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SPRING COLLEGE IN MATERIALS SCIENCE
ON
"METALLIC MATERIALS"
(11 May - 19 June 1987)

DISLOCATIONS (Part I)

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DISLOCATIONS

SPRING COLLEGE MATERIALS SCIENCE
ICTP - Trieste MAY 1987

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OUTLINE.

1. DEFECTS IN CRYSTALS
2. OBSERVATION OF DISLOCATIONS
3. MOVEMENT OF DISLOCATIONS
4. ELASTIC PROPERTIES OF DISLOCATIONS
5. DISLOCATIONS IN FACE-CENTRED CUBIC METALS
6. Dislocations in other crystal structures
   - hexagonal close-packed metals
   - Body-centred cubic metals
   - dislocations in superlattices
   - dislocations in covalent crystals
   - dislocations in ionic crystals
   - dislocations in polymer crystals
7. Dislocations dynamics
   - nuclear spin-relaxation theory
   - spin relaxation due to dislocation motion
   - moving dislocations in ionic materials
   - moving dislocations in metals
   - moving dislocations in alloys.

1. Defects in crystals.

1.1. Crystalline materials

The arrangement of atoms in a crystal can be described with respect to a three-dimensional net of straight lines.
→ "space lattice"
Every point of a space lattice has identical surroundings.

The positions of the planes, directions and point sites are described by reference to the unit cell in the space lattice. The usual notation (Miller indices) is to take the reciprocals of the ratios of the intercepts to the corresponding unit cell dimensions

NOTE:
Brackets [ ] and ( ) imply specific directions and planes respectively, and < > and { } refer respectively to directions and planes of the same type.

1.2. Simple Crystal structures.

simple cubic structure: the atoms touch along $\langle 001 \rangle$

body-centred cubic structure: the atoms touch along $\langle 111 \rangle$

The stacking sequence of $\{100\}$ and $\{110\}$ planes is ABABAB...

The stacking sequence of $\{112\}$ planes is ABCDEFG AB....

face-centred cubic structure: the atoms touch along the $\langle 011 \rangle$ close packed directions.

The stacking sequence of $\{100\}$ and $\{110\}$ planes is: ABAB AB ...
The stacking sequence of $\{111\}$ planes is ABC ABC ...

The close packed hexagonal structure: stacking basal plane ABAB...

$\frac{c}{a} = 1.633$

Miller-Bravais indices: (h, k, i, l)

Basal plane (0001) $\quad i = -(h+k)$

Prism plane $(1\bar{1}00)$

1.3. DEFECTS

ⓐ point-defects.

Change of free energy ΔG associated with the introduction of n-vacancies:

$$\Delta G = n E_f^v - T \Delta S$$

$$\Delta S = \Delta S^{vib} + \underbrace{\Delta S^{conf}}_{k \ln \frac{(N+n)!}{N!\, n!}}$$

Equilibrium

$$\frac{\delta \Delta G}{\delta n} = 0$$

$$\Rightarrow \quad \frac{n}{N+n} \propto C_v(T) = e^{\frac{\Delta S^{vib}}{k}} e^{-\frac{\Delta E_f^v}{kT}}$$

Cu: $E_f^v = 1.3\,eV$ $\quad C_v(T = 1300k) = 10^{-5}$

$C_v(T = 300k) = 10^{-22}$

$$E_f^{Interstitial} >> E_f^{vacancy}$$

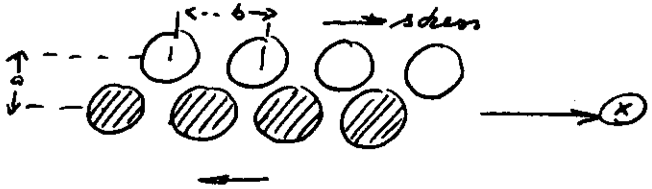
$$C_I(T) << C_v(T)$$

Dislocations belong to the microstructure, i.e. no thermal equilibrium concentrations. The same accounts for grain boundaries.

1.4. Dislocations.

Strong evidence arose from attempts to reconcile theoretical and experimental values of the applied shear stress required to plastically deform a single crystal.

Assume that there is a periodic shearing force required to move the top row of atoms across the bottom row:



$$\tau = \frac{\mu b}{2\pi a}\sin\left(\frac{2\pi x}{b}\right)$$

μ = shear modulus.

$$\tau_{max} = \frac{\mu b}{2\pi a}$$

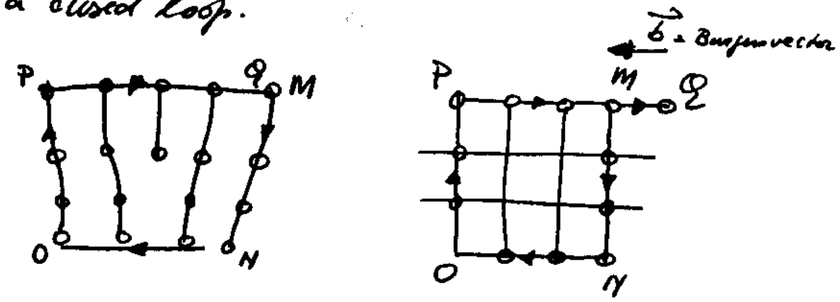
since $b \simeq a$: $\tau_{theo} \simeq$ fraction of μ.

$\tau_{observed} = 10^{-4} - 10^{-8}\mu$.

1934 OROWAN, POLANYI, TAYLOR
CONCEPT OF DISLOCATION.

GEOMETRY OF DISLOCATIONS.

The most useful definition of a dislocation is given in terms of the Burgers circuit. A Burgers circuit is any atom-to-atom path taken in a crystal containing dislocations which forms a closed loop.

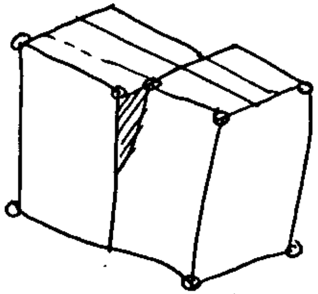


imperfect

perfect

The vector required to complete the closed circuit is called the "Burgers vector" $\vec b$

The Burgers vector $\vec b$ of an edge dislocation is normal to the line of the dislocation $\vec \xi$.



The Burgers vector of a screw dislocation is parallel to the line of the dislocation.

In most general case the dislocation line lies at an arbitrary angle to $\vec{b}$: mixed edge and screw character.

REMARKS:

(a) the circuit is taken in a clockwise fashion.

(b) $\vec{b}$ is taken to run from the finish to the start point of the reference circuit in the perfect crystal.

(c) Dislocations with the same sign but opposite $\vec{b}$ are physically opposite.

(d) reversing the line sense reverses the direction of $\vec{b}$ for a given dislocation.

Dislocation lines can end at the surface of a crystal and at grain boundaries, but never inside a crystal.

Thus, dislocations must either form closed loops or branch into other dislocations.

dislocation density:

$$\rho = \frac{\text{line length}}{\text{volume}} = [m^{-2}]$$

well annealed: $\rho = 10^4 - 10^6\ mm^{-2}$

semiconductors: $\rho \cong 0.1\ mm^{-2}$

plastically deformed: $\rho \cong 10^{+9}\ m^{-2}$

2. OBSERVATION OF DISLOCATIONS

2.1. The techniques can be devided in five main groups:

- a surface methods, in which the point of emergence of a dislocation at the surface of a crystal is revealed.
- b Decoration methods, in which dislocations in bulk specimens transparent to light are decorated with precipitate particles to show up their positions.
- c TEM.
- d X-ray topography
- e Field Ion Microscopy.
- f Nuclear Magnetic Resonance techniques (dynamics)

Except for e, and isolated examples in c these techniques reveal not-directly the arrangement of atoms but rely on such features as the strain field.

2.2. Surface methods.

The difference in the rate of removal of atoms due to chemicals arises from:

- a lattice distortion and strain field of the dislocation
- b geometry of planes associated with a screw dislocation
- c concentration of impurity atoms at the dislocation which changes the chemical composition.

methods:
- chemical and electrolytic etching
- thermal etching (at low pressure)
- sputtering (atom bombardment)

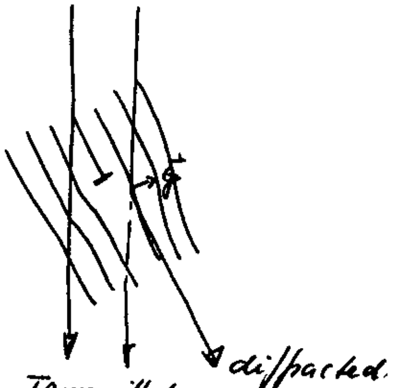
2.3. Decoration methods

There are a number of crystals which are transparent to visible light and infrared radiations. The dislocations in these crystals are not normally visible. However it is possible to decorate the dislocations by inducing precipitation along the dislocation line.

- KCl (by adding AgCl to the melt)
- Si (by adding Cu, Al, infrared)

2.4. Electron microscopy.

(See lecture notes M.L. Jenkins).



Screw dislocation.

In an isotropic medium, planes parallel to the line remain flat, for $\vec{u}$ (displacement vector) is parallel to $\vec{b}$. Hence, $\vec{g}$ is perpendicular to $\vec{b}$, $\vec{g}\cdot\vec{u} = \vec{g}\cdot\vec{b} = 0$, and the invisibility criterion is satisfied.

Edge dislocation

all ~~linear~~ planes parallel to the line are bent, and $\vec{u}$ is non-zero in all directions perpendicular to the line. In this case, both $\vec{g}\cdot\vec{b}$ and $\vec{g}\cdot(\vec{b}\times\vec{\xi})$ be zero, where $\vec{\xi}$ is a vector along the line. It is satisfied

only when $\vec{g}$ is parallel to the line, for only planes perpendicular to the line remain flat.

REMARK:

(a) For the mixed dislocation there is no combination for which $\vec{g}\cdot\vec{u}$ is exactly zero.

(b) In anisotropic crystals no planes remain flat around edge and screw dislocations, except in a few special cases. Thus the invisibility method for determining $\vec{b}$ often relies on finding $\vec{g}$ which results in weak contrast rather than complete invisibility.

2.5. X-ray diffraction topography

similar to Electron diffraction, but with a greatly reduced resolution.
image width is $1\mu m$

- Consequently, applicable only to study dislocations in crystals with low dislocation density.
- Advantage: Bulk technique.

2.6. Field Ion Microscopy.

tip radius : 5 – 100 nm
magnification: $10^6 - 10^9$

Atom probe technique : chemical composition can be analysed at the atomic level

(see lecture notes : P. Haasen).

2.7. Nuclear magnetic resonance techniques

see # 7 (Part II of the lecture notes)

3. Movement of Dislocations

3.1. Concept of slip

There are two basic types of dislocation movement.

ⓐ glide or conservative motion
in which the dislocation moves in the area which contains both $\vec{\xi}$ and $\vec{b}$.

ⓑ climb or non-conservative motion
in which the dislocation moves out of the glide area normal to $\vec{b}$.

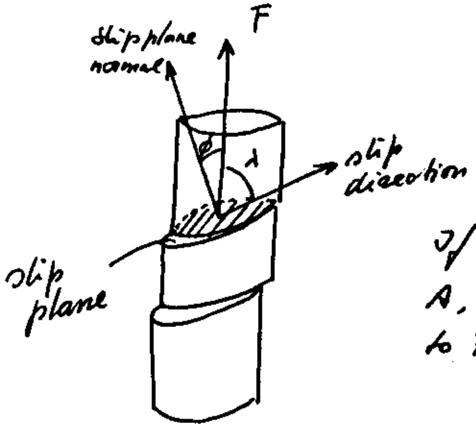
slip plane is normally the plane with the highest density of atoms and the direction of slip is the direction in the slip plane in which the atoms are most closely packed.

f.c.c. slip plane: $\{111\}$
slip direction: $\langle 110\rangle$

b.c.c. slip planes $\{110\}\ \{112\}\ \{123\}$
slip direction: $\langle 111\rangle$

h.c.p. slip plane : $\{0001\}$
slip direction: $\langle \bar{1}2\bar{1}0\rangle$

A characteristic shear stress is required for slip:



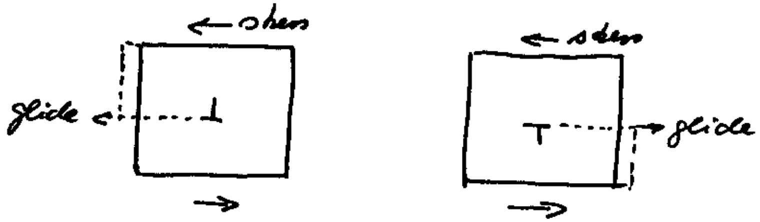
If the cross-sectional area is A, the tensile stress parallel to F is $\boxed{\sigma = \frac{F}{A}}$

The force has components $F\cos\lambda$ in the slip direction. This force $F\cos\lambda$ acts over the slip surface which has an area $\frac{A}{\cos\phi}$. Then the shear stress τ, resolved on the slipplane in the slip direction is:

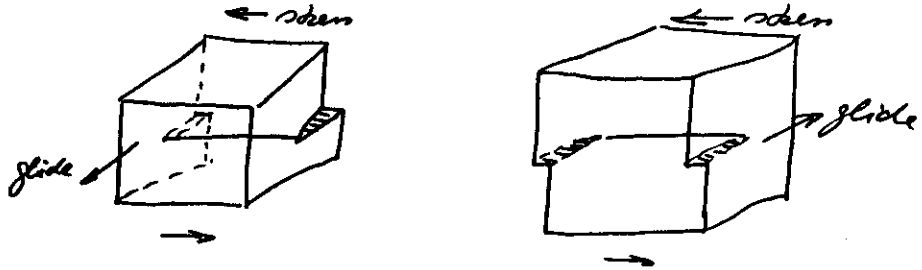
$$\tau = \frac{F\cos\lambda}{A/\cos\phi} = \frac{F}{A}\underbrace{\cos\phi\cos\lambda}$$

is called Schmid factor.

The direction in which a dislocation glides under stress can be determined by physical reasoning.



a positive edge dislocation glides to the left
a negative edge dislocation glides to the right



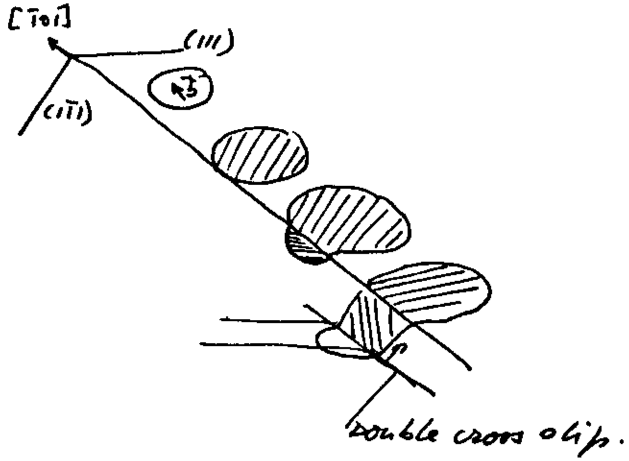
a right-handed screw dislocation glides to the front. a left-handed screw dislocation glides towards the back.
It demonstrates that:

ⓐ dislocations of opposite sign glide in opposite directions under the same stress

ⓑ for dislocation glide a shear stress must act on the slipplane in the direction of $\vec{b}$.

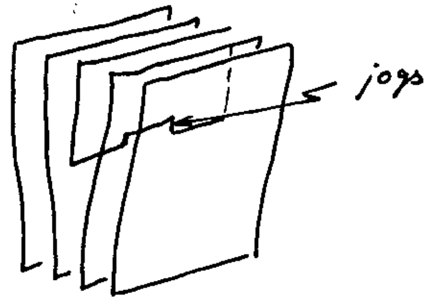
3.2. Cross-slip.

In general screw dislocations tend to move in certain crystallographic planes. In f.c.c. the screw dislocations move in $\{111\}$ planes but can switch from one $\{111\}$ type to another. This process is called cross slip.



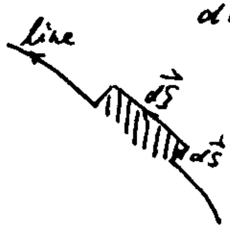
3.3. Climb

At low temperatures where diffusion is difficult, and in the absence of a non-equilibrium concentration of point defects, the movement of dislocations is almost entirely restricted to glide. At higher temperatures an edge dislocation can move out of its slip plane by a process called "climb"



REMARK:

If a small segment $d\vec{\xi}$ of a dislocation line undergoes a small displacement $d\vec{s}$, the local change in volume is:



$$dV = \vec{b} \cdot d\vec{\xi} \times d\vec{s} = \vec{b} \times d\vec{\xi} \cdot d\vec{s}$$

The glide plane is by definition perpendicular to $\vec{b} \times d\vec{\xi}$ and so when either $d\vec{s}$ is perpendicular to $\vec{b} \times d\vec{\xi}$ or $\vec{b} \times d\vec{\xi} = 0$ (screw), $\boxed{dV = 0}$

This is the condition for conservative motion.

For other cases, $dV \neq 0$, the volume is not conserved. The motion is climb and the number of point defects required is

$$\frac{dV}{\Omega}, \quad \Omega = \text{volume per atom.}$$

<u>Jogs</u> are steps on the dislocation which move it out of the slipplane. Steps which displace it on the <u>same</u> slip plane are called <u>kinks</u>.

<u>kinks:</u>

edge

screw

kinks do <u>not</u> impede glide of the line (in fact it may assist it)

<u>jogs</u>

<u>edge</u>

jogs on edge do not effect glide

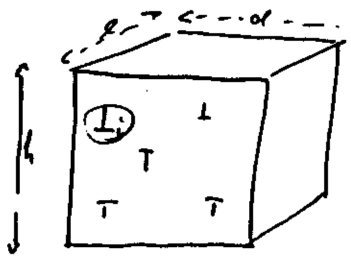
<u>screw</u>

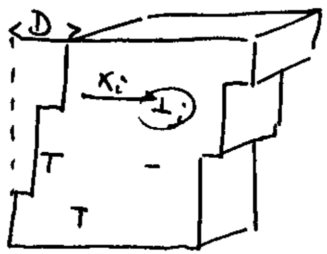
jogs on screw dislocation has <u>edge</u> character movement at right angles to $\vec{b}$ requires <u>climb</u>

3.4. Plastic strain due to dislocation movement.

Consider a crystal of volume hld containing edge dislocations. Under an applied stress dislocation will glide, positive ones to the right, negative ones to the left. The top surface is therefore displaced plastically relative to the bottom surface a distance D. If a dislocation moves completely across the slipplane through the distance d, it contributes b to D. Since b is small in comparison with d and h, the contribution which moves a distance x_i may be taken as the fraction $\frac{x_i}{d}$ of b. Thus if the number of dislocations which move is N, the total displacement is

$$\boxed{D = \frac{b}{d} \sum_i^N x_i}$$





dislocation i has moved a distance x_i.

The macroscopic shear strain ε is given by:

$$\varepsilon = \frac{D}{h} = \frac{b}{hd}\sum_i^N x_i$$

average distance moved by a dislocation:

$$\bar{X} = \frac{1}{N}\sum_i^N x_i$$

mobile dislocation density:

$$\rho_m = \frac{Nl}{hld}$$

$$\varepsilon = \frac{b}{hd}\sum_i^N x_i = \frac{bN}{hd}\bar{X} = b\rho_m\bar{X}$$

The strain rate

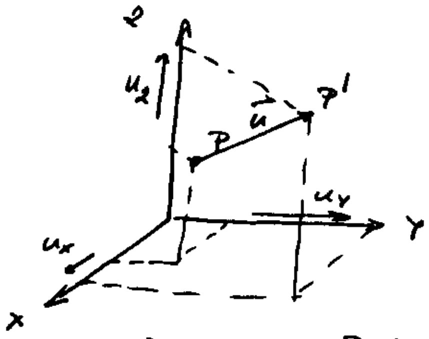
$$\boxed{\dot{\varepsilon} = \frac{d\varepsilon}{dt} = b\rho_m\bar{V}}$$

4. Elastic properties of dislocations.

4.1. Elements of elasticity theory

The displacement of a point in a strained body from its position in the unstrained state is represented by the vector:

$$\vec{u} = [u_x, u_y, u_z]$$



displacement of P to P' by $\vec{u}$.

STRAIN

In linear elasticity, the nine components of strain are given in terms of the first derivatives of $\vec{u}$.

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial u_y}{\partial y}, \quad \varepsilon_{zz} = \frac{\partial u_z}{\partial z}$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad i = x, y, z$$

partial differentials are used since in general $\vec{u} = f(x, y, z)$

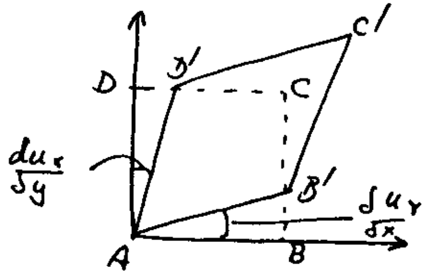
ε_{ij} components of a second rank tensor.

since:

$$\Delta u_i = \sum_j \frac{\partial u_i}{\partial x_j}\Delta x_j = \sum_j \varepsilon_{ij}\Delta x_j$$

vector components.

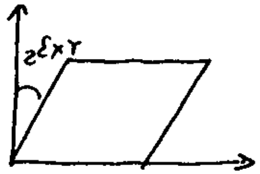
The six-components $\varepsilon_{xz}, \varepsilon_{zx}, \varepsilon_{xy}, \varepsilon_{yx}, \varepsilon_{yz}, \varepsilon_{zy}$ have simple physical meanings:



pure shear.

ABCD strained to AB'C'D' without change of area.

The angles between AB and AD has decreased by $\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} = 2\varepsilon_{xy}$. By rotating, but not deforming the element is it seen that the element has undergone simple shear.



simple shear.

the volume change:

$$(V+\Delta V) = V(1+\varepsilon_{xx})(1+\varepsilon_{yy})(1+\varepsilon_{zz})$$

The fractional change in volume Δ, known as dilatation:

$$\Delta = \frac{\Delta V}{V} = (\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz})$$

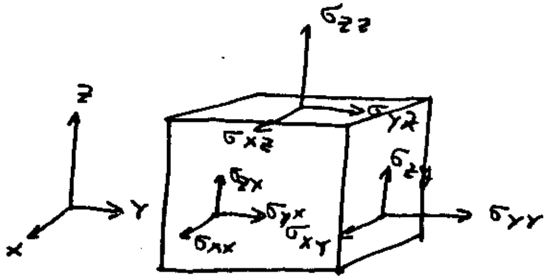
STRESS

stress = force per unit area of surface.

nine components:

σ_{ij} ($i,j = x\,y\,z$)

force per unit area in the positive i direction on a face with outward normal in the positive j-direction.

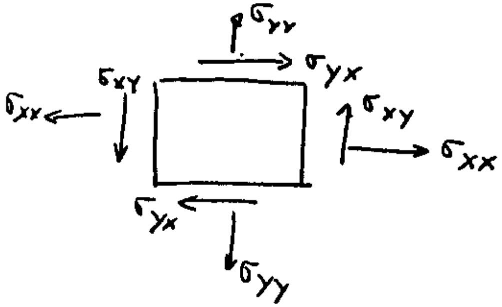


(+) Tensile stresses: $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$

(−) compressive stresses:

shear stresses: $\sigma_{yx}, \sigma_{xy}, \sigma_{zx}, \sigma_{xz}, \sigma_{yz}, \sigma_{zy}$

because $\sum \vec{M} = 0$, $\sigma_{ij} = \sigma_{ji}$



Hooke's law

$$\sigma_{ij} = c_{ijkl}\,\varepsilon_{kl}$$

$$\varepsilon_{ij} = s_{ijkl}\,\sigma_{kl}$$

(Einstein notation) implies summation over kl)

s = compliance, stiffness

c = (elastic) constant

In total 81 coefficients.

Since: $\sigma_{kl} = \sigma_{lk}$

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk}$$

81 → reduces to 36.

Helmholtz free energy:

$$(dF)_T = \sigma_{ij}\, d\varepsilon_{ij} = c_{ijkl}\,\varepsilon_{kl}\, d\varepsilon_{ij}$$

$$\frac{\partial^2 F}{\partial \varepsilon_{kl}\,\partial \varepsilon_{ij}} = \frac{\partial^2 F}{\partial \varepsilon_{ij}\,\partial \varepsilon_{kl}}$$

follows: $c_{ijkl} = c_{klij}$

36 reduces to 21.

notation: $c_{ijkl} \rightarrow c_{mn}$

$ij, kl \rightarrow$ 11 22 33 23 31 12 tensor notation

$\downarrow \quad \downarrow$

$m, n \rightarrow$ 1 2 3 4 5 6 matrix notation

$c_{2312} = c_{46}$ etc.

$$\{\sigma_{ij}\} = (ij) \xrightarrow{(kl)} \{c_{ijkl}\}\ \{\varepsilon_{kl}\}$$

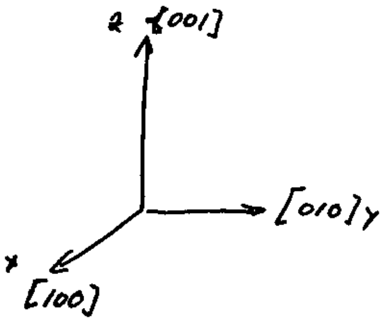
reduces to:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{21} \\ \sigma_{32} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{14} & c_{15} & c_{16} \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \end{bmatrix} \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ e_{23} \\ e_{31} \\ e_{21} \\ e_{32} \\ e_{13} \\ e_{12} \end{bmatrix}$$

because of symmetry:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix} \begin{bmatrix} e_{11} \\ e_{22} \\ e_{33} \\ 2e_{23} \\ 2e_{13} \\ 2e_{12} \end{bmatrix}$$

The number of <u>independent</u> elastic constants can be reduced further based on symmetry-considerations:



x, y, z : twofold and fourfold axes of rotation which leave the cubic <u>invariant</u>.

twofold axis around y:

	ijkl notation	m,n notation
x → −x	11 → 11	1 → 1
y → y	22 → 22	2 → 2
z → −z	33 → 33	3 → 3
	23 → −23	4 → −4
	13 → 13	5 → 5
	12 → −12	6 → −6

$$\{C_{mn}\} \xrightarrow[\text{axis around } Y]{2\text{ fold}} \begin{bmatrix} 11 & 12 & 13 & -14 & +15 & -16 \\ & 22 & 23 & -24 & +25 & -26 \\ & & 33 & -34 & 35 & -36 \\ & & & 44 & -45 & 46 \\ & & & & 55 & -56 \\ & & & & & 66 \end{bmatrix}$$

Invariant: $C_{14} \to -C_{14}$ therefore $C_{14} = 0$
$C_{15} \to -C_{15}$ therefore $C_{15} = 0$
etc.

$$\{C_{mn}\} = \begin{bmatrix} 11 & 12 & 13 & 0 & 15 & 0 \\ & 22 & 23 & 0 & 25 & 0 \\ & & 33 & 0 & 35 & 0 \\ & & & 44 & 0 & 46 \\ & & & & C_{55} & 0 \\ & & & & & 66 \end{bmatrix}$$

$$\{C_{mn}\} \xrightarrow[\text{around } \hat{y}]{4\text{ fold}} \begin{bmatrix} 33 & 23 & 13 & -36 & -35 & 34 \\ & 22 & 12 & -26 & -25 & 24 \\ & & 11 & -16 & -15 & 14 \\ & & & 66 & 56 & -46 \\ & & & & 55 & -45 \\ & & & & & 44 \end{bmatrix}$$

$x \to z$
$y \to Y$
$z \to -X$

combine: $\hat{C}_2(\hat{y})$ and $\hat{C}_4(\hat{y})$:

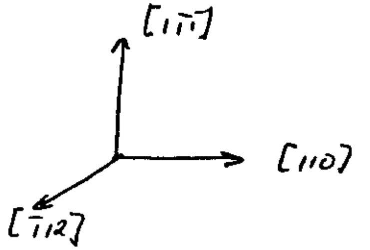
$$\hat{C}_4(\hat{Y}): \begin{bmatrix} 11 & 12 & 13 & 0 & -15 & 0 \\ & 22 & 12 & 0 & 0 & 0 \\ & & 11 & 0 & +15 & 0 \\ & & & 44 & 0 & 0 \\ & & & & 55 & 0 \\ & & & & & 44 \end{bmatrix}$$

⟨100⟩{100}

$$\begin{array}{ccc} \hat{C}_4(x) & \hat{C}_4(Y) & \hat{C}_4(z) \\ \begin{bmatrix} 11 & 12 & 12 & 0 & 0 & 0 \\ & 22 & 23 & 24 & 0 & 0 \\ & & 22 & -24 & 0 & 0 \\ & & & 44 & 0 & 0 \\ & & & & 55 & 0 \\ & & & & & 55 \end{bmatrix} & \begin{bmatrix} 11 & 12 & 13 & 0 & -15 & 0 \\ & 22 & 12 & 0 & 0 & 0 \\ & & 11 & 0 & +15 & 0 \\ & & & 44 & 0 & 0 \\ & & & & 55 & 0 \\ & & & & & 44 \end{bmatrix} & \begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 16 \\ & 11 & 13 & 0 & 0 & -16 \\ & & 33 & 0 & 0 & 0 \\ & & & 44 & 0 & 0 \\ & & & & 44 & 0 \\ & & & & & 66 \end{bmatrix} \end{array}$$

$$\begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{bmatrix} \quad \text{3 independent}$$

isotropy: $C_{44} = \frac{1}{2}(C_{11} - C_{12})$ 2 independent slip system: $\{111\}$



result in 7 independent c_{ij}

$$
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\
c_{12} & c_{22} & c_{12} & 0 & 0 & 0 \\
c_{13} & c_{12} & c_{11} & -c_{14} & 0 & 0 \\
c_{14} & 0 & -c_{14} & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{55} & -c_{14} \\
0 & 0 & 0 & 0 & c_{14} & c_{44}
\end{bmatrix}
$$

General:

$$
c_{ijrs} = \underbrace{a_{ip}\ a_{iq}\ a_{rl}\ a_{sm}}\ c_{pqlm}
$$

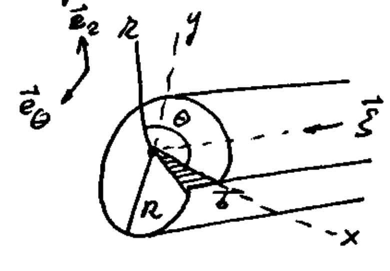
in dislocation system

elements of unitary - orthogonal transformation matrix (Euler transformation) matrix.

in cubic

4.2. Stress field of a straight dislocation:

Consider a screw dislocation along the axis of a cylinder of radius R and length L.



A reasonable guess for the displacement in the z direction is:

$$
u_z = \frac{b}{2\pi} \tan^{-1}\left(\frac{y}{x}\right)
$$

If a circuit is made about the dislocation line, the arctan function changes 2π, and thus u_z changes by the amount of b.

The elastic strains around the screw dislocation are:

$$
\varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) = -\frac{b}{4\pi}\ \frac{y}{x^2+y^2}
$$

$$
\varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right) = \frac{b}{4\pi}\ \frac{x}{x^2+y^2}
$$

$$
\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = 0
$$

The stress fields are:

$$\sigma_{xz} = 2\mu \varepsilon_{xz} = -\frac{\mu b}{2\pi} \frac{y}{x^2+y^2}$$

$$\sigma_{yz} = 2\mu \varepsilon_{yz} = \frac{\mu b}{2\pi} \frac{x}{x^2+y^2}$$

$$\sigma_{xx} = \sigma_{yy} = \sigma_{xy} = 0.$$

or written in polar coordinates:

$$\sigma_{\theta z} = -\sigma_{xz} \sin\theta + \sigma_{yz} \cos\theta = \frac{\mu b}{2\pi r}$$

$$\sigma_{rz} = \sigma_{13} \cos\theta + \sigma_{23} \sin\theta = 0$$

$$\sigma_{r\theta} = \sigma_{rr} = \sigma_{\theta\theta} = \sigma_{zz} = 0$$

$\sigma_{\theta z}$ means the stress in the z direction acting on a radial plane, i.e. a plane normal to $\vec{e}_\theta$.

The stress field has radial symmetry around the dislocation, $\sigma_{\theta z} = \frac{\mu b}{2\pi r}$ and is independent of θ.

Stationary edge dislocation

According to Newton's law the force in the x-direction will produce an acceleration $\frac{\partial^2 u_x}{\partial t^2}$ in the x-direction:

$$\rho \frac{\partial^2 u_x}{\partial t^2} = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z}$$

In the case of a stationary dislocation, $\frac{\partial^2 u_x}{\partial t^2}$ must set equal to zero. The equations reduce to:

$$(\lambda+2\mu)\frac{\partial^2 u_x}{\partial x^2} + \mu \frac{\partial^2 u_x}{\partial y^2} + (\lambda+\mu)\frac{\partial^2 u_y}{\partial x \partial y} = 0$$

$$\mu \frac{\partial^2 u_y}{\partial x^2} + (\lambda+2\mu)\frac{\partial^2 u_y}{\partial y^2} + (\lambda+\mu)\frac{\partial^2 u_x}{\partial x \partial y} = 0$$

$$\mu \left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} \right) = 0$$

The displacement of atoms that produced the edge dislocation is in the x-direction rather than in the z direction (screw). We anticipate (see screw) that the displacement u_x is given by $u_x = \frac{b}{2\pi} \tan^{-1}\left(\frac{y}{x}\right)$.

However, by itself the arctan function

does not satisfy the above mentioned equations. In order to satisfy both it is necessary to set:

$$u_x = \frac{b}{2\pi}\left[\tan^{-1}\left(\frac{y}{x}\right) + \frac{\lambda+\mu}{\lambda+2\mu}\frac{xy}{x^2+y^2}\right]$$

$$u_y = \frac{b}{2\pi}\left[-\frac{\mu}{2(\lambda+2\mu)}\ln\left(\frac{x^2+y^2}{c}\right) + \frac{\lambda+\mu}{\lambda+2\mu}\frac{y^2}{x^2+y^2}\right]$$

The elastic displacements give rise to strains:

$$\varepsilon_{xx} = -\frac{by}{2\pi}\frac{\mu y^2 + (2\lambda+3\mu)x^2}{(\lambda+2\mu)(x^2+y^2)^2}$$

$$\varepsilon_{yy} = \frac{by}{2\pi}\frac{(2\lambda+\mu)x^2 - \mu y^2}{(\lambda+2\mu)(x^2+y^2)^2}$$

$$\varepsilon_{xy} = \frac{b}{4\pi(1-\nu)}\frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

where $\nu = \frac{\lambda}{2(\lambda+\mu)}$ Poisson's ratio.

The stresses calculated are:

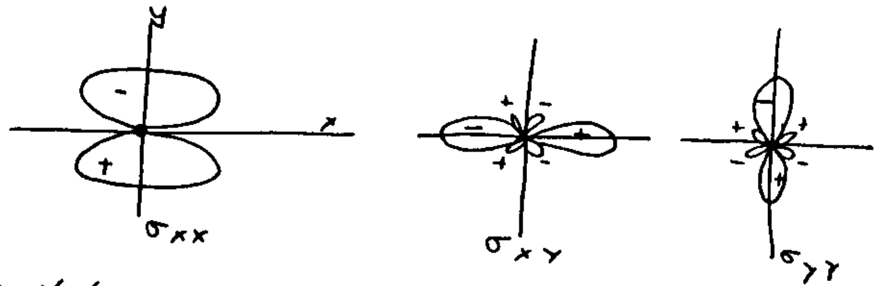
$$\sigma_{xx} = \frac{-\mu b}{2\pi(1-\nu)}\frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$

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

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

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

$$\sigma_{xz} = \sigma_{yz} = 0.$$



Limitations:

(a) elastic solutions apply to a ring of isotropic material. A real crystal is not an isotropic continuum.

(b) σ varies as $1/r$. It will rise to infinity at $r=0$. There exists a limiting radius r_c below which the elastic solutions do not apply.

4.3 Strain energy of a dislocation.

$$E_{tot} = E_{core} + E_{elastic\text{-}strain}.$$

For a screw dislocation the elastic work done in displacing the faces of a crystal unit length by a distance b along the slip direction relative to eachother is:

$$E_{el}^{(s)} = \frac{1}{2}\int_{r_c}^{r_1} \sigma^{o}_{\theta z}\, b\, dr$$

$\sigma^{o}_{\theta z}$: stress acting in z direction on radial plane perpendicular to $\hat{e}_\theta$.

$$\sigma^{o}_{\theta z} = \frac{\mu b}{2\pi r}$$

$$E_{el}^{(screw)} = \frac{1}{2}\int_{r_c}^{r_1} \frac{\mu b^2}{2\pi r}\, dr = \frac{\mu b^2}{4\pi} \ln \frac{r_1}{r_c}$$

Elastic energy depends on size of the crystal!!

The corresponding equations for an edge dislocation:

$$E_{el}^{(edge)} = \frac{1}{2}\int_{r_c}^{r_1} \sigma^{o}_{r\theta}\, b\, dr$$

$$\sigma_{r\theta} = \frac{\mu b}{2\pi(1-\nu)} \frac{\cos\theta}{r}$$

For a slit cut along the slipplane $\cos\theta = 1$

$$E_{el}^{(edge)} = \frac{1}{2}\int_{r_c}^{r_1} \frac{\mu b^2}{2\pi(1-\nu)} \frac{dr}{r} = \frac{\mu b^2}{4\pi(1-\nu)} \ln\left(\frac{r_1}{r_c}\right)$$

Conclusion

$E_{elastic}$ (dislocations) $\propto \underline{\underline{\mu b^2}}$

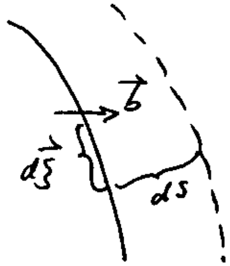
(order of 8 eV/plane)

Consider the reaction:

$$\frac{1}{2}[1\bar{1}\bar{1}] + \frac{1}{2}[111] \rightarrow [100]$$
$$\vec{b}_1 + \vec{b}_2 \rightarrow \vec{b}$$

According to $E_{elastic}$, the elastic strain energies are proportional to b_1^2, $\vec{b}_1^2$ and b^2. Since $b_1^2 + b_2^2 > b^2$ it follows that when the dislocations meet, the reaction results in a reduction of strain energy.

4.4. Forces on dislocations



consider a dislocation moving in the direction of $\vec{b}$. When an element $d\vec{\xi}$ moves forward a distance ds the crystal above and below the slipplane will be displaced relative to each other. The average shear displacement produced is:

$$\left(\frac{d\xi\, ds}{A}\right) b$$

A : area slip plane. The applied force giving the stress τ is $A\tau$ so that the work done is:

$$dW = A\tau \cdot \left(\frac{d\xi\, ds}{A}\right) b = \tau b\, d\xi\, ds$$

In addition to the force due to an externally applied stress, a dislocation has a line tension: ($E_{elastic} \approx \mu b^2$ per unit length)

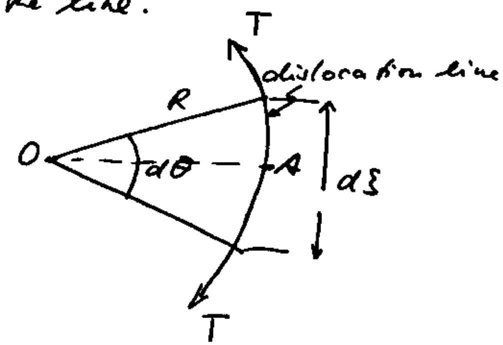
The line tension, which may be defined as the increase in energy per unit increase in the length of a dislocation line, will be

$$T = \alpha \mu b^2$$

(compare: surface tension $= \dfrac{E_{surface}}{\text{unit area}}$

line tension $= \dfrac{\text{line energy}}{\text{unit length}}$)

The line tension will produce a force tending to straighten the line and so reduce the total energy of the line.



- Outward force along OA due to the applied stress: $\tau_0\, b\, d\xi$
- Opposing inward force along OA due to line tension T:

$$2T \sin\left(\frac{d\theta}{2}\right) \approx T d\theta$$

Equilibrium:

$$T\,d\theta = \tau_0\, b\, d\xi$$

$$\tau_0 = \frac{T}{bR} \qquad (d\xi = R\,d\theta)$$

$T = \alpha \mu b^2$

$$\boxed{\tau_0 = \frac{\alpha \mu b}{R}}$$

The force required to bend a dislocation to a radius R. (orowan stress)

4.5. Forces between dislocations

In general, dislocations with opposite sign will attract each other; dislocations with the same sign will repel each other.

Screw dislocations

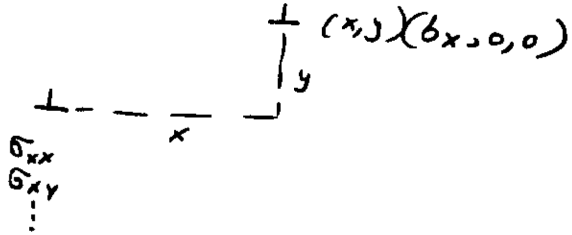
stress field has radial symmetry:

$$F_r = \tau_{\theta r}\cdot b = \frac{\mu\, \vec{b}\cdot\vec{b}}{2\pi r}$$

The force is attractive for dislocations of opposite sign and repulsive for dislocations of the same sign.

edge dislocations

$$\vec{F} = \frac{dW}{ds} = \left(\overline{\overline{\Sigma}}\cdot\vec{b} \times d\vec{\xi}\right)$$



$$\begin{bmatrix} \sigma_{11}\hat{x}\hat{x} & \sigma_{12}\hat{x}\hat{y} & 0 \\ \sigma_{12}\hat{y}\hat{x} & \sigma_{22}\hat{y}\hat{y} & 0 \\ 0 & 0 & \sigma_{33}\hat{z}\hat{z} \end{bmatrix} \cdot \begin{bmatrix} \hat{x} b_x \\ 0 \\ 0 \end{bmatrix}$$

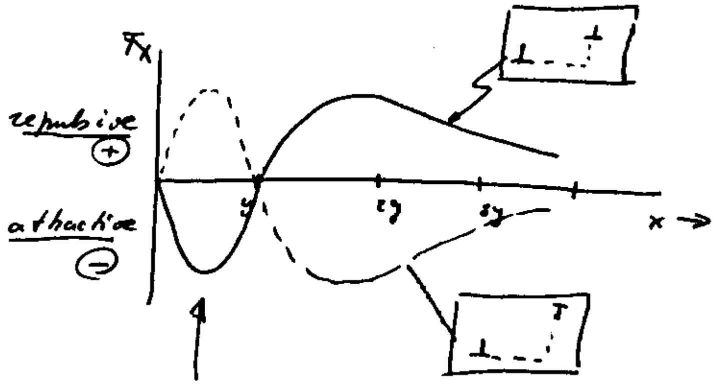
$$(b_x \sigma_{11}\hat{x} + b_x\sigma_{12}\hat{y}) \times d\vec{\xi} \rightarrow \hat{x}\sigma_{21} b_x - \hat{y}\sigma_{11} b_x$$

$$F_x = \sigma_{21} b_x$$

$$F_y = -\sigma_{11} b_x$$

$$\vec{F} = \frac{\mu b^2}{2\pi(1-\nu)}\frac{x(x^2-y^2)}{(x^2+y^2)^2}\hat{x} + \frac{\mu b^2}{2\pi(1-\nu)}\frac{y(3x^2+y^2)}{(x^2+y^2)^2}\hat{y}$$

$$F_x = \frac{\mu\,\vec{b}\cdot\vec{b}}{2\pi(1-\nu)}\;\frac{x(x^2-y^2)}{(x^2+y^2)^2}$$



The dislocations will repel each other for all values $x > y$ when both dislocations have positive signs. For dislocations of opposite signs $F_x < 0$ for $x > y$ and the dislocations will attract each other.