terms in square brackets on R.H.S. does not depend on $N_U$ or $N_L$.

$$\therefore \boxed{[\![ u(N) ]\!]_S = \underset{\sim}{b} + \underline{W}\, \underset{\sim}{x}(N)}$$ where $\underset{\sim}{b}$ & $\underline{W}$ are uniform on $S$.

# Continuously Distributed Dislocations
## Elastic Theory of Dislocations

J.F. Nye - Acta Metallurgica,
Vol 1, 1953, 153-162.

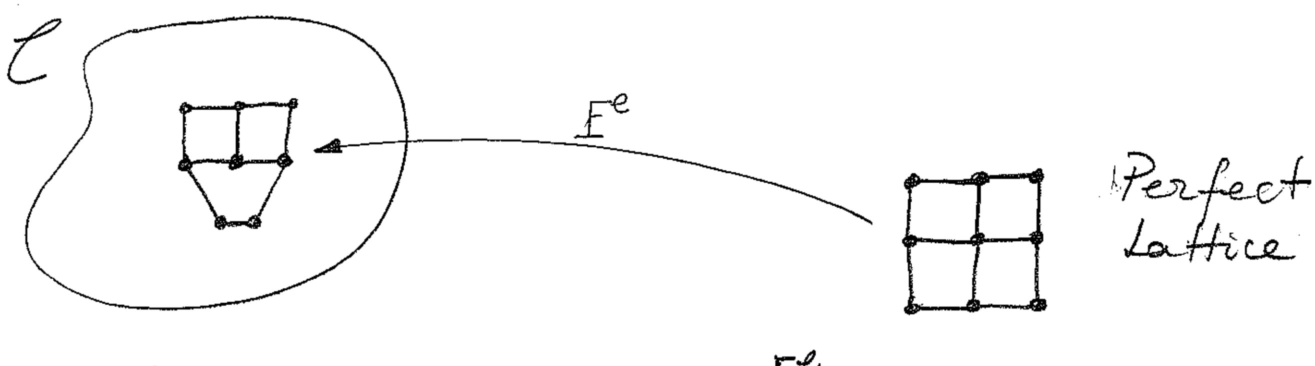
Dislocation Density Tensor: At the point $\underset{\sim}{x}$, let $N_\ell$ be the number of dislocation lines along the unit direction $\underset{\sim}{\ell}$ per unit area perpendicular to $\underset{\sim}{\ell}$. Let these dislocations have true Burgers vector in the direction $\underset{\sim}{b}_\ell$. Then the contribution to the dislocation density tensor from these dislocations is

$$N_\ell\, \underset{\sim}{b}_\ell \otimes \underset{\sim}{\ell}$$

At the point $\underset{\sim}{x}$, the total dislocation density tensor is the sum of all such dyads:

$$\underset{-}{\alpha} = \sum_k N_\ell^k\, \underset{\sim}{b}_\ell^k \otimes \underset{\sim}{\ell}^k .$$

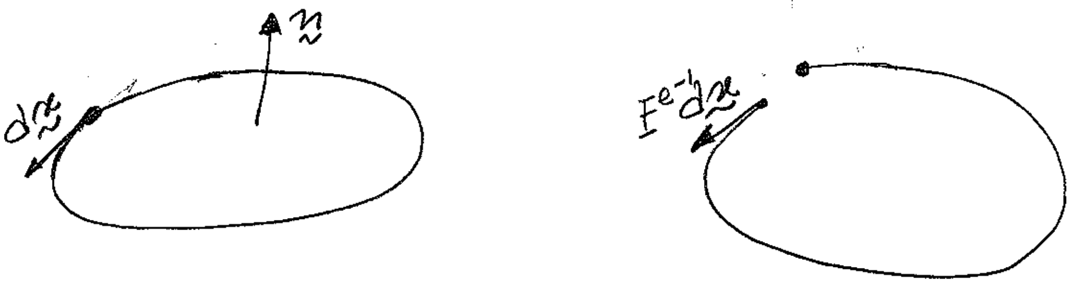
For describing a single dislocation by the Nye tensor field see the paper "Elementary observations ...." Acharya & Chapman, Section 2.//




Lattice deformation $\longrightarrow \underset{-}{F}^e$.

- with dislocation present - closed lattice curve in $\mathcal{C}$
  → open curve in the perfect lattice.

## The Lattice distortion Incompatibility Equation:




$$\oint_C \underline{F}^{e^{-1}} d\underset{\sim}{x} = \int_A \operatorname{curl} \underline{F}^{e^{-1}} \underset{\sim}{n}\, da = -\int_A \underbrace{\underline{\alpha}\, \underset{\sim}{n}}\, da \quad \forall \ A \text{ patches}$$

(gives S-F) (Gives F-S $\rightarrow$ $\therefore$ -ve sign).

LHS $\rightarrow$ Calculus gives closure deficit along closed curve ; RHS $\rightarrow$ physical interpretation of $\underline{\alpha}$ characterizing closure deficit of a circuit having threading dislocations

equality LHS = RHS is a physical modeling statement linking the lattice distortion to the dislocation density.

$$\Rightarrow \boxed{\operatorname{curl} \underline{F}^{e^{-1}} = -\underline{\alpha}} \longrightarrow \text{kinematics.}$$

(Notation: $(\operatorname{div} \underline{T}) \cdot \underset{\sim}{c} = \operatorname{div}(\underline{T}^T \underset{\sim}{c}) \ \forall$ constant fields $\underset{\sim}{c}$.
$(\operatorname{curl} \underline{T})^T \underset{\sim}{c} = \operatorname{curl}(\underline{T}^T \underset{\sim}{c}) \ \forall$ constant fields $\underset{\sim}{c}$)

Stress : $\boxed{\operatorname{div} \underline{T} = \underset{\sim}{0}} \rightarrow$ equilibrium

$\underline{T} = \hat{\underline{T}}(\underline{F}^e) \rightarrow$ elastic constitutive response.

Governing Equations:- (Willis-1967, Intl. J. of Engg. Sci, V.5, p.171-190).

$$\left.\begin{aligned} \text{curl } \underline{F}^{e^{-1}} &= -\underline{\alpha} \\ \underline{T} &= \hat{\underline{T}}(\underline{F}^e) \\ \text{div } \underline{T} &= \underset{\sim}{0} \end{aligned}\right\} \text{ ignoring body forces. on } C.$$

Condition for existence $\longrightarrow$ $\text{div}\,\underline{\alpha} = \underset{\sim}{0}$.

B.C.s:- $\underline{T}\underset{\sim}{n} = \underset{\sim}{t}$ } on $\partial C$.

[For equilibrium need to have $\int_{\partial C} \underset{\sim}{t}\, da = \underset{\sim}{0}$ ]

$\longrightarrow$ 9 variables — 12 eqns!?.

literature:- because $\text{div}\,\underline{\alpha} = \underset{\sim}{0}$ $\rightarrow$ 3 eqns.

$$\left.\begin{aligned} \text{curl } \underline{F}^{e^{-1}} &= \underline{\alpha} \\ \text{div } \underline{T} &= \underset{\sim}{0} \end{aligned}\right\} \cdot 12 \text{ eqns}$$

$\rightarrow$ $12 - 3 = 9$ eqns & 9 variables.

But such logic does not always work —

Consider $\text{grad}\,\varphi = \underset{\sim}{v}$

for existence we need $\text{curl}\,\underset{\sim}{v} = 0$.

We need to solve for one variable $\varphi$.

$\text{curl}\,\underset{\sim}{v} = 0 \rightarrow 3$ eqns.

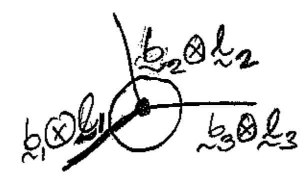
$\text{grad}\,\varphi = \underset{\sim}{v} \rightarrow 3$ eqns.

Then $3 - 3 = 0$ — but solns still exist!

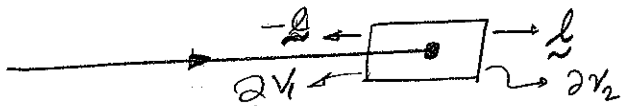
Going back to case of dislocations

$\text{div}\,\underline{\alpha} = \underset{\sim}{0}$ is a condition for existence of solns to $\text{curl}\,\underline{F}^{e^{-1}} = \underline{\alpha}$.

$\operatorname{div}\underline{\alpha} = \underset{\sim}{0}$ $\Rightarrow$ a) dislocation lines cannot end in the body. b) The sum of Burgers Vector at a junction has to vanish.




$\underset{\sim}{b}_1 + \underset{\sim}{b}_2 + \underset{\sim}{b}_3 = \underset{\sim}{0}$:




$$\underline{\alpha} = \tilde{\underset{\sim}{b}} \otimes \underset{\sim}{l}$$

$$\int_V \operatorname{div}\underline{\alpha}\, dv = \int_V \underset{\sim}{0}\, dv$$

$$\Rightarrow \int_{\partial V} \underline{\alpha}\, \underset{\sim}{n}\, da = \underset{\sim}{0}.$$

$$-\int_{\partial V_1} \tilde{\underset{\sim}{b}}(\underset{\sim}{l}\cdot\underset{\sim}{l})\, da = \underset{\sim}{0} \quad \Rightarrow \int_{\partial V_1} \tilde{\underset{\sim}{b}}\, da = \underset{\sim}{0} \;//.$$

whereas

$$-\int_{\partial V_1} \tilde{\underset{\sim}{b}}(\underset{\sim}{l}\cdot\underset{\sim}{l})\, da + \int_{\partial V_2} \tilde{\underset{\sim}{b}}(\underset{\sim}{l}\cdot\underset{\sim}{l})\, da = 0 \;//.$$

## The linear theory:

Define $\underline{U}^e := \underline{F}^e - \underline{I}$.

$$A^{-1}_{ij} A_{jk} = \delta_{ik}$$

$$\frac{\partial A^{-1}_{ij}}{\partial A_{rl}} A_{jk} = -A^{-1}_{ij}\, \delta_{rj}\, \delta_{kl}$$

So
$$\frac{\partial A^{-1}_{im}}{\partial A_{rl}} = -A^{-1}_{ir}\, \delta_{kl}\, A^{-1}_{km}$$
$$= -A^{-1}_{ir}\, A^{-1}_{lm}.$$

⑤

So $\underline{A}^{-1}(\underline{I}+\underline{U}^e) = \underline{A}^{-1}(\underline{I}) + \frac{\partial \underline{A}^{-1}}{\partial \underline{A}}(\underline{I}):[\underline{U}^e] + \cdots$

$$A^{-1}_{im}(\underline{I}+\underline{U}^e) \approx \delta_{im} + (-1)\delta_{ir}\delta_{\ell m} U^e_{r\ell} + \cdots$$
$$= \delta_{im} - U^e_{im} + \cdots$$

So $\underline{F}^{e^{-1}} \approx \underline{I} - \underline{U}^e$.

Then
$$\left.\begin{array}{l} \operatorname{curl}(\underline{I}-\underline{U}^e) = -\underline{\alpha} \\ \underline{T} = \underline{\underline{C}}\,\underline{U}^e. \\ \text{if } \hat{\underline{T}}(\underline{I}) = \underline{\underline{0}} \ \& \ \underline{\underline{C}} = \frac{\partial \hat{\underline{T}}}{\partial \underline{F}^e}(\underline{I}). \\ \& \quad \operatorname{div} \underline{T} = \underset{\sim}{0}. \end{array}\right\}$$

Need $\operatorname{div}\underline{\alpha} = \underset{\sim}{0}$.

+ b.c. $\underline{T}\,\underset{\sim}{n} = \underset{\sim}{t}$ on $\partial C$.

So. governing eqns for linear case.

$$\left.\begin{array}{l} \operatorname{Curl} \underline{U}^e = \underline{\alpha} \\ \underline{T} = \underline{\underline{C}}\,\underline{U}^e \\ \operatorname{div} \underline{T} = \underset{\sim}{0} \end{array}\right\} \text{ on } C. \qquad -(4).$$

B.C. $\underline{T}\underset{\sim}{n} = \underset{\sim}{t}$ on $\partial C$.

need $\operatorname{div}\underline{\alpha} = \underset{\sim}{0}$ !. (up to a spatially uniform skew tensor field)

Uniqueness: $\exists$ at most one solution to the system (4) for given $\underline{\alpha}$ satisfying $\operatorname{div}\underline{\alpha} = \underset{\sim}{0}$ & $\underline{T}\underset{\sim}{n} = \underset{\sim}{t}$ on $\partial C$.

We assume $C$ is simply connected.

Proof: Let there be two solutions $\underline{U}_1$ & $\underline{U}_2$.

Then $\underline{U} := \underline{U}_1 - \underline{U}_2$.

& $$\left.\begin{array}{l} \operatorname{curl} \underline{U} = \underline{0} \\ \operatorname{div}[\underline{\underline{C}}\, \underline{U}] = \underset{\sim}{0} \end{array}\right\} \text{ on } \mathcal{C}.$$

$$(\underline{\underline{C}}\, \underline{U}) \underset{\sim}{n} = \underset{\sim}{0} \text{ on } \partial\mathcal{C}.$$

domain simply connected

then $$\left.\begin{array}{l} \operatorname{curl} \underline{U} = \underline{0} \Rightarrow \underline{U} = \operatorname{grad} \underset{\sim}{\varphi} \\ \operatorname{div}[\underline{\underline{C}} \operatorname{grad} \underset{\sim}{\varphi}] = \underset{\sim}{0} \end{array}\right\} \text{ on } \mathcal{C}.$$

$$(\underline{\underline{C}} \operatorname{grad} \underset{\sim}{\varphi}) \underset{\sim}{n} = \underset{\sim}{0} \text{ on } \partial C.$$

This implies $$\int_{\mathcal{C}} \varphi_i \, (C_{ijkl}\, \varphi_{k,l})_{,j} \, dv = 0$$

$$\Rightarrow \int_{\mathcal{C}} \{\varphi_i\, C_{ijkl}\, \varphi_{k,l}\}_{,j} \, dv - \int_{\mathcal{C}} \varphi_{i,j}\, C_{ijkl}\, \varphi_{k,l}\, dv = 0.$$

$$\Rightarrow \int_{\mathcal{C}} \varphi_i [C_{ijkl}\, \varphi_{k,l}] n_j \, da - \int_{\mathcal{C}} \varphi_{i,j}\, C_{ijkl}\, \varphi_{k,l}\, dv = 0.$$

$$\Rightarrow \int_{\mathcal{C}} \varphi_{i,j}\, C_{ijkl}\, \varphi_{k,l}\, dv = 0.$$

Since $C_{ijkl}$ is +ve definite & has minor symmetries

$$\varphi_{i,j}\, C_{ijkl}\, \varphi_{kl}(\underset{\sim}{x}) \geq 0 \text{ at all } \underset{\sim}{x}.$$

$$\Rightarrow \quad \varphi_{i,j} = \omega_{ij} \rightarrow \text{skew symmetric}.$$

But $\mathcal{C}$ & $\{\underset{\sim}{x} : \underset{\sim}{x} = \underset{\sim}{X} + \underset{\sim}{\varphi}(\underset{\sim}{X}),\ \underset{\sim}{X} \in \mathcal{C}\}$ have the same strain w.r.t. $\mathcal{C}$ $\{\underset{\sim}{\varepsilon} = \underset{\sim}{0}\}$

$\Rightarrow \omega_{ij}(\underset{\sim}{X}) = \omega^0_{ij} \rightarrow$ spatially uniform.

$$\therefore \quad \boxed{\underline{U}_1 - \underline{U}_2 = \underline{\omega}^\circ} \qquad \square$$

## Some Remarks on the general Nature of Solutions

\# Note that the strain field is unique & hence the stress $\underline{T} = \underline{\underline{C}}\,\underline{U}^e$ & $\underline{\underline{C}}$ has minor symmetries.

\# Suppose $\underline{A}$ is a particular soln to

$$\text{curl}\, \underline{U}^e = \underline{\alpha}.$$

Then $\underline{A} + \text{grad}\, \underline{\varphi}$ for any $\underline{\varphi}$ is a soln too.

So try this as a soln to (L).

$$\text{div}\left[\underline{\underline{C}}\,(\underline{A} + \text{grad}\,\underline{\varphi})\right] = \underset{\sim}{0}$$

$$\underline{\underline{C}}\,(\underline{A} + \text{grad}\,\underline{\varphi})\,\underset{\sim}{n} = \underset{\sim}{t} \text{ on } \partial\mathcal{C}.$$

where $\displaystyle\int_{\partial C} \underset{\sim}{t}\, da = \underset{\sim}{0}.$

$$\Rightarrow \quad \text{div}\left(\underline{\underline{C}}\,\text{grad}\,\underline{\varphi}\right) = -\,\text{div}\left(\underline{\underline{C}}\,\underline{A}\right) \quad \text{on } \mathcal{C}.$$

$$\left\{\underline{\underline{C}}\,\text{grad}\,\underline{\varphi}\right\}\underset{\sim}{n} = \underset{\sim}{t} - \left(\underline{\underline{C}}\,\underline{A}\right)\underset{\sim}{n} \quad \text{on } \partial C$$

Necessary condition for linear elastic Neumann problem is

$$\int_{\partial\mathcal{C}} \left(\underline{\underline{C}}\,\text{grad}\,\underline{\varphi}\right)\underset{\sim}{n}\, da = -\int_{\partial C} \left(\underline{\underline{C}}\,\underline{A}\right)\underset{\sim}{n}\, da,$$

which require that $\displaystyle\int_{\partial C} \underset{\sim}{t}\, da = \underset{\sim}{0}$ which is satisfied.

\# So the problem becomes a standard linear elasticity problem — the dislocations become body forces. //

equivalently, (25), (27) and (28) with $\mathbf{U} = \mathbf{0}$. In the nonlinear case, (5), (7) and (8) will be solved.

To proceed analytically, the Riemann–Graves integral operator is introduced for generating particular solutions to exterior differential equations on star-shaped domains (Edelen, 1985; Edelen and Lagoudas, 1988). This is a class of differential equations to which equations of the form $\operatorname{curl} X = \beta$ can be shown to belong. As pointed out in Edelen and Lagoudas (1988), solutions to such equations for data with compact support have very general spatial decay properties. Such properties have a remarkable resemblance to dislocation fields derived from linear elasticity.

Let $\beta_{ij}$ be a matrix function satisfying $\beta_{ij,j}=0$ on a star-shaped domain whose points are generically denoted by $x := (x_j, j = 1,3)$. Corresponding to $\beta_{ij}$, the skew-symmetric functions $\hat{\beta}_{rjk} := e_{jkm}\beta_{rm}$ are defined. For an arbitrarily chosen fixed point $x^0$, the integral $H\beta$ (to be interpreted as one symbol) is now introduced as

$$H\beta_{ik}(x;x^0) := (x_j - x_j^0)\int_0^1 \hat{\beta}_{ijk}(x^0 + \lambda(x - x^0))\,\lambda\,\mathrm{d}\lambda. \tag{31}$$

It is now to be demonstrated that

$$A_{ijk} := H\beta_{ik,j} - H\beta_{ij,k} = \hat{\beta}_{ijk} \tag{32}$$

which implies

$$\operatorname{curl} H\beta = \beta; \quad e_{rjk}H\beta_{ik,j} = \beta_{ir}. \tag{33}$$

Since

$$\begin{aligned} H\beta_{ik,j} &= \int_0^1 \hat{\beta}_{ijk}(x^0 + \lambda(x - x^0))\,\lambda\,\mathrm{d}\lambda \\ &\quad + (x_m - x_m^0)\int_0^1 \hat{\beta}_{imk,j}(x^0 + \lambda(x - x^0))\lambda^2\,\mathrm{d}\lambda, \end{aligned} \tag{34}$$

$$\begin{aligned} A_{ijk} &= 2\int_0^1 \hat{\beta}_{ijk}(x^0 + \lambda(x - x^0))\,\lambda\,\mathrm{d}\lambda \\ &\quad + (x_m - x_m^0)\int_0^1 \{\hat{\beta}_{imk,j}(x^0 + \lambda(x - x^0)) - \hat{\beta}_{imj,k}(x^0 + \lambda(x - x^0))\}\,\lambda^2\,\mathrm{d}\lambda, \end{aligned} \tag{35}$$

where a subscript comma followed by a letter, say $j$, represents partial differentiation with respect to $x_j$. Integrating the first term by parts,

$$A_{ijk} = \hat{\beta}_{ijk}(x) + \int_0^1 \{(x_m - x_m^0)(\hat{\beta}_{imk,j} - \hat{\beta}_{imj,k}) - (x_r - x_r^0)\hat{\beta}_{ijk,r}\}\lambda^2\,\mathrm{d}\lambda. \tag{36}$$

The constraint $\beta_{ij,j} = 0$ translates to

$$\hat{\beta}_{i23,1} + \hat{\beta}_{i31,2} + \hat{\beta}_{i12,3} = 0. \tag{37}$$

A direct expansion of the integrand of the second term on the right-hand side of (36) and use of (37) now yields the desired result (32) which is independent of the choice of $x^0$ in (31).

# Elastic Theory of Dislocations

## Kröner's Method for Isotropic Elasticity

* Infinite Medium
* Isotropic Elasticity $\therefore$ $\sigma_{ij} = \lambda \varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}$

We assume there exists a solution to

$$e_{ijk} U_{lk,j} = \alpha_{li} \quad \left(\begin{matrix}\text{where}\\ \alpha_{li,i}=0\end{matrix}\right) \qquad (*)$$

and

$$\sigma_{ij,j} = 0 \qquad (**)$$

$\underline{\underline{\sigma}}$ formed from strain, i.e. $\text{sym}(\underline{\underline{U}}) = \underline{\underline{\varepsilon}}$

also define $\text{skw}(\underline{\underline{U}}) = \underline{\underline{\omega}}$.

$$(*) \Rightarrow e_{rsl}\, e_{ijk}\, U_{lk,js} = e_{rsl}\, \alpha_{li,s}$$

Now $\frac{1}{2}\left(e_{rsl}\alpha_{li,s} + e_{isl}\alpha_{lr,s}\right)$

$$= \frac{1}{2}\left(e_{rsl}e_{ijk}U_{lk,js} + e_{isl}e_{rjk}U_{lk,js}\right)$$

$$= \frac{1}{2}\left(e_{rsl}e_{ijk}\varepsilon_{lk,js} + e_{isl}e_{rjk}\varepsilon_{lk,js}\right) + \frac{1}{2}\left(e_{rsl}e_{ijk}\omega_{lk,js} + e_{isl}e_{rjk}\omega_{lk,js}\right)$$

$$= \frac{1}{2}\left(e_{rsl}e_{ijk}\varepsilon_{lk,js} + e_{ijk}e_{rsl}\varepsilon_{kl,sj}\right) + \frac{1}{2}\left(e_{rsl}e_{ijk}\omega_{lk,js} + \underbrace{e_{ijk}e_{rsl}\omega_{kl,sj}}_{= -e_{ijk}e_{rsl}\omega_{lk,sj}}\right)$$

$$\Rightarrow \frac{1}{2}\left(e_{rsl}\alpha_{li,s} + e_{isl}\alpha_{lr,s}\right) = e_{rsl}e_{ijk}\varepsilon_{lk,js}$$

Define $\frac{1}{2}\left(e_{rse}\alpha_{ei,s} + e_{ise}\alpha_{er,s}\right) = \eta_{ri}$

and $e_{rse}e_{ijk}\varepsilon_{ek,js} = (\text{inc}\,\underline{\underline{\varepsilon}})_{ri}$,

We have

$$\eta = \boxed{\text{inc}\,\underline{\underline{\varepsilon}} = \text{sym}\left(\text{curl}\,\underline{\underline{\alpha}}^T\right)} \quad \text{—} (1)$$

Let us now also assume that there exists a fn $\underline{\underline{\chi}}$ which is related to $\underline{\underline{\sigma}}$ as follows: (assume $\underline{\underline{\chi}}$ is symmetric)

$$\sigma_{ij} = e_{ike}e_{jrs}\chi_{es,rk} \quad \text{———} (***)$$

Now $\sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}$

$$\sigma_{ee} = (3\lambda+2\mu)\varepsilon_{ee}$$

$$\therefore \varepsilon_{ij} = \frac{1}{2\mu}\left(\sigma_{ij} - \frac{\lambda}{(3\lambda+2\mu)}\sigma_{kk}\delta_{ij}\right)$$

Now $(\text{inc}\,\underline{\underline{\varepsilon}})_{mn} = e_{mpi}e_{nqj}\varepsilon_{ij,pq}$

$$= \frac{1}{2\mu}\left[e_{mpi}e_{nqj}\sigma_{ij,pq} - \frac{\lambda}{(3\lambda+2\mu)}e_{mpi}e_{nqj}\delta_{ij}\sigma_{kk,pq}\right]$$

Substituting (***)

$$(\text{inc}\,\underline{\underline{\varepsilon}})_{mn} = \frac{1}{2\mu}\left[e_{mpi}e_{nqj}e_{ike}e_{jrs}\chi_{es,rkpq} - \frac{\lambda}{(3\lambda+2\mu)}e_{mpi}e_{nqi}e_{jke}e_{jrs}\chi_{es,rkpq}\right]$$

$$= \frac{1}{2\mu}\Big[ (\delta_{mk}\delta_{pl} - \delta_{ml}\delta_{pk})(\delta_{nr}\delta_{qs} - \delta_{ns}\delta_{qr}) \chi_{ls,rkpq}$$

$$- \frac{\lambda}{(3\lambda+2\mu)} (\delta_{mn}\delta_{pq} - \delta_{mq}\delta_{pn})(\delta_{kr}\delta_{ls} - \delta_{ks}\delta_{lr}) \chi_{ls,rkpq} \Big]$$

$$= \frac{1}{2\mu}\Big[ (\chi_{ps,rmpq} - \chi_{ms,rppq})(\delta_{nr}\delta_{qs} - \delta_{ns}\delta_{qr})$$

$$- \frac{\lambda}{(3\lambda+2\mu)} (\chi_{ss,rrpq} - \chi_{rs,rspq})(\delta_{mn}\delta_{pq} - \delta_{mq}\delta_{pn}) \Big]$$

$$= \frac{1}{2\mu}\Big[ \chi_{pq,nmpq} - \chi_{pn,qmpq} - \chi_{mq,nppq} + \chi_{mn,qppq}$$

$$- \frac{\lambda}{(3\lambda+2\mu)} (\chi_{ss,rrpq} - \chi_{rs,rspq})(\delta_{mn}\delta_{pq} - \delta_{mq}\delta_{pn}) \Big]$$

$$= \frac{1}{2\mu}\Big[ \chi_{pq,pqnm} - \chi_{pn,qqmp} - \chi_{mq,ppnq} + \chi_{mn,qqpp}$$

$$- \frac{\lambda}{(3\lambda+2\mu)} \big( \chi_{ss,rrqq}\delta_{mn} - \chi_{ss,rrnm}$$

$$- \chi_{rs,rsqq}\delta_{mn} + \chi_{rs,rsmn} \big) \Big]$$

$$\Rightarrow (\mathrm{inc}\,\underline{\underline{\varepsilon}})_{mn}$$

$$= \frac{1}{2\mu}\Big[ \chi_{mn,qqpp} - \frac{\lambda}{(3\lambda+2\mu)} \chi_{ss,qqpp}\delta_{mn} \Big] \quad \text{— (A)}$$

$$+ \frac{1}{2\mu}\Big[ \chi_{pq,qpmn} - \chi_{np,pmqq} - \chi_{mq,qnpp}$$

$$- \frac{\lambda}{(3\lambda+2\mu)} \big( - \chi_{ss,rrmn} - \chi_{rs,rsqq}\delta_{mn} + \chi_{rs,rsmn} \big) \Big]$$

Let us further assume that there exists a function (symmetric tensor valued fn) $\underline{\underline{X}}'$ that is related to $\underline{\underline{X}}$ as

$$X'_{mn} = \alpha\left[X_{mn} - \beta X_{aa}\delta_{mn}\right] \quad -(G)$$

and which has vanishing divergence, i.e. $X'_{mn,n} = 0$.

($\alpha$ & $\beta$ are ~~...~~ two scalar constants).

Then $X_{mn,n} = \beta X_{aa,n}\delta_{mn}$

$$\Rightarrow X_{mn,n} = \beta X_{aa,m}.$$

Substituting in (A).

$$(\mathrm{inc}\,\underline{\underline{\varepsilon}})_{mn} = \frac{1}{2\mu} X_{mn,qqpp} - \frac{\lambda}{2\mu(3\lambda+2\mu)} X_{ss,qqpp}\delta_{mn}$$

$$+\frac{1}{2\mu}\Big[\beta X_{aa,ppmn} - \beta X_{aa,qqmn} - \beta X_{aa,ppmn}$$

$$-\frac{\lambda}{(3\lambda+2\mu)}\Big\{-X_{aa,rrmn} - \beta X_{aa,rrqq}\delta_{mn} + \beta X_{aa,rrmn}\Big\}\Big]$$

$$\Rightarrow (\mathrm{inc}\,\underline{\underline{\mathcal{E}}})_{mn} = \frac{1}{2\mu} X_{mn,qqpp}$$

$$+ \frac{\lambda}{2\mu(3\lambda+2\mu)}\left[-1+\beta\right] X_{ss,rrqq}\,\delta_{mn}$$

$$+ \left[-\frac{\lambda\beta}{(3\lambda+2\mu)} + \frac{\lambda}{(3\lambda+2\mu)2\mu} - \frac{\beta}{2\mu}\right] X_{aa,qqmn}.$$

$$= \frac{1}{2\mu}\left[X_{mn,qqpp} - \frac{\lambda}{(3\lambda+2\mu)}(1-\beta) X_{ss,qqpp}\,\delta_{mn}\right]$$

$$+ \frac{1}{2\mu}\underbrace{\left[-\frac{\lambda\beta}{(3\lambda+2\mu)} + \frac{\lambda}{(3\lambda+2\mu)} - \beta\right]}_{C} X_{aa,qqmn}$$

Let $\beta$ in (G) be such that

$$C = 0$$

$$\Rightarrow \cancel{-}\beta\left[\frac{\lambda}{(3\lambda+2\mu)} + 1\right] = \cancel{-}\frac{\lambda}{(3\lambda+2\mu)}$$

$$\Rightarrow \beta \cdot 2(2\lambda+\mu) = \lambda$$

$$\Rightarrow \boxed{\beta = \frac{\lambda}{2(2\lambda+\mu)}}.$$

Then

$$(\mathrm{inc}\,\underline{\underline{\mathcal{E}}})_{mn} = \frac{1}{2\mu}\left[X_{mn,qqpp} - \frac{\lambda}{\cancel{(3\lambda+2\mu)}}\cdot\frac{\cancel{(3\lambda+2\mu)}}{2(2\lambda+\mu)} X_{ss,qqpp}\,\delta_{mn}\right]$$

Let $\alpha$ in (G) be $\alpha = \frac{1}{2\mu}$.

Then $\boxed{(\mathrm{inc}\,\underline{\underline{\mathcal{E}}})_{mn} = X'_{mn,qqpp}}$

i.e. $$\boxed{(\text{inc}\,\underline{\underline{\varepsilon}}) = \nabla^4 \underline{\underline{\chi}}'} \quad \text{— (2)}$$

where $\nabla^4 \phi = \text{divgrad}\{\text{divgrad}\,\phi\}$ for a scalar field $\phi$.

Combining (1) & (2)

$$\underline{\underline{\eta}} = \text{inc}\,\underline{\underline{\varepsilon}} = \text{sym}(\text{curl}\,\underline{\underline{\alpha}}^T)$$

$$\text{inc}\,\underline{\underline{\varepsilon}} = \nabla^4 \underline{\underline{\chi}}'$$

$$\Rightarrow \boxed{\nabla^4 \underline{\underline{\chi}}' = \underline{\underline{\eta}}} \quad \text{— (S1)}$$

where $\underline{\underline{\chi}}'$ has been assumed to satisfy $\text{div}\,\underline{\underline{\chi}}' = \underline{0}$.

The above was a derivation of necessary conditions for existence of a solution to (*) & (**), making various assumptions of $\underline{\underline{\chi}}'$ & $\underline{\underline{\chi}}$.

We now show that if (S1) is satisfied by $\underline{\underline{\chi}}'$ then there indeed exists a solution ~~to~~ $\underline{\underline{\varepsilon}}$ that satisfies (1) and (**).

Assuming $\underset{\sim}{\eta} \to 0$ very rapidly as

$$|\underset{\sim}{x}| = |x_i \underset{\sim}{e}_i| \to \infty$$

A standard solution to the biharmonic equation (S1) is

$$\boxed{\chi'_{ij}(\underset{\sim}{x}) = -\frac{1}{8\pi}\int_V |\underset{\sim}{x}-\underset{\sim}{x}'|\,\eta_{ij}(\underset{\sim}{x}')\,dV'} \qquad \text{(S2)}$$

i.e. $-\frac{1}{8\pi}|\underset{\sim}{x}-\underset{\sim}{x}'|$ is the Green's function for $\nabla^4 \phi(\underset{\sim}{x}) = \delta(\underset{\sim}{x})$.

Since $\underset{\sim}{\eta}$ vanishes at infinity

$$\chi'_{ij,j}(\underset{\sim}{x}) = -\frac{1}{8\pi}\int_V |\underset{\sim}{x}-\underset{\sim}{x}'| \frac{\partial \eta_{ij}}{\partial x'_j}(\underset{\sim}{x}')\,dV'$$

(integrate by parts).

But going back to the definition of $\underset{\sim}{\eta}$ on pg. 2

$$\chi'_{ij,j}(\underset{\sim}{x}) = \frac{\partial \chi'_{ij}}{\partial x_j}(\underset{\sim}{x}) = 0$$

since $\alpha_{\ell i,i} = 0$ [a requirement of $\underset{\sim}{\alpha}$]

From (G) & the values of $\alpha$, $\beta$, derived,

$$X_{mn} = \frac{1}{\alpha} X'_{mn} + \beta X_{aa} \delta_{mn}.$$

$$\Rightarrow X_{aa} = \left(3\beta + \frac{1}{\alpha}\right) X'_{aa}$$

$$\Rightarrow \boxed{X_{mn} = \frac{1}{\alpha} X'_{mn} + \left(3\beta + \frac{1}{\alpha}\right) X'_{aa} \delta_{mn}} \quad \text{(S3)}$$

Using the soln (S2) define $\underline{\underline{X}}'$ from (S3).
We now define $\underline{\underline{\sigma}}$ from $\underline{\underline{X}}$ using (***).
Clearly $\sigma_{ij,j} = 0$. so (**)
is satisfied by our solution.
Now, because $X'_{ij,j} = 0$ and
$\underline{\underline{X}}$ & $\underline{\underline{X}}'$ satisfy (G), then
following the steps in the derivation
of the necessary condition we find
that $\underline{\underline{\varepsilon}}$ defined from $\underline{\underline{\sigma}}$ defined from
$\underline{\underline{X}}$ defined from $\underline{\underline{X}}'$ satisfies.

$$(\text{inc}\, \underline{\underline{\varepsilon}}) = \underline{\underline{\eta}}.$$

And consequently we have constructed a ~~solu~~ $\underset{=}{\varepsilon}$ to the system

$$\left\{\begin{aligned} (\mathrm{inc}\,\underset{=}{\varepsilon}) &= \underset{=}{\eta} \\ \underset{=}{\sigma} &= \lambda\, \mathrm{tr}(\underset{=}{\varepsilon})\,\mathbb{I} + 2\mu\, \underset{=}{\varepsilon} \\ \mathrm{div}\,\underset{=}{\sigma} &= 0 \end{aligned}\right\}$$

where $\underset{=}{\eta}$ is defined from a given dislocation density field $\underset{=}{\alpha}$ satisfying $\mathrm{div}\,\underset{=}{\alpha} = \underset{-}{0}$.

"Transformation Strain & Inclusion Problems"

"The determination of the elastic field of an ellipsoidal inclusion, and related problems."
Proc. Roy. Soc. A 241., 1957, J.D. Eshelby.

Explicit Solutions.

(1) The transformation Strain Problem:

"A region (the 'inclusion') in an infinite homogeneous isotropic elastic medium undergoes a change in shape & size which, but for the constraint imposed by its surroundings (the 'matrix'), would be an arbitrary homogeneous strain. What is the elastic state of inclusion & matrix?

(2) The Inhomogeneity Problem:

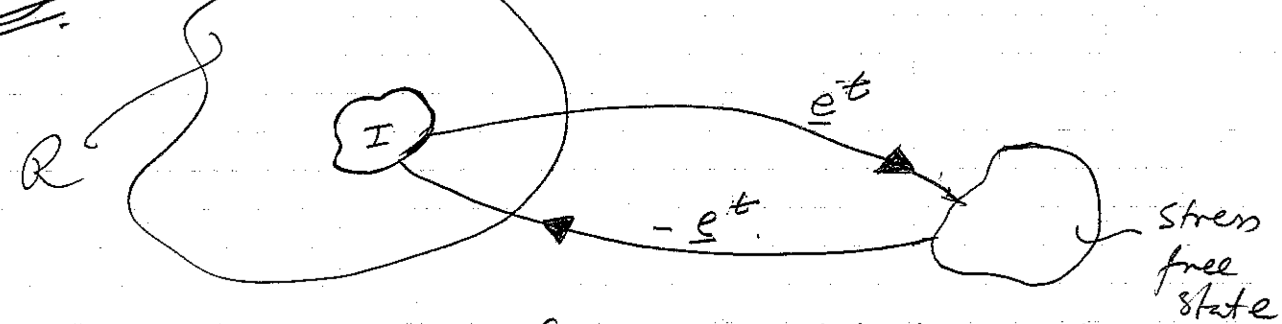
"An ellipsoidal region in a solid has elastic constants differing from those of the remainder (cf, in particular, the constants are zero within the ellipsoid we have the case of the cavity). How is an applied stress, uniform at large distances, disturbed by this inhomogeneity?

Note: 2nd Problem can be computed approximately with modern numerical methods.

1st problem: not even clear how the frame it.

Transformation strain / inclusion problem:

**I**




① Remove inclusion; let it undergo homogeneous stress-free strain. $\underline{e}^t$.

② Let $\underline{T}^t := \lambda\, tr(\underline{e}^t)\underline{I} + 2\mu\underline{e}$.

Put surface traction $-\underline{T}^t \underset{\sim}{n}$ on surface of stress-free inclusion. Then it fits back in 'hole' in $R$.

③ - Weld the inclusion to matrix keeping the surface traction on. Matrix is stress-free at this stage; inclusion has stress $-\underline{T}^t$.

~~④~~ Release the surface traction. Matrix feels constraint due to inclusion & vice-versa. Let body relax. Call the displacement field on $R$ $\underset{\sim}{u}^c$.

- Then strain in inclusion $\underline{e}^c - \underline{e}^t$

" " matrix $\underline{e}^c$

Calculate stresses from constitutive assumption.

* In stage 3 there is a traction discontinuity in R. This can happen only in the presence of a singular body force distribution for statics. See page 3a.

* After the end of 4 displacements & tractions are continuous. So the apparent body force is negated by the process of relaxation. Thus $\underset{\sim}{u}^c$ is the solution to

$$\operatorname{div} \underline{T}^c - \underset{\sim}{f} = 0.$$

$$\text{where } -\underset{\sim}{f} = \underline{T}^t \underset{\sim}{n} \text{ on } \underline{S}_I.$$

Thus $\underline{T} = \underline{T}^c - \underline{T}^t$ in inclusion.

$\underline{T} = \underline{T}^c$ in matrix

Eshelby provides a formula for $\underset{\sim}{u}^c$.

* If inclusion is ellipsoidal, $\underline{T}^c$ is homogeneous within inclusion.

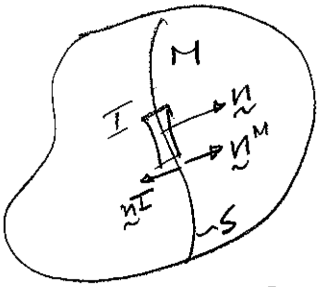
True even for linear elastic anisotropic material.

# Notes for Eshelby problem.

3a

$$\operatorname{div} \underset{\sim}{T} + \underset{\sim}{b} = \underset{\sim}{0} \qquad \text{(A)}$$

on regions without discontinuities.




$$\int_S T^M \underset{\sim}{n}^M + T^I \underset{\sim}{n}^I da + \int_{\Delta V \to S} \underset{\sim}{b}\, dV = \underset{\sim}{0}$$

on interface with discontinuous fields.

Let $\underset{\sim}{n}^M = -\underset{\sim}{n}^I = \underset{\sim}{n}$.

Then $\int_S \left( T^M - T^I \right) \underset{\sim}{n}\, da + \int_{\Delta V \to S} \underset{\sim}{b}\, dV = \underset{\sim}{0} \Rightarrow [\![T]\!] \underset{\sim}{n} + \underset{\sim}{b}^* = \underset{\sim}{0}$. (++)

Remarks: at this level we could have put the $\underset{\sim}{b}$ on the other side of the equality to begin with. We use what we do here because we will use the Kelvin pt. load soln later where the body force appears as in (A) above apart from the fact that when summing forces for balance of linear momentum $\int_{\partial V} T \underset{\sim}{n}\, da + \int_V \underset{\sim}{b}$ appear on the same side.

(++) Here $\underset{\sim}{b}^*$ is to be thought of as a completely known force per unit area distribution given by $T^M \underset{\sim}{n}^M + T^I \underset{\sim}{n}^I$. //

So at end of step 3 we have

$$\operatorname{div} T^{(3)} + \underset{\sim}{b} = 0$$

where $\underset{\sim}{b}$ is singular.

where the singular body force distribution may be taken as $-[\![T]\!] \underset{\sim}{n} = \underset{\sim}{b}^*$.

So in step 4, to negate this,

$$\operatorname{div} T^c - \underset{\sim}{f} = \underset{\sim}{0} \quad \text{where } -\underset{\sim}{f} = -\underset{\sim}{b}^*$$

So that $\operatorname{div} T^{(3)} + \operatorname{div} T^c = 0$ on $S$

$$= -[\![T]\!] \underset{\sim}{n}$$

$$= \left( T^M - T^I \right) \underset{\sim}{n}^M$$

$$= -T^I \underset{\sim}{n}^M = T^t \underset{\sim}{n}^M,$$

Since $T^I = -T^t$ //

Inhomogeneity Problem: [Restricted to ellipsoids].

- Suppose for now that we have an inclusion with at transformation strain $\underline{e}^t$.
- On the relaxed state superimpose a uniform strain $\underline{e}^A$.

Then strain in inclusion is

$$\underline{e}^c + \underline{e}^A - \underline{e}^t.$$

In matrix $\underline{e}^c + \underline{e}^A$.

If inclusion ellipsoidal, $\underline{e}^t$ homogeneous within inclusion.

Suppose we want to equate final stress state to that of an inhomogeneous material with different elastic constants in inclusion subjected to the strain field $\underline{e}^c + \underline{e}^A$ to the reference.

So $\underline{\underline{C}}^i(\underline{e}^c + \underline{e}^A) = \underline{\underline{C}}(\underline{e}^c + \underline{e}^A - \underline{e}^t)$ in all $\mathcal{R}$.

Since R.H.S. satisfies equilibrium L.H.S does & latter can be considered the stress field in the body due to the presence of the inhomog. subjected to uniform far-field stress corresponding to strain field $\underline{e}^A$.

For ellipsoidal inclusion within inclusion $\underline{e}^c = \underline{\underline{S}}\,\underline{e}^t$, spatially homogeneous.

So $$\underline{\underline{C}}^i(\underline{\underline{S}}\,\underline{e}^t + \underline{e}^A) = \underline{\underline{C}}\,(\underline{\underline{S}}\,\underline{e}^t + \underline{e}^A - \underline{e}^t)$$

within inclusion

$\therefore$ equivalent transformation strain

$$\left[(\underline{\underline{C}} - \underline{\underline{C}}^i)\underline{\underline{S}} - \underline{\underline{C}}\right]\underline{e}^t = \left[\underline{\underline{C}}^i - \underline{\underline{C}}\right]\underline{e}^A.$$

$$\Rightarrow \boxed{\underline{e}^t = \left[(\underline{\underline{C}} - \underline{\underline{C}}^i)\underline{\underline{S}} - \underline{\underline{C}}\right]^{-1}\left[\underline{\underline{C}}^i - \underline{\underline{C}}\right]\underline{e}^A.}$$

(Note, spatial homog. of $\underline{e}^c$ within inclusion is essential to argument].

Once obtained,

$\underset{\sim}{u}^c$ is given as a formula in terms of $\underline{e}^t$.

$$\underset{\sim}{u}^c = \mathcal{F}\left[\underline{e}^t(\cdot)\right].$$

- So can evaluate and then evaluate stress field in matrix & inclusion.

* $\underline{\underline{C}}^i = \underline{\underline{0}}$ can figure out stress field of a ~~body~~ body with an ellipsoidal cavity under applied far-field uniform stress field $\underline{T}^A$.

Kelvin Solution: Point load in an isotropic elastic infinite medium.

Define $2\mu \underset{\sim}{u} = \text{grad}\, \Phi + \text{curl}\, \underset{\sim}{A}$

(Stokes Helmholtz).

$$2\mu u_i = \Phi_{,i} + e_{ijk} A_{k,j}.$$

$$2\mu u_{i,i} = \Phi_{,ii}.$$

$$\sigma_{ij} = \lambda u_{k,k} \delta_{ij} + \mu (u_{i,j} + u_{j,i}).$$

$$\sigma_{ij,j} = \lambda u_{k,kj} \delta_{ij} + \mu (u_{i,jj} + u_{j,ij})$$

$$= \lambda u_{k,ki} + \mu (u_{j,ji} + u_{i,jj})$$

$$= (\lambda+\mu)(u_{k,k})_{,i} + \mu u_{i,jj}$$

Now $\boxed{\lambda + \mu = \dfrac{\mu}{(1-2\nu)}}$

So $$\mu u_{i,jj} + \frac{\mu}{(1-2\nu)} u_{k,ki} + F_i = 0 \text{ in } V$$

equilibrium.

$$2\mu u_{i,jj} + \frac{2\mu}{(1-2\nu)} u_{k,ki} = -2F_i.$$

$$\left[\Phi_{,i} + e_{irk} A_{k,r}\right]_{,jj} + \frac{1}{(1-2\nu)} \Phi_{,kki} = -2F_i.$$

$$\Rightarrow \boxed{\left[\frac{2(1-\nu)}{(1-2\nu)} \Phi_{,i} + e_{irk} A_{k,r}\right]_{,jj} = -2F_i}$$

Define $\psi_i = -\frac{1}{2(1-2\nu)}\Phi_{,i} - \frac{1}{4(1-\nu)}\,\mathrm{curl}_i\,\underset{\sim}{A}$.

Then $\boxed{\psi_{i,jj} = \frac{F_i}{2(1-\nu)}}$ Poisson Eqn. Can solve. (Green's fn $\frac{1}{r}$)

Now $\psi_{i,i} = -\frac{1}{2(1-2\nu)}\Phi_{,ii}$.

But $(x_r\psi_r)_{,ii} = (\psi_i + x_r\psi_{r,i})_{,i}$

$= \underbrace{\psi_{i,i} + \psi_{i,i}} + x_r\psi_{r,ii}$.

$\therefore \frac{1}{(1-2\nu)}\Phi_{,ii} = -2\psi_{i,i} = x_r\psi_{r,ii} - (x_r\psi_r)_{,ii}$.

$\Rightarrow \left[\frac{1}{(1-2\nu)}\Phi + x_r\psi_r\right]_{,ii} = x_r\psi_{r,ii} = \frac{x_r F_r}{2(1-\nu)}$

Define $\boxed{\varphi := -\frac{\Phi}{(1-2\nu)} - x_r\psi_r.}$

Then $\boxed{\varphi_{,ii} = -\frac{x_r F_r}{2(1-\nu)}}$ Poisson Eqn Can solve.

Now determine $\mathrm{curl}_i\,\underset{\sim}{A}$ from $\varphi, \underset{\sim}{\psi}$.

$\mathrm{curl}_i\,\underset{\sim}{A} = -4(1-\nu)\psi_i - \frac{2(1-\nu)}{(1-2\nu)}\Phi_{,i}$.

$= -4(1-\nu)\psi_i + 2(1-\nu)(\varphi + x_r\psi_r)_{,i}$.

$\therefore 2\mu u_i = \Phi_{,i} + \mathrm{curl}_i\,\underset{\sim}{A}$.

$2\mu u_i = -4(1-\nu)\psi_i - \frac{2(1-\nu)}{(1-2\nu)}\Phi_{,i} + \Phi_{,i}$

Now $\left[-\frac{2(1-\nu)}{(1-2\nu)}+1\right]\Phi_{,i} = \left(\frac{-2+\cancel{2\nu}+1-\cancel{2\nu}}{\cancel{1-2\nu}}\right)(-\varphi+x_r\psi_r)_{,i}\cancel{(-1)(1-2\nu)}$

$$= (\varphi + x_r\psi_r)_{,i}$$

$$\therefore \boxed{2\mu u_i = (\varphi + x_r\psi_r)_{,i} - 4(1-\nu)\psi_i}$$

Paptkovich-Neubier representation

Particular Integral for body force:

$$\nabla^2\varphi = -\frac{x_i F_i}{2(1-\nu)} \quad ; \quad \nabla^2\psi_i = \frac{F_i}{2(1-\nu)}.$$

P.I : $\varphi(\underset{\sim}{x}) = \frac{1}{8\pi(1-\nu)}\int_V \frac{\xi_i F_i(\underset{\sim}{\xi})}{|\underset{\sim}{x}-\underset{\sim}{\xi}|}\,d\underset{\sim}{\xi}$

$$\psi_i(\underset{\sim}{x}) = -\frac{1}{8\pi(1-\nu)}\int_V \frac{F_i(\underset{\sim}{\xi})}{|\underset{\sim}{x}-\underset{\sim}{\xi}|}\,d\underset{\sim}{\xi}.$$

$$\boxed{\begin{aligned} 2\mu u_i &= (\varphi_{,i} + \psi_i + x_r\psi_{r,i}) - 4(1-\nu)\psi_i \\ &= \varphi_{,i} - (3-4\nu)\psi_i + x_r\psi_{r,i}. \end{aligned}}$$

For $F_i(\underset{\sim}{\xi}) = L_i\,\delta(\underset{\sim}{\xi})$

$$\psi_i(\underset{\sim}{x}) = \frac{-L_i}{8\pi(1-\nu)}\frac{1}{|\underset{\sim}{x}|}$$

$$\varphi_{,i} = \frac{1}{8\pi(1-\nu)}\int_V \frac{\partial}{\partial x_i}\left(\frac{1}{|\underset{\sim}{x}-\underset{\sim}{\xi}|}\right)\xi_i L_i\,\delta(\underset{\sim}{\xi})\,d\underset{\sim}{\xi}.$$

$$= 0.$$

$$\psi_{r,i} = -\frac{1}{8\pi(1-\nu)}\int_V L_r\,\delta(\underset{\sim}{\xi})\frac{\partial}{\partial x_i}\left(\frac{1}{|\underset{\sim}{x}-\underset{\sim}{\xi}|}\right)d\underset{\sim}{\xi}$$

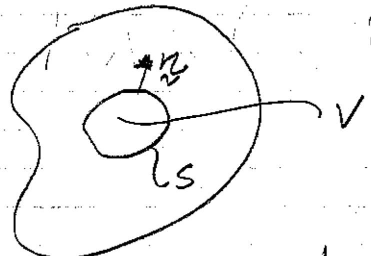
$$\psi_{r,i} = -\frac{1}{8\pi(1-\nu)} L_r \left(\frac{1}{|x|}\right)_{,i}$$

$$\boxed{2\mu u_i(x) = \frac{1}{8\pi(1-\nu)}\left[(3-4\nu)\frac{L_i}{|x|} \;\cancel{+}\; - \; x_r L_r \left(\frac{1}{|x|}\right)_{,i}\right]}$$

So for a pt. load $L_j$ at pt. $x'$

$$\boxed{16\pi\mu(1-\nu)\, u_i(x) = \frac{L_j}{|x-x'|}\underbrace{\left[(3-4\nu)\delta_{ij} + \frac{(x_j-x_j')(x_i-x_i')}{|x-x'|^2}\right]}_{\text{fundamental soln. / Green's fn.}}}$$

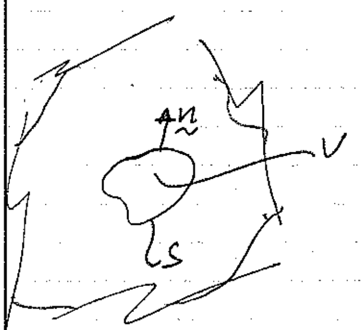
Returning to Eshelby Inclusion problem.




$$u_i^e(x) = \frac{1}{16\pi\mu(1-\nu)}\int_S T^t_{jk}\, n_k(x')\left[(3-4\nu)\delta_{ij} + \frac{(x_j-x_j')(x_i-x_i')}{|x-x'|^2}\right] da'$$

$$= \frac{1}{16\pi\mu(1-\nu)}\, T^t_{jk}\int_V \left[(3-4\nu)\delta_{ij} + \frac{(x_j-x_j')(x_i-x_i')}{|x-x'|^2}\right]_{,k} dV'$$

# Eshelby Inclusion




$$u_i^c(x) = \frac{1}{16\pi\mu(1-\nu)} \int_S T^t_{jk} \frac{n_k(x')}{|x-x'|}\left[(3-4\nu)\delta_{ij} + \frac{(x_i-x_i')(x_j-x_j')}{|x-x'|^2}\right] dx'$$

$$u_i^c(x) = \frac{1}{16\pi\mu(1-\nu)} T^t_{jk}\int_V \left[\frac{1}{|x-x'|}\left\{(3-4\nu)\delta_{ij} + \frac{(x_j-x_j')(x_i-x_i')}{|x-x'|^2}\right\}\right]_{,k} dV'$$

Can show (HW).

$$u_i^c(x) = \frac{T^t_{jk}}{16\pi\mu(1-\nu)}\int_V \frac{dV'}{r^2} f_{ijk}(l) = \frac{e^t_{jk}}{8\pi(1-\nu)}\int_V \frac{dV'}{r^2} g_{ijk}(l)$$

where $r = |x - x'|$

$$l = \frac{x - x'}{|x - x'|}$$

and $f_{ijk} = (1-2\nu)(\delta_{ij} l_k + \delta_{ik} l_j) - \delta_{jk} l_i + 3 l_i l_j l_k$

$g_{ijk} = (1-2\nu)(\delta_{ij} l_k + \delta_{ik} l_j - \delta_{jk} l_i) + 3 l_i l_j l_k$.

## Ellipsoidal Inclusion

Consider integration

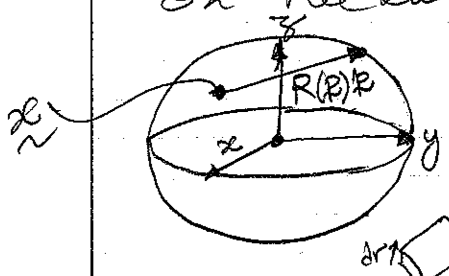
$$u_i^c = \frac{e^t_{jk}}{8\pi(1-\nu)} \int_V \frac{dv'}{r^2}\, g_{ijk}(\underset{\sim}{l}).$$

Define $\quad -\underset{\sim}{l} = \dfrac{\underset{\sim}{x}'-\underset{\sim}{x}}{|\underset{\sim}{x}'-\underset{\sim}{x}|} = \underset{\sim}{p}.$

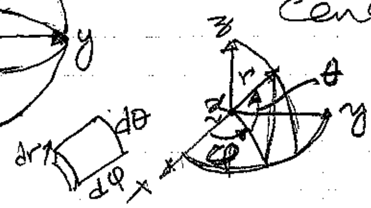
Then $\quad u_i^c(\underset{\sim}{x}) = -\dfrac{e^t_{jk}}{8\pi(1-\nu)} \displaystyle\int_V \frac{dv'}{r^2}\, g_{ijk}(\underset{\sim}{p}).$

where $V$ is now ellipsoidal domain defined by $\quad \dfrac{X^2}{a^2} + \dfrac{Y^2}{b^2} + \dfrac{Z^2}{c^2} = 1.$

where we choose origin of coordinates at center of ellipsoid & $(X, Y, Z)$ is a pt. on the surface of ellipsoid.




Integrate in spherical coords. centered at $\underset{\sim}{x}$.




$$dv' = (r\,d\theta)(r\sin\theta\, d\varphi)\, dr$$

$$\int_V \frac{dv'}{r^2}\, g_{ijk}(\underset{\sim}{p})$$

$$= \int_{\theta=-\pi}^{\theta=\pi} \int_{\varphi=0}^{\varphi=2\pi} g_{ijk}(\underset{\sim}{p}(\theta,\varphi))\, R(\underset{\sim}{p}(\theta,\varphi)) \sin\theta\, d\varphi\, d\theta$$

where $R(\theta,\varphi)$ is +ve root of:

$$(x_1 + R p_1)^2/a^2 + (x_2 + R p_2)^2/b^2 + (x_3 + R p_3)^2/c^2 = 1.$$

(HW) Can show that $\quad \{\lambda_1 = p_1/a^2;\ \lambda_2 = p_2/b^2;\ \lambda_3 = p_3/c^2\}$

$$u_i^c(\underset{\sim}{x}) = \frac{x_m e^t_{jk}}{8\pi(1-\nu)} \int_{\theta=-\pi}^{\theta=\pi} \int_{\varphi=0}^{\varphi=2\pi} \frac{\lambda_m g_{ijk}}{g} \sin\theta\, d\varphi\, d\theta.$$

where $g = p_1^2/a^2 + p_2^2/b^2 + p_3^2/c^2$.

$\therefore\ e^c_{ik}(\underset{\sim}{x}) = S_{ikmn}\, e^T_{mn}$ where $S$ does not depend on $\underset{\sim}{x}$.

## Recap Inhomogeneity Problem (Ellipsoidal inhomogeneity).

- Suppose inclusion is made of different material ($\underset{=}{C}^i$).
- Suppose we apply far field b.c.s. that in the homogeneous body would result in a homogeneous strain field $\underset{=}{e}^A$.
- Under the same applied loading let the strainfield of the inhomogeneous composite be $\underset{=}{e}^c + \underset{=}{e}^A$ {where $\underset{=}{e}^c$ needs to be determined}.
- So stress in composite $\underset{=}{C}^i(\underset{=}{e}^c + \underset{=}{e}^A)$.

- Suppose we think of a fictitious transf. strain problem for the homogeneous material which produces the same stress field for the same deformation of the reference configuration (at this pt., don't know if this is possible).
(so need $\underset{=}{e}^c$ ~~of~~ inhom. problem to be the $\underset{=}{e}^c$ of the transformation strain problem).

Then stress in homogeneous-material inclusion problem is $\underset{=}{C}(\underset{=}{e}^c + \underset{=}{e}^A - \underset{=}{e}^t)$.

In ellipsoid $\rightarrow$ $\underset{=}{e}^c = \underset{=}{S}\,\underset{=}{e}^t$.

$$\underset{=}{C}(\underset{=}{S}\,\underset{=}{e}^t + \underset{=}{e}^A - \underset{=}{e}^t) = \underset{=}{C}^i(\underset{=}{S}\,\underset{=}{e}^t + \underset{=}{e}^A).$$

Solve for $\underset{=}{e}^t$.

# Reciprocal Theorem & Interaction Energy in Linear Elasticity

## Reciprocal Theorem (Betti)

For two equilibrium states with displacements $u_i, u_i'$ for body forces and tractions $F_i, T_i$ and $F_i', T_i'$ respectively

We have.

(*) — $$\int_S T_i u_i' \, ds + \int_V F_i u_i' \, dv = \int_S T_i' u_i \, ds + \int_V F_i' u_i \, dv$$

Assume $C_{ijkl} = C_{klij}$.

Proof: L.H.S. $$\int_S \tau_{ij} n_j u_i' \, ds + \int_V F_i u_i' \, dv$$

$$= \int_V (\tau_{ij} u_i')_{,j} \, dv + \int_V F_i u_i' \, dv$$

$$= \int_V \tau_{ij} u'_{i,j} \, dv + \underbrace{\int_V F_i u_i' \, dV + \int_V \tau_{ij,j} u_i' \, dv}_{=0}$$

$$= \int_V \tau_{ij} u'_{i,j} \, dv$$

Now $$\tau_{ij} u'_{i,j} = \frac{1}{2} \tau_{ij} (u'_{i,j} + u'_{j,i})$$

$$= \tau_{ij} e'_{ij}$$

$$= C_{ijkl} e_{kl} e'_{ij}$$

$$= C_{klij} e_{kl} e'_{ij}$$

$$= \tau'_{kl} e_{kl} = \tau'_{ij} u_{i,j}$$

& ∴ (*) holds by symmetry.

- ~~Both~~ (*) & (**) $\int_V \tau_{ij} e'_{ij} \, dv = \int_V \tau'_{ij} e_{ij} \, dv$

are useful.

- ~~Holds~~ for inhomogeneous bodies, for composites if $u_i$ & $T_i$ are continuous at the interfaces.

Betti used theorem to get change in volume in terms of applied loads

take $u'_i = e x_i$ (homog. defmn). $F'_i = 0$.

$$\tau'_{ij} = \lambda e'_{kk} \delta_{ij} + 2\mu e'_{ij}$$

$$= 3\lambda e \delta_{ij} + 2\mu e \delta_{ij}$$

$$= 3ke \delta_{ij}.$$

So $\int_V \tau'_{ij} u_{i,j} \, dv = \int_S T_i u'_i ds + \int_V F_i u'_i ds$.

$$= \int_V 3ke \, u_{i,i} \, dv = e\int_S T_i x_i \, ds + e\int_V F_i x_i \, dV.$$

$$\Rightarrow \int_V e_{kk} \, dV = \frac{1}{3k} \left[ \int_S T_i x_i \, ds + \int_V F_i x_i \, dV \right]$$

## Interaction Energy.

$$E(A,B) = E(A) + E(B) + E_{int}(A,B)$$

where $E$ is total energy of an elastic body & $A, B$ refer to 'sources' of elastic strain/stress.

The total energy includes strain energy plus the potential energy of applied loads.

If Energy Minimization is considered a physical principle then the knowledge of the $E_{int}$ can be used to predict certain configurations of defects. e.g.

Suppose $E(A) > 0$ & $E(B) > 0$. (generally true).

but $E_{int}(A,B)$ can have any sign.

So if A and B & solely A are competing states (e.g. body with a straight dislocation of 1-sign vs. body with a dipole).

If $|E_{int}(A,B)| > |E(B)|$

& $E_{int}(A,B) < 0$.

then $E(A) > E(A,B)$.

& ∴ A and B is what will be observed i.e. a dipole will be observed. and, in fact, in the absence of external stress will annihilate.

Elastic Energy of dislocation distributions:-

Infinite medium. (no external loads).

$(\sigma_{ij}^A, \varepsilon_{ij}^A)$ $(\sigma_{ij}^B, \varepsilon_{ij}^B)$ → elastic states corresponding to two dislocation distributions, say $\underline{\alpha}_A$ & $\underline{\alpha}_B$.

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$

$$E_{tot}(A,B) = \frac{1}{2}\int_V (\sigma_{ij}^A + \sigma_{ij}^B)(\varepsilon_{ij}^A + \varepsilon_{ij}^B)\,dV.$$

$$= \underbrace{\frac{1}{2}\int_V \sigma_{ij}^A \varepsilon_{ij}^A\,dV}_{E_{tot}(A)} + \underbrace{\frac{1}{2}\int \sigma_{ij}^B \varepsilon_{ij}^B\,dV}_{E_{tot}(B)} + \underbrace{\int \underbrace{\sigma_{ij}^A \varepsilon_{ij}^B}_{C_{ijkl}\varepsilon_{kl}^A\varepsilon_{ij}^B}\,dV}_{E_{int}(A,B)}$$

$$C_{ijkl}\varepsilon_{kl}^A\varepsilon_{ij}^B = C_{klij}\varepsilon_{ij}^B\varepsilon_{kl}^A = \sigma_{kl}^B\varepsilon_{kl}^A.$$

$$E_{int}(A,B) = \int \chi_{ij}^A \eta_{ij}^B\,dV.$$

{after two integration by parts & having boundary terms vanish}.

# A note on Interaction Energy Analysis

In Eshelby's analysis one often comes across integrals of the form

$$\int_V p^S_{ij}\, u^T_{i,j}\, dv$$

where $u^T_i$ is a continuous vector field in $V$ but $p^S_{ij}$ can have singularities.

The integral above is often converted by Eshelby to

$$\int_V p^S_{ij}\, u^T_{i,j}\, dv = \int_{\partial V} p^S_{ij}\, u^T_i\, n_j\, da$$

This may be justified as follows:

Let the singularity be located at $x \in V$.

Then $$\int_V p^S_{ij}\, u^T_{i,j}\, dv = \int_{V \setminus B^r_x} p^S_{ij}\, u^T_{i,j}\, dv + \int_{B^r_x} p^S_{ij}\, u^T_{i,j}\, dv.$$

where $B^r_x$ is a ball of radius $r$ around $\underline{x}$.

$$R.H.S = \int_{\partial V} p^S_{ij}\, u^T_i\, n_j\, da - \int_{\partial B^r_x} p^S_{ij}\, u^T_i\, n_j\, da + \int_{B^r_x} p^S_{ij}\, u^T_{i,j}\, dv.$$

Assume $u^T_i$ & $u^T_{i,j}$ as continuous fns. So in the limit

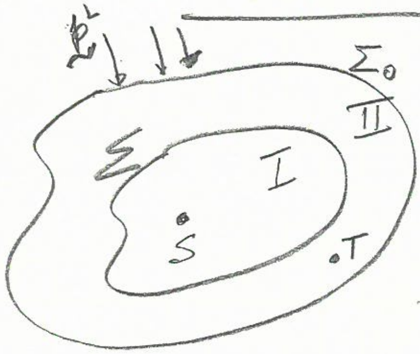
$r \to 0$ $\quad R.H.S = \int_{\partial V} p^S_{ij}\, u^T_i\, n_j\, da - u^T_i \int_{\partial B^r_x} p^S_{ij}\, n_j\, da + u^T_{i,j} \int_{B^r_x} p^S_{ij}\, dv.$

For disloc. soln $\int_{\partial B^r_x} p^S_{ij}\, n_j\, da = 0$. We also assume $\int_{B^r_x} p^S_{ij}\, dv = 0$.

e.g. $\int_{B^r_x} \frac{c}{r}\, r\, dr\, d\theta \approx cr \to 0$ as $r \to 0$ //.

(Eshelby, 1956)

# Interaction Energy & Force on a dislocation




Let S & T be two sources of internal stress. Let $p^L$ be applied traction field on $\Sigma_0$. Let us call stress tensors by symbol $p_{ij}$.

$$E_{tot} = \frac{1}{2}\int_V (p_{ij}^S + p_{ij}^T + p_{ij}^L)(\varepsilon_{ij}^S + \varepsilon_{ij}^T + \varepsilon_{ij}^L)\,dv - \int_{\Sigma_0} p_{ij}^L(u_i^S + u_i^L + u_i^T)n_j\,da$$

$$= \frac{1}{2}\int_V p_{ij}^S \varepsilon_{ij}^S\,dv + \frac{1}{2}\int_V p_{ij}^L \varepsilon_{ij}^L\,dv + \frac{1}{2}\int_V p_{ij}^T \varepsilon_{ij}^T\,dv$$

$$+ \frac{1}{2}\int_V p_{ij}^S \varepsilon_{ij}^T\,dv + \frac{1}{2}\int_V p_{ij}^S \varepsilon_{ij}^L\,dv.$$

$$+ \frac{1}{2}\int_V p_{ij}^T \varepsilon_{ij}^S\,dv + \frac{1}{2}\int_V p_{ij}^T \varepsilon_{ij}^L\,dv$$

$$+ \frac{1}{2}\int_V p_{ij}^L \varepsilon_{ij}^S\,dv + \frac{1}{2}\int_V p_{ij}^L \varepsilon_{ij}^T\,dv$$

$$- \int_{\Sigma_0} p_{ij}^L u_i^S n_j\,da - \int_{\Sigma_0} p_{ij}^L u_i^L n_j\,da - \int_{\Sigma_0} p_{ij}^L u_i^T n_j\,da$$

If we were to be interested in changes in energy due to changes only in the field $\varepsilon_{ij}^S$ & $p_{ij}^S$ (due to motion of defects) the only terms that change in the total energy are

$$E_{int}(S;T,L) = \frac{1}{2}\int_V p_{ij}^S \varepsilon_{ij}^T\,dv + \frac{1}{2}\int_V p_{ij}^T \varepsilon_{ij}^S\,dv$$
$$+ \frac{1}{2}\int_V p_{ij}^S \varepsilon_{ij}^L\,dv + \frac{1}{2}\int_V p_{ij}^L \varepsilon_{ij}^S\,dv - \int_{\Sigma_0} p_{ij}^L u_i^S n_j\,da$$

(2)

(and we ignore the quadratic term $\frac{1}{2}\int_V p^S_{ij}\varepsilon^S_{ij}\,dv$)

a) often before & after change they are infinite).

b) or we assume that after integration on the domain before & after change the quantity is unchanged).

# So for studying changes in total energy due to motion of defects we simply study $E_{int}(S;T,L)$.

# Let the singularities of S be distributed within $\Sigma$ & those of T in the region between $\Sigma_0$ & $\Sigma$.

Now because of elastic const. assumption & major symmetry

$$\varepsilon^S_{ij}p^T_{ij} = C_{ijkl}\varepsilon^T_{kl}\varepsilon^S_{ij} = C_{klij}\varepsilon^S_{ij}\varepsilon^T_{kl} = p^S_{kl}\varepsilon^T_{kl}.$$

$\therefore$ the volume integrals $1^{st}$ & $2^{nd}$ are equal & $3^{rd}$ & $4^{th}$ are equal.

$$\therefore \underbrace{\frac{1}{2}\int_V p^S_{ij}\varepsilon^T_{ij}\,dv + \frac{1}{2}\int_V p^T_{ij}\varepsilon^S_{ij}\,dv}_{A} = \int_V p^S_{ij}\varepsilon^T_{ij}\,dv = \int_V p^T_{ij}\varepsilon^S_{ij}\,dV.$$

$$= \int_I p^S_{ij}\varepsilon^T_{ij}\,dv + \int_{II} p^T_{ij}\varepsilon^S_{ij}\,dv.$$

But in I $\varepsilon^T_{ij} = \frac{1}{2}(u^T_{i,j} + u^T_{j,i})$ & in II $\varepsilon^S_{ij} = \frac{1}{2}(u^S_{i,j}+u^S_{j,i})$

So that $$A = \int_\Sigma p^S_{ij}u^T_i n_j\,da + \int_{\Sigma_0} p^T_{ij}n_j u^S_i\,da - \int_\Sigma p^T_{ij}u^S_i n_j\,da$$

But $p^T_{ij} n_j = 0$ on $\Sigma_0$

So $$\boxed{A = \int_{\Sigma} \left[ p^S_{ij} u^T_i - p^T_{ij} u^S_i \right] n_j \, da.}$$

Similarly, let's denote

$$B = \frac{1}{2}\int_V p^S_{ij} \varepsilon^L_{ij} dv + \frac{1}{2}\int_V p^L_{ij} \varepsilon^S_{ij} dv$$

$$= \int_V p^S_{ij} \varepsilon^L_{ij} dv = \int_{\Sigma_0} p^S_{ij} u^L_i n_j da$$

But $p^S_{ij} n_j = 0$ on $\Sigma_0$

$\therefore \quad B = 0$

Now, consider $C = -\int_{\Sigma_0} p^L_{ij} u^S_i n_j \, da.$

$$= -\left[ \int_{II} (p^L_{ij} u^S_i)_{,j} dv - (-1)\int_{\Sigma} p^L_{ij} u^S_i n_j da \right].$$

$$= -\left[ \int_{II} p^L_{ij} u^S_{i,j} dv + \int_{\Sigma} p^L_{ij} u^S_i n_j da \right]$$

$$= -\left[ \int_{II} p^S_{ij} u^L_{i,j} dv + \int_{\Sigma} p^L_{ij} u^S_i n_j da \right].$$

$$= -\left[ -\int_{\Sigma} p^S_{ij} u^L_i n_j da + \int_{\Sigma} p^L_{ij} u^S_i n_j da \right] \left\{ \because p^S_{ij} n_j = 0 \text{ on } \Sigma_0. \right.$$

④

$\therefore$ $E_{int}(S;T,L) =$

$$\int_{\Sigma} \left[ p^S_{ij}\left(u^L_i + u^T_i\right) - \left(p^T_{ij} + p^L_{ij}\right) u^S_i \right] n_j \, da .$$

# The 'force' on a dislocation segment due to another stress field.

# We do not use explicit expressions for the field of a dislocation.

Assumptions:

(i) The displacement jump on any point of the slip surface is a constant and given by $b_i$, having chosen an orientation for the surface.

ii) If $\underset{\sim}{x}$ is the position vector from any fixed point on the dislocation line then

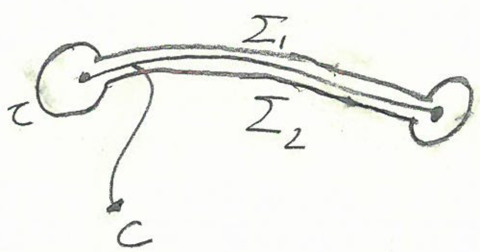
$$\lim_{r \to 0} r\, u_i^s(\underset{\sim}{x}) = 0.$$

iii) The integral $\int_\Sigma p_{ij}^s n_j \, da$ vanishes even when taken over the surface bounding a volume traversed by dislocation line. (including end caps of surface).

Let $C$ be any cap bounded by the dislocation line.

Use formula

$$E_{int}(S,T) = \int_\Sigma \left(p_{ij}^s u_i^T - p_{ij}^T u_i^s\right) n_j \, da$$




Let us assume that $b_i = u_i^2(\underset{\sim}{x} \in C) - u_i^1(\underset{\sim}{x} \in C)$. //.

\# As radius of $\tau$ goes to zero, $2^{nd}$ term in $E_{int}(S,T)$ vanishes (for integral on $\tau$) since $p^T_{ij}$ is continuous & we use ii).

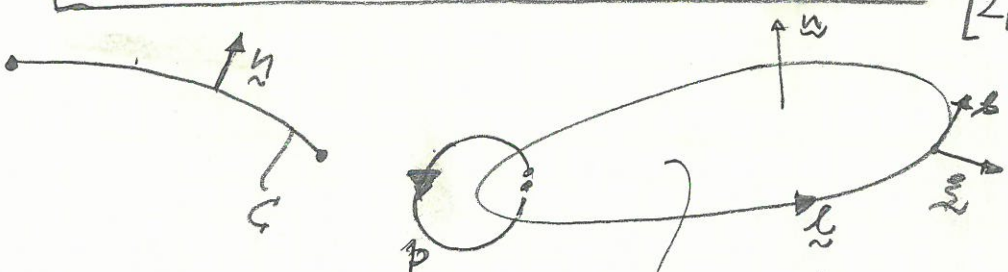
\# Using (iii) & cutting $\tau$ into many small pieces, first term also vanishes (using continuity of $u^T_i$ also). (important that (iii) hold on end caps too).

So we are left with contributions from $\Sigma_1$ & $\Sigma_2$.

\# Since $p^S_{ij}$ & $u^T_i$ are continuous on $C$ the contribution from first term vanishes.

So we are left with $\quad b_i = [\![u_i]\!] \Big|_{\text{for } \underset{\sim}{x} \in C}$, $\quad [\![\ ]\!] = 2 - 1$

$$\boxed{E_{int}(S,T) = b_i \int_C p^T_{ij}\, n_j\, da} = -\left[\int_{\Sigma_1} p^T_{ij}\, u^1_i\, n_j\, da - \int_{\Sigma_2} p^T_{ij}\, u^2_i\, n_j\, da\right]$$




$$\oint_p u_{i,j}\, dx_j = b_i$$

\# For a displacement of $\underset{\sim}{\xi}$ of an element of loop $l\,\underset{\sim}{s}$ the change in

$$\delta E_{int}(S,T) = b_i\, p^T_{ij}\, e_{jek}\, l\, \xi_e\, s_k$$

$\therefore$ Force per unit length $\dfrac{1}{l}\dfrac{\partial E_{int}(S,T)}{\partial \xi_l} = b_i\, p^T_{ij}\, e_{kje}\, s_k$

$\Rightarrow -\dfrac{1}{l}\dfrac{\partial E_{int}(S,T)}{\partial \xi_l} = e_{ljk}(b_i\, p^T_{ij})\, s_k$ $\longrightarrow$ Peach-Koehler force.

# *3.40 Lecture Summary*

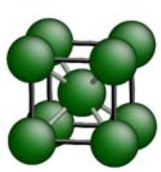
September 16, 2009

Department of Materials Science and Engineering

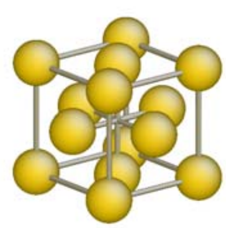
## Basic Crystallography

*BCC, FCC, and HCP Crystals*

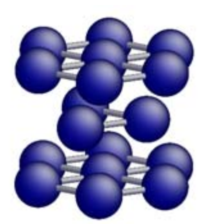
1 BCC



2 FCC



3 HCP



| BCC Metals | FCC Metals | HCP Metals |
|---|---|---|
| Fe, W, V, Mo | Cu, Ag, Au, Pt, Al, Ni, Pb | Ti,Zr, Mg, Zn, Be, Cd |
| At high temps: Ti, Zr | At high temps: Fe | -- |

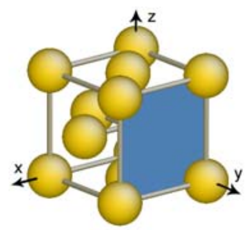
[1] Li, J. Modeling Simul. Mater. Sci. Eng. 11 (2003) 173. (AtomEye Visualization Software)
[2] NRL. Lattice Crystal Structures (2008)<http://cst-www.nrl.navy.mil/lattice/>.
[3] Abbaschian, R. et al. Physical Metallurgy Principles 4th ed. (2009).

1

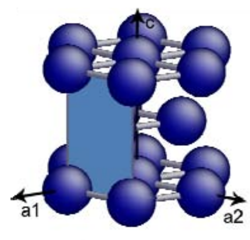
# Basic Crystallography

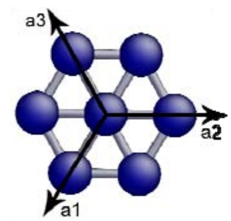
## *Miller Indices*

① Cubic Lattices




② Hexagonal Lattices




| (010) | a | b | c |
|---|---|---|---|
| Intercept Length | ∞ | 1 | ∞ |
| Reciprocal | 0 | 1 | 0 |

| (1010) | a1 | a2 | a3 | c |
|---|---|---|---|---|
| Intercept Length | 1 | ∞ | -1 | ∞ |
| Reciprocal | 1 | 0 | -1 | 0 |

[1] Li, J. Modeling Simul. Mater. Sci. Eng. 11 (2003) 173. (AtomEye Visualization Software)

2

# Basic Crystallography

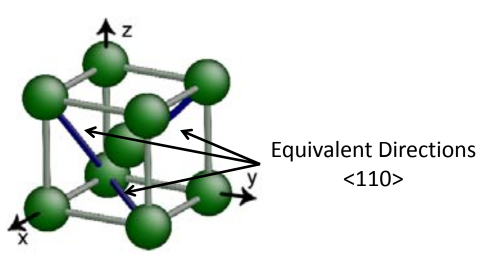
## *Crystal Symmetry*

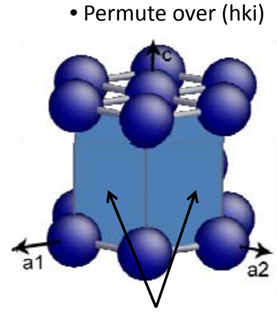
① Cubic Lattice Symmetry

- Crystallographic families
  - Directions: <hkl>
  - Plane: {hkl}
  - Implies permutation rule

② Hexagonal Lattice Symmetry

- Why (hkil) indexing scheme?
  - Allows permutation rule!
  - (hkil)
  - Permute over (hki)




Equivalent Planes: {$10\bar{1}0$}

[1] Li, J. Modeling Simul. Mater. Sci. Eng. 11 (2003) 173. (AtomEye Visualization Software)

3

# Basic Crystallography

## *Crystal Symmetry and Stereographic Projection*

1. What symmetry exists in cubic crystals?
   - o Rotational
     - 2 fold - ⬬
     - 3 fold - ▲
     - 4 fold – ■

Image removed due to copyright restrictions.
Please see p. 3 in Schlom, Darrell G.
"Stereographic Projection."
MatSE535 Course Notes, 2009.

2. What symmetry exists in hexagonal crystals?
   - o Rotational
     - 6 fold – ⬢

Image removed due to copyright restrictions.
Please see Fig 16.4
in Henderson, David, and Daina Taimina.
*Experiencing Geometry: Euclidean and Non-Euclidean With History.*
3rd Ed. Upper Saddle River, NJ: Prentice-Hall, 2005.

3. How do we keep track of crystal symmetries?
   - o Answer: Stereographic Projection

[4]Schlom, D. G. Stereographic Projection Notes. <http://www.ems.psu.edu/~schlom/MatSE535/StereoProjection.pdf>.
[5] Henderson, D. W. (1999) <http://www.math.cornell.edu/~dwh/books/eg99/Ch16/Ch16.html



# Basic Crystallography

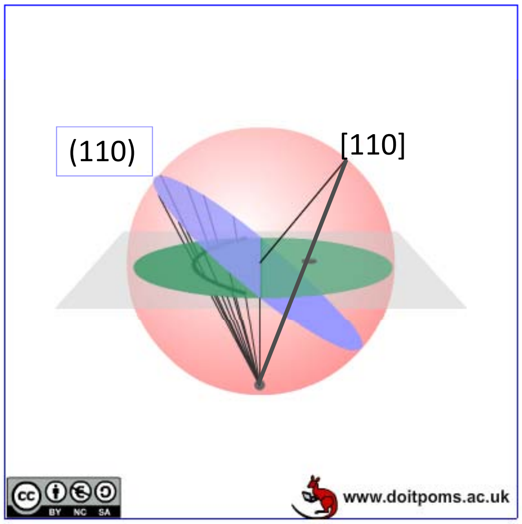
## *Stereographic Projection of Crystal Directions*

Image removed due to copyright restrictions.
Please see p. 3, 10 in Schlom, Darrell G.
"Stereographic Projection."
MatSE535 Course Notes, 2009.

**[1] www.ems.psu.edu/~schlom/MatSE535/StereoProjection.pdf**

# Basic Crystallography

## *Stereographic Projection of Crystal Planes*

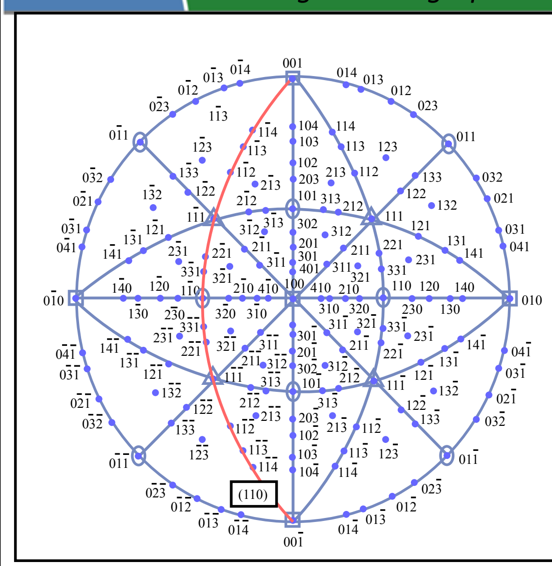



[1] http://www.doitpoms.ac.uk/tlplib/stereographic/index.php



# Basic Crystallography

## *Reading a Stereographic Projection*




1. The plane is 90 degrees from the pole direction on a longitudinal line
2. The directions on a plane are in the plane
3. Symmetry markers reflect the point symmetry of the crystal

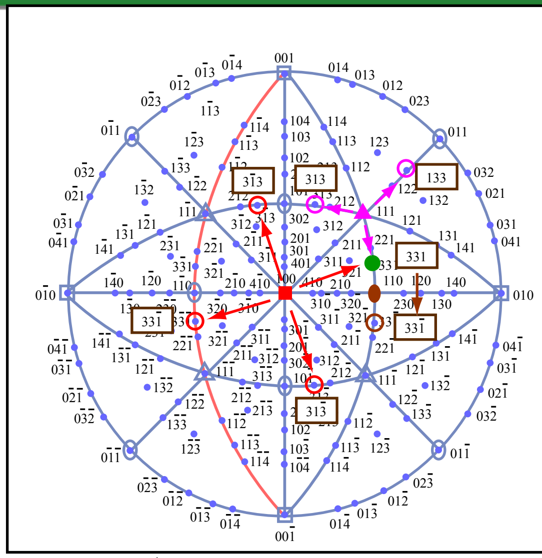
Figure by MIT OpenCourseWare.

Adapted from Fig. 1.33 in Reed-Hill and Abbaschian, *Physical Metallurgy Principles*

[1 Abbaschian, R. et al. Physical Metallurgy Principles 4th ed. (2009).

## Basic Crystallography

### *Symmetry on the Stereographic Projection*



Adapted from Fig. 1.33 in Reed-Hill and Abbaschian, *Physical Metallurgy Principles*

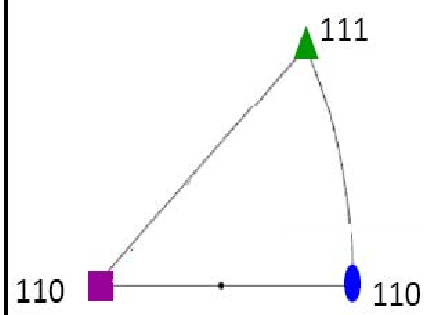
8

[1] Abbaschian, R. et al. Physical Metallurgy Principles 4th ed. (2009).

Figure by MIT OpenCourseWare.

## Basic Crystallography

### *Standard Stereographic Triangle*



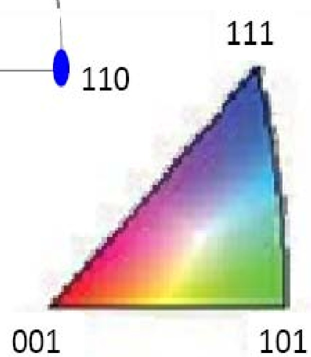





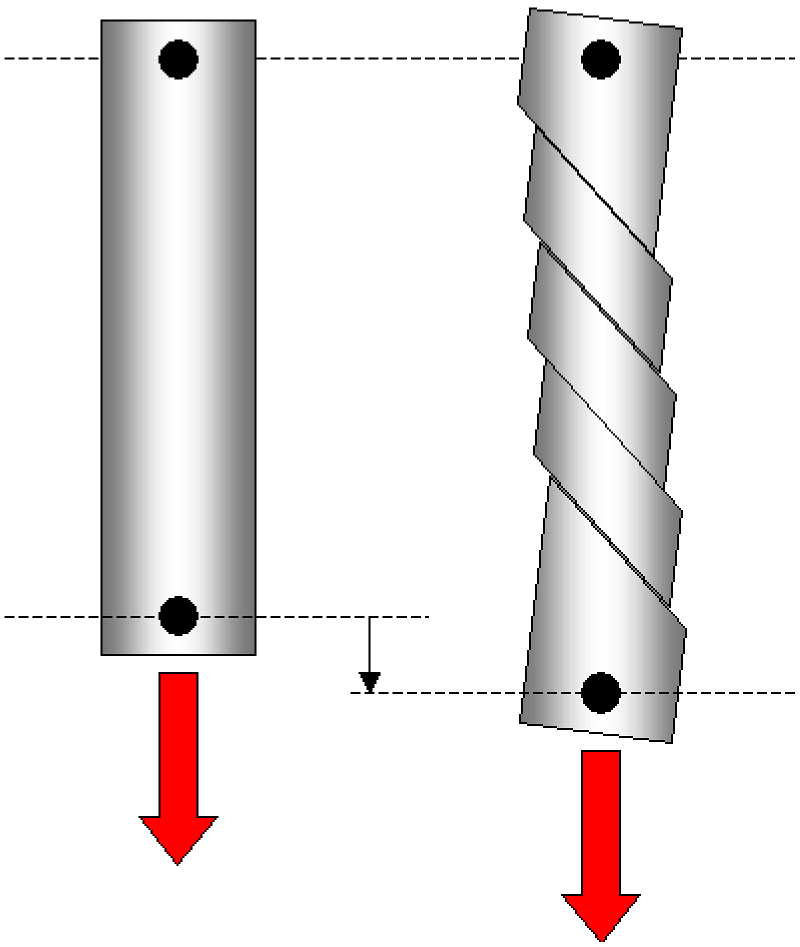
Image courtesy of U.S. Naval Research Laboratory.


[1] Geltmacher.,A.B. et al. Image-based Modeling of Naval Steels (2003) http://www.nrl.navy.mil/content.php?P=03REVIEW163

[2] Ferry, Michael. "Appendix B - Representation of Textures and their Interpretation". Direct Strip Casting of Metals and Alloys: Processing, Microstructure and Properties. Woodhead Publishing. (2006)


9

# An Interesting Experiment

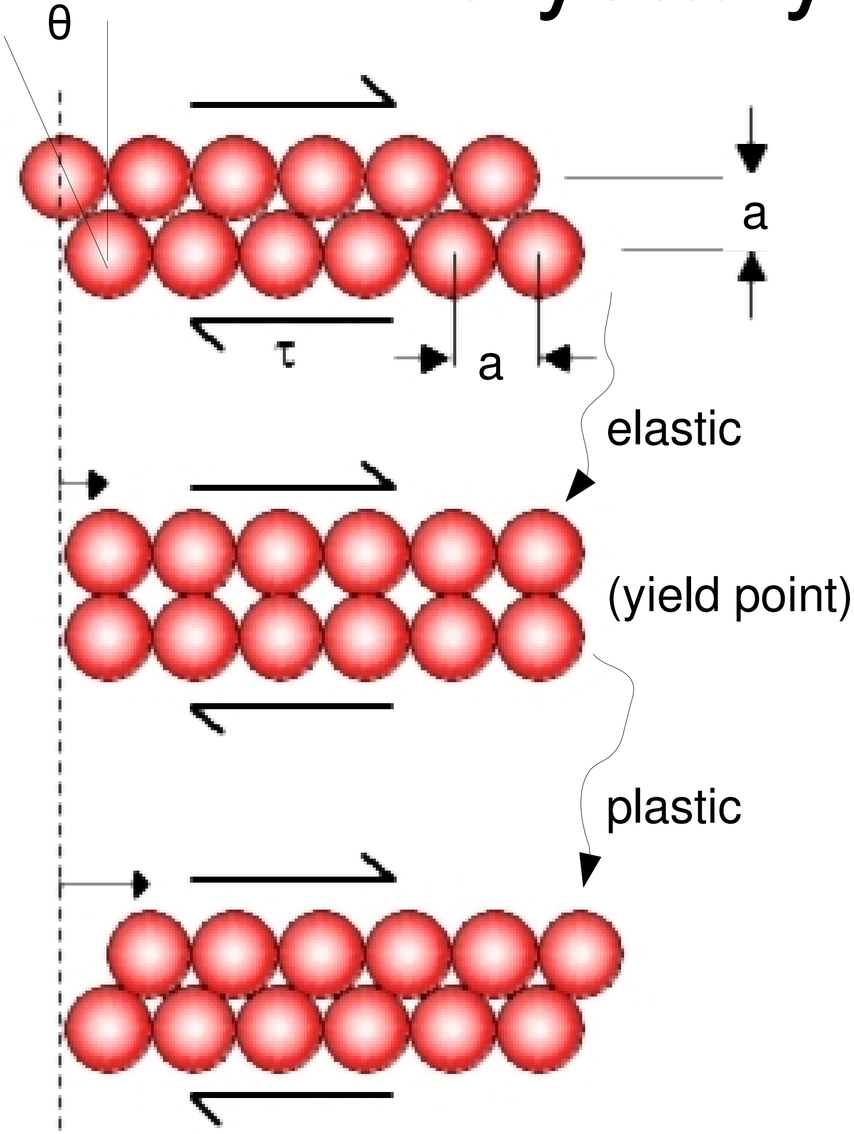


Courtesy of DoITPoMS, University of Cambridge. Used with permission.

- Take a single-crystal metal sample, and measure its stress-strain curve in tension
- Deformed sample exhibits slip steps
- The slip is always along crystallographic planes
- What is the slip mechanism?

<http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html>

# Initial (and incorrect) theory of crystal yield under shear




- Under shear stress, planes of atoms slide past one another, moving as a unit
- By Hooke's Law: $\tau = \mu \gamma$
- From the proposed geometry:

$$\tau_y = \mu \gamma_y \simeq \mu \tan(\theta) = \frac{\mu}{\sqrt{3}}$$

- ~$10^4$ - $10^5$ discrepancy between theory and experiment!
- There **must** be a lower-energy way to shear the lattice



<http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html>

# Crystal yield under shear (how it really happens)

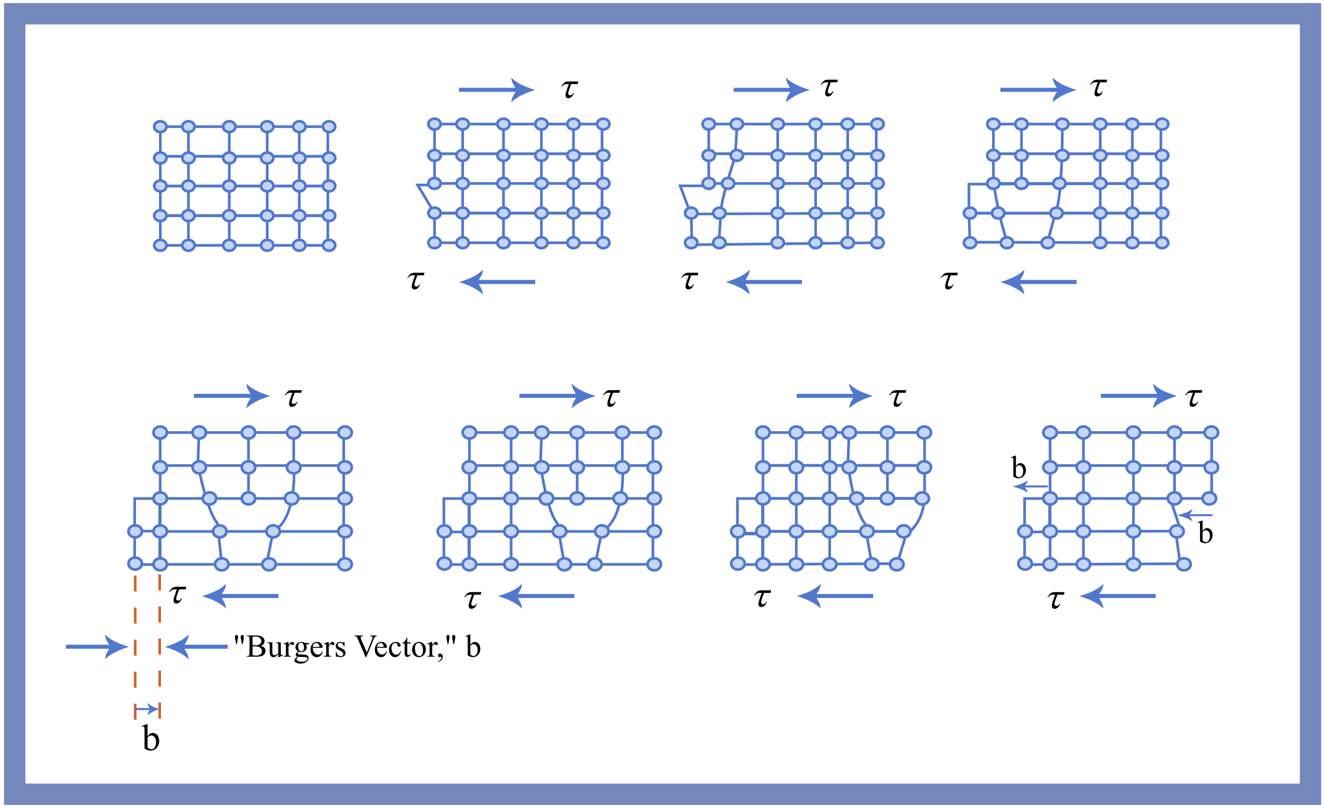
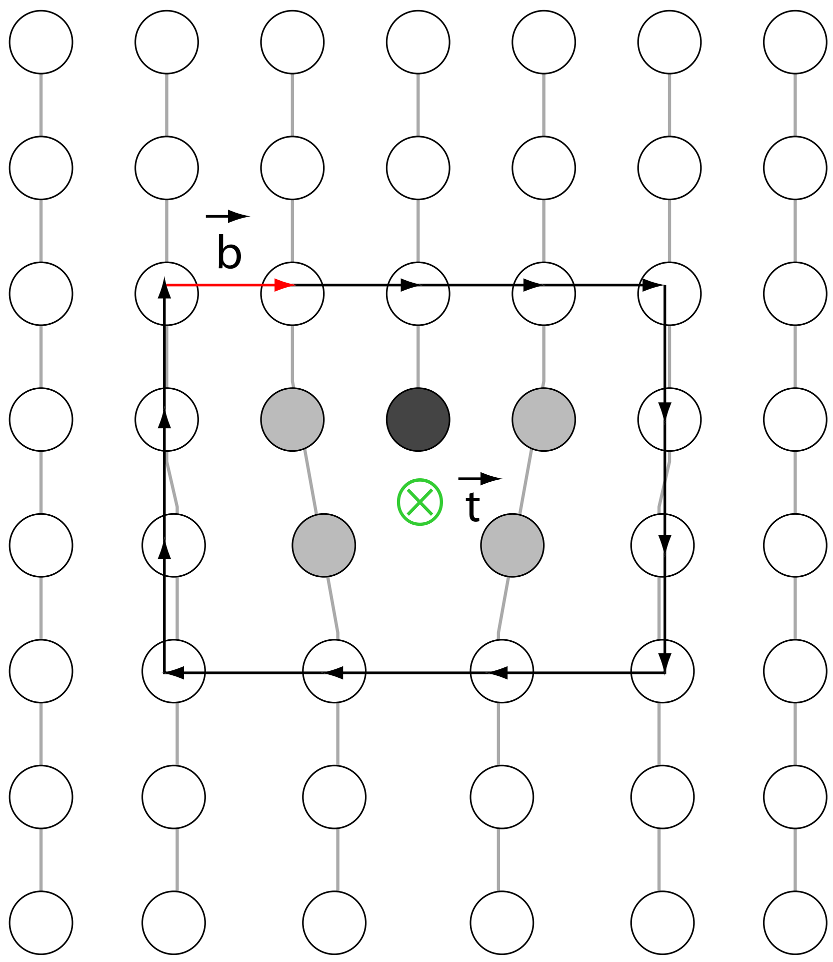



Figure by MIT OpenCourseWare. Adapted from Fig. 9.4 in Ashby, M. F., and D. R. H. Jones. *Engineering Materials 1*. Boston, MA: Elsevier Butterworth-Heinemann,2005.

- The dislocations generates a local strain field that makes it easier to shear the lattice
- Displacement ripples through the crystal, moving one column at a time

<http://courses.eas.ualberta.ca/eas421/lecturepages/microstructures.html>

# The Burgers Vector (RHFS Convention)




- Define a line axis $\vec{t}$
- Construct a right-handed loop about $\vec{t}$
- $\vec{b}$ is the vector that heals the closure in the finish-to-start direction



<http://courses.eas.ualberta.ca/eas421/lecturepages/microstructures.html>

# Dislocation Characteristics

- Have a single, constant $\vec{b}$ over their entire length
- Slip occurs always in the plane defined by $\vec{b}$ and $\vec{t}$
- Dislocation characterized by $\vec{b}$ and $\vec{t}$ together, not just by $\vec{b}$ alone
- Dislocations cannot terminate in a crystal

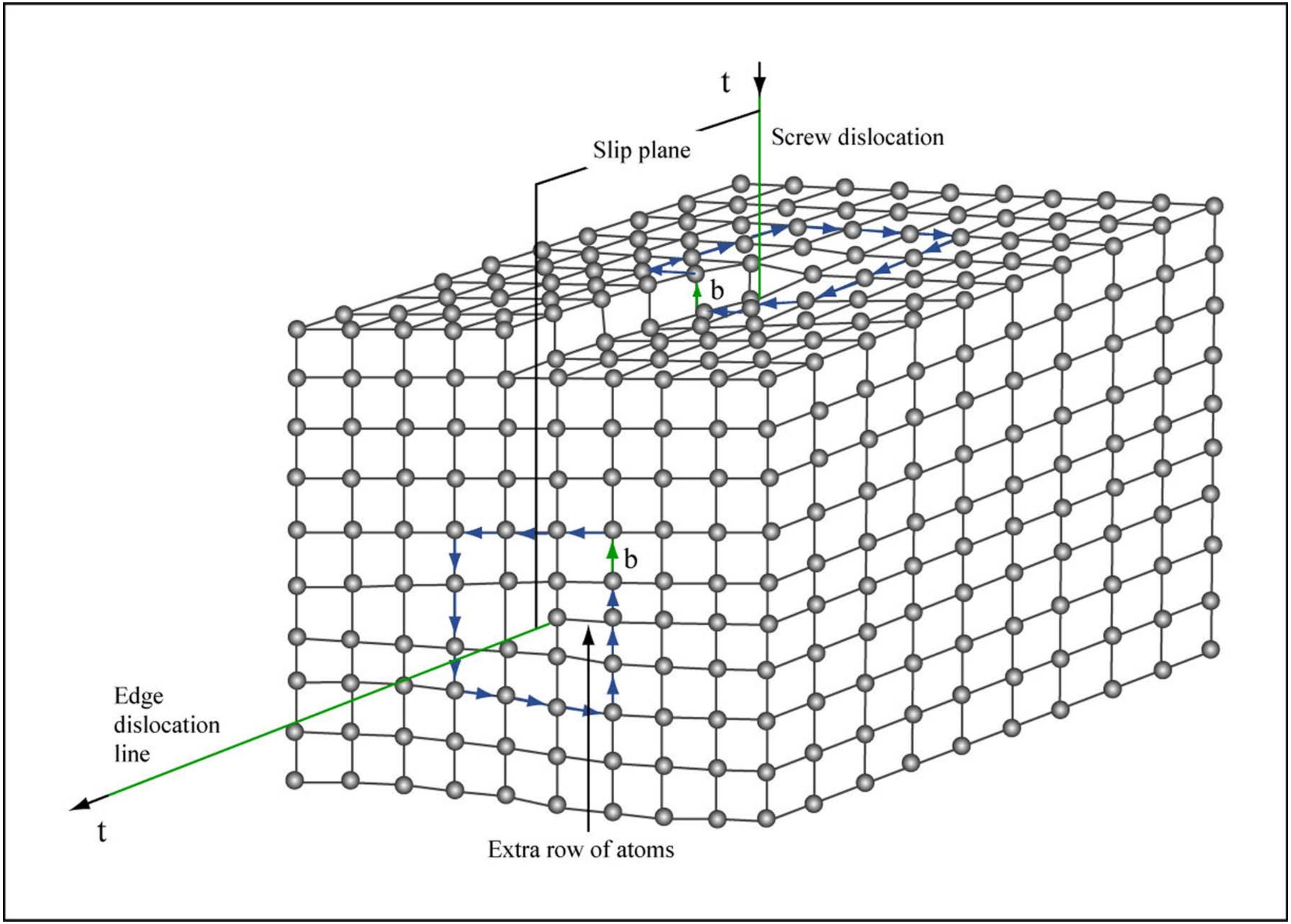
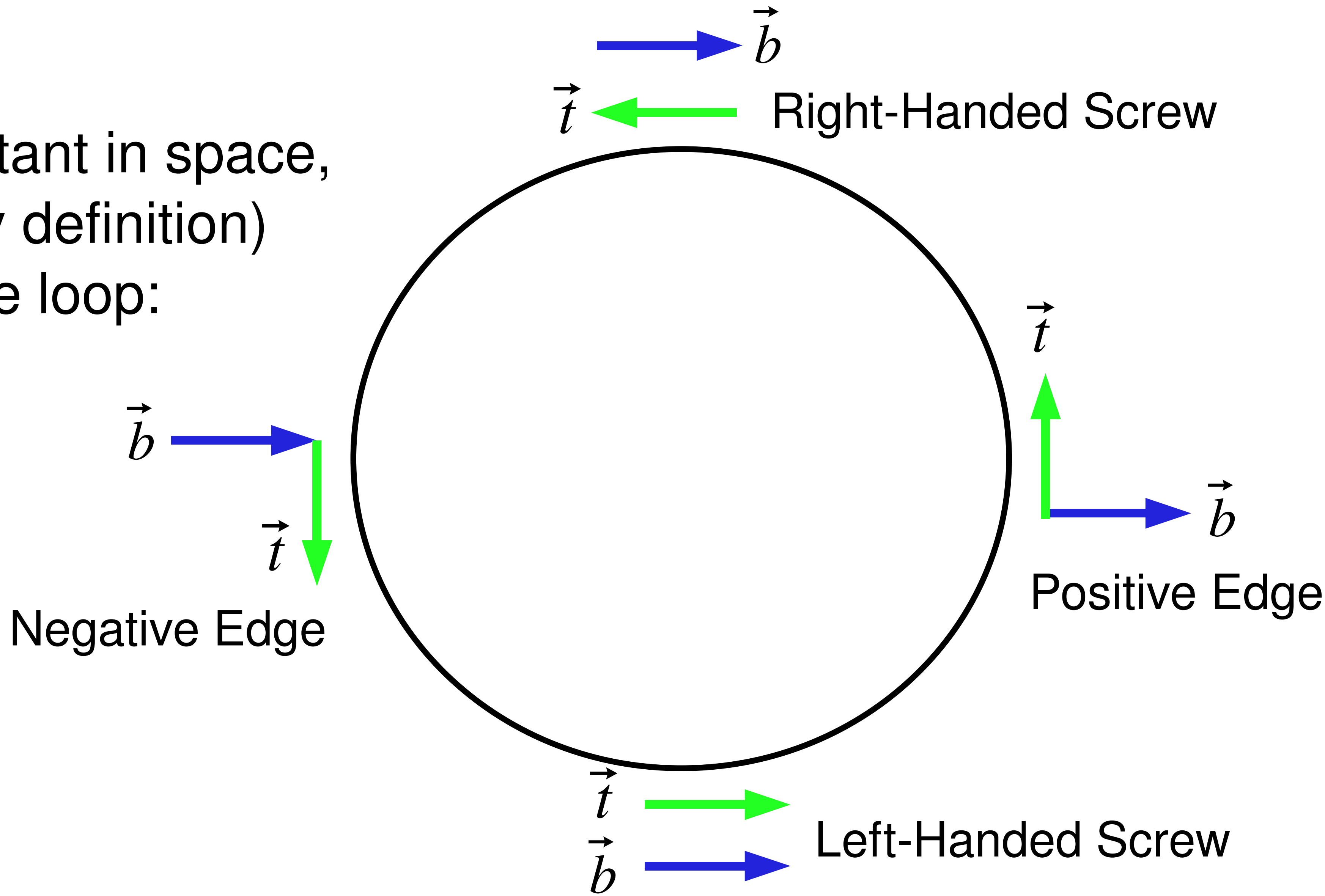



Figure by MIT OpenCourseWare.

Adapted from <http://courses.eas.ualberta.ca/eas421/lecturepages/microstructures.html>

# Loop Dislocation

$\vec{b}$ is constant in space, and $\vec{t}$ (by definition) follows the loop:



# Loop Dislocation

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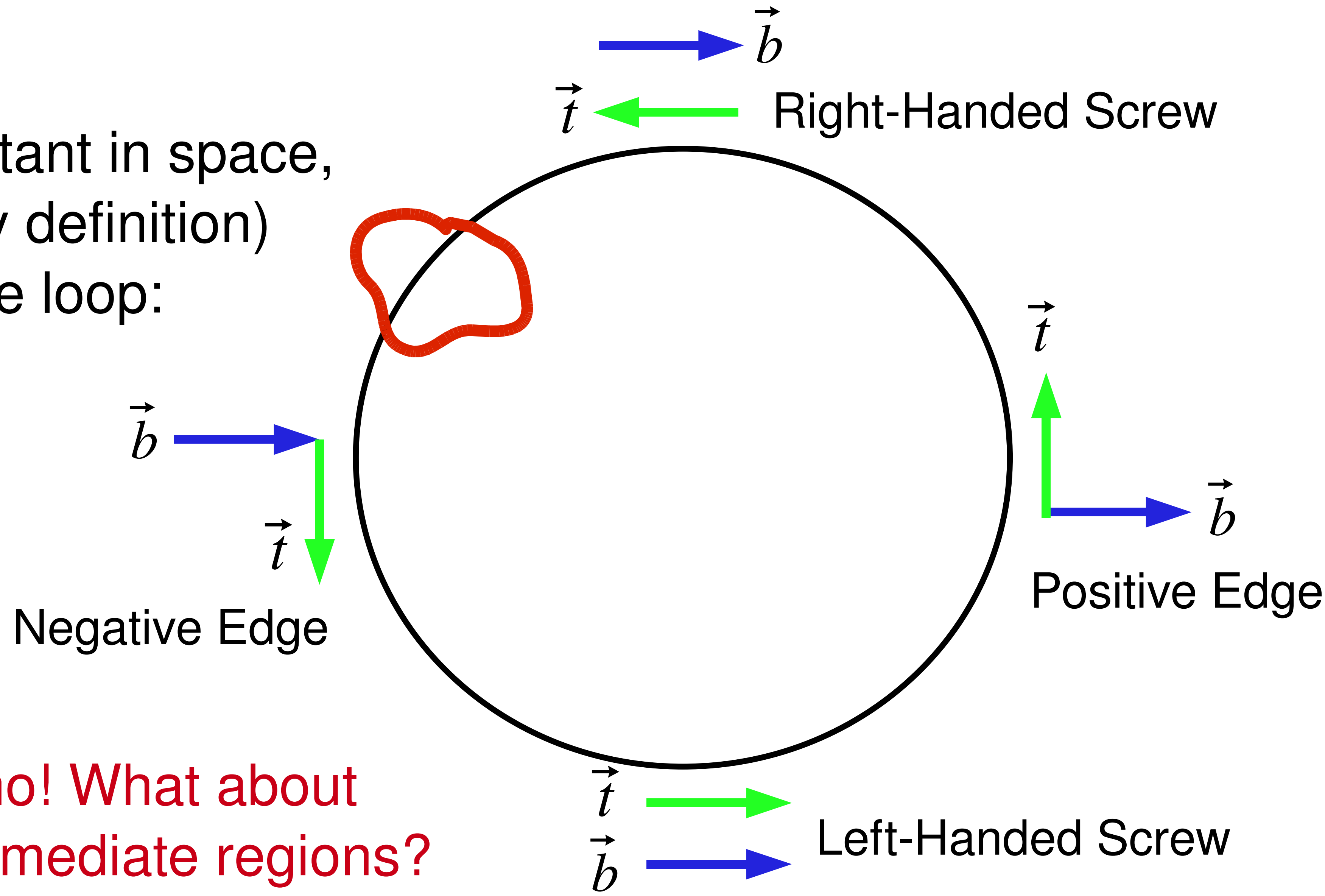
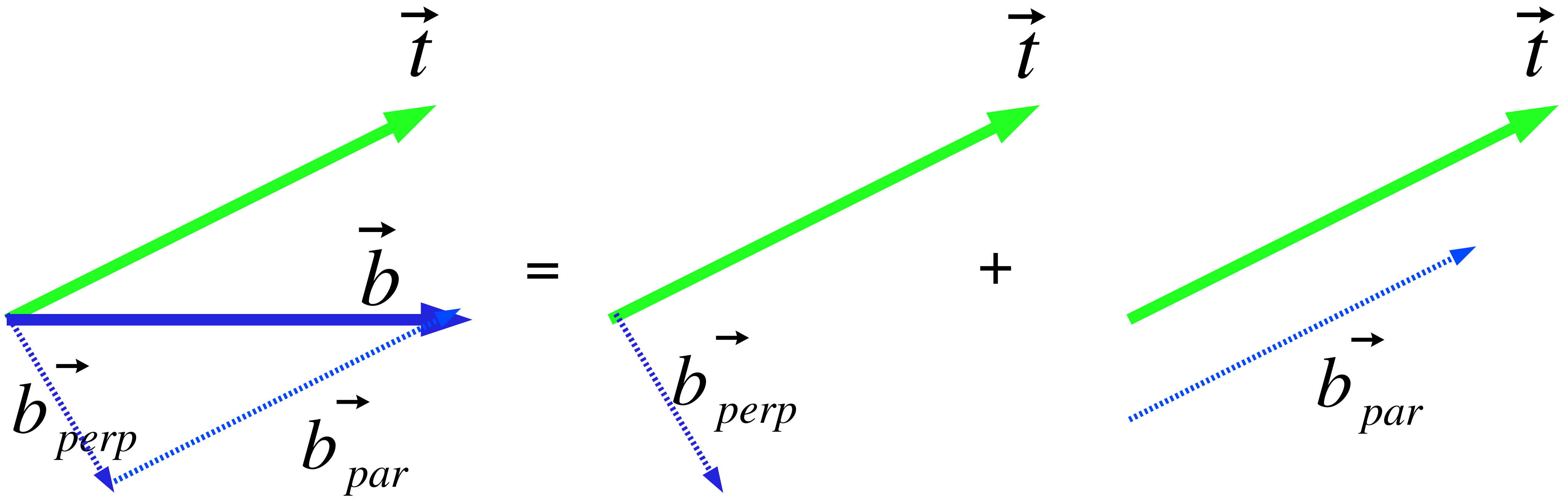
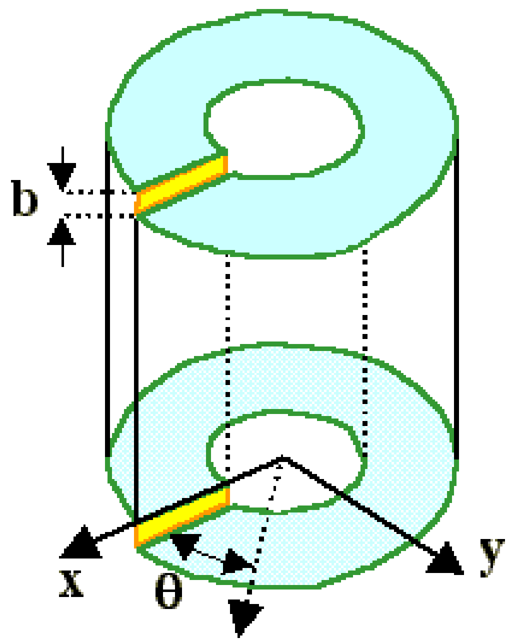



But oh no! What about the intermediate regions?

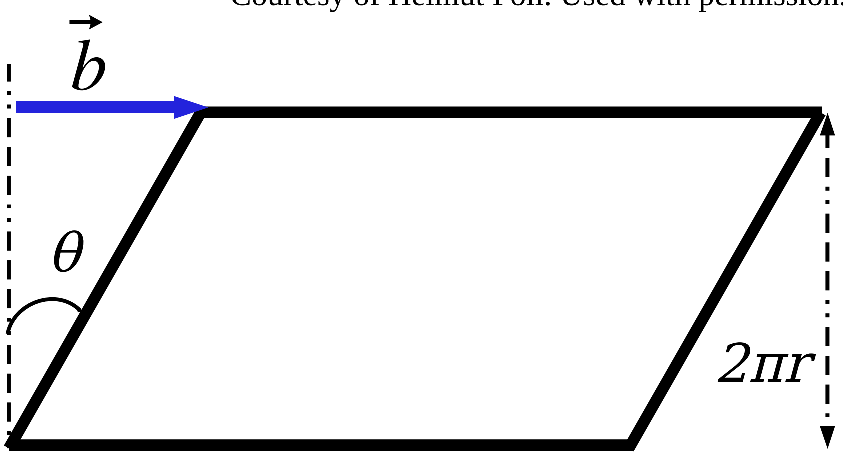
- Mixed dislocations: when $\vec{b}$ and $\vec{t}$ are neither parallel, antiparallel, or perpendicular
- Characterize them by decomposing $\vec{b}$ into parallel and perpendicular components



# Stress-Strain around Dislocations




Courtesy of Helmut Föll. Used with permission.

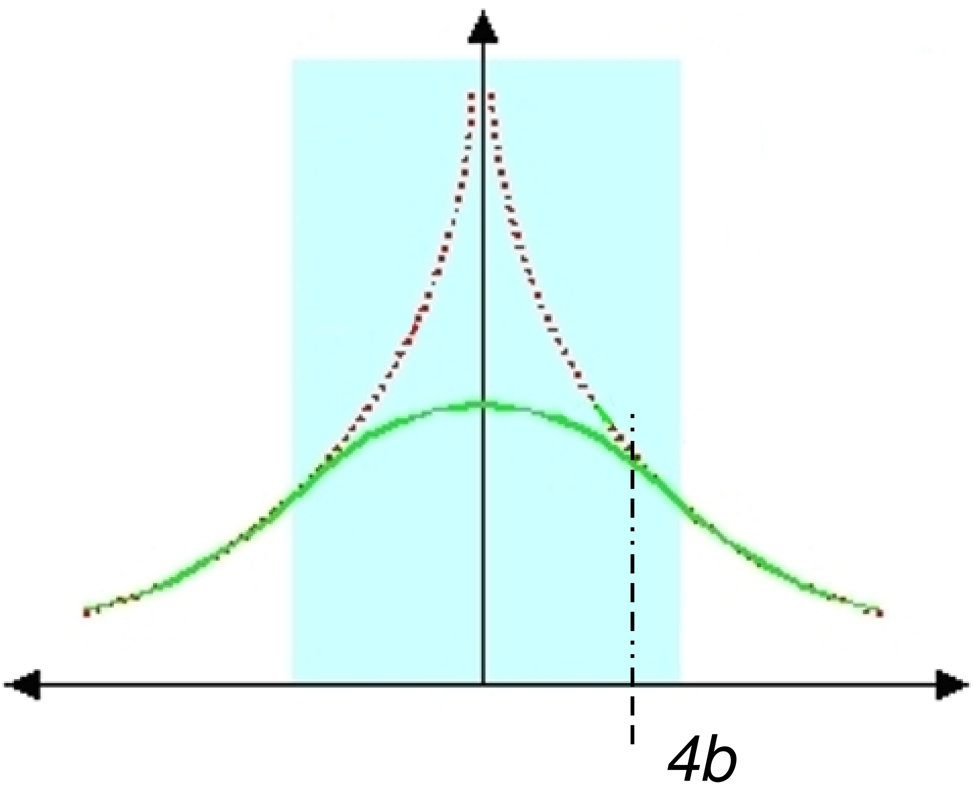



- Displacement → strain → stress → energy
- Construct a cylinder around the dislocation axis
- Unwrapping the cylinder produces a parallelogram
- $\gamma_{rz}^{screw} = \dfrac{b}{2\pi r} = \gamma_{zr}^{screw}$

$$\underline{\gamma} = \begin{bmatrix} \gamma_{rr} & \gamma_{zr} & \gamma_{\theta r} \\ \gamma_{rz} & \gamma_{zz} & \gamma_{\theta z} \\ \gamma_{r\theta} & \gamma_{z\theta} & \gamma_{\theta\theta} \end{bmatrix}$$

<http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html>

# Stress-Strain around Dislocations




Courtesy of Helmut Föll. Used with permission.

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<http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html>

# Dislocation Energy

$$W = E = \int_0^{\gamma} \tau d\gamma = \frac{1}{2}\tau\gamma_{rz} = \frac{1}{2}\mu\gamma_{rz}^2$$

$$W_{screw} = \int_z \int_r \frac{\mu b^2}{8\pi^2 r^2}$$

$$W/V = \frac{\mu b^2}{8\pi^2 r^2}$$

$$W = l\frac{\mu b^2}{4\pi}\ln(\frac{r_{outer}}{r_{inner}})$$

**Screw**

$$\boxed{\frac{W}{l} \sim \mu b^2}$$

**Edge**

$$\boxed{\frac{W}{l} \sim \frac{\mu b^2}{1-\nu}}$$

- Energy of dislocation proportional to length
  - Same dimensions as F, "line tension"
- Edge dislocation always higher energy
  - (1-ν)<1
- Crystals try to form long screw dislocations
  - Dislocations often zigzag to accommodate screw

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_2_3.html

# Mixed Dislocations

| Stress | Edge | Screw |
|---|---|---|
| $\sigma_{xx}$ | $-\dfrac{\mu b_y}{2\pi(1-\nu)}\dfrac{3x^2+y^2}{(x^2+y^2)^2}$ | 0 |
| $\sigma_{yy}$ | $\dfrac{\mu b_y}{2\pi(1-\nu)}\dfrac{x^2-y^2}{(x^2+y^2)^2}$ | 0 |
| $\sigma_{zz}$ | $\nu(\sigma_{xx}+\sigma_{yy})$ | 0 |
| $\tau_{xy}$ | $\dfrac{\mu b_x}{2\pi(1-\nu)}\dfrac{x^2-y^2}{(x^2+y^2)^2}$ | 0 |
| $\tau_{xz}$ | 0 | $\dfrac{\mu b}{2\pi r}\cos\Theta$ |
| $\tau_{yz}$ | 0 | $\dfrac{\mu b}{2\pi r}\sin\Theta$ |

# Stress Fields

- Dislocations can interact
- Imagine them like charges: similar dislocations repel, opposites attract

Image of stress fields around two dislocations removed due to copyright restrictions.

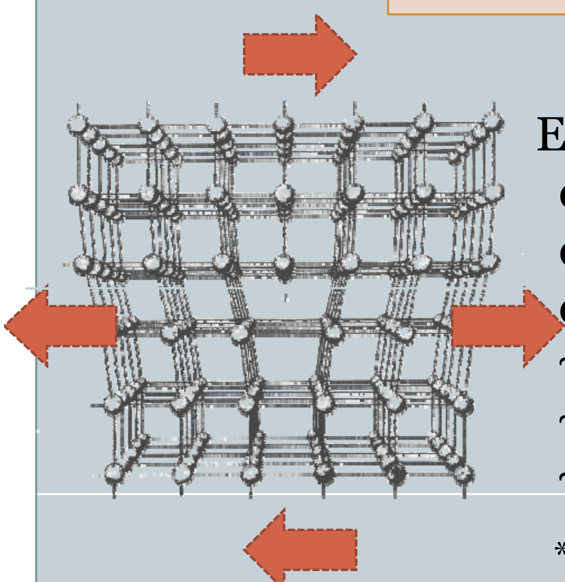
http://www.matter.org.uk/matscicdrom/manual/images/image109.gif

# Dislocation Motion

- Peach-Koehler Equation

$$F_x = b_x \sigma_{xy} + b_y \sigma_{yy} + b_z \sigma_{zy}$$

$$F_y = -\left(b_x \sigma_{xx} + b_y \sigma_{xy} + b_z \sigma_{xz}\right)$$



| Edge Dislocation | Screw Dislocation |
| --- | --- |
| $\sigma_{xx} \longrightarrow F \downarrow$ | $\sigma_{xx} \longrightarrow F = 0$ |
| $\sigma_{yy} \longrightarrow F = 0$ | $\sigma_{yy} \longrightarrow F = 0$ |
| $\sigma_{zz} \longrightarrow F = 0$ | $\sigma_{zz} \longrightarrow F = 0$ |
| $\tau_{xy} \longrightarrow F \rightarrow$ | $\tau_{xy} \longrightarrow F = 0$ |
| $\tau_{xz} \longrightarrow F = 0$ | $\tau_{xz} \longrightarrow F \downarrow$ |
| $\tau_{yz} \longrightarrow F = 0$ | $\tau_{yz} \longrightarrow F \rightarrow$ |

*assumes pos Edge, RH Screw

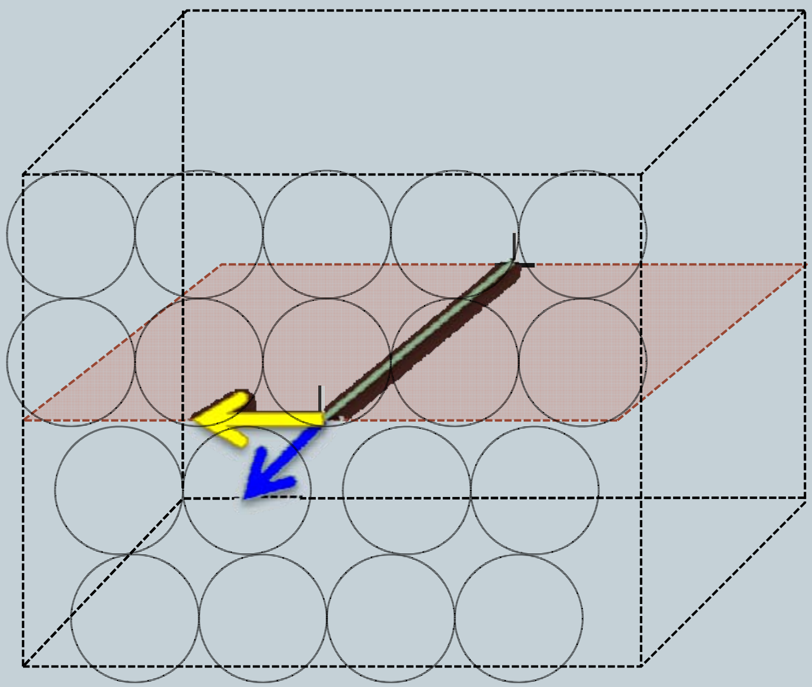
Image removed due to copyright restrictions. Please see the cover of *Nature Physics* 5 (April 2009).

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/dislocation_3dim.jpg

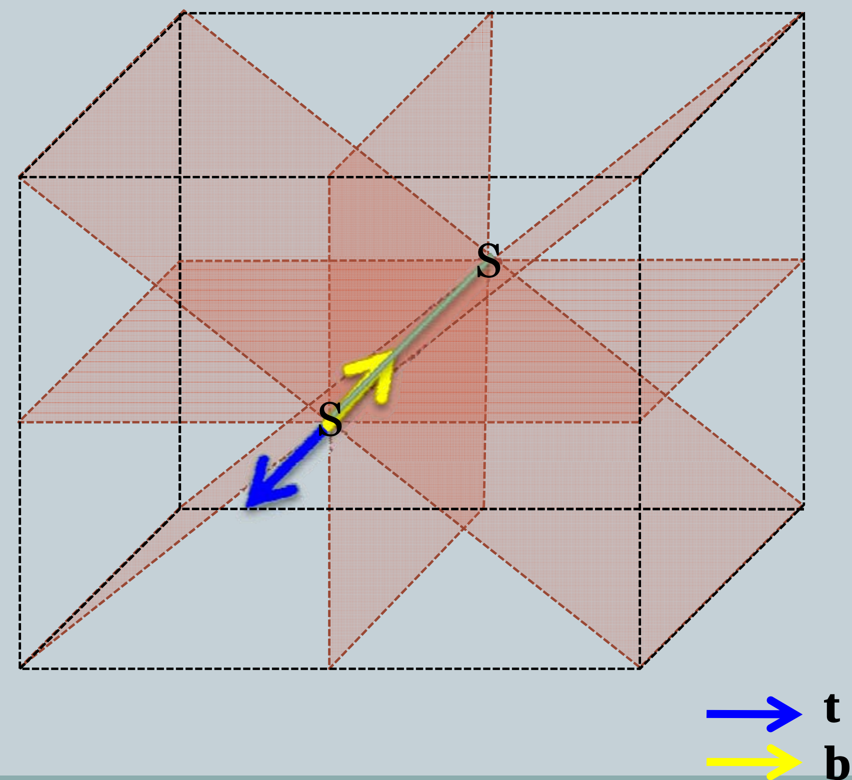
# Dislocation Motion

- Dislocation moves along plane containing **b, t**

**Edge**



**Screw**



# 1. Interactions between dislocations :

❖ General rule :

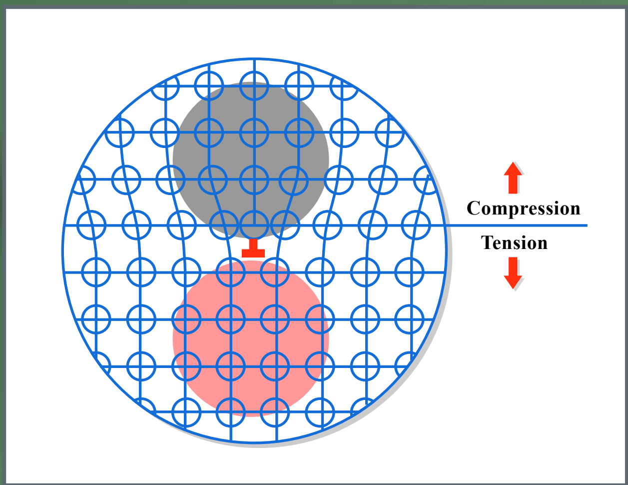
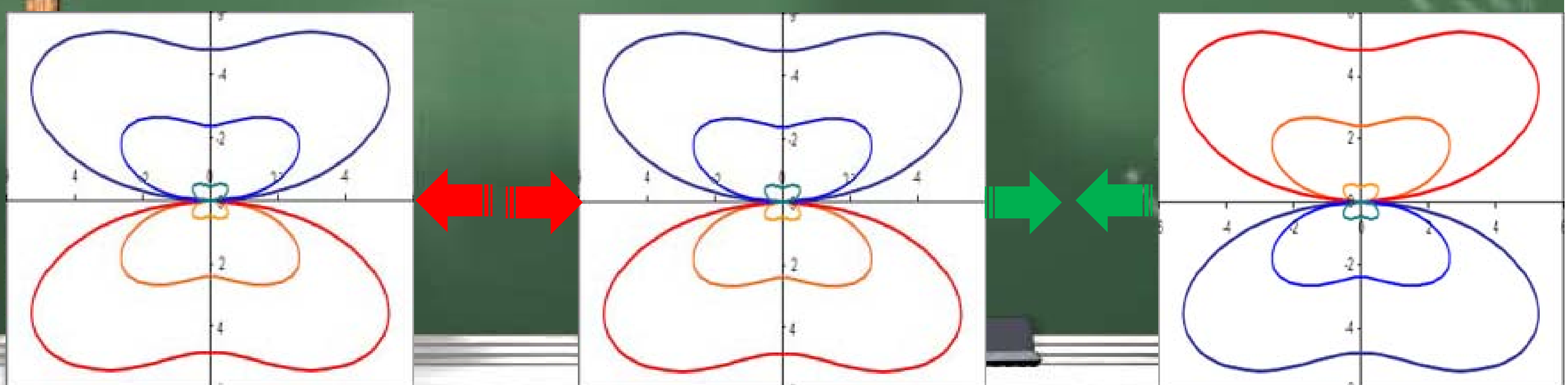



Figure by MIT OpenCourseWare.

□ □ Peach-Koehler equation :

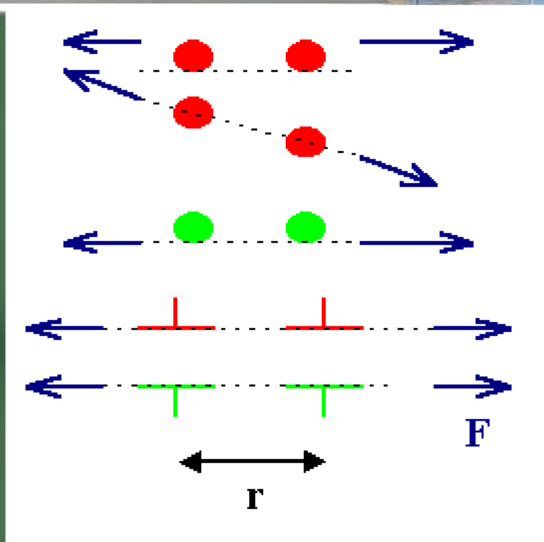
$$F_x = b_x\sigma_{xy} + b_y\sigma_{yy} + b_z\sigma_{zy}$$

$$F_y = -(b_x\sigma_{xx} + b_y\sigma_{xy} + b_z\sigma_{xz})$$



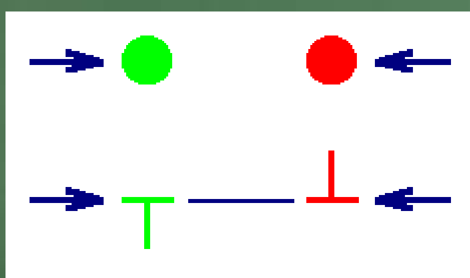
http://www.soton.ac.uk/~engmats/xtal/deformation/dislocation.html

## ❖ Main results :




Repulsion $F \sim b^2/r$

Courtesy of Helmut Föll. Used with permission.



Attraction $F \sim - b^2/r$

Courtesy of Helmut Föll. Used with permission.


No interaction

http://www.tf.uni-kiel.de/matwis/amat/

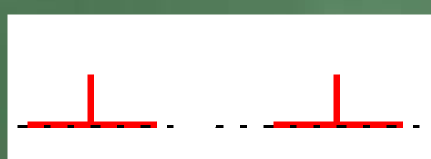
# 2. Effects on material behavior:

- Same plane, same sign ⇨ **PILE UP**

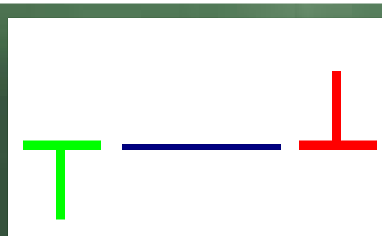
Please see videos of pileup and annihilation from Groupe Matériaux Cristallins sous sous Contrainte, CNRS.

- Same plane, opposite sign ⇨ **ANNIHILATION**

**Frank's rule :** $$\overline{b_3} = \overline{b_1} + \overline{b_2}$$



⇨ 2b



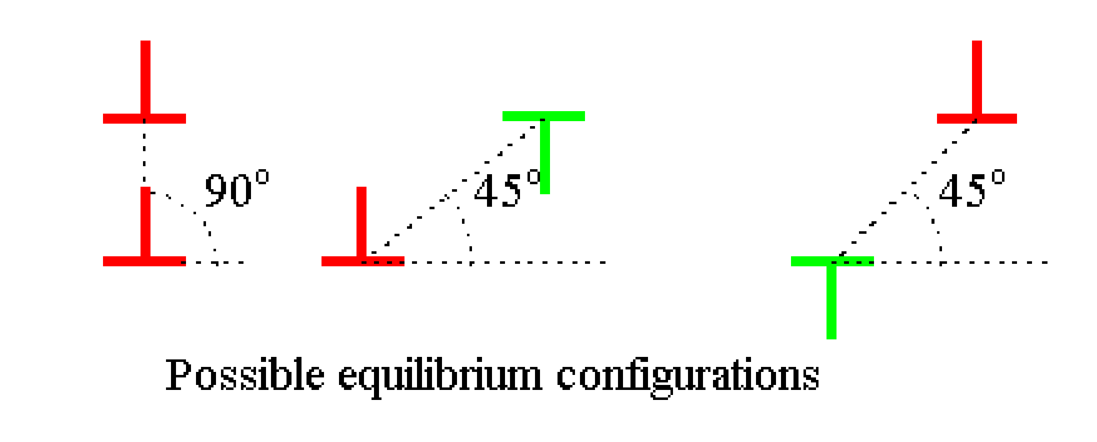
⇨ 0

Courtesy of Helmut Föll. Used with permission.

http://www.cemes.fr/r2_rech/r2_sr3_mc2

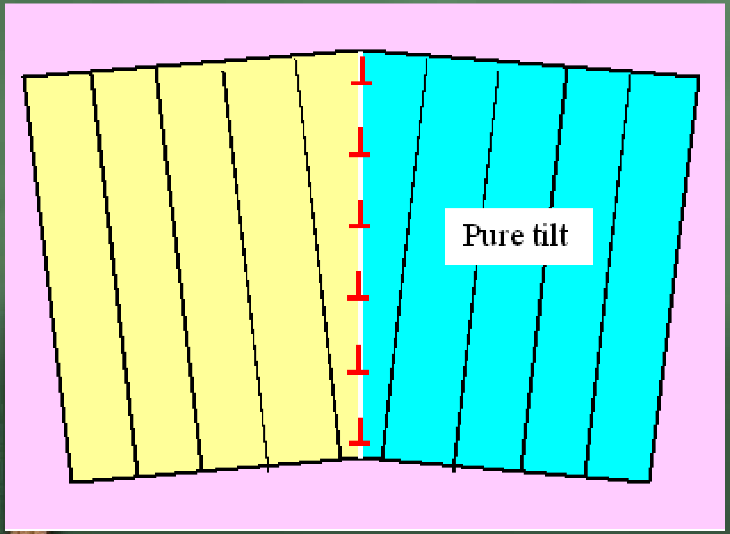
## ❖ Low energy configurations:

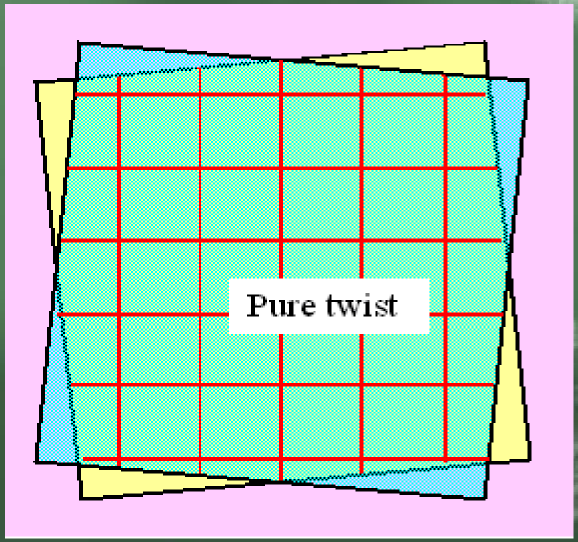
**Dislocation dipole :**




Courtesy of Helmut Föll. Used with permission.

**Grain boundaries :**



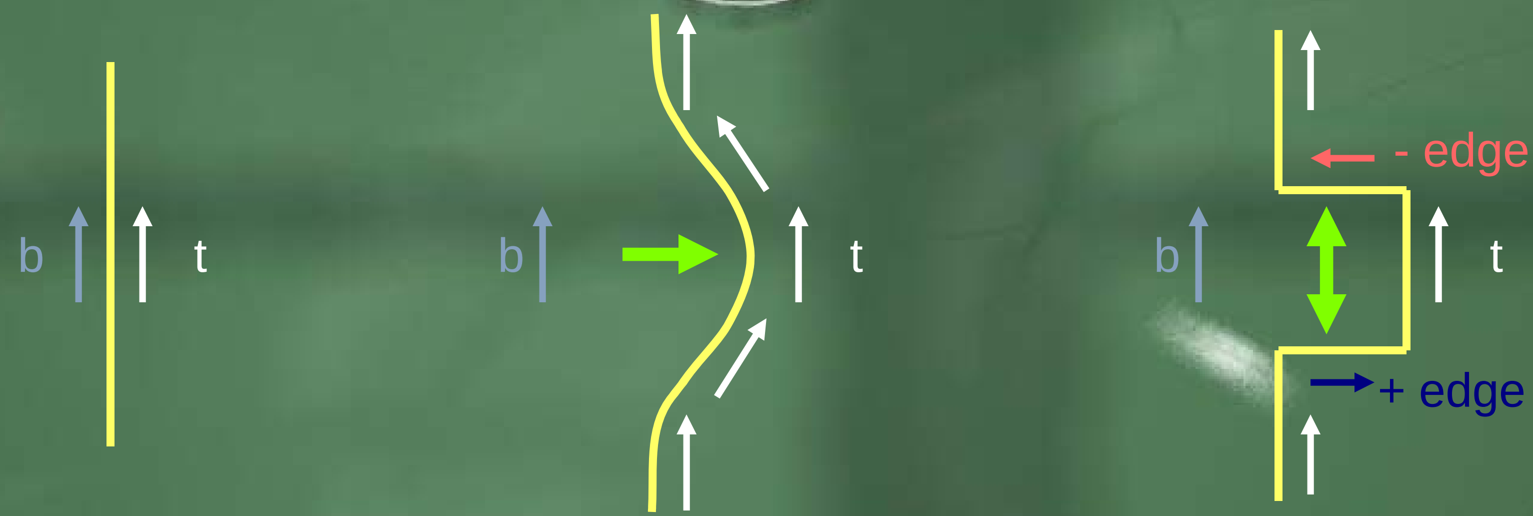




$$D = \frac{b}{\theta}$$

http://www.tf.uni-kiel.de/matwis/amat

Courtesy of Helmut Föll. Used with permission.

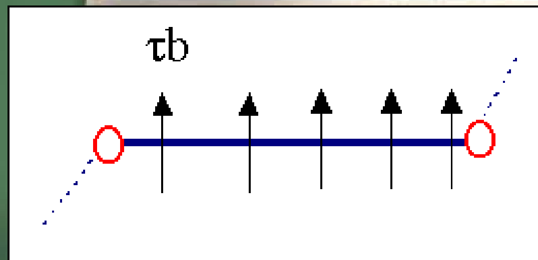
# 3. Line Tension

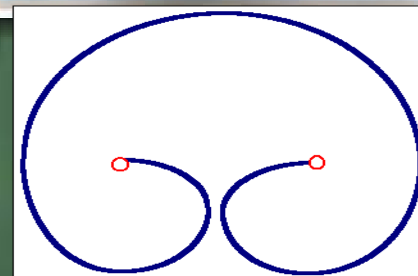



- Restoring force promotes straight dislocations
- Sharp bends are not favorable

# 4. Dislocation Multiplication

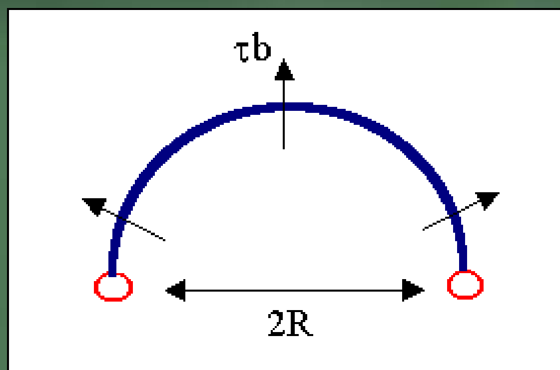
Pinned ends
Shear stress

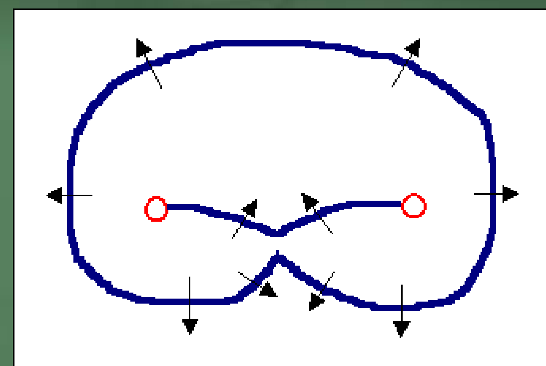


Two opposite segments meet and annihilate

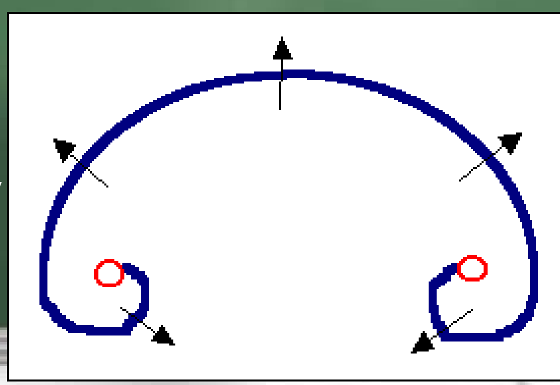
Dislocation bows out

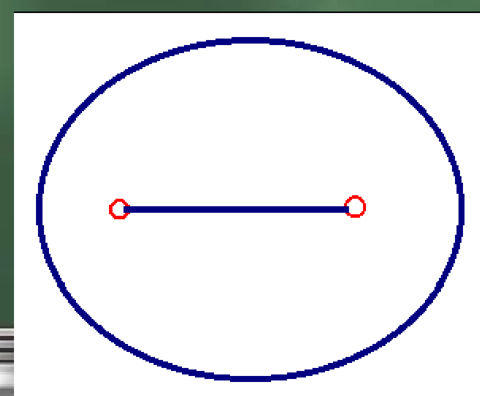


Loop and segment separate

Dislocation spontaneously grows





Loop expands

Line straightens

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_3_2.html

# Frank-Read Source

- Dislocation is pinned at both ends
- Shear stress is exerted on slip plane
- Force causes dislocation to lengthen and bend
- Dislocation spontaneously grows when
  - Shear stress overcomes restoring force
  - Past the semicircular equilibrium state
- Generate many dislocations on slip planes

Image removed due to copyright restrictions.

Please see http://commons.wikimedia.org/wiki/File:Frank-Read_Source.png

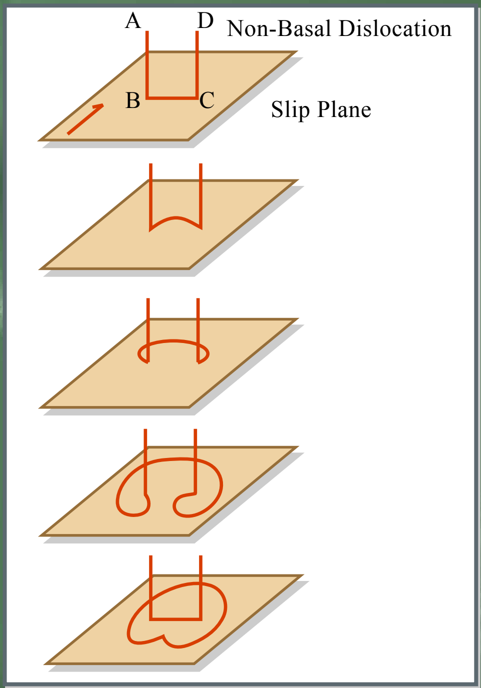
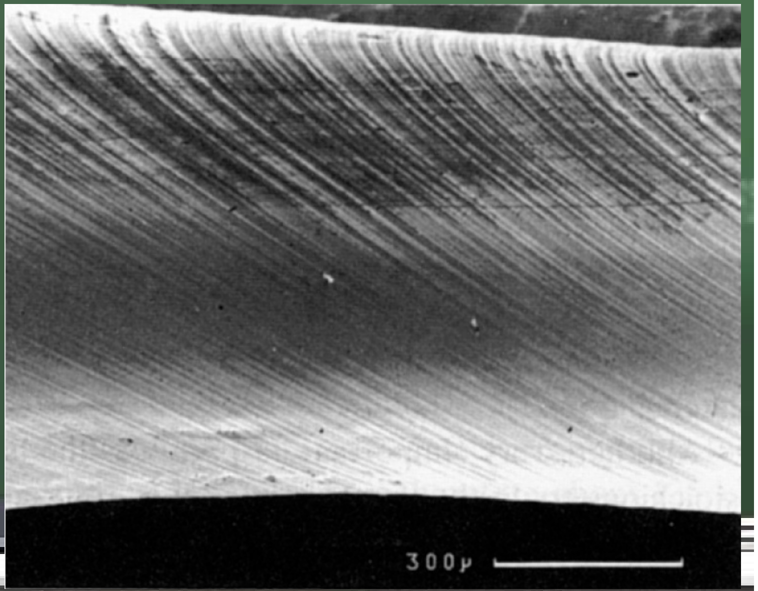



Figure by MIT OpenCourseWare.

http://web.earthsci.unimelb.edu.au/wilson/ice1/generations.html
http://en.wikipedia.org/wiki/Frank-Read_Source

# 5. Dislocation Observation

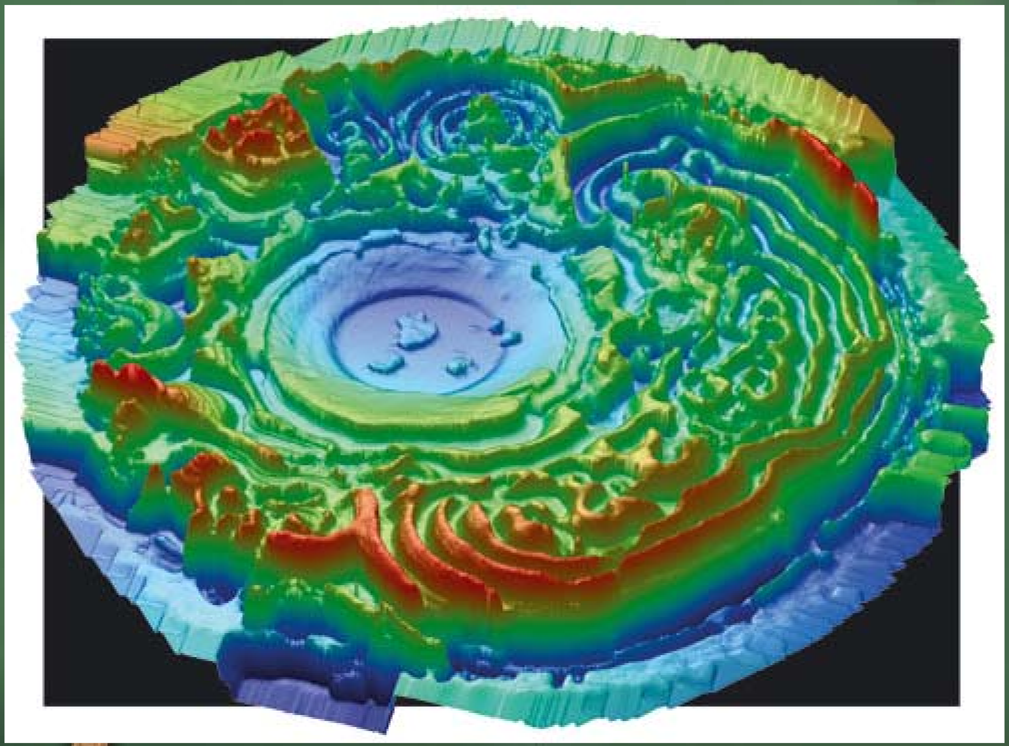
- Dislocations are sub-nm features
- Frank-read source generates many dislocations in one plane
- Therefore, it allows macroscopic observation of dislocations
  - Slip steps




Courtesy of DoITPoMS, University of Cambridge. Used with permission.

http://www.msm.cam.ac.uk/doitpoms/tlplib/miller_indices/printall.php

# Dislocation Observation



Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

- White light interferometer image from an optical profiler
- Partially decomposed crystalline GaN around a Ga droplet
- characteristics suggestive of a Frank-Read dislocation source
- Millimeter scale feature

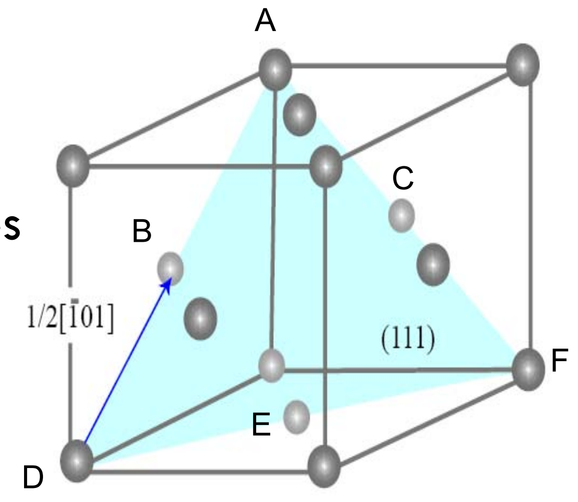
http://materialstoday.com/covercomp2008.html

# Key Lecture Topics

- **Crystal Structures in Relation to Slip Systems**
- **Resolved Shear Stress**
- **Using a Stereographic Projection to Determine the Active Slip System**

# Slip Planes and Slip Directions

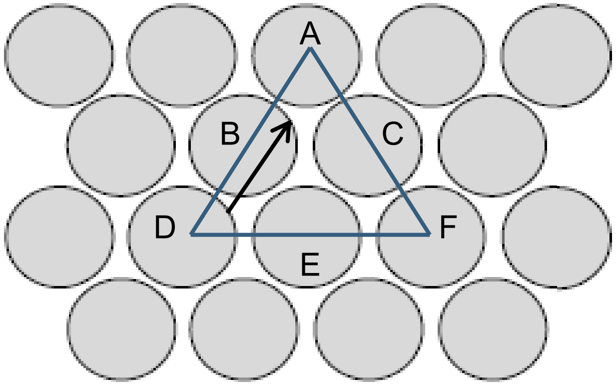
- *Slip Planes*
  - Highest Planar Density
    - Corresponds to most widely spaced planes
- *Slip Directions*
  - Highest Linear Density
- *Slip System*
  - Slip Plane + Slip Direction




Slip Plane: {111}

Figures by MIT OpenCourseWare.

The FCC unit cell has a slip system consisting of the {111} plane and the <110> directions.



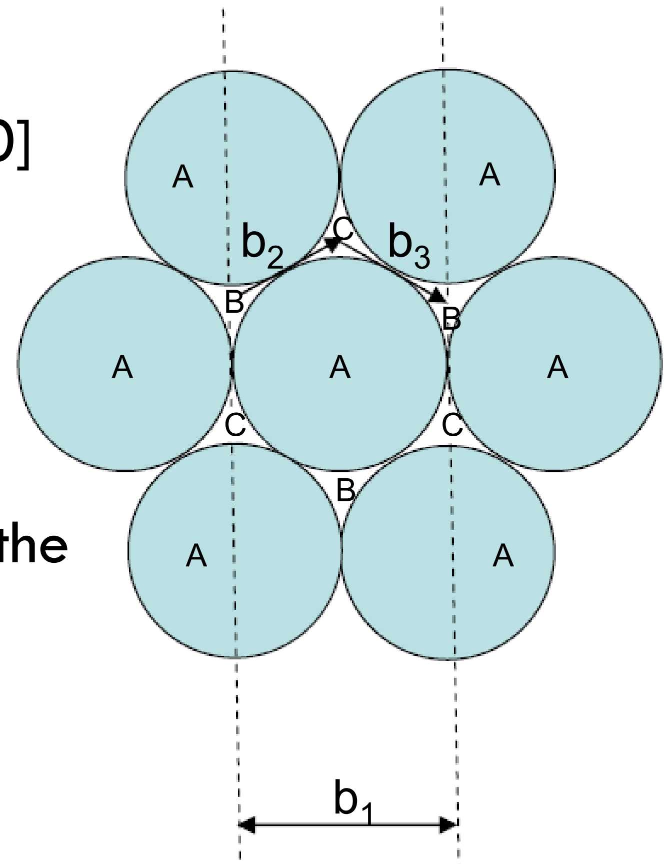
# Face Centered Cubic Slip Systems

FCC (eg. Cu, Ag, Au, Al, and Ni)

**Slip Planes** {111} **Slip Directions** [110]

- The shortest lattice vectors are ½[110] and [001]
- According to Frank's rule, the energy of a dislocation is proportional to the square of the burgers vector, $b^2$
- Compare energy
  - ½[110] dislocations have energy $2a^2/4$
  - [001] dislocations have energy $a^2$
  - → Slip Direction is [110]

Figure by MIT OpenCourseWare.




Partial dislocations along {111} planes in FCC metals.

# More Slip Systems

| *Metals* | *Slip Plane* | *Slip Direction* | *Number of Slip Systems* |
|---|---|---|---|
| Cu, Al, Ni, Ag, Au | **FCC** {111} | $<1\bar{1}0>$ | 12 |
| α-Fe, W, Mo | **BCC** {110} | $<\bar{1}11>$ | 12 |
| α-Fe, W | {211} | $<\bar{1}11>$ | 12 |
| α-Fe, K | {321} | $<\bar{1}11>$ | 24 |
| Cd, Zn, Mg, Ti, Be | **HCP** {0001} | $<11\bar{2}0>$ | 3 |
| Ti, Mg, Zr | $\{10\bar{1}0\}$ | $<11\bar{2}0>$ | 3 |
| Ti, Mg | $\{10\bar{1}1\}$ | $<11\bar{2}0>$ | 6 |

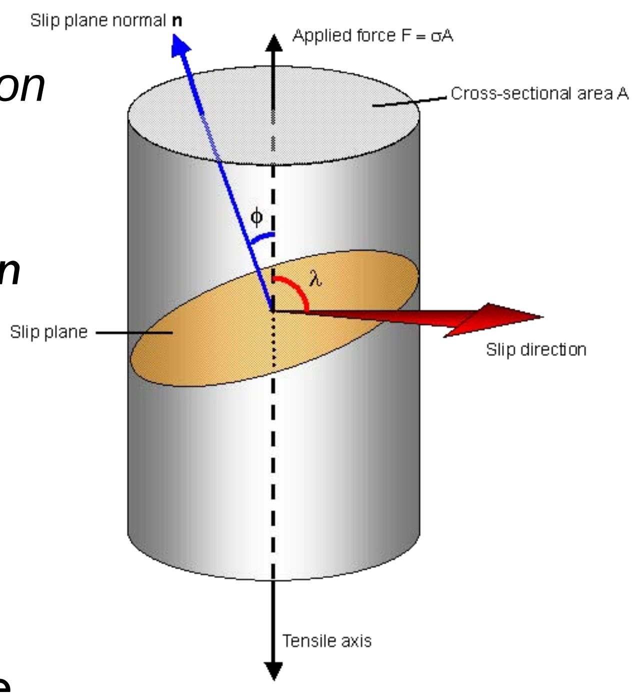
# Resolved Shear Stress

- What do we need to move dislocations?
  - **A Shear Stress!**

$$\sigma = F / A$$

$F \cos\lambda$ *Component of force in the slip direction*

$A / \cos\phi$ *Area of slip surface*




Courtesy of DoITPoMS, University of Cambridge. Used with permission.

  - *Thus the shear stress τ, resolved on the slip plane in the slip direction*

$$\tau = F / A \cos\phi \cos\lambda = \sigma \boxed{\cos\phi \cos\lambda}$$

**Schmid Factor**

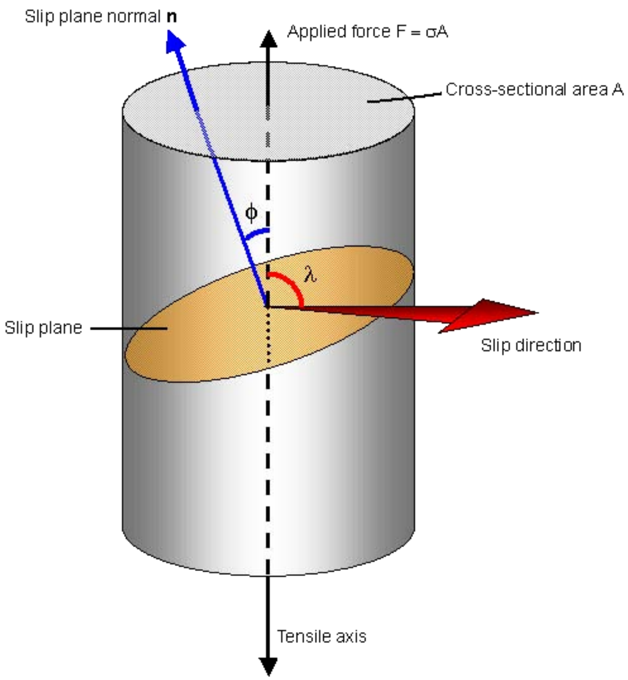
  - *Note that Φ + λ ≠ 90 degrees because the tensile axis, slip plane normal, and slip direction do not always lie in the same plane*

# Critical Resolved Shear Stress

- *Critical Resolved Shear Stress,* $\tau_{CRSS}$ - the minimum shear stress required to begin plastic deformation or slip.
  - Temperature, strain rate, and material dependent
  - The system on which slip occurs has the largest Schmid factor

$$\tau = F / A \cos\phi \cos\lambda = \sigma \cos\phi \cos\lambda$$

- The minimum stress to begin yielding occurs when $\lambda = \Phi = 45°$
  - $\sigma = 2\tau_{CRSS}$

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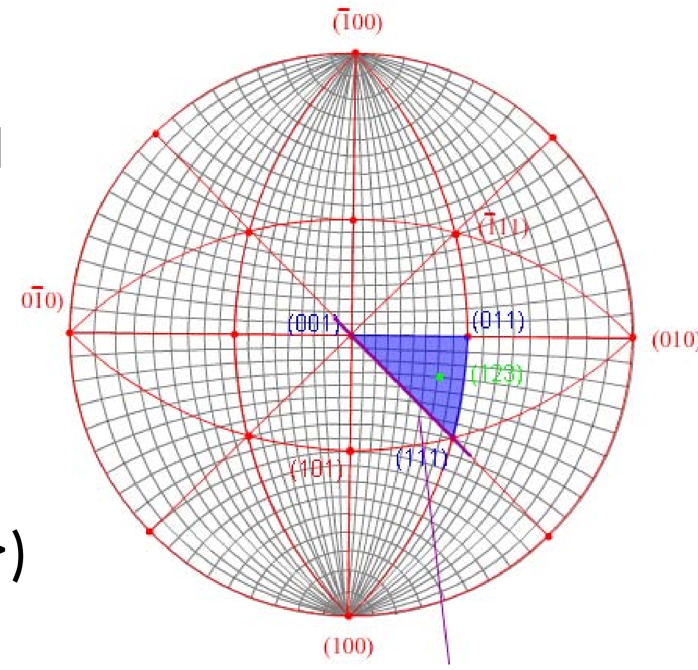
# Determining Active Slip System

- There are two methods to determine which slip system is active
  - *Brute Force Method*- Calculate angles for each slip system for a given load and determine the maximum Schmid Factor
  - *Elegant Method*- Use stereographic projection to determine the active slip system graphically

# Stereographic Projection Method

1. **Identify the triangle** containing the tensile axis
2. **Determine the slip plane** by taking the pole of the triangle that is in the family of the slip planes (i.e. for FCC this would be {111}) and reflecting it off the opposite side of the specified triangle
3. **Determine the slip direction** by taking the pole of the triangle that is in the family of directions (i.e. for FCC this would be <1-10>) and reflecting it off the opposite side of the specified triangle

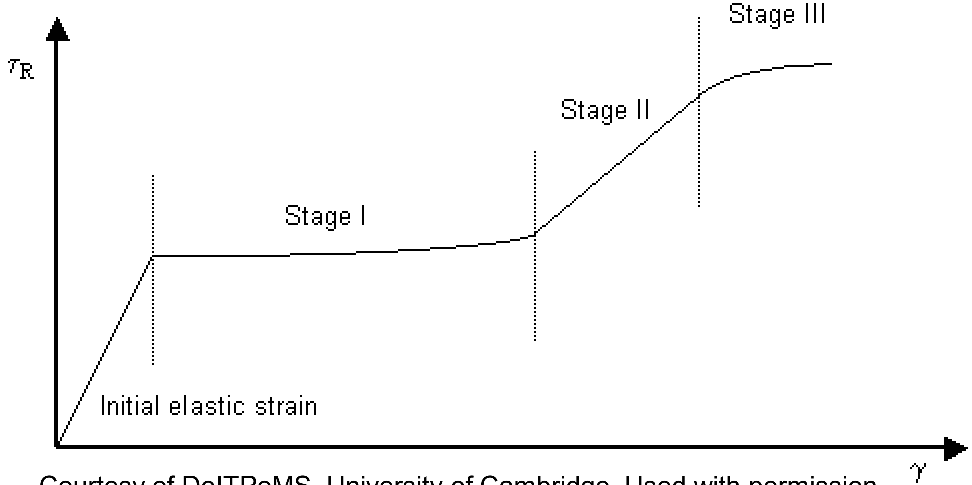
Courtesy of DoITPoMS, University of Cambridge.



# Rotation of Crystal Lattice Under an Applied Load

- With increasing load, the slip plane and slip direction align parallel to the tensile stress axis
- This movement may be traced on the stereographic projection
- The tensile axis rotates toward the slip direction eventually reaching the edge of the triangle
  - Note that during compression the slip direction rotates away from the compressive axis
- At the edge of the triangle a second slip system is activated because it has an equivalent Schmid factor

# More Physical Examples




Courtesy of DoITPoMS, University of Cambridge. Used with permission.

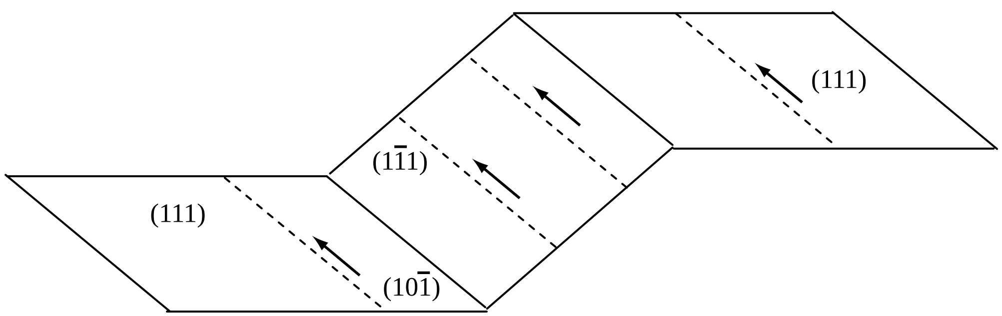
- *Initial Elastic Strain*- results from bond stretching (obeys Hooke's Law)
- *Stage I (easy glide)*- results from slip on one slip system
- *Stage II*- Multiple slip systems are active. A second slip system becomes active when it's Schmid factor increases to the value of the primary slip system
- In some extreme orientations of HCP crystals, the material fractures rather than deforms plastically

# 3.40 Sept 30th Lecture Highlights

- Cross-slip
- Applied stress:
  - Stress axis & slip systems
- Dislocation Locking Interactions
  - Intersections
  - Combinations
- Partial Dislocations

# Cross-slip

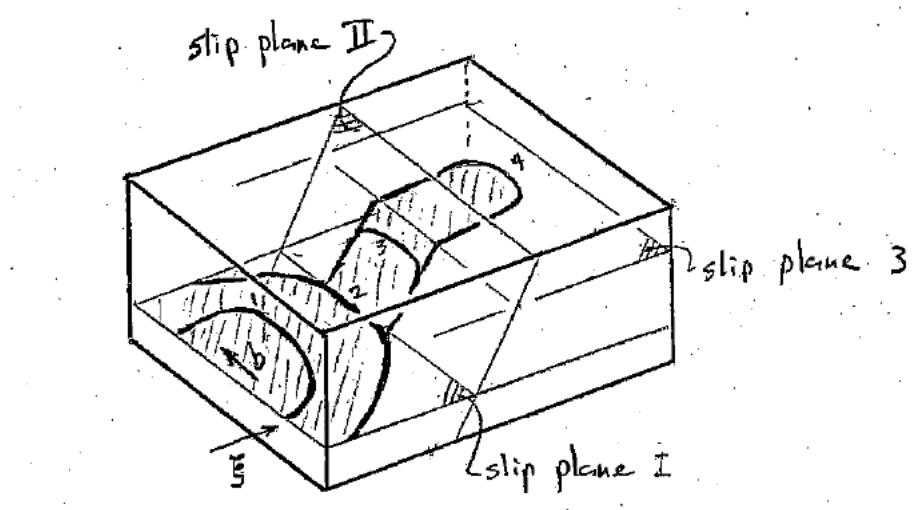
- Overcome an obstacle in primary slip plane
  - Screw dislocation: no uniquely defined slip plane
  - Transfer to intersecting slip plane <u>with same **b**</u>
  - Returns to initial slip plane (double cross slip)
  - Conservative: length of dislocation line unchanged




W. Hosford. Mechanical behavior of materials. Cambridge. 2005



Please also see Fig. 10.8 in Hosford, William F. *Mechanical Behavior of Materials*. New York, NY: Cambridge University Press, 2005.



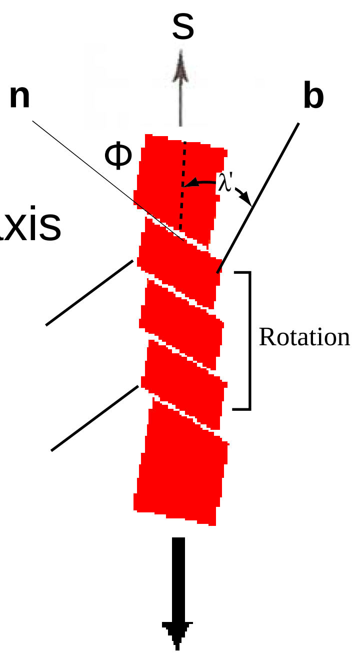

S Baker. MS&E 402 course notes 2006. Cornell University

# Effects of Stress

Reorientation of stress axis

Tension: **s** towards slip direction **b**

Compression: **s** towards slip plane **n**




Changes Schmid factors:

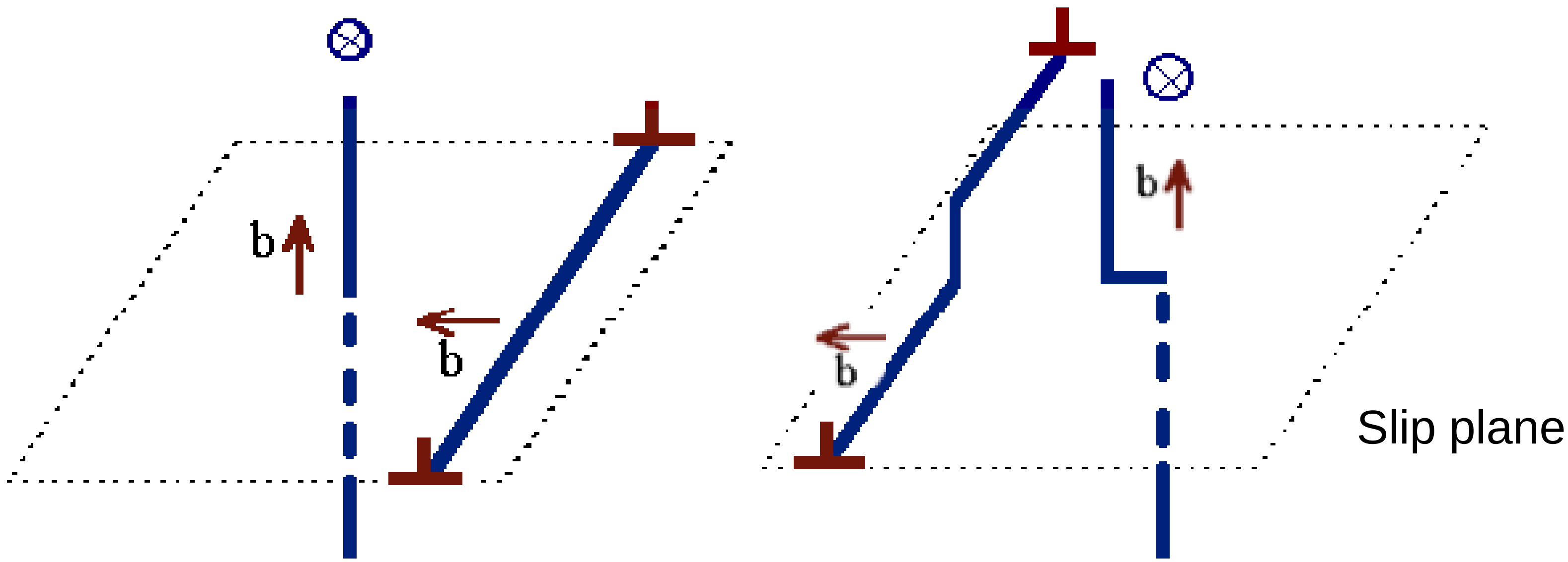
Activates new slip systems

Image removed due to copyright restrictions.
Please see Fig. 5.31 in Reed-Hill and Abbaschian, *Physical Metallurgy Principles*. Boston, MA: PWS Publishing, 1994.

FCC <110>{111} slip system
Tension applied

T. Courtney. Mechanical behavior of materials. 2000   R. Abbaschian, R Hill. Physical metallurgy principles. Cengage Learning. 2008

# Dislocation Intersections

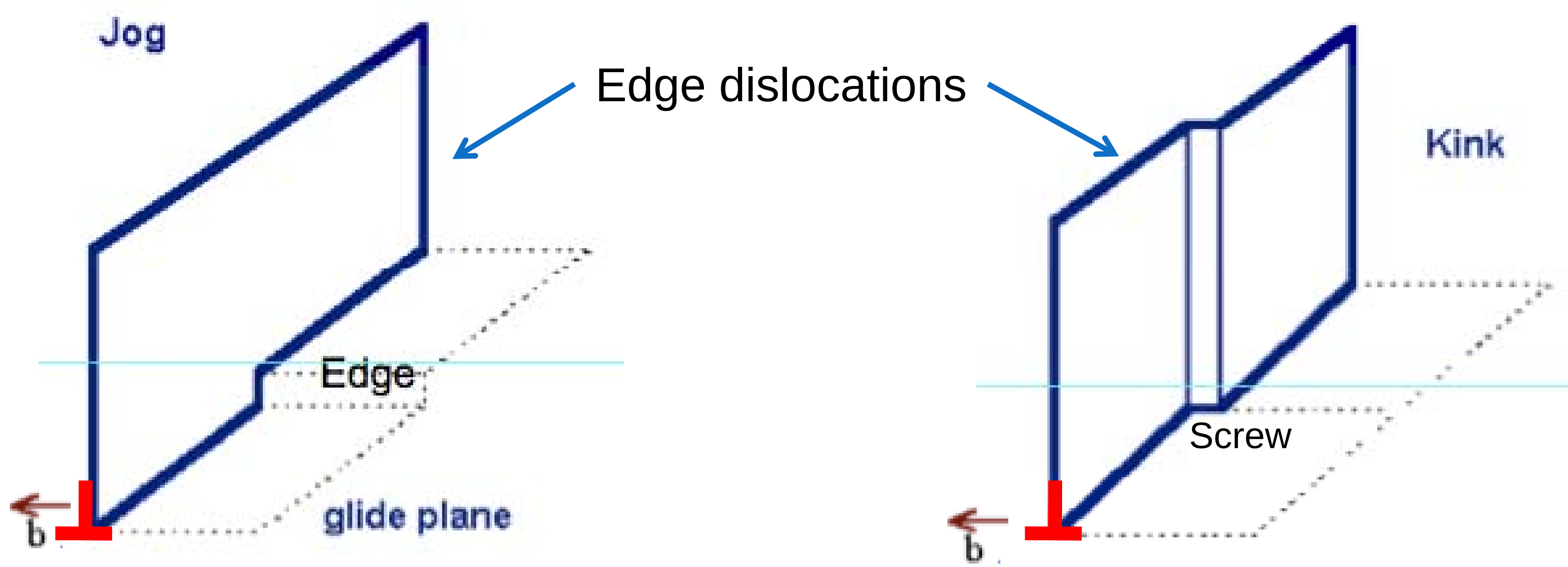



Courtesy of Helmut Föll. Used with permission.

- Dislocation acquires a step
  - Equal in direction and magnitude to intersecting dislocations burgers vector
    - Exception: **b** || dislocation line: Nothing happens
  - May have different character and glide plane than original dislocation

http://www.bss.phy.cam.ac.uk/~amd3/teaching/A_Donald/Crystalline_solids_2.htm

# Steps in Dislocations




| Step normal to slip plane | Step in slip plane |
| --- | --- |
| Changes glide plane | Constant glide plane |
| Pinning point (glissile) | Mobile (sessile) |



http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html

# Steps in Dislocations- Visual

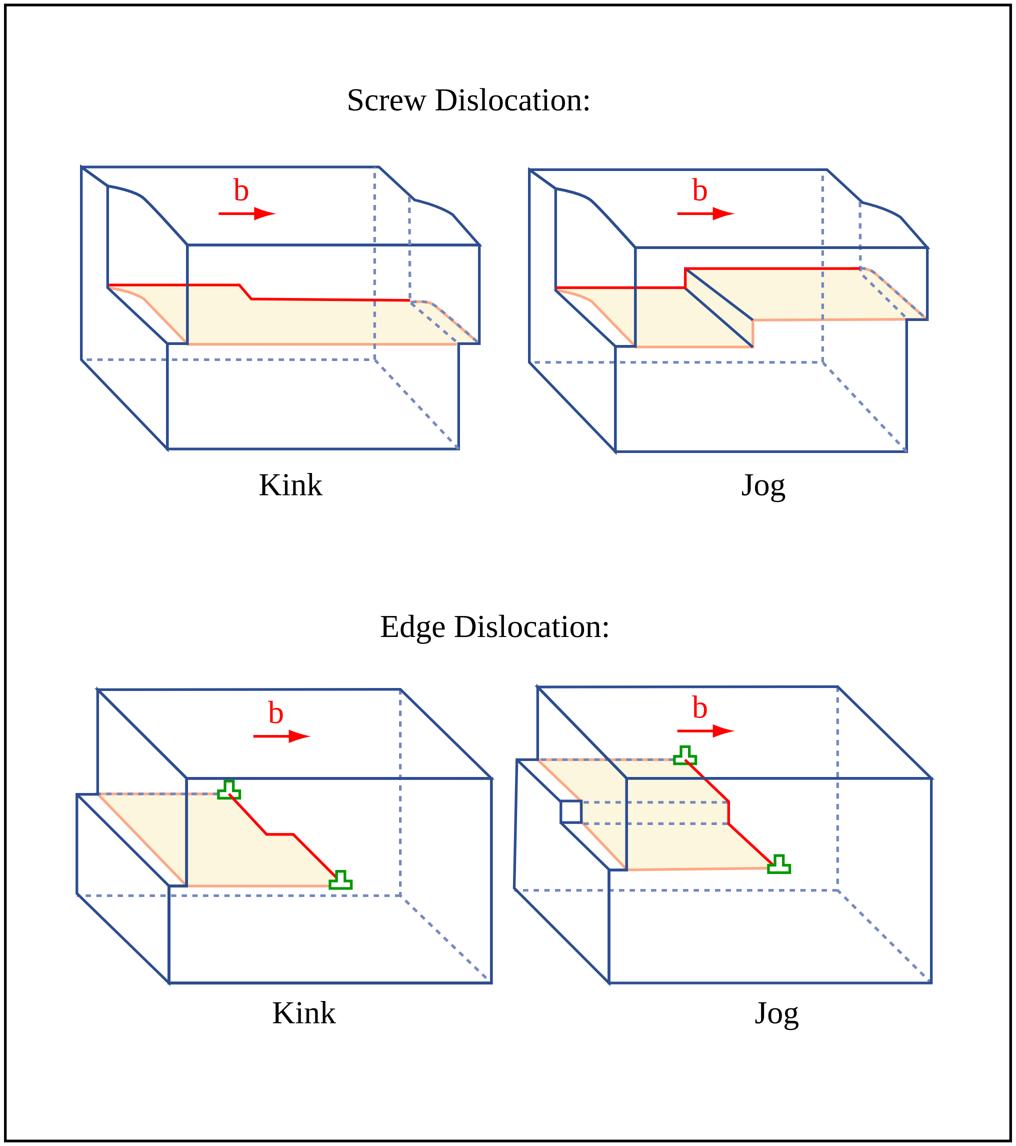
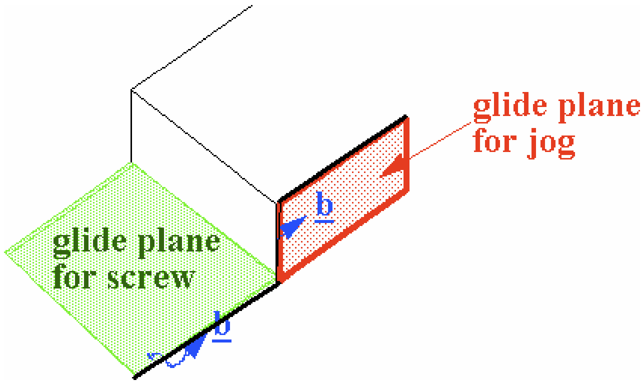



Figure by MIT OpenCourseWare




Courtesy of A. M. Donald. Used with permission.

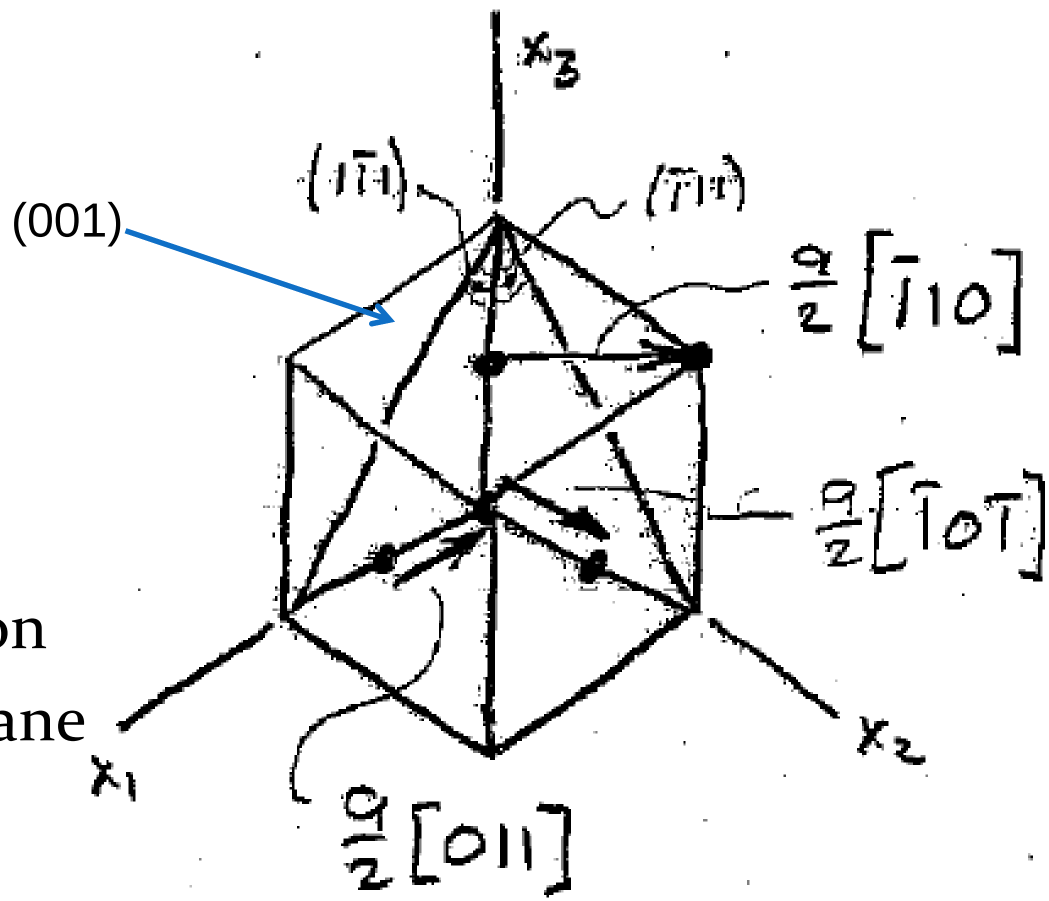
web.nchu.edu.tw/~jyuan/handout/3_3%20Dislocation.pdf

# Lomer Lock: Combination

- 2 Dislocations on primary slip planes combine

$$\frac{a^2}{2}+\frac{a^2}{2}>\frac{a^2}{2}$$

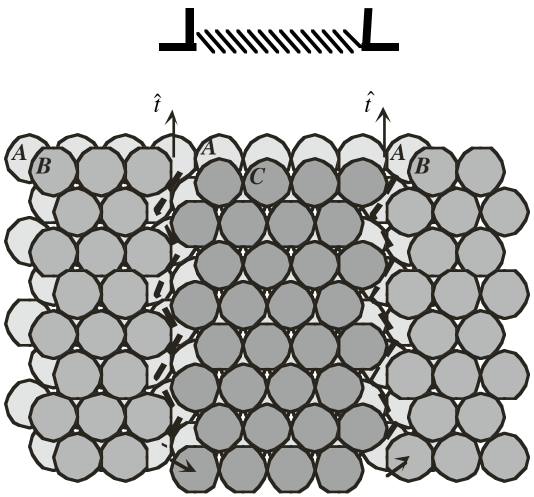
- new dislocation:
  - **b** primary slip direction
  - **n** non-primary slip plane
- Dislocation becomes immobile “locked”





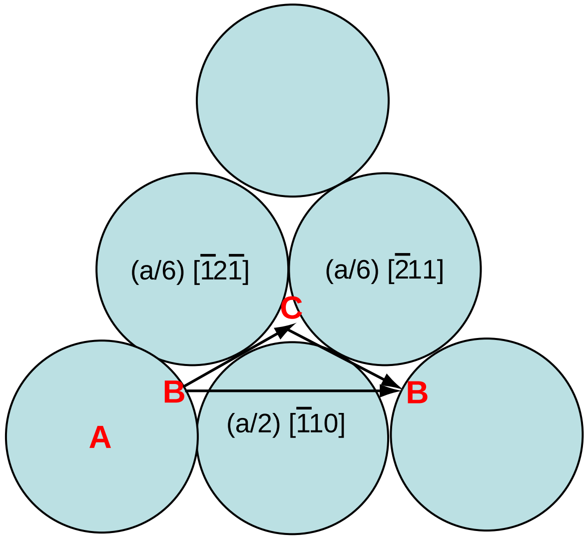

S Baker. MS&E 402 course notes 2006. Cornell University

# Partial Dislocations




Partial dislocation

Single dislocation → 2 partials & stacking fault




$E_{disloc} \cong \mu b^2/2$

$$\frac{E_{partials}}{E_{Perfect}} \frac{\frac{a^2}{6}+\frac{a^2}{6}}{\frac{a^2}{2}} = \frac{2}{3}$$

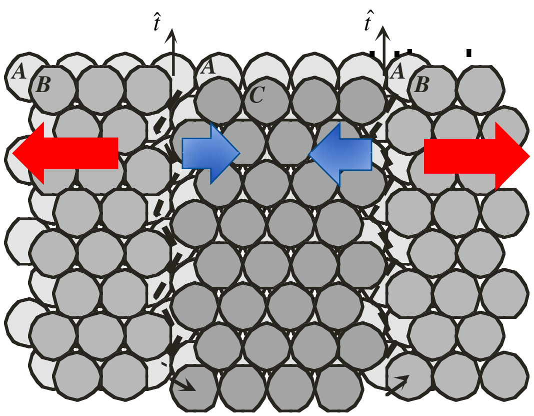

Please also see Fig. 9.20 and 9.25 in Hosford, William F. *Mechanical Behavior of Materials*. New York, NY: Cambridge University Press, 2005.

A. Putnis. Introduction to mineral sciences. Cambridge Univ. Press. 1992

# Partial Dislocations

Dislocations repel

Stacking fault resists




Partial dislocation

- Stacking Fault Energy $\gamma_{SF}$ (mJ/m$^2$)
- Ag: 22   Cu: 78   Ni: 128

- Low $\gamma_{SF}$ = large separation
- Hinders partial recombination
    - Limits cross-slip
    - Easier work hardening

$$\gamma_{SF}\ \Delta x \propto \frac{\mu b^2}{\gamma_{SF}}$$

$$\gamma_{SF} = b\tau$$

$$\tau = \frac{\mu b}{2\pi\Delta x}(screw)\frac{\mu b}{2\pi(1-\nu)\Delta x}(edge)$$



Please also see Fig. 9.25 in Hosford, William F. *Mechanical Behavior of Materials*. New York, NY: Cambridge University Press, 2005.

A. Putnis. Introduction to mineral sciences. Cambridge Univ. Press. 1992

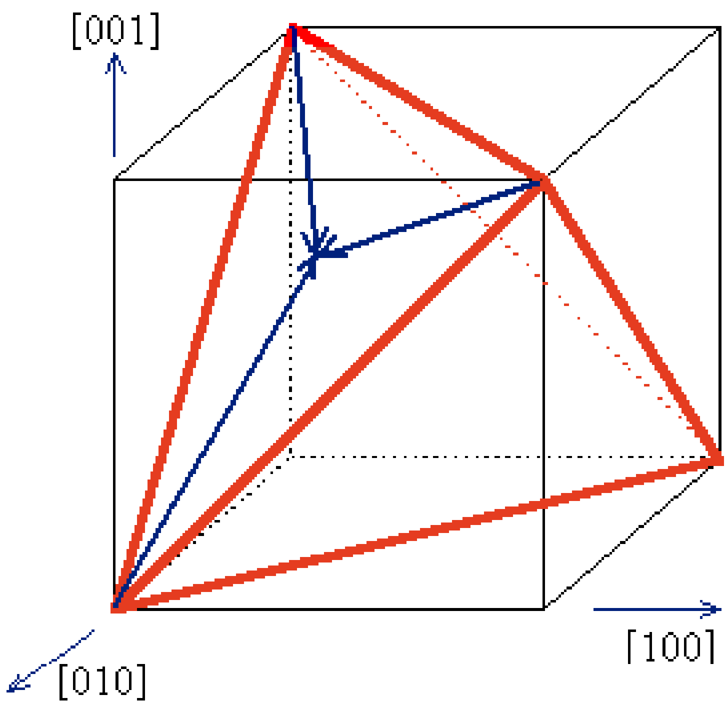
L. E. Murr, Interfacial Phenomena in Metals and Alloys(Addison Wesley, Reading MA, 1975).

# Thompson's Tetrahedron

- Notation for all slip planes, directions, and partials.

  <u>Example: FCC</u>

- Triangles are slip planes
  - {111}
- Edges are slip directions
  - <110>
- Blue arrows:
  - Partial dislocations

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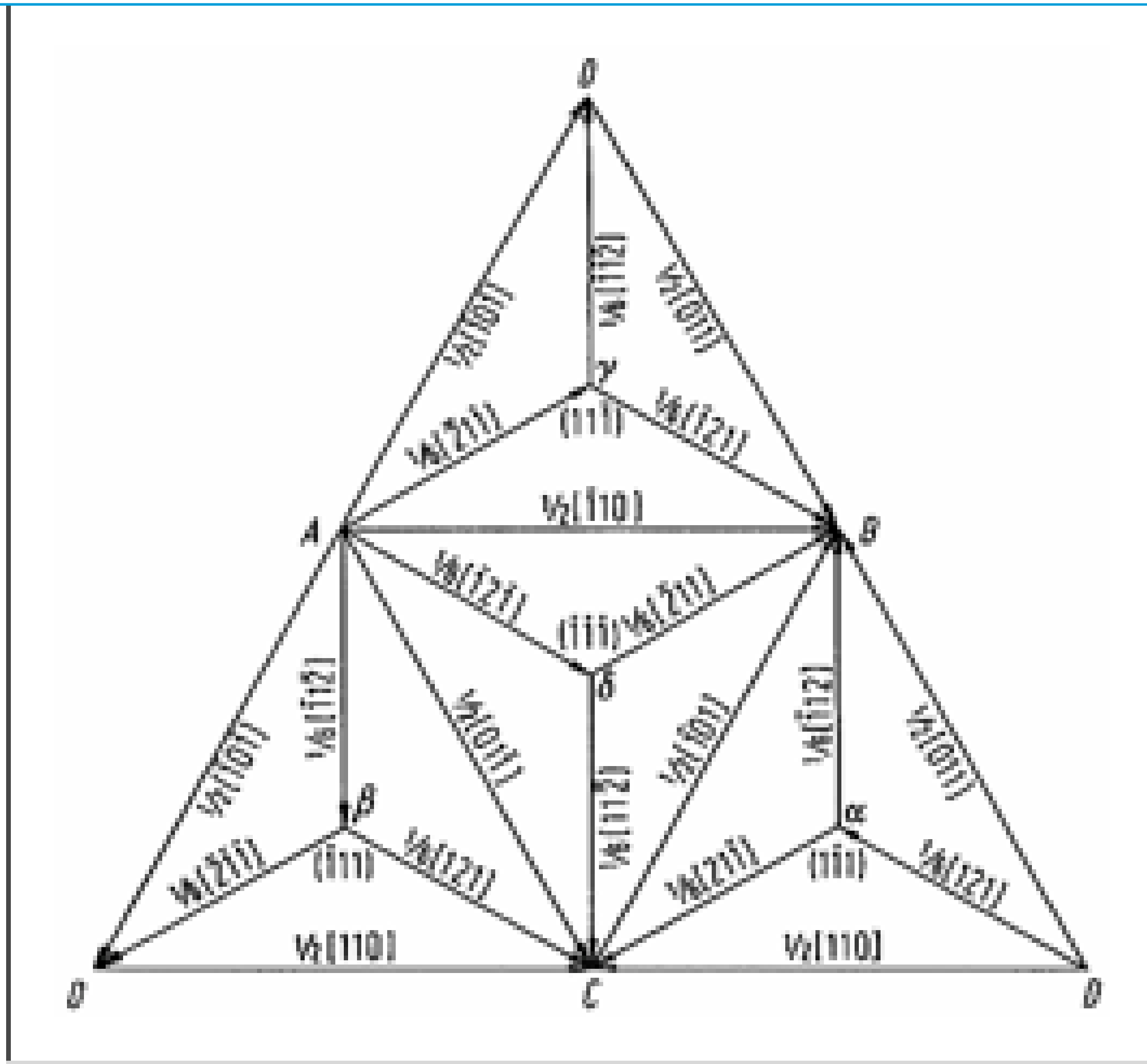
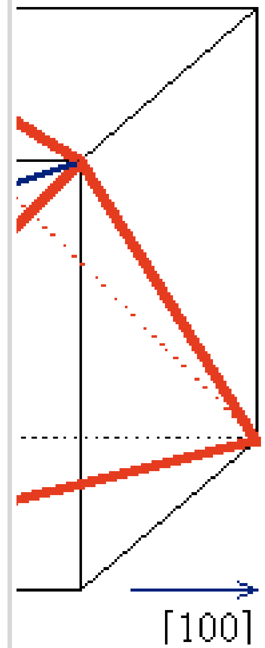
http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/i5_4_5.html

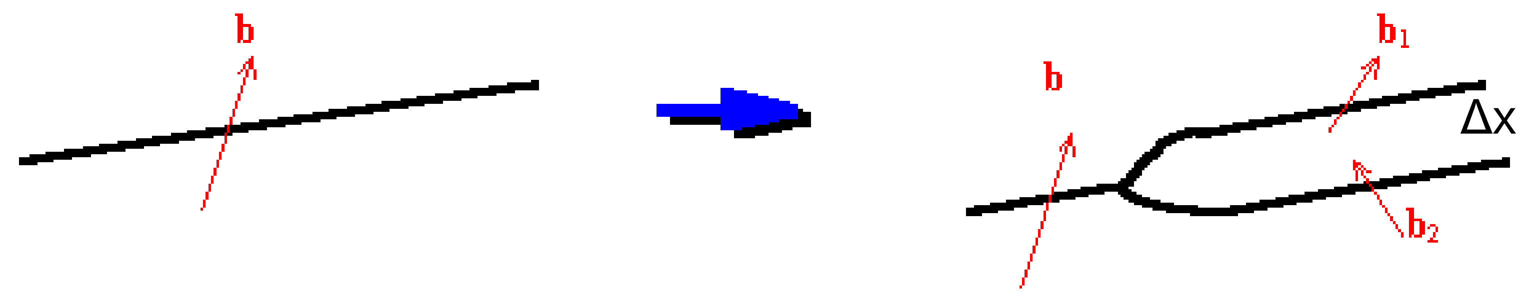
# Thompson's Tetrahedron

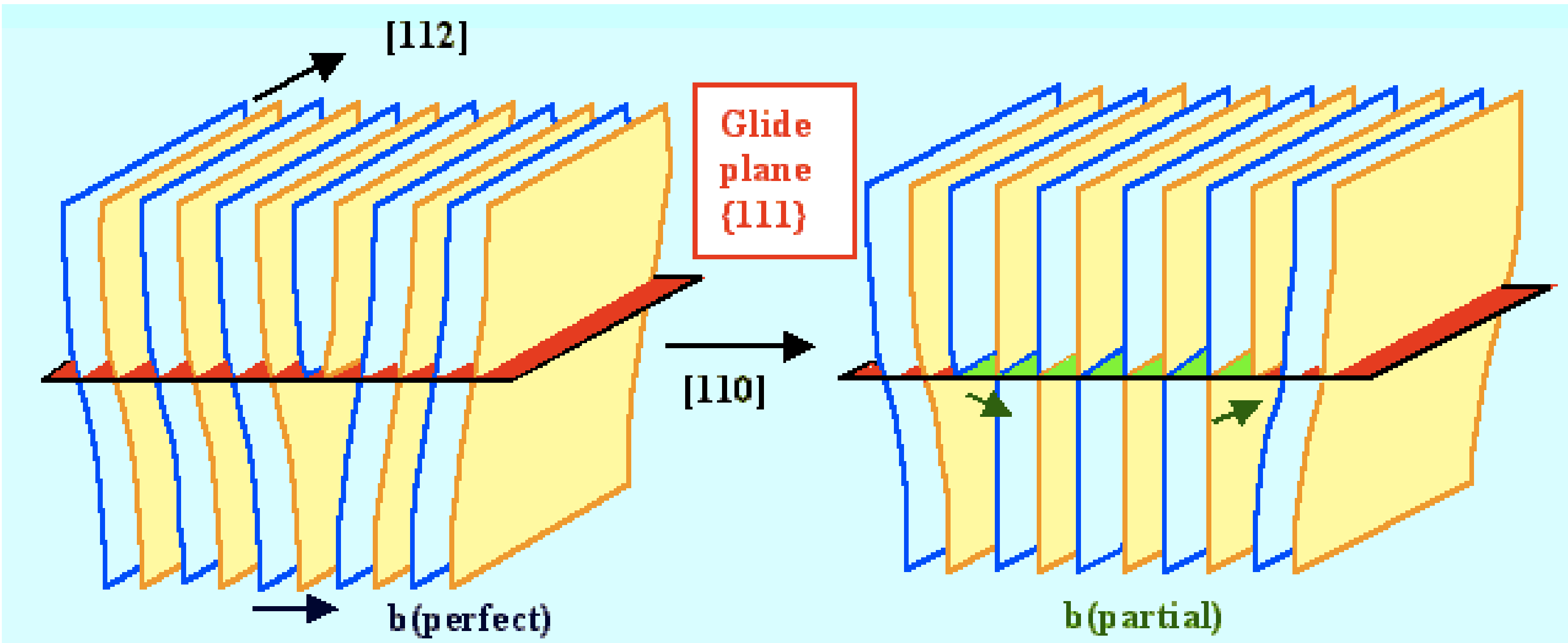
- Exam
- Trian
  - {111
- Edges
  - <11
- Blue a
  - Par




http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/i5_4_5.html




Courtesy of Helmut Föll. Used with permission.

View from below
Glide plane

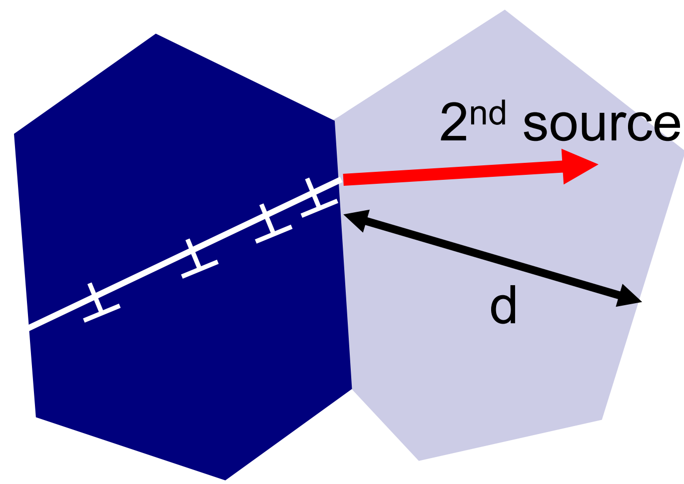
Image removed due to copyright restrictions.
Please see Fig. 5.8b in Hull, D., and D. J. Bacon.
*Introduction to Dislocations*. Boston, MA: Butterworth-Heinemann, 2001.

# DISLOCATION INTERACTIONS

- Dislocations reduce the stress required to plastically deform materials
- Dislocations interact with
  - Forests of Dislocations
  - Grain Boundaries
    - Hall - Petch Relationship

$$\tau_y \propto \frac{1}{\sqrt{d}}$$

  - Precipitates
  - Solutes




Courtesy of Markus Buehler. Used with permission.

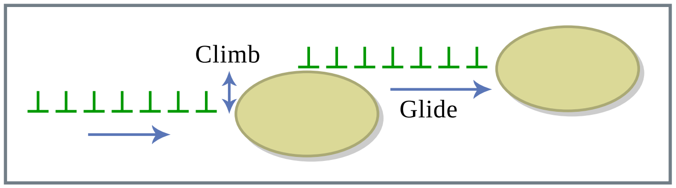
**Schematic of a Dislocation Pile up at a Grain Boundary**

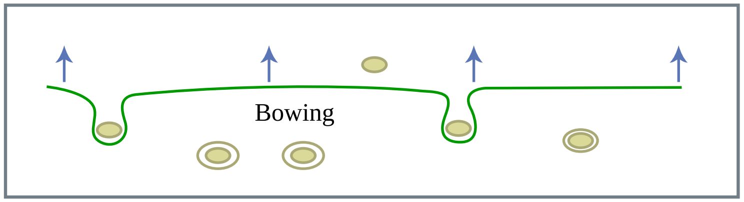
Mechanical Metallurgy, Dieter G., 3rd Edition

http://en.wikipedia.org/wiki/File:Dislocation_pileup.png

# OROWAN LOOPING

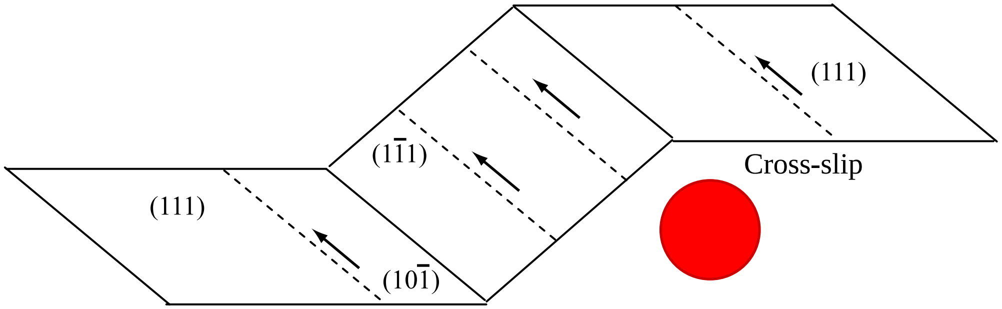
- Precipitates act as pinning points for dislocations




Figures by MIT OpenCourseWare.

- Bowing leads to unpinning leaving behind dislocation loops around the particles




Courtesy of Krystyn Van Vliet. Used with permission.

Please also see "Strengthening Processes: Dispersion Hardening." *aluMATTER*, University of Liverpool.

**Dislocation bypass around precipitates**

http://www.cemes.fr/r2_rech/r2_sr3_mc2/videos

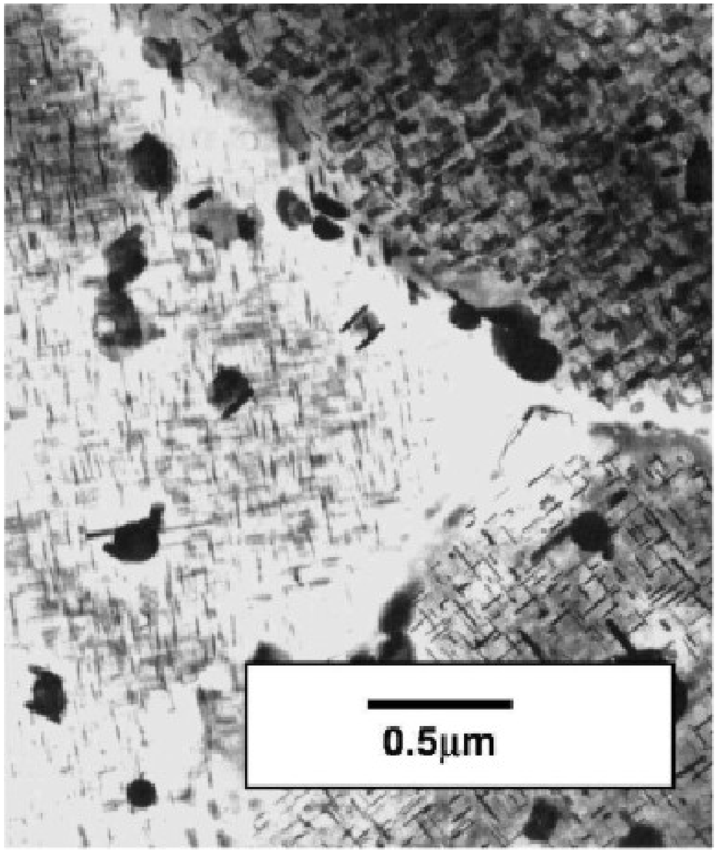
http://aluminium.matter.org.uk/

# OROWAN LOOPING

- Yield Stress to overcome obstacles:

$$\tau_y \approx \frac{\mu b}{L} = \alpha \mu b \sqrt{\rho_\perp}$$

- Dislocation density has units of 1/Area
- Ageing  Treatment
  - Precipitation Hardening
  - eg. Al – Cu alloys
  - “Overageing”




**Microstructure of an aged Al – 4 % Cu alloy showing CuAl2 precipitates**
http://aluminium.matter.org.uk/

Fig. 1204.03.18 in Jacobs, M. H. "1204 Precipitation Hardening." *Introduction to Aluminium Metallurgy*. TALAT, 1999.

# WORK HARDENING

- Orowan's Equation:

$$\tau_y \approx \alpha' \mu \sqrt{b\gamma} \approx K\sqrt{\gamma}$$

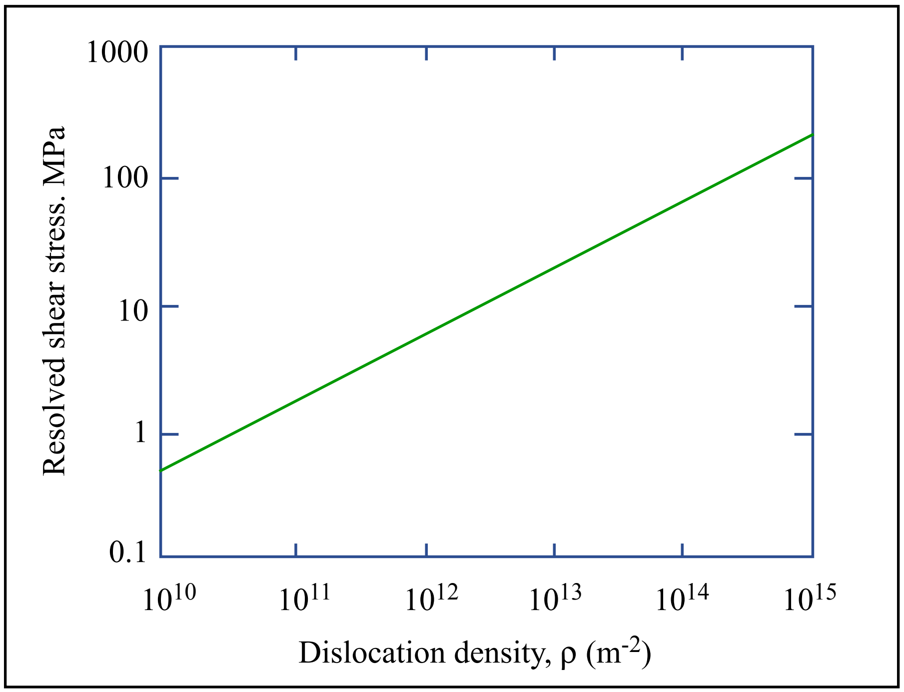
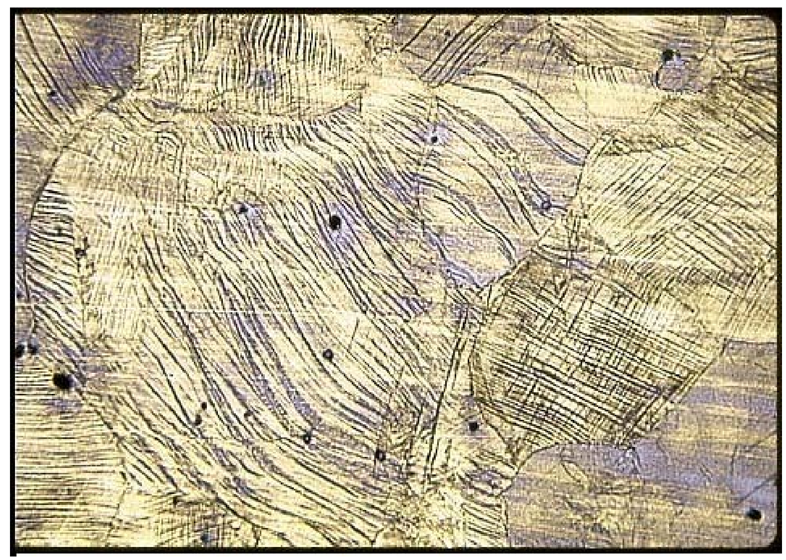



Figure by MIT OpenCourseWare.



Courtesy of George Langford. Used with permission.

**Heavily Cold Worked Steel Microstructure**

Microstructures, George Langford, MIT

**Schematic of a Stress Strain Curve**

http://en.wikipedia.org/wiki/File:Work_HArd.png

# WORK HARDENING

- Holloman Power Law Hardening

$$\tau_y = K\gamma^n$$

- n – Strain Hardening Exponent
- K – Strength Coefficient

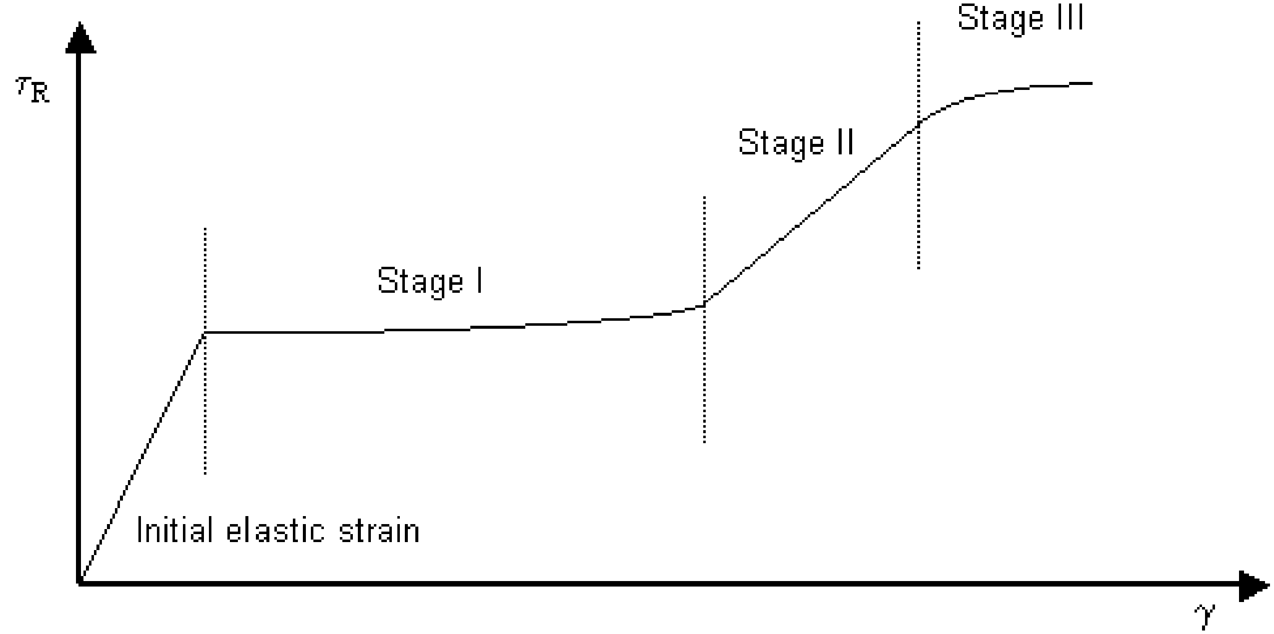


**Values of n and K for certain selected metals**

Handbook of Workability and Process design, Dieter GE

# WORK HARDENING

- Stages in a single crystal
  - Stage I : Single Slip
  - Stage II : Work Hardening Stage
  - Stage III : Saturation of Work Hardening




http://www.doitpoms.ac.uk/tlplib/slip/slip_in_ccp.php

# POLYCRYSTAL DEFORMATION

- Multiple Slip Regime
  - Elastic Anisotropy
    - Local stress state is complicated
  - Accommodation of Plasticity
    - Shape compatibility must be satisfied
    - Nucleates "Geometrically Necessary Dislocations" to remove the incompatibility
    - Stage II is absent

Image removed due to copyright restrictions. Please see Fig. 4.23c in Courtney, Thomas. *Mechanical Behavior of Materials*. Long Grove, IL: Waveland Press, 2005.

**Removal of Shape Incompatibilities during deformation**

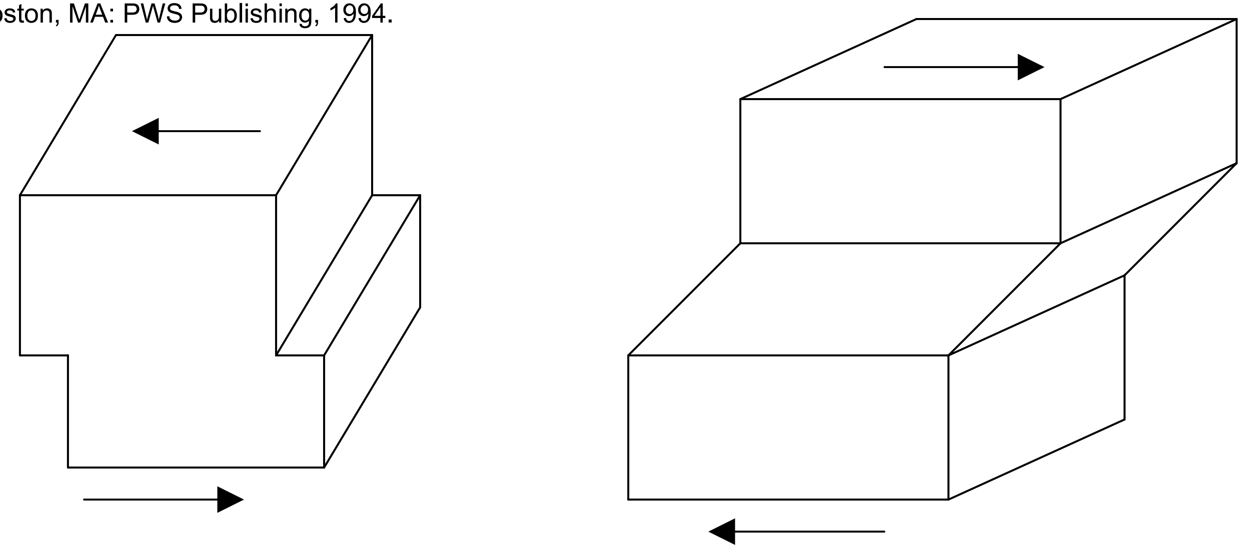
Mechanical Metallurgy, Dieter G., 3rd Edition

# Lecture Summary 10/07/09 “Twinning”

# Glide vs Twinning Comparison

| | Glide | Twinning |
|---|---|---|
| **Atomic movement** | Atoms move a whole number of atomic spacing on a single plane. | Planes of atoms move fractional atomic spacing. Distributed over entire volume. |
| **Microscopic appearance** | Thin lines | Wide bands or broad lines |
| **Lattice orientation** | No change in lattice orientation. The steps are only visible on the surface of the crystal and can be removed by polishing. After polishing there is no evidence of slip. | Lattice orientation changes. Surface polishing will not destroy the evidence of twinning. |

Image removed due to copyright restrictions. Please see Fig. 17.2 in Reed-Hill, Robert E., and Reza Abbaschian. *Physical Metallurgy Principles.* 3rd ed. Boston, MA: PWS Publishing, 1994.



http://info.lu.farmingdale.edu/depts/met/met205/plasticdeformation.html

# Characteristics of Twinning

- Distributed over entire volume and not confined to a single plane
- Happens very quickly (speed of sound in material)
- Cooperative motion of many planes of atoms with each plane moving only a small distance

- Lattice is rotated not distorted » <u>NOT</u> a phase transformation

# Rules for Twinning

- Fundamental Rule: crystal orientation is rotated but crystal is not distorted -Crystal structure is unchanged as a result of twinning
  - Basis vectors maintain same mutual angles and length
  - Solving for the vector combinations that follow the above rules yields the twinning system

# Rule Development

Image removed due to copyright restrictions. Please see Fig. 17.5, 17.7 in Reed-Hill, Robert E., Reza Abbaschian, and Lara Abbaschian. *Physical Metallurgy Principles.* 3rd ed. Boston, MA: PWS Publishing, 1994.

Reed-Hill, Physical Metallurgy Principles 3rd Edition, PWS Publishing Company, 1994

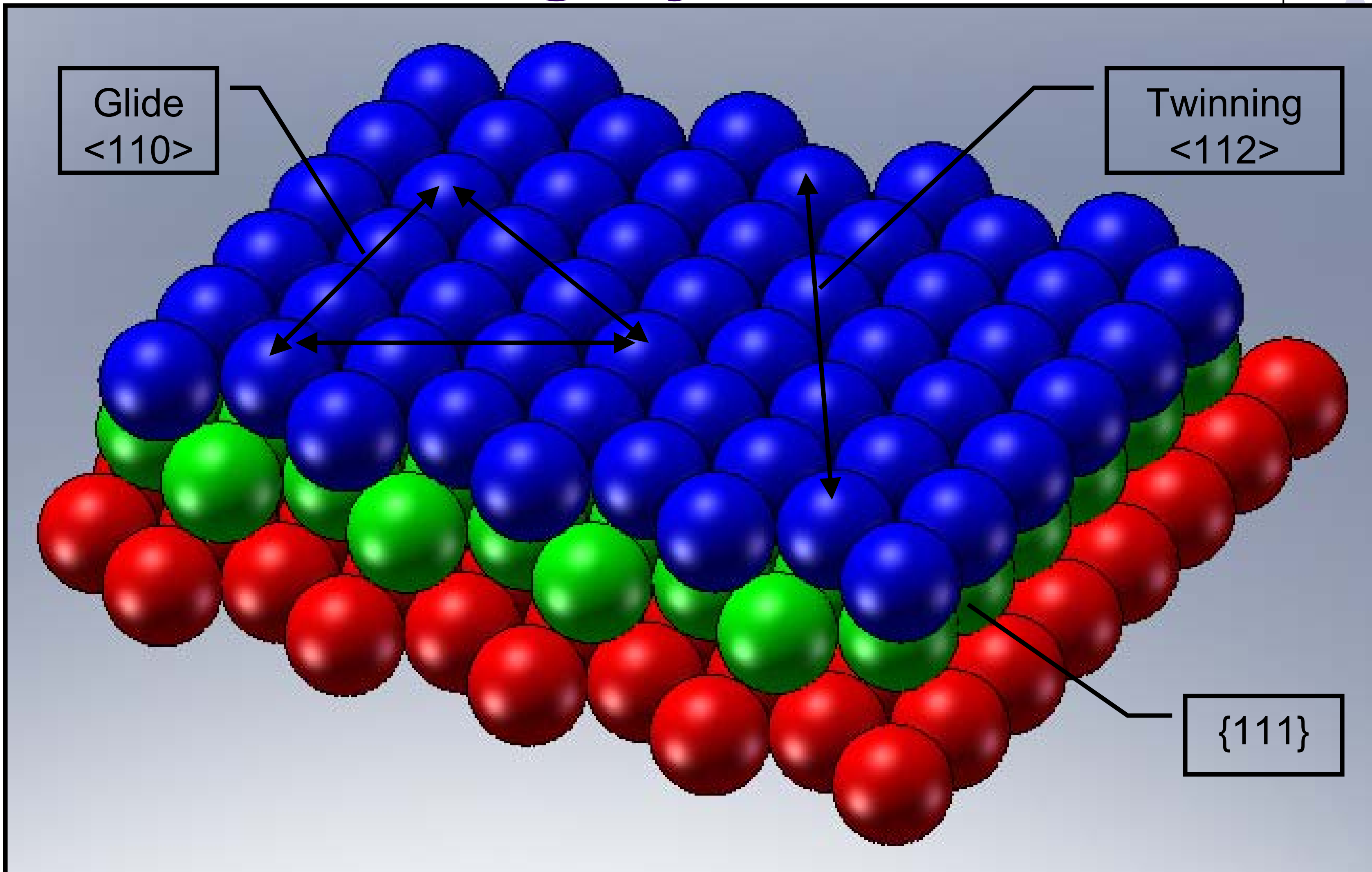
# Rules for Twinning

- Twin is completely defined when $K_1$, $K_2$, $\eta_1$, $\eta_2$ are all known

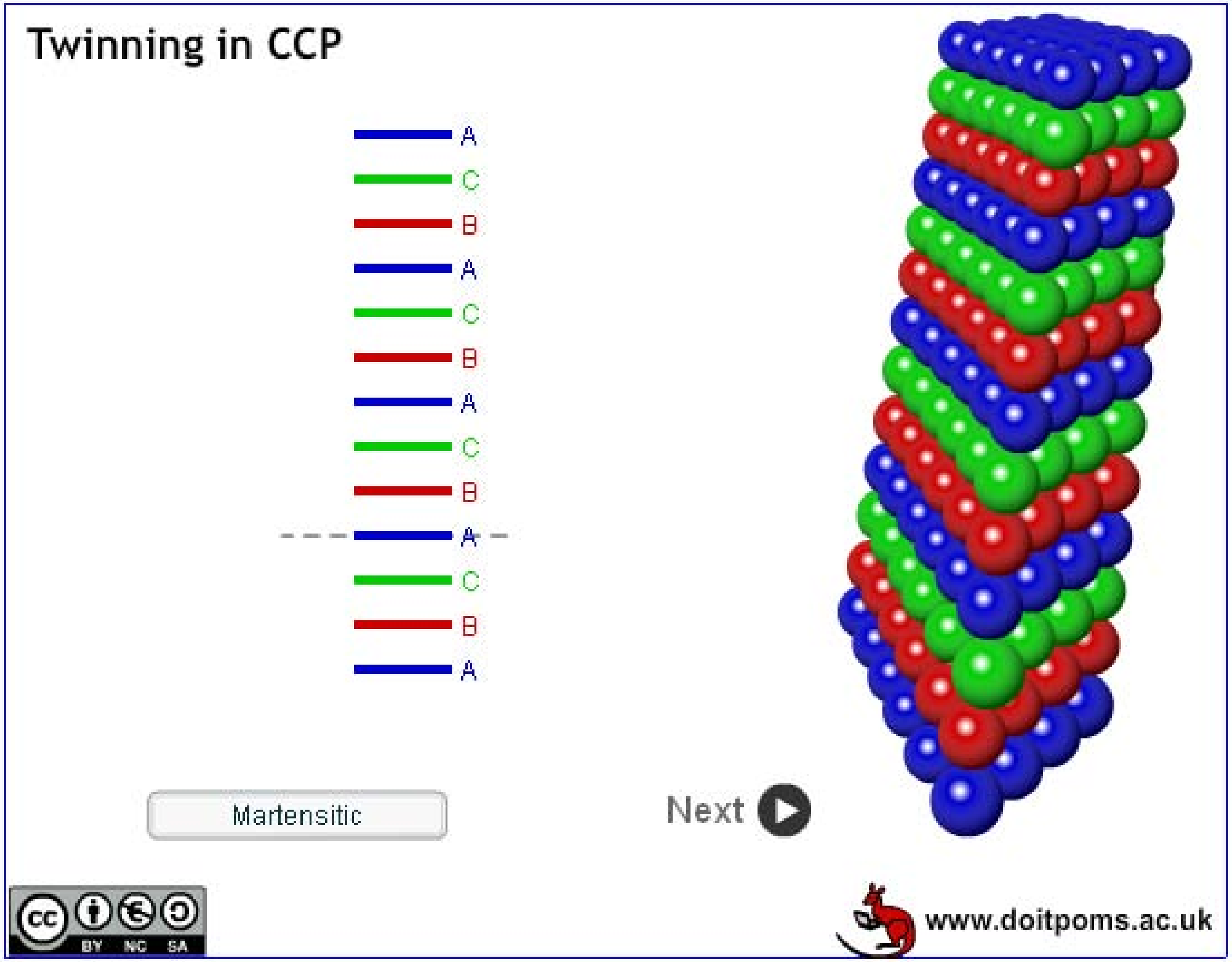
- $\eta_1$ and $\eta_2$ must lie in the same plane

- $\eta_1$ and $\eta_2$ must be perpendicular to the intersection of the $K_1$ and $K_2$ planes

# FCC Twinning System

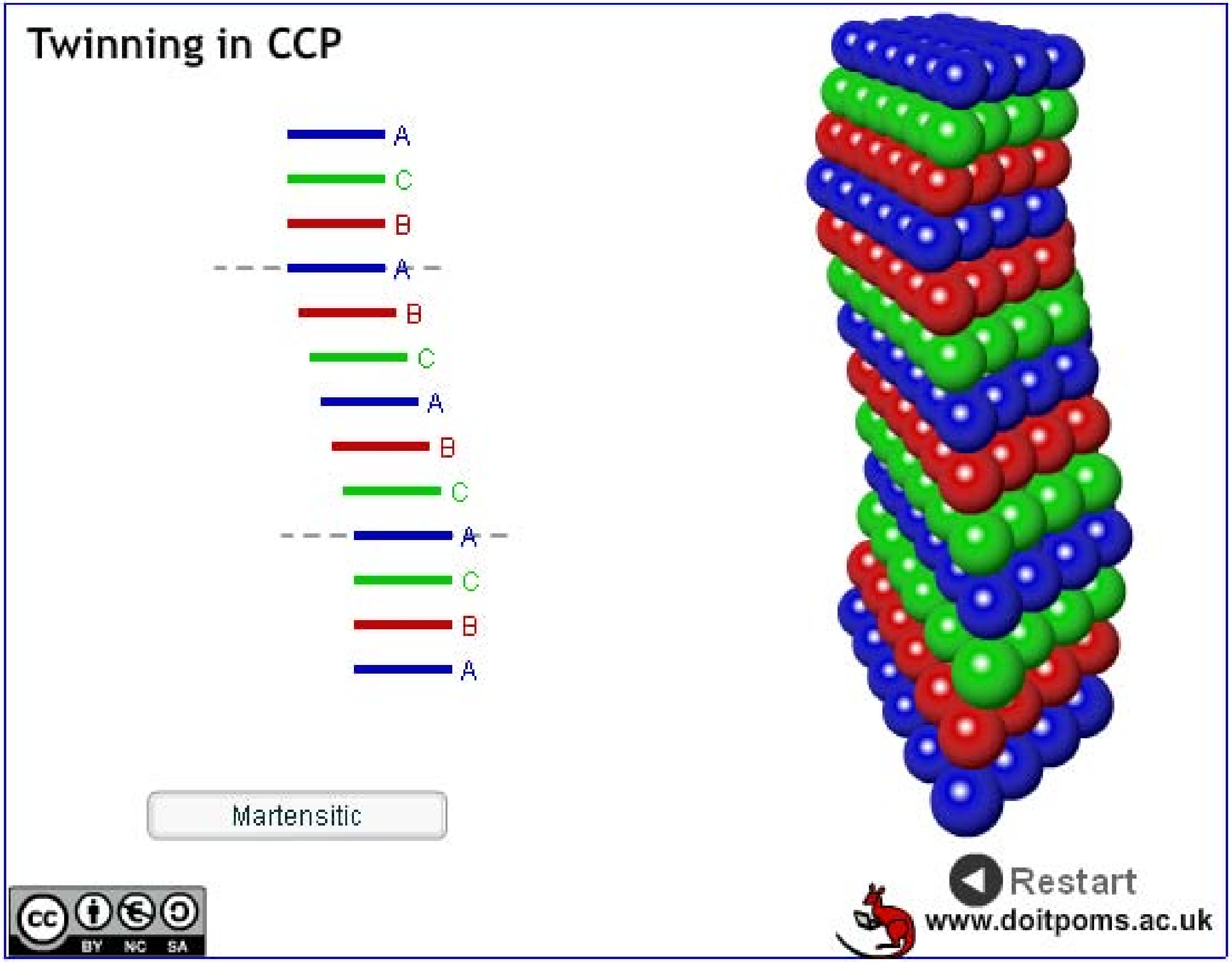


# Cubic Close Packed Twinning




Courtesy of DoITPoMS, University of Cambridge. (Online)

# Cubic Close Packed Twinning




Courtesy of DoITPoMS, University of Cambridge. (Online)

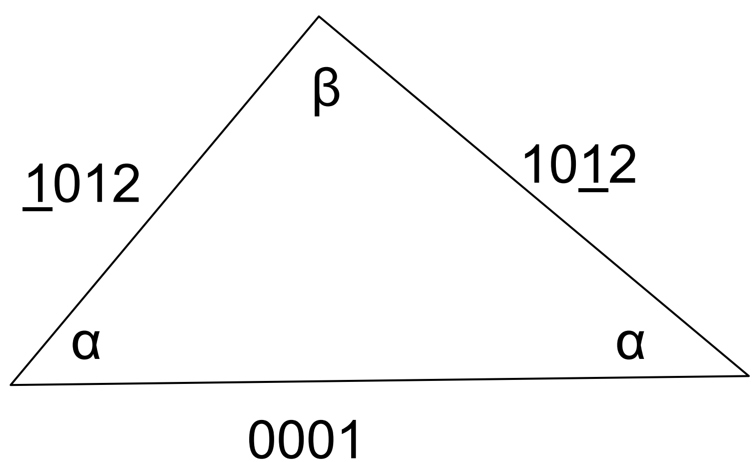
# Twinning Systems

| Type of Metal | $K_1$ | $\eta_1$ | $K_2$ | $\eta_2$ |
|---|---|---|---|---|
| BCC | $\{112\}$ | $\langle 11\underline{1} \rangle$ | $\{11\underline{2}\}$ | $\langle 111 \rangle$ |
| FCC | $\{111\}$ | $\langle 11\underline{2} \rangle$ | $\{11\underline{1}\}$ | $\langle 112 \rangle$ |
| HCP *(Mg, Ti)* | $\{10\underline{1}1\}$ | $\langle 10\underline{1}\underline{2} \rangle$ | $\{10\underline{1}\underline{3}\}$ | $\langle 30\underline{3}2 \rangle$ |
| *(Be, Cd, Hf, Mg, Ti, Zn, Zr)* | $\{10\underline{1}2\}$ | $\langle 10\underline{1}\underline{1} \rangle$ | $\{10\underline{1}\underline{2}\}$ | $\langle 10\underline{1}\underline{1} \rangle$ |
| *(Mg)* | $\{10\underline{1}3\}$ | $\langle 30\underline{3}\underline{2} \rangle$ | $\{10\underline{1}\underline{1}\}$ | $\langle 10\underline{1}2 \rangle$ |
| *(Hf, Ti, Zr)* | $\{11\underline{2}1\}$ | $\langle 11\underline{2}\underline{6} \rangle$ | $\{0002\}$ | $\langle 11\underline{2}0 \rangle$ |
| *(Ti, Zr)* | $\{11\underline{2}2\}$ | $\langle 11\underline{2}\underline{3} \rangle$ | $\{11\underline{2}\underline{4}\}$ | $\langle 22\underline{4}3 \rangle$ |

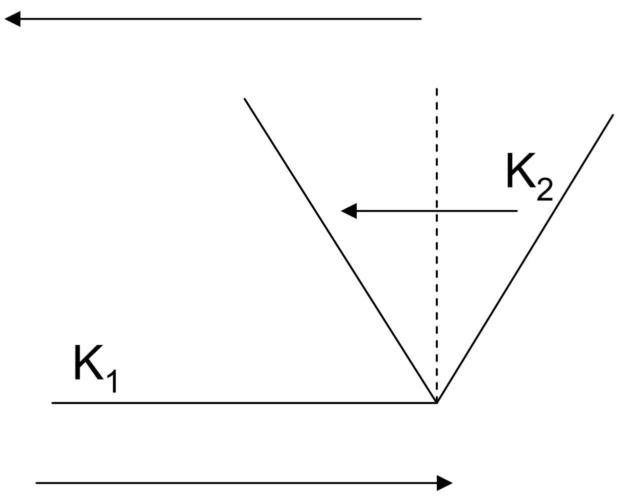
"Physical Metallurgy Principles" Appendix E

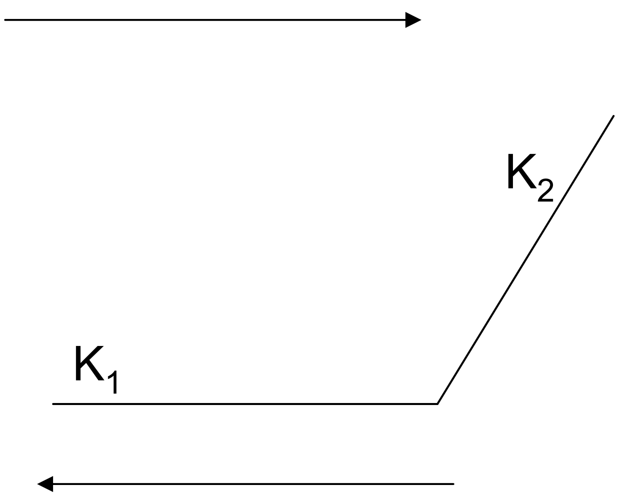
# Hexagonal Metals

- Twinning system is often $\{10\underline{1}2\}$ $\langle\underline{1}011\rangle$, corresponding to $K_1=(10\underline{1}2)$, $K_2=(\underline{1}012)$
- Zn: c/a=1.86, β=86°
- Mg: c/a=1.62, β=94°



# Twinning & Stress Sign
# Obtuse β



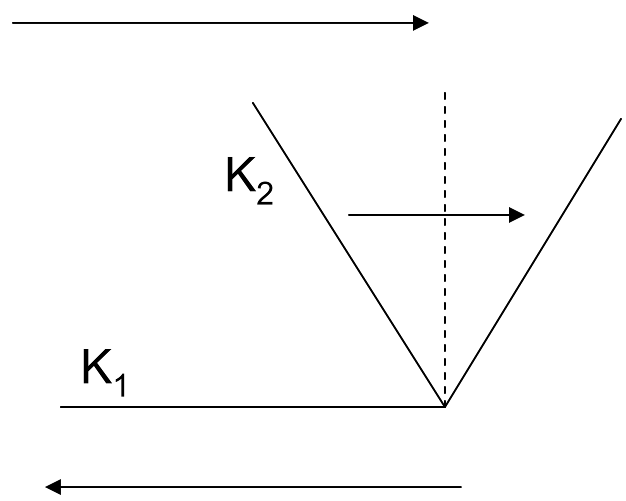

Twinning **will** occur

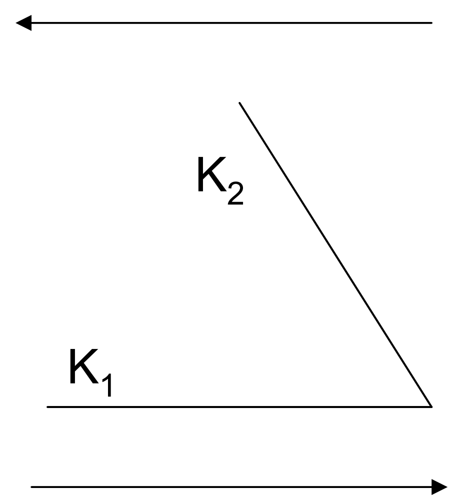
•Mg in compression

Twinning will **not** occur → fracture

•Mg in tension

# Twinning & Stress Sign Acute β



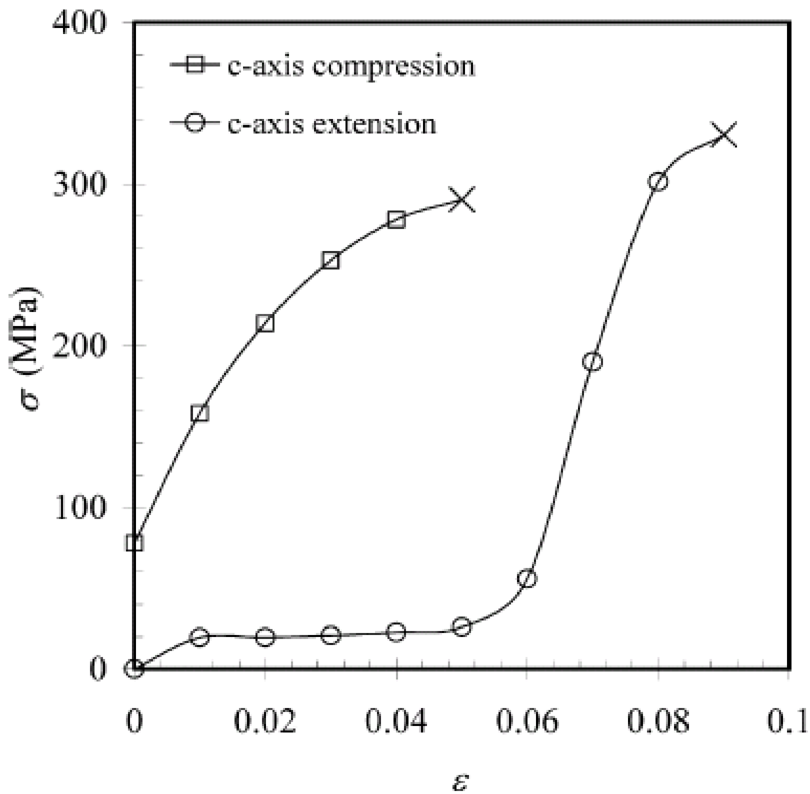

Twinning **will** occur

•Zn in tension

Twinning will **not** occur → fracture

•Zn in compression

# Magnesium Twinning




Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

M. R. Barnett, 2007

# Titanium Twinning

Image removed due to copyright restrictions.

Please see Fig. 9 in Zhong, Yong, Fuxing Yin, and Kotobu Nagai.

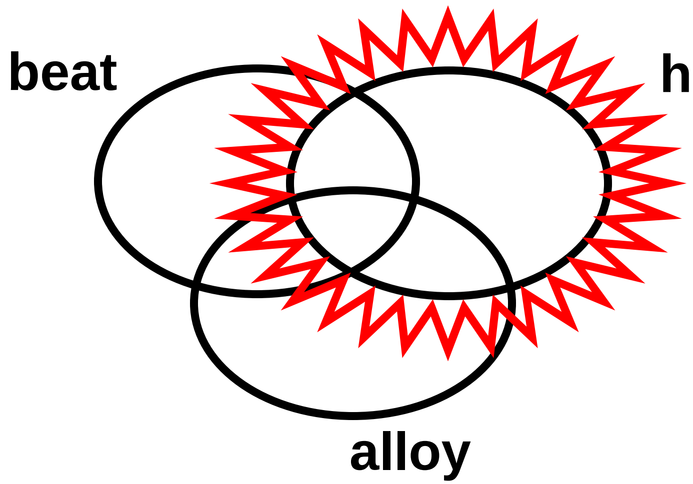
"Role of deformation twin on texture evolution in cold-rolled commercial-purity Ti."

*Journal of Materials Research* 23 (November 2008): 2954-2966.

Zhong et al., 2008

# Physical Metallurgy

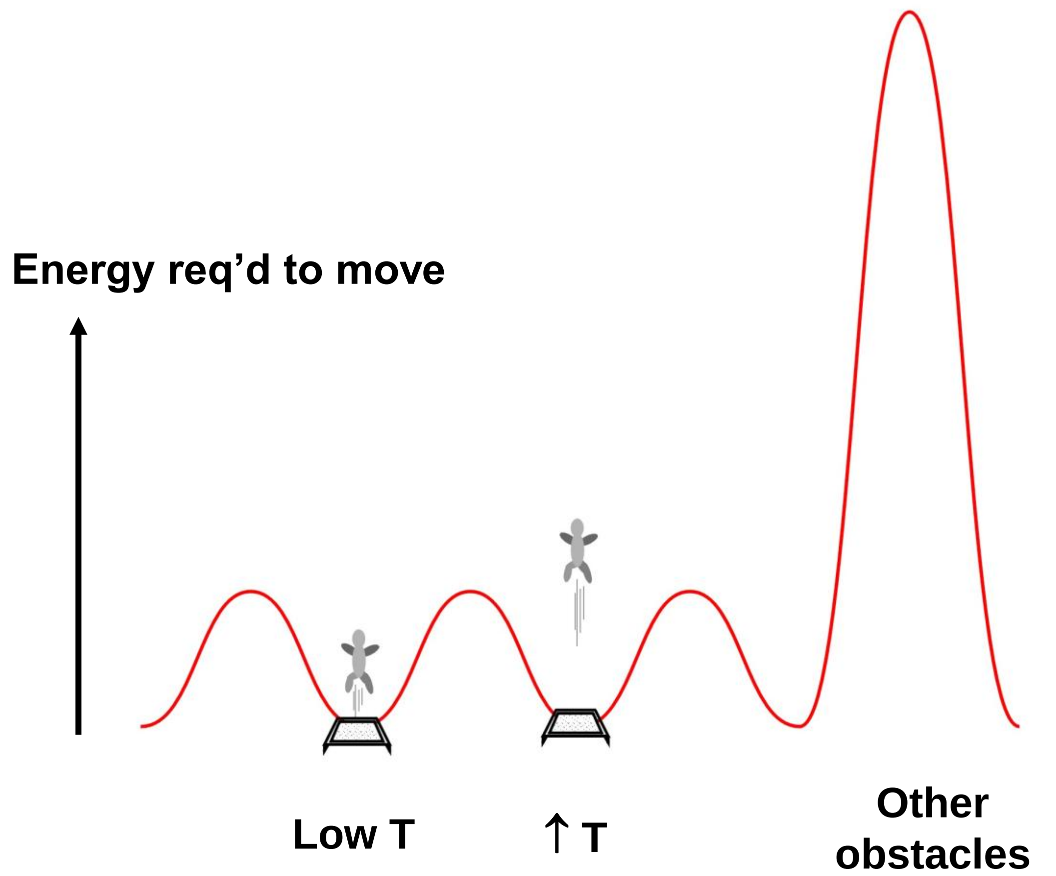
*10/13-10/14 Lecture Review*




Dept. of Mechanical Engineering, MIT

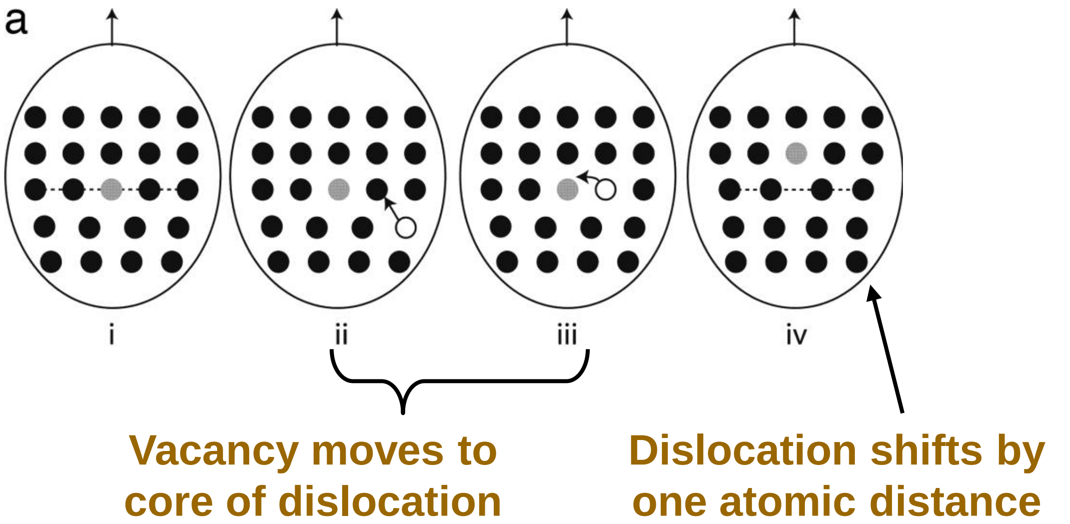
# With increasing temperature

- Glide becomes easier
- Apparent activation barrier is lower



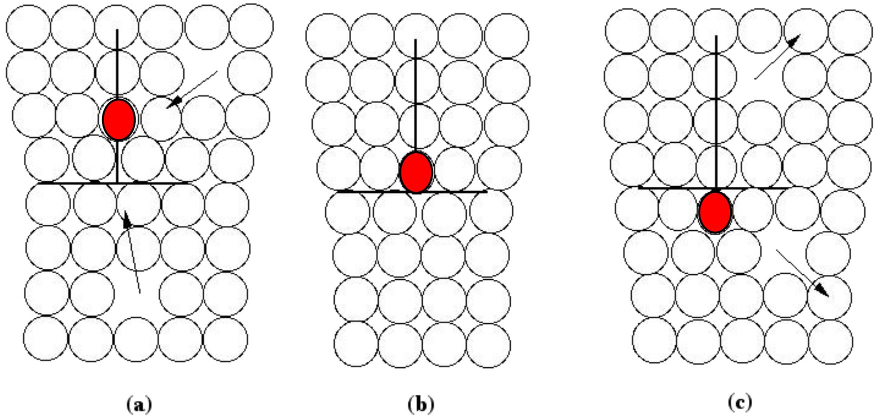

http://www.msm.cam.ac.uk/wjc/coursef/Lecture5.htm

# Dislocation climb





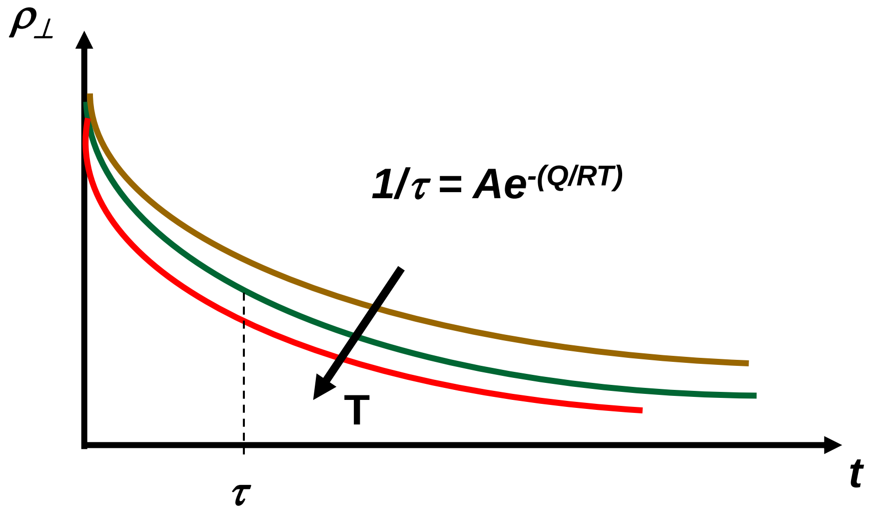

- Edge dislocations can leave their slip plane
- $\perp$ climb can absorb or emit vacancies
- Increase T = increase vacancies






Vitelli V et al. PNAS 2006;103:12323-12328
http://neon.materials.cmu.edu/rohrer/defects_lab/polygoniz_bg.html

# Recovery (Annealing)




- Recovery of $\rho_\perp$, stored $\perp$ energy
- $T \geq 1/3\ T_{melt}$
- Heat + mobility = $\perp$ annihilation

# Recovery: Polygonization

- ⊥ of like sign assemble into boundaries
- Subgrain formation of low-angle grain boundaries
- Localizes lattice curvature into polygonal regions

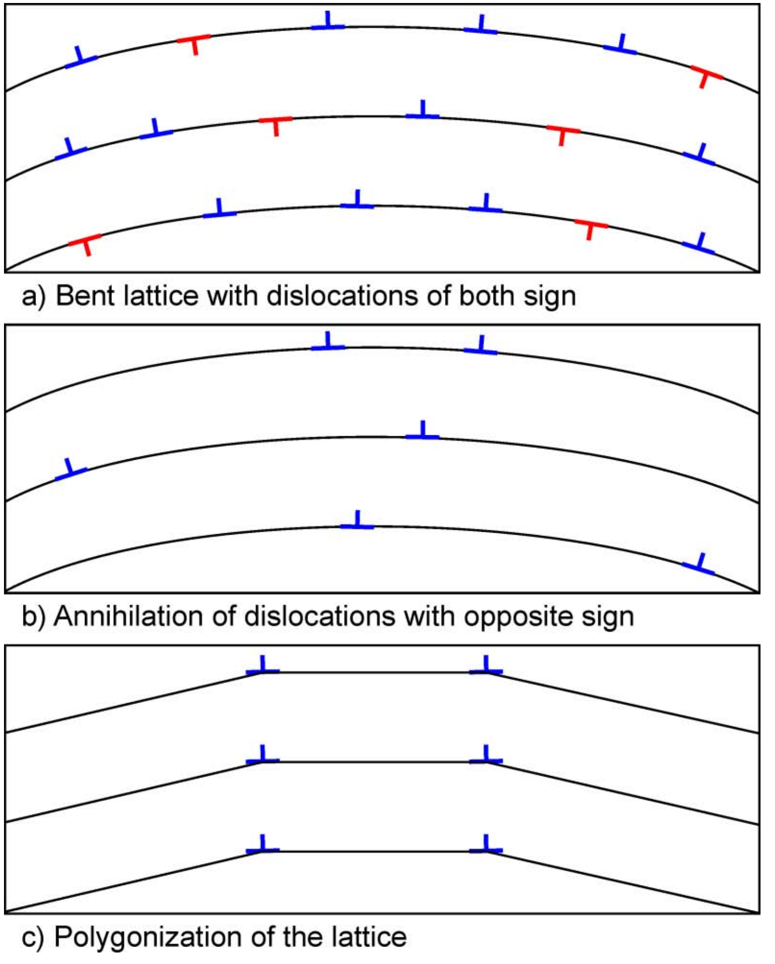
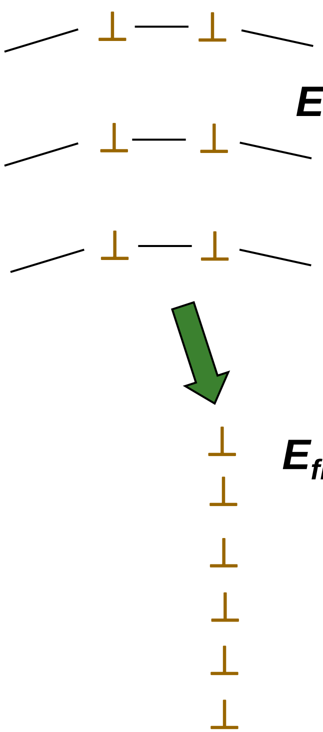



Image removed due to copyright restrictions.
Please see Fig. 6.82 in Totten, George E.
*Steel Heat Treatment Handbook: Metallurgy and Technologies*. Vol. 1. Boca Raton, FL: Taylor & Francis, 2007.

Steel heat treatment: metallurgy and technologies, Totten (2006)
http://en.wikipedia.org/wiki/Recovery_%28metallurgy%29

# Recovery: Coarsening

- Loss of boundary area to reduce interaction energy



$E_{initial} \sim \mu b^2$

$E_{final} \sim \mu b^2/2$

Image removed due to copyright restrictions.

Please see Fig. 3 in Gutierrez-Urrutia, I., M. A. Muñoz-Morris, and D. G. Morris. "Recovery of deformation substructure and coarsening of particles on annealing severely plastically deformed Al-Mg-Si alloy and analysis of strengthening mechanisms." *Journal of Materials Research* 21 (February 2006): 329-342.

Gutierrez-Urrutia et al (2006) J. Materials Research

# Recrystallization: ReX

- Nucleation of new, ⊥-free grains
- Heterogeneous process, complex kinetics
- Original microstructure <u>erased</u>

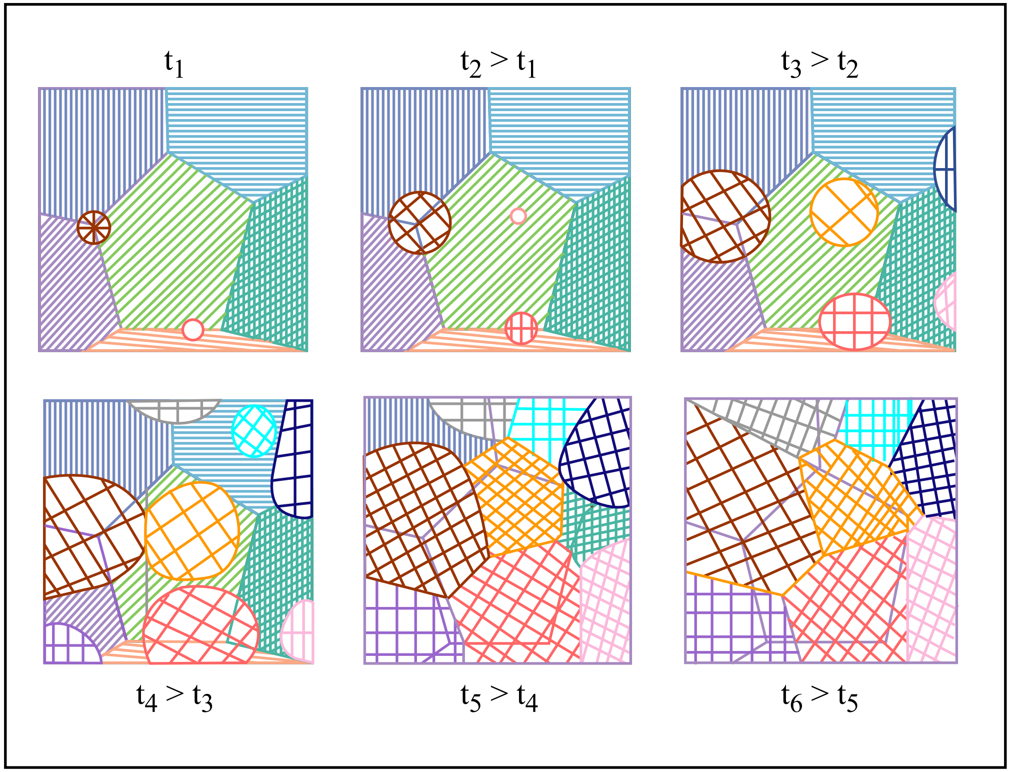



Figure by MIT OpenCourseWare. Adapted from Fig. 6.85 in Totten, George E. *Steel Heat Treatment Handbook: Metallurgy and Technologies*. Vol. 1. Boca Raton, FL: Taylor & Francis, 2007.

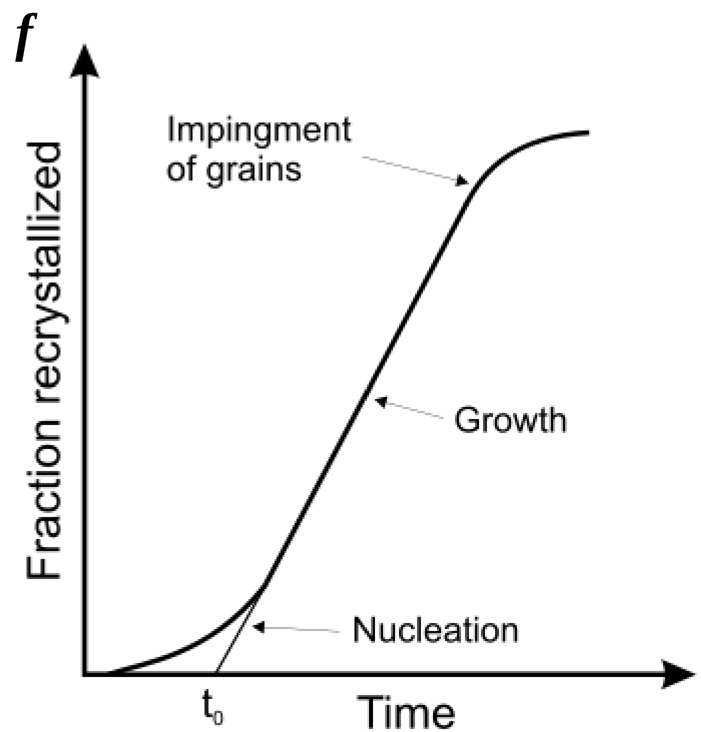
**nucleation** → **growth** → **impingement**

Steel heat treatment: metallurgy and technologies, Totten (2006)

# Recrystallization: JMAK analysis

Johnson-Mehl-Avrami-Kolmogorov Theory

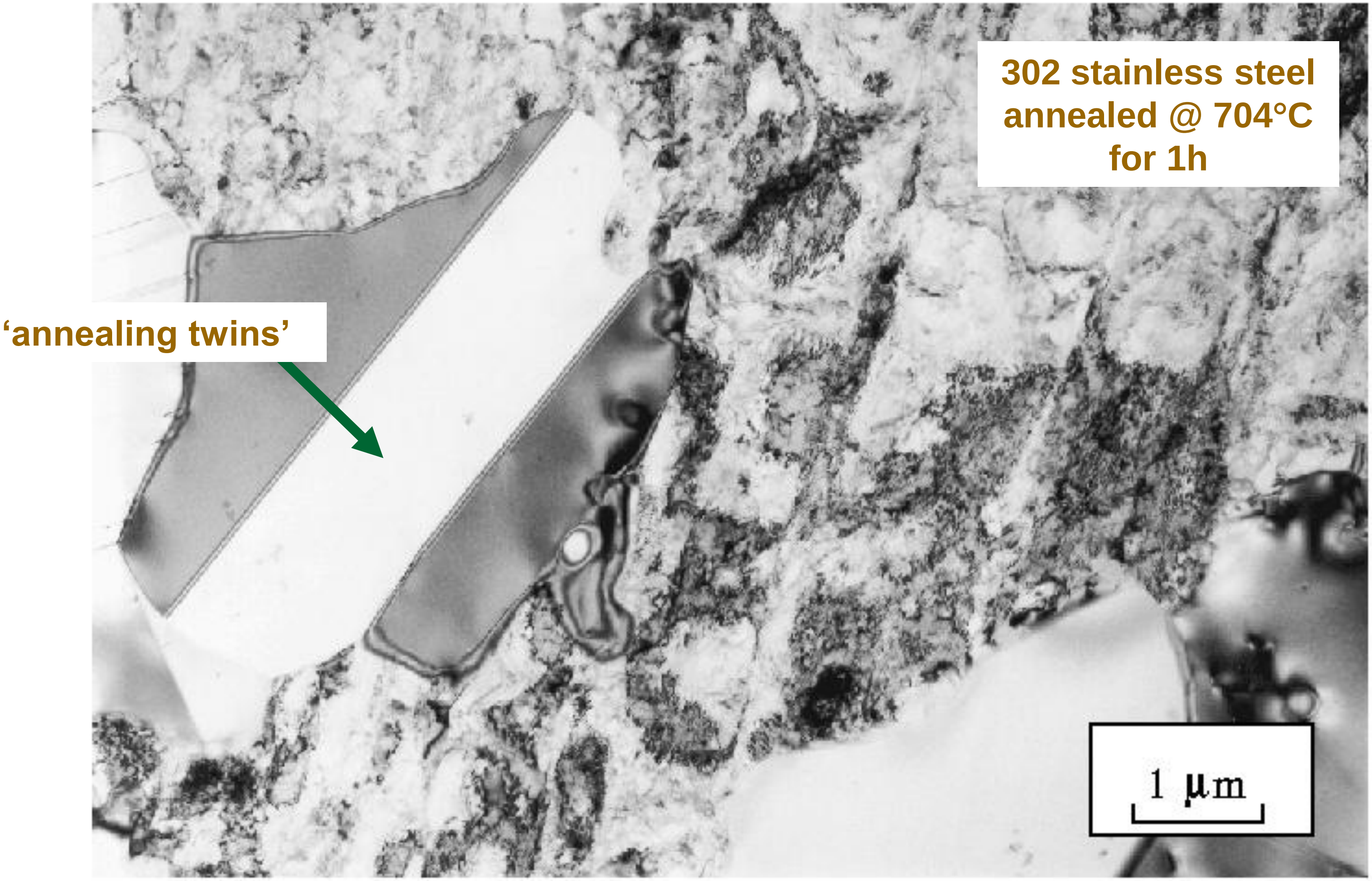
- Nucleation
  - $N$ = nucleation rate
- Growth
  - $G$ = constant growth rate
- Impingement
  - $df = df_{ex}\,(1-f)$




| | |
|---|---|
| **Spherical grains** | $f = 1 - \exp\left(-\frac{\pi}{3}\dot{N}G^3t^4\right)$ |
| **General form** **(*n = d + 1*)** | $f = 1 - \exp(-K\,t^{n})$ |

http://en.wikipedia.org/wiki/Recrystallization_%28metallurgy%29

# Recrystallization: ReX




http://www.doitpoms.ac.uk/miclib/full_record.php?id=772

Courtesy of H. K. D. H. Bhadeshia and DoITPoMS, University of Cambridge.

# Annealing of stainless steel bellows

Please see MazzolaTermomacchine.
"Stainless Steel Bellows End Annealing." March 12, 2009.
YouTube. Accessed May 5, 2010. http://www.youtube.com/watch?v=VJNY-68ulGk

http://www.youtube.com/watch?v=VJNY-68ulGk

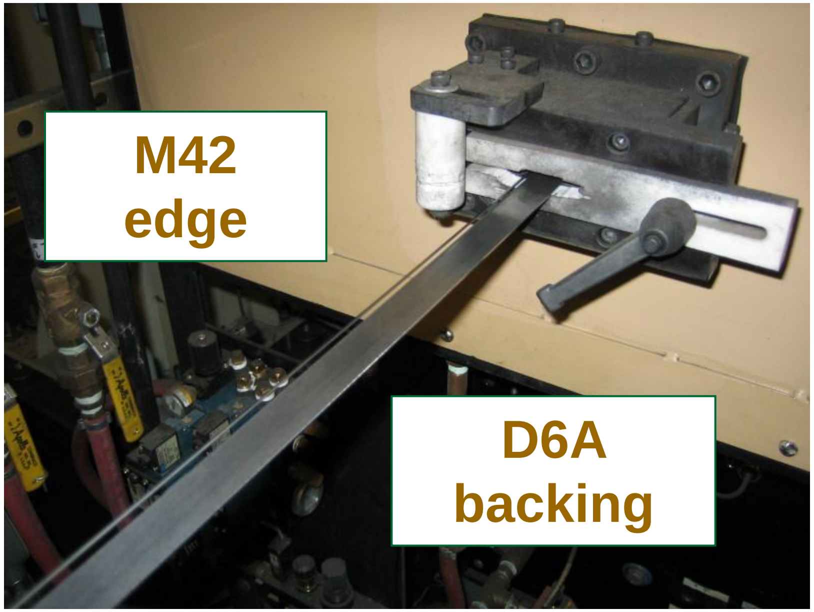
# Recrystallization! (copper(II) sulfate)

Please see mikishima. "Recrystallization of Copper Vitriol." April 4, 2007. YouTube. Accessed May 5, 2010. http://www.youtube.com/watch?v=erjXD1iUXKo

# Heat Treatment

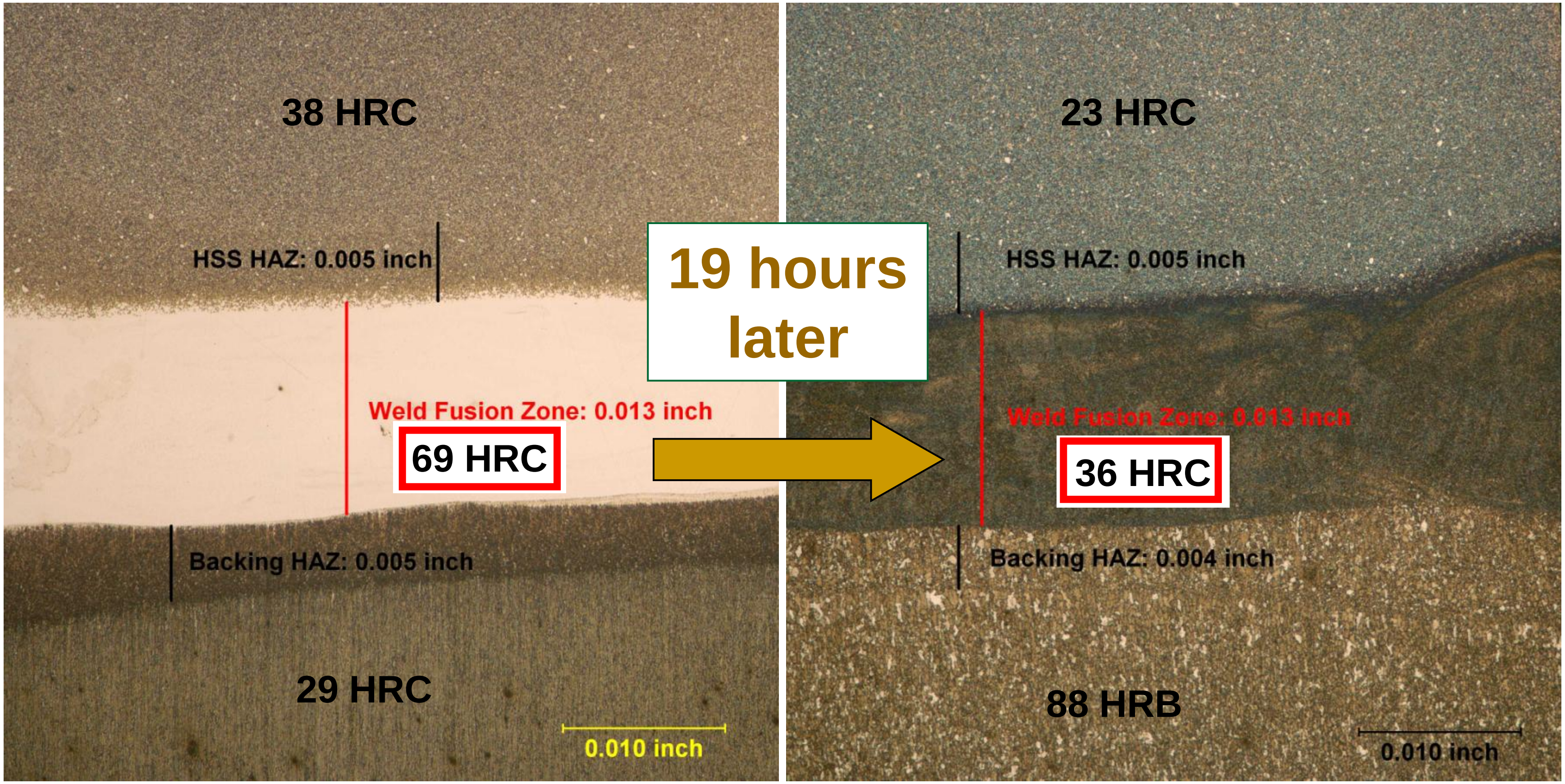
Please see dziadunio. "Heat Treatment." February 29, 2008.
YouTube. Accessed May 5, 2010. http://www.youtube.com/watch?v=rAm2Y0wGRF4

# Bandsaw blade manufacturing




Vacuum pit furnace

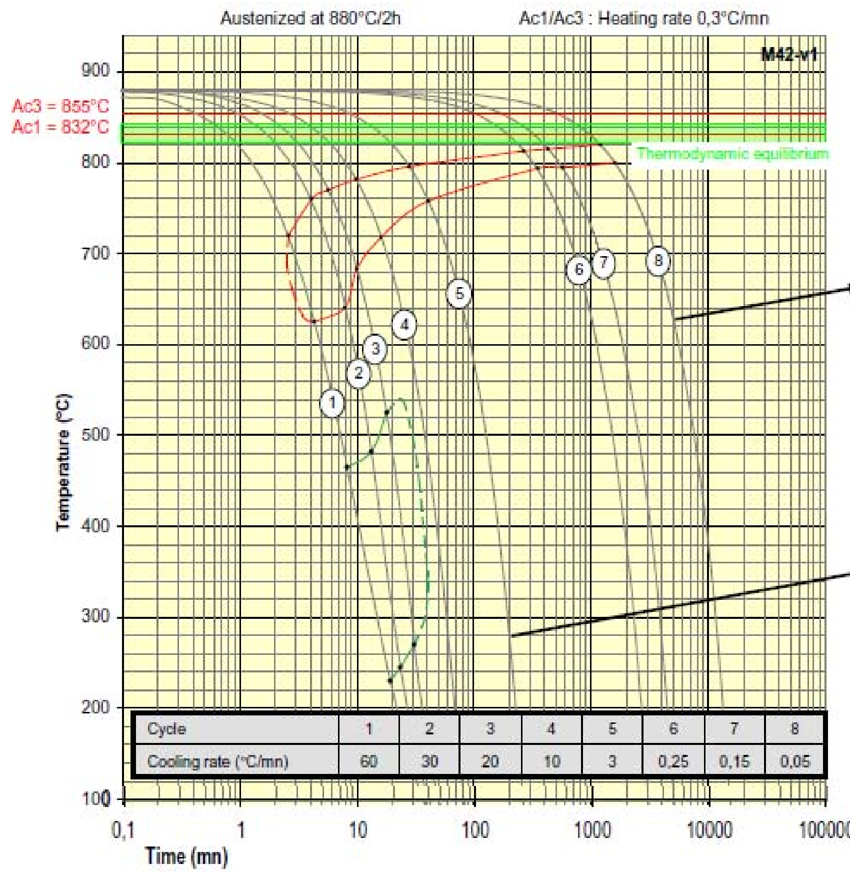
# Bandsaw blade annealing



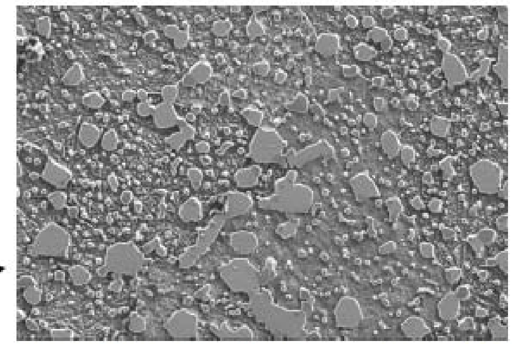

**Before Anneal** **After Anneal**

# Recovery time vs. hardness

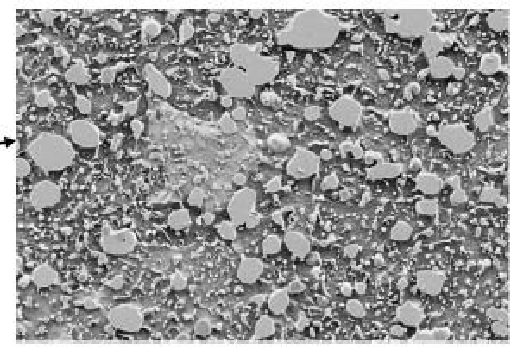
## ER projects on annealing




| Cycle | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| Cooling rate (°C/mn) | 60 | 30 | 20 | 10 | 3 | 0,25 | 0,15 | 0,05 |

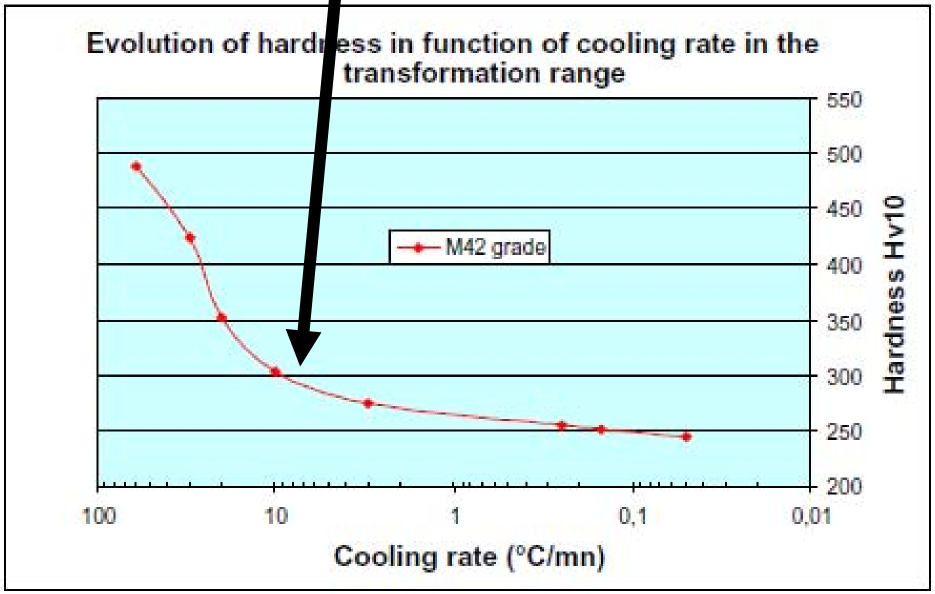


0.05°C/mn = 3°C/h → 244 Hv10



3°C/mn = 180°C/h → 275 Hv10

# Familiar looking curve?



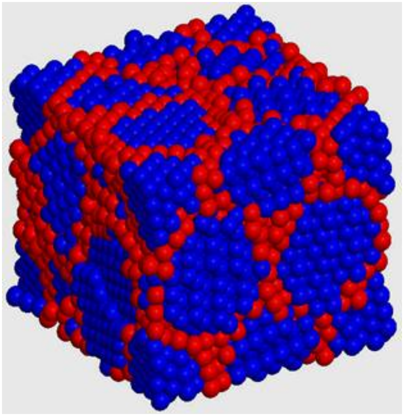

| Cooling rate | Hardness |
|---|---|
| °C/mn | Hv10 |
| 0,05 | 244 |
| 0,15 | 251 |
| 0,25 | 255 |
| 3 | 275 |
| 10 | 304 |
| 20 | 352 |
| 30 | 424 |
| 60 | 489 |

| softwares | Temperature | $M_2C$ | $M_6C$ | MC | $M_{23}C_6$ | $M_7C_3$ | Ferrite | Austenite |
|---|---|---|---|---|---|---|---|---|
| THERMO-CALC | 750°C | 6.36 | 7.02 | 0.91 | - | 5.31 | 80.41 | - |
| | 880°C | 6.73 | 6.27 | 0.81 | - | 1.5 | - | 84.70 |
| MAT-CALC | 750°C | 10.94 | 0.16 | 1.70 | 3.29 | - | 83.92 | - |
| | 880°C | 7.78 | 2.92 | 2.21 | - | - | - | 87.08 |

# Physical Metallurgy

## *12/09 Lecture Review*

# Nanocrystalline Metals



Courtesy of Chris Schuh.
Used with permission.

Dept. of Mechanical Engineering, MIT

http://schuh.mit.edu/research/images/nanox_3Datomicstruct.jpg

# nanocrystalline metals

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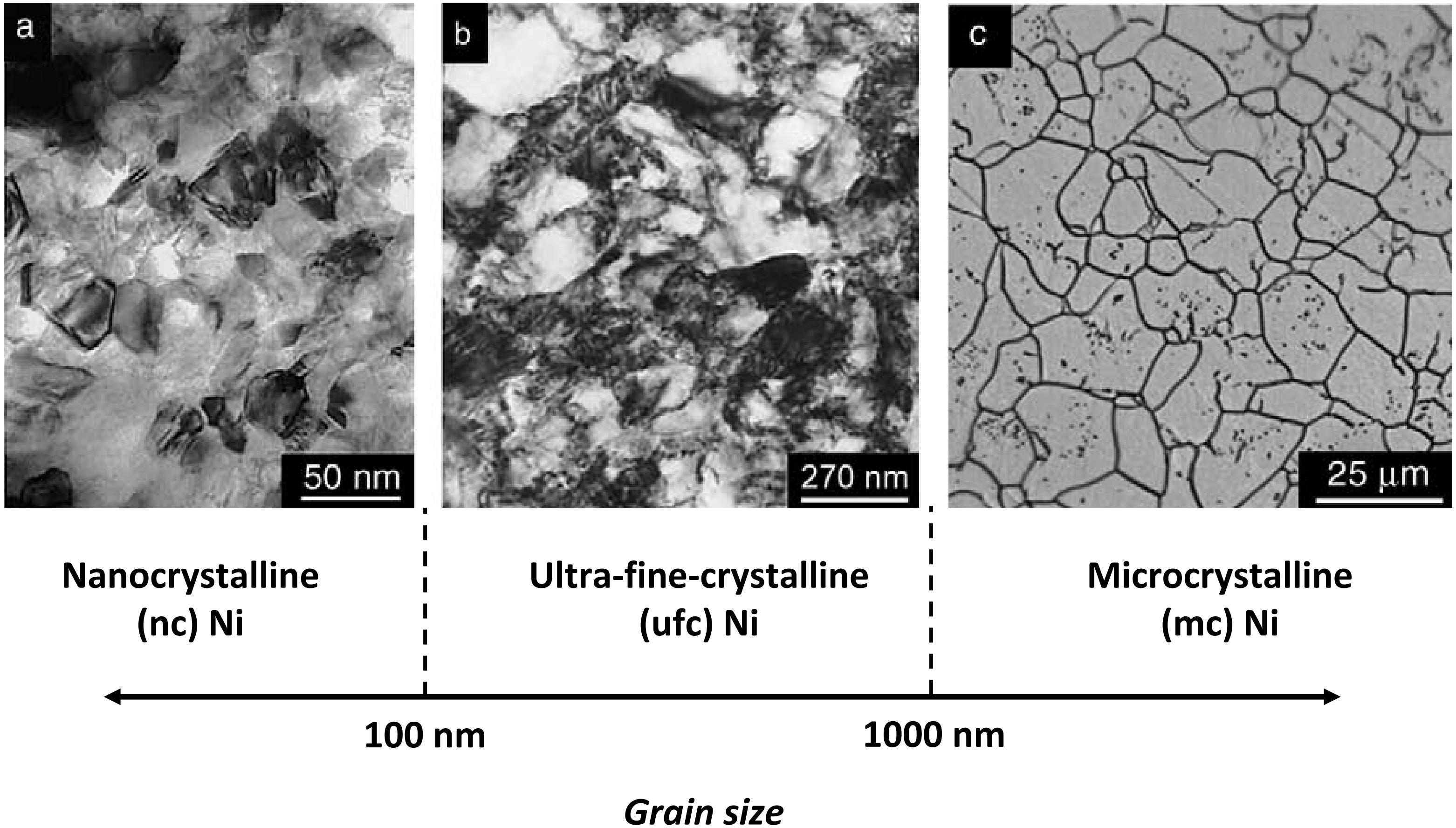
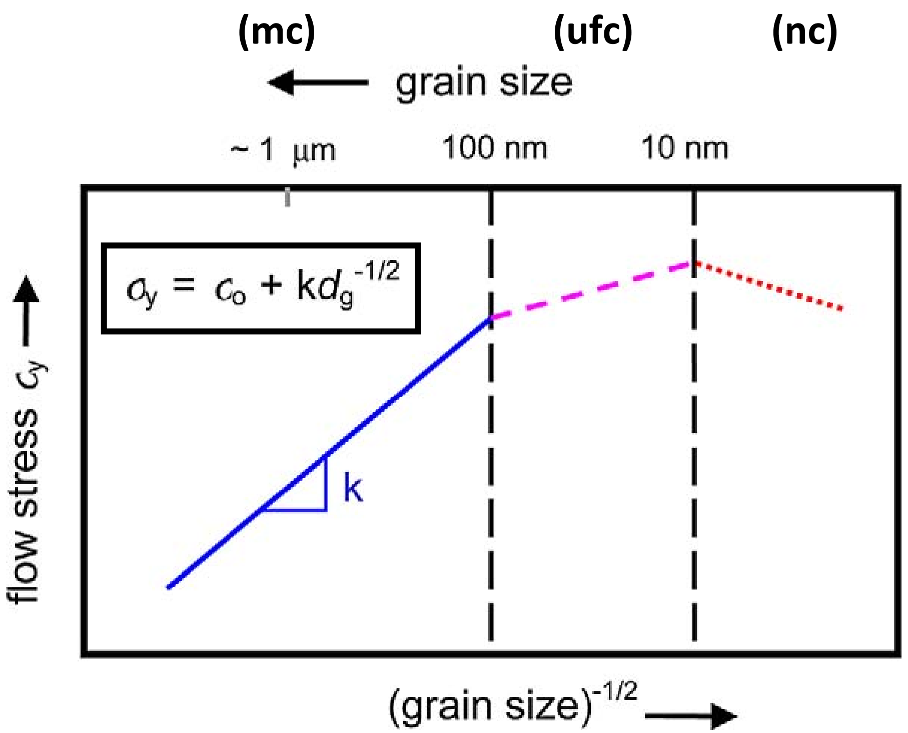



T. Hanlon, Y.-N. Kwon, S. Suresh (2003) Scripta Materialia

# strengthening effects of grain size




Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

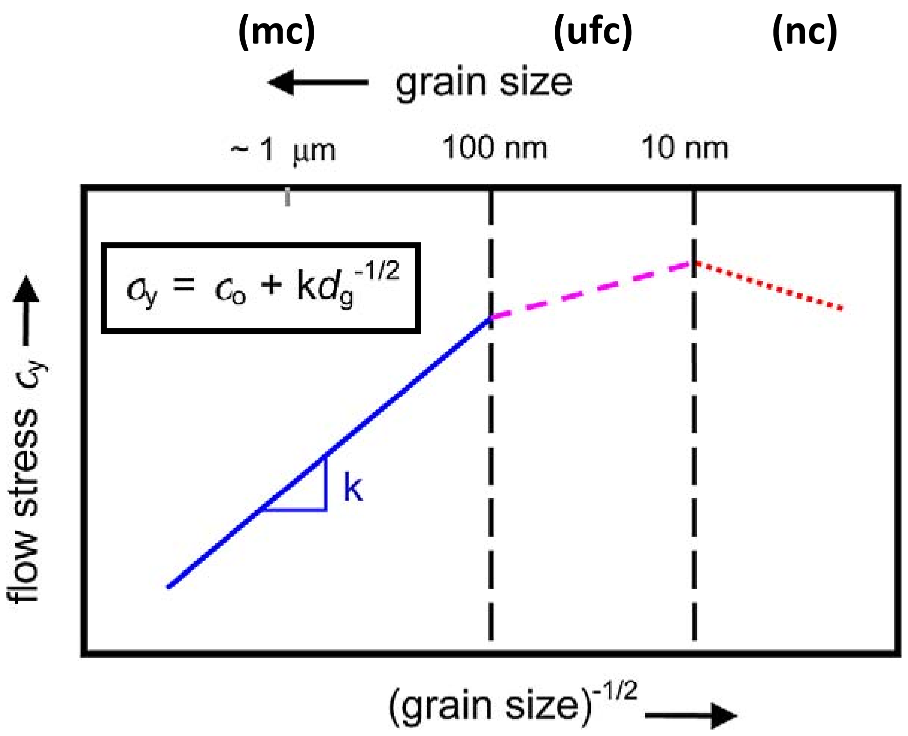
- mc

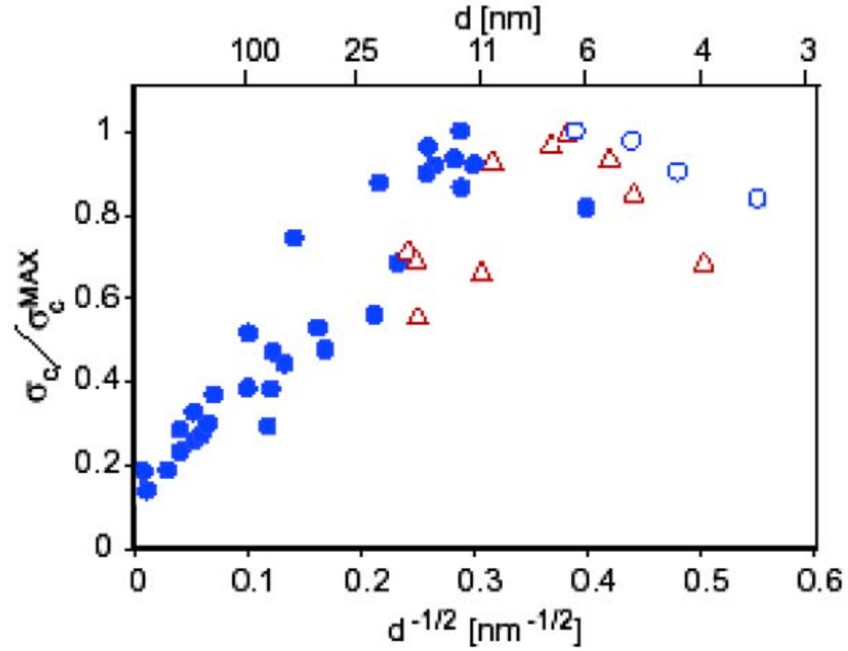
  Hall-Petch relationship ($\sigma \sim d^{-1/2}$ )
- ufc

  σ ↑ as d ↓, but not like H-P
- nc

  σ plateau or decreasing!

# strengthening effects of grain size

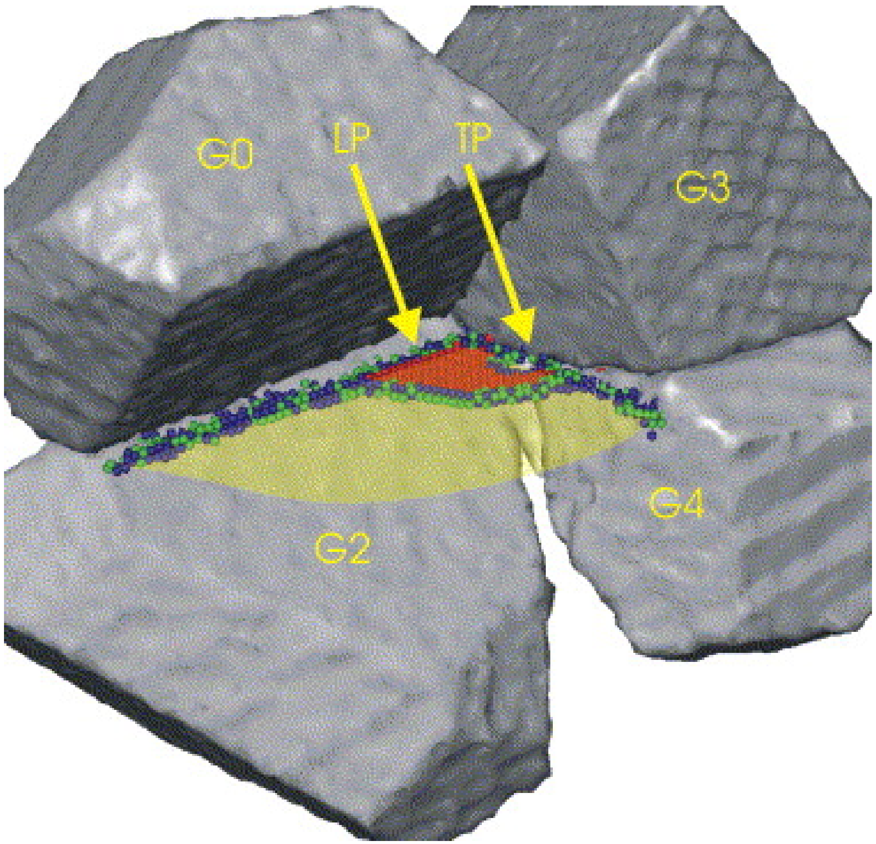





K. S. Kumar, H. Van Swygenhoven and S. Suresh (2003) Acta Materialia

# dislocation motion in nc materials





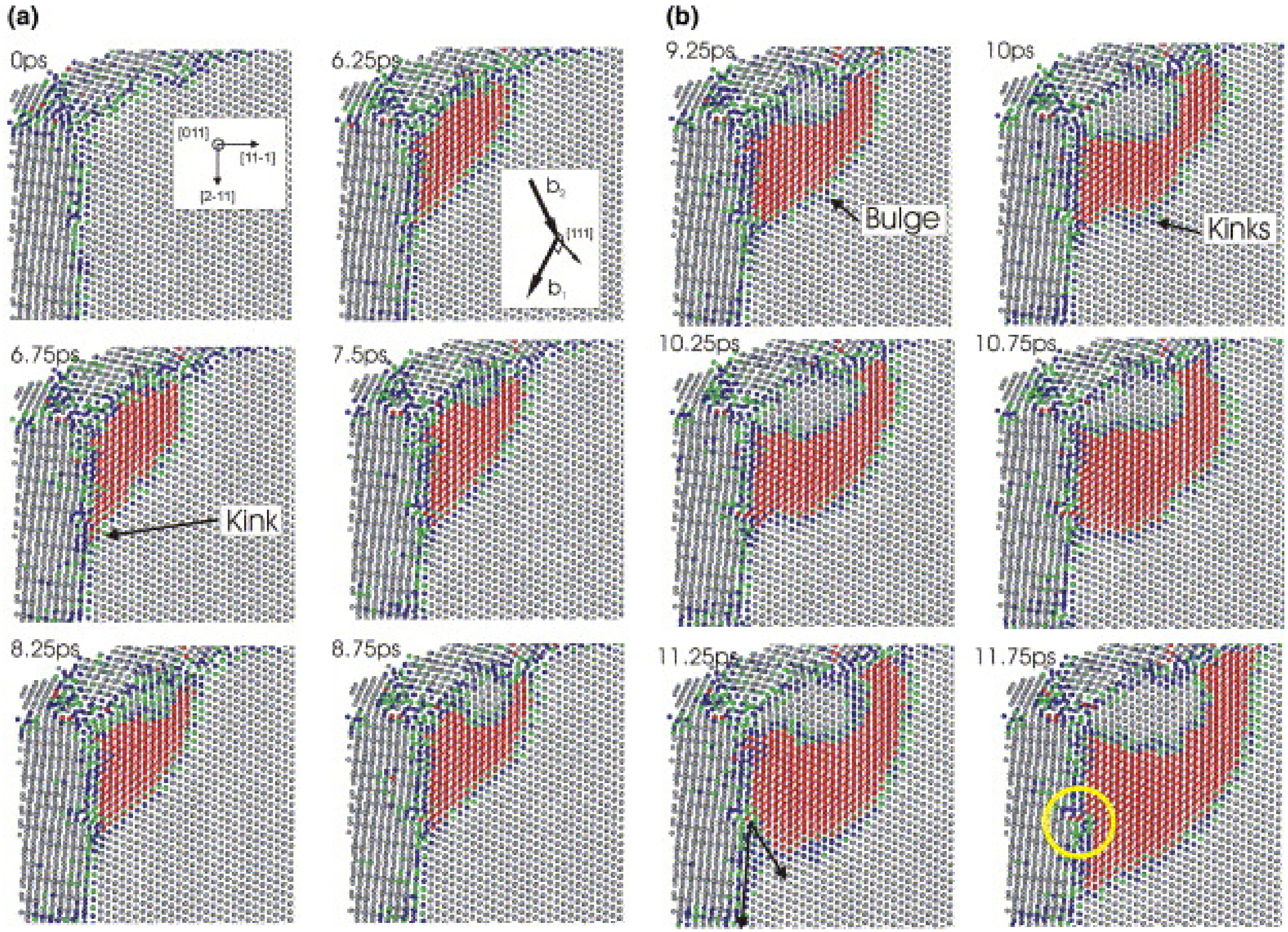

Grain Boundaries (GB) can act as dislocation sources

3 step process:

- Nucleation
- Propagation
- Reabsorbed at GB

H. Van Swygenhoven, P.M. Derlet and A.G. Frøseth (2006) Acta Materialia

# nc (partial) dislocation emission

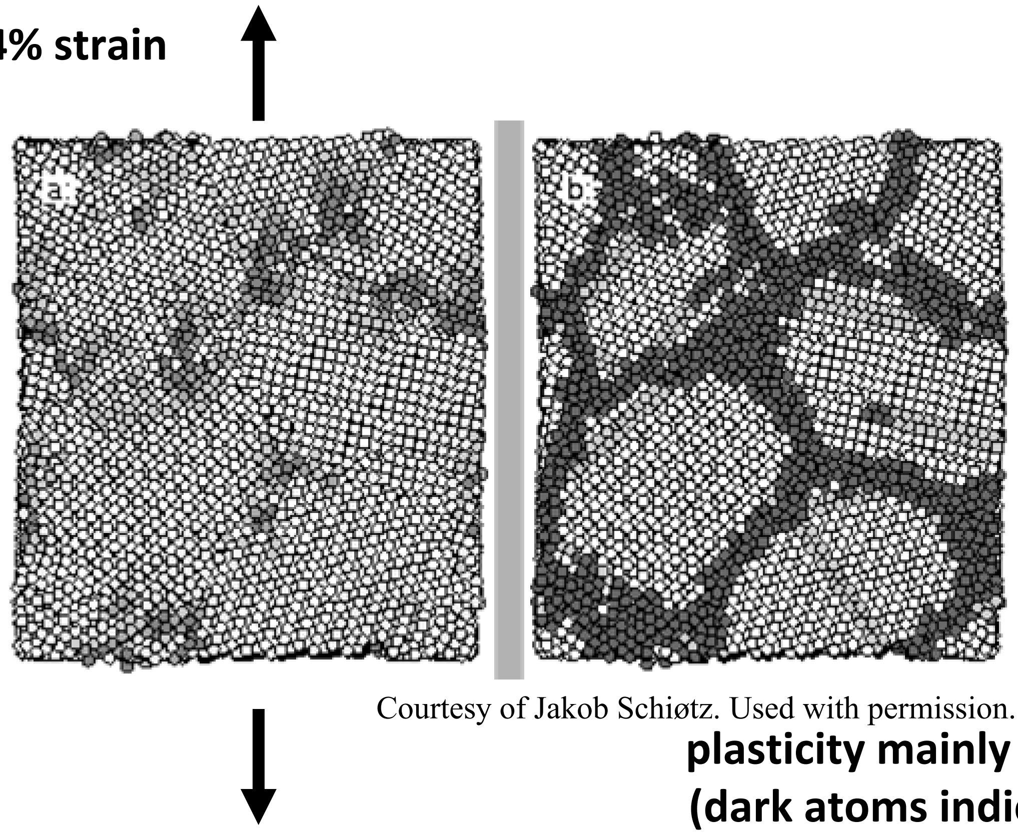





H. Van Swygenhoven, P.M. Derlet and A.G. Frøseth (2006) Acta Materialia

# with very fine nc grains (d < 10 nm)

0.4% strain



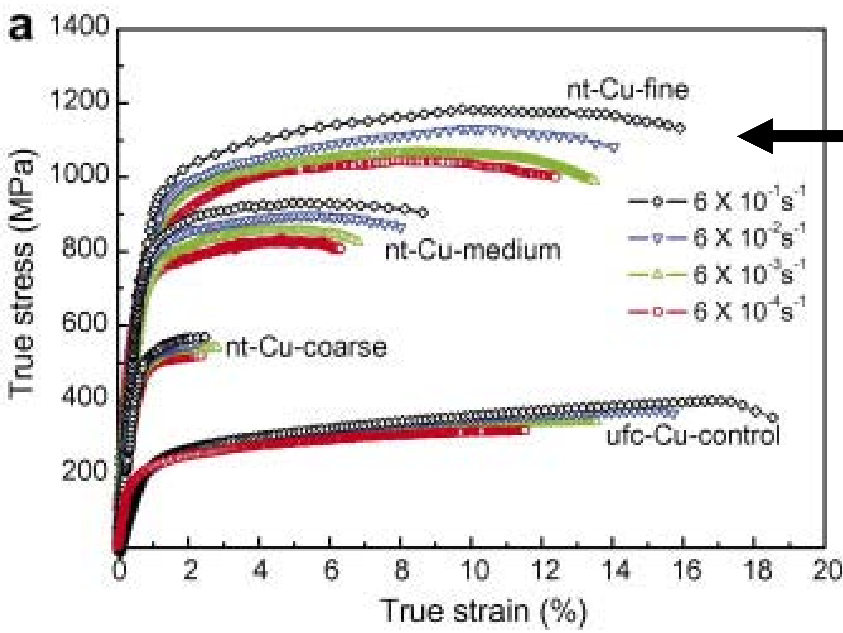

Courtesy of Jakob Schiøtz. Used with permission.

**plasticity mainly occuring @ GB's**
**(dark atoms indicate movement)**

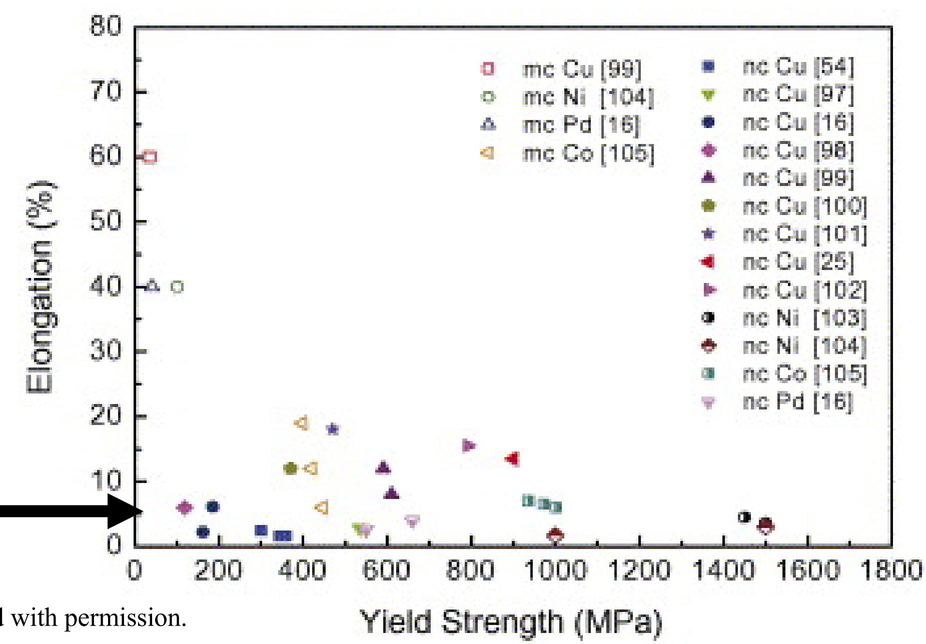
***before*** ***after***

H. Van Swygenhoven, P.M. Derlet and A.G. Frøseth (2006) Acta Materialia

# nc tensile testing data




**increased strain rate sensitivity**

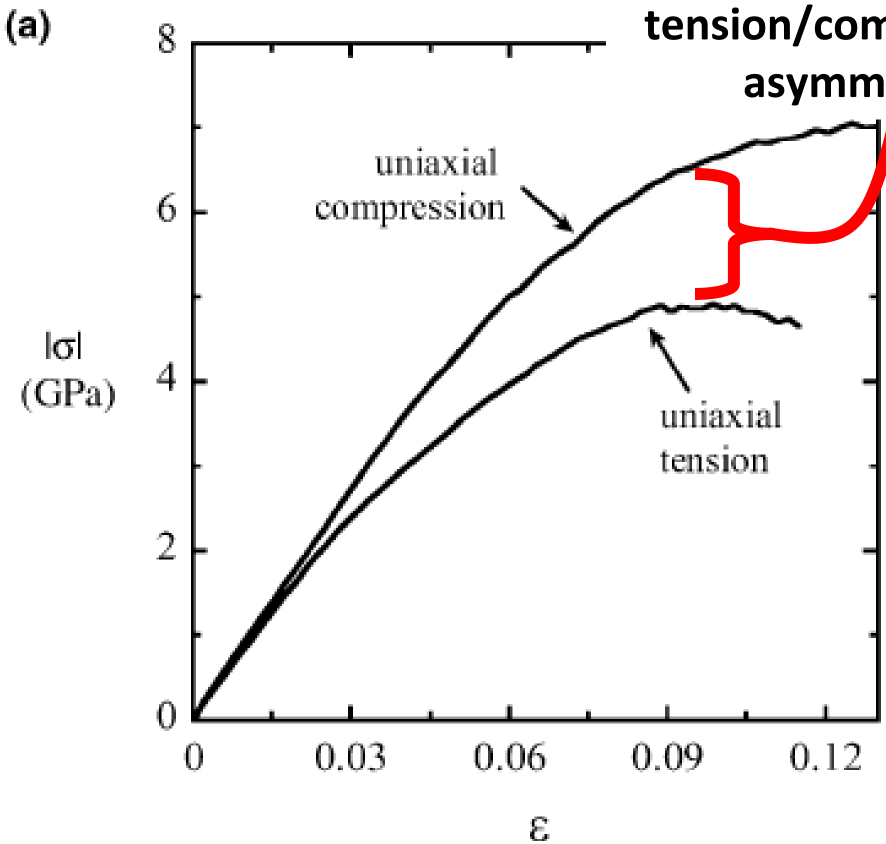



**very low ductility (<10%)**

Courtesy of Elsevier, Inc., http://www.sciencedirect.com. Used with permission.

M. Dao, L. Lu, R.J. Asaro, J.T.M. De Hosson, E. Ma, Toward (2007) Acta Materialia

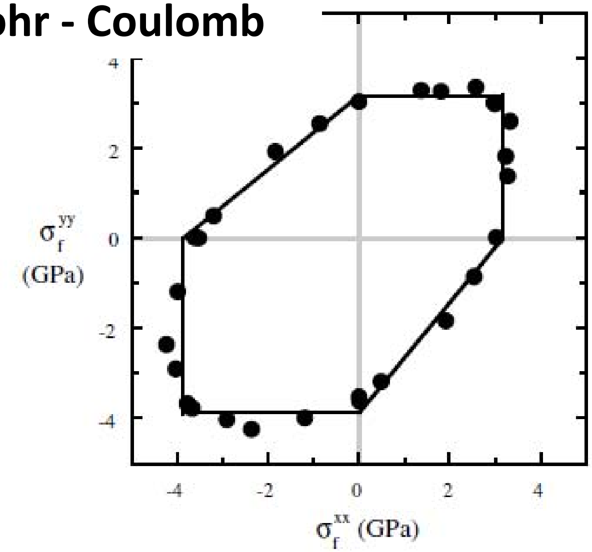
# nc yield criteria



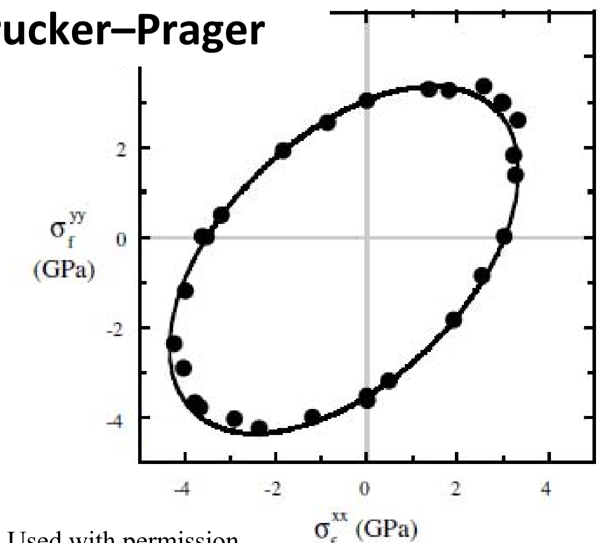

**tension/compression asymmetry**

***atomistic simulations for d = 4 nm***

**Mohr - Coulomb**



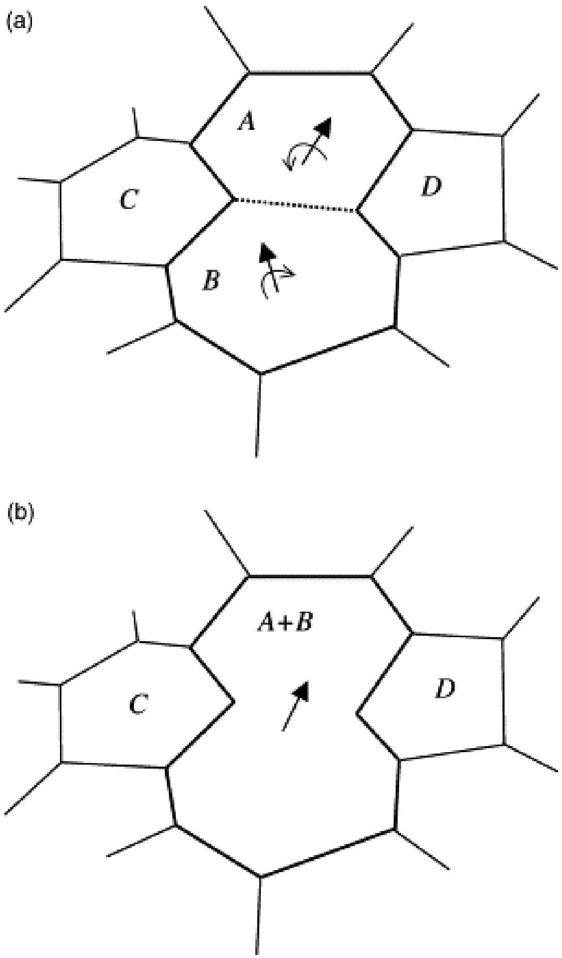

**Drucker–Prager**






A.C. Lund, C.A. Schuh (2005) Acta Materialia

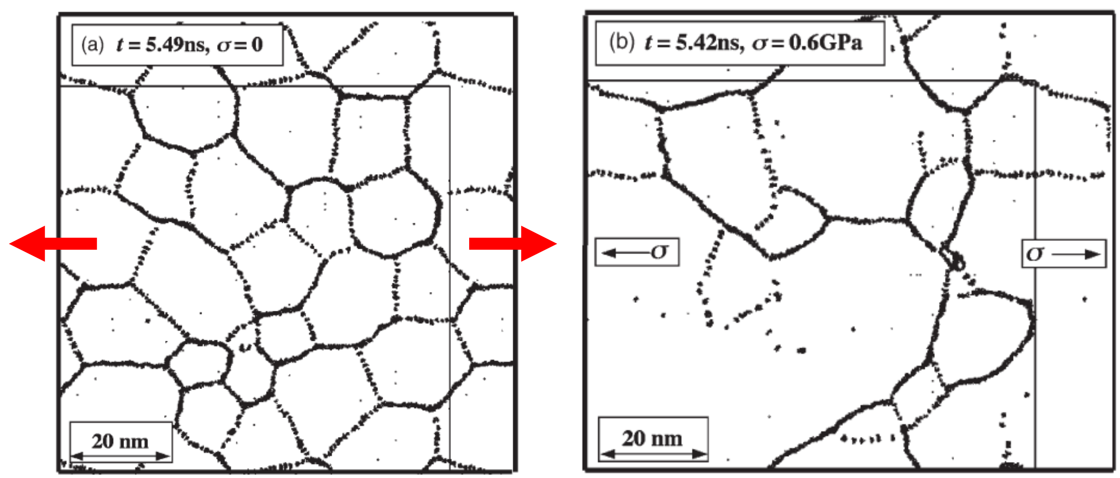
# mechanically-induced grain growth




*GB rotation*

Driven by mechanical force

- GB migration
- GB rotation




*before* *after*



D. Moldovan, D. Wolf, S. R. Phillpot, A. J. Haslam (2002) Acta Materialia
A.J. Haslam, D. Moldovan, V. Yamakov, D. Wolf, S.R. Phillpot, H. Gleiter (2003) Acta Materialia

# “Nanovated” material

**“Integran’s patented Nanovating process, creates materials with 1000 times smaller grain sizes.”**

**“Integran’s Grain Boundary Engineering (GBE®) process enhances reliability and durability by altering the internal structure of materials on the nanometre-scale.”**



**conventional grains** **average “nanovated” grain size ~ 20 nm**

http://www.integran.com/tech/nanovate.htm

# video – nc testing

- Atomistic simulation of nc Al:

  Psuedo1ntellectual. "Mechanical Properties of Nano-phase Metals (Tensile test)." August 7, 2007. YouTube. Accessed May 14, 2010. http://www.youtube.com/watch?v=QVJ1DOIDl2A

- Bending test of nc Ni-W coating on steel:

  TJRupert. "Bending test – 25 nm grain size – Nanocrystalline nickel-tungsten." October 6, 2009. YouTube. Accessed May 14, 2010. http://www.youtube.com/watch?v=xl8Ziy3H8CI