Dislocation loops

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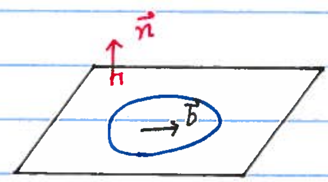
1. Formation of loops

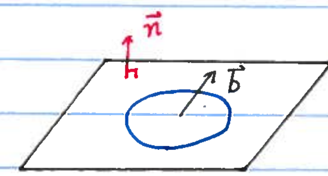
· The actual forms of dislocations in materials.
·· Not straight, circle, ...

· The main part of dislocations formed during plastic deformation is in the form of loops.

· Two kinds of dislocation loop.
i) slip loops ; $\vec{b} \cdot \vec{n} = 0$
ii) prismatic loops ; $\vec{b} \cdot \vec{n} \neq 0$



[slip loop]

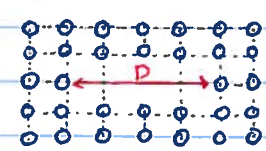


[prismatic loop]

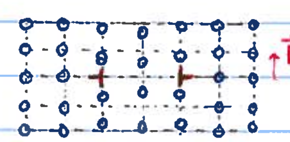
– Slip loops
·· usually formed under external stress or by stress concentration on inhomogeneities
·· can further extend up to $1\mu \sim 100\mu$

– Prismatic loops.
··· first proposed by Nabarro (1947)

· vacancy precipitation forms discs.



· collapse of the vacancy disc.
··· can glide along its slip cylinder
··· can only move on its plane by climb



·· formed after quenching, which produces a high supersaturation of vacancies.
and during subsequent annealing, which enables diffusion and precipitation of vacancies.

-- average $D \sim 300$Å

- <u>Precipitation of vacancies (FCC).</u>
  - Assume that the disc of vacancies is form in (111)
  - Energy of disc (E_0)

$$E_0 = 2\pi R^2 \gamma_0$$

(γ_0 ; surface energy density).

  - Prismatic loop can be formed by the collapse of disc.
  - The Burgers vector of the loop.

$\vec{b}_1 = \frac{1}{3}[111]$ ~ normal to the loop plane.

  - The loop is formed by a partial dislocation and encloses a staking fault.
  - The energy of the loop (E_1)

$$E_1 = E_1' + E_1'' = \text{Total staking fault } E + \left(\begin{array}{l}\text{Elastic energy} \\ \text{Core } \text{''}\end{array}\right)$$

$$= \pi R^2 \gamma + E_1''$$

  - if $E_1 \leq E_0$ ∴ disc will collapse.
  - R_c (critical radius) ~ few atomic distance in F.CC
  - ∴ After further growth, a partial dislocation loop can change into a dislocation loop with a complete Burgers vector $\vec{b} = \frac{1}{2}[110]$ without staking fault
  - if $E_2 \leq E_1$ ∴ transformation occurs.

R_{c_2} ~ 100Å

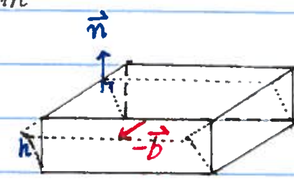
$$\begin{cases} R > R_{c_2} \therefore \text{Complete } \vec{b} \\ R < R_{c_2} \therefore \text{Partial } \vec{b} \end{cases}$$

∴ as $\gamma\uparrow$ ∴ $R_{c_2}\downarrow$ ∴ complete Burgers vector

- The process of vacancy precipitation ~ purity, defects, thermal treatm
- Prismatic loops can be formed by punching effect
  (Annealing the crystal containing precipitates with different thermal expansion cofficient)
- Prismatic loops are also formed in plastically defomed crystals by the motion of screw dislocations with large jogs.

2. Infinitesimal loops.

- Displacement & Stress field around it.
- Consider a plate-like region T with an area δA and a thickness h.



I. Take T out of the body & transform it (upper side will be displaced by $-\vec{b}$

- plastic displacement ; $u_k = -\frac{b_k}{h}(x_l' - x_l^{0\prime})\, n_l$

x_l' : coordinates of a point of the region
$x_l^{0\prime}$; " " " " on the lower side

- plastic strain

$$e^T_{kj} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_j'} + \frac{\partial u_j}{\partial x_k'}\right)$$

$$= -\frac{1}{2h}\left(b_k n_j + b_j n_k\right)$$

- Stress in T = "0"

Stress formally calculated from Hooke's law using e^T_{kj}

$$\sigma^T_{kj} = \lambda e^T_{ll}\delta_{kj} + 2\mu e^T_{kj}$$

II. · Apply $-\sigma^T_{kj}\nu_k$ on the surface of T
(ν_k ; unit normal to the surface of T)
It brings the region back to the original shape.
· Put it back in the body & join across the whole surfac
· Then, the surface forces have now become a layer of body force spread over A

III. Let these body forces relax. or
Apply a futher distribution $+\sigma^T_{kj}\nu_k$ over A
The displacement component u_i at point $\vec{x}$, due to the component F_j of a point force acting at the point $\vec{x}'$: $u_i = U_{ij}F_j$

$$U_{ij} = \frac{1}{16\pi\mu(1-\nu)}\left[\delta_{ij}\frac{1}{\rho}(3-4\nu) + \frac{\rho_i\rho_j}{\rho^3}\right]$$

$$\rho_i = x_i - x_i'$$
$$\rho = \sqrt{(x_1-x_1')^2 + (x_2-x_2')^2 + (x_3-x_3')^2}$$

- The displacement u_i from a surface distribution of forces $+\sigma_{kj}^T \nu_k$

$$u_i = \iint_{(A)} U_{ij} \underbrace{\sigma_{kj}^T \, dA_k}_{dF_j}$$

or, Using the Gauss theorem

$$u_i = \iiint_{(V)} \sigma_{kj}^T U_{ij,k'} \, dV' = \sigma_{kj}^T \iiint_{(V)} U_{ij,k'} \, dV'$$

σ_{kj}^T ; constant inside T

At a large distance from T, the displacement

$$u_i = U_{ij,k'} \, \sigma_{kj}^T \, V' \qquad (V' = \delta A \cdot h)$$

The $U_{ij,k'}$ is taken with respect to the coordinate x_k' of an internal point of T. Let's take center of T as x_k'

$$\boxed{u_i = -\frac{1}{8\pi(1-\nu)\rho^2} \left\{ \frac{1-2\nu}{\rho} [n_i b_k \rho_k + b_i n_k \rho_k - \rho_i b_k n_k] + \frac{3\rho_i b_k \rho_k n_l \rho_l}{\rho^3} \right\} \delta A} \quad (2.9)$$

$\therefore$ not depend on h (thickness)

$\therefore$ $\lim_{h \to 0} u \Rightarrow T$; dislocation loop

u ; displacement at a large distance from (finite) dislocation loop

- For an infinitesimal area δA the loop can be infinitesimal

$$du_i = -\frac{1}{8\pi(1-\nu)\rho^2} \{ \cdots \} \, dA$$

- The stress tensor σ_{ij} at a large distance from a finite loop or $d\sigma_{ij}$ around an infinitesimal loop.

$$\boxed{\begin{aligned} \sigma_{ij} = \frac{-\mu}{4\pi\rho^3(1-\nu)} \Big\{ &\Big[\frac{3(1-2\nu)}{\rho^2} b_k \rho_k n_l \rho_l + (4\nu-1) b_k n_k \Big] \delta_{ij} + (1-2\nu)(b_i n_j + n_i b_j) \\ &+ \frac{3\nu}{\rho^2} [b_k \rho_k (n_i \rho_j + \rho_i n_j) + n_k \rho_k (b_i \rho_j + \rho_i b_j)] \\ &+ \frac{3(1-2\nu)}{\rho^2} b_k n_k \rho_i \rho_j - \frac{15}{\rho^4} b_k \rho_k n_l \rho_l \rho_i \rho_j \Big\} \delta A \end{aligned}} \quad (2.11)$$

- Displacement decreases with distance ρ as $1/\rho^2$
  Stresses $\sim 1/\rho^3$
- The displacements and stresses of a general dislocation are given as surface integrals over its area δA

$$u_i = \iint_{(\delta A)} du_i \qquad (2.12)$$

$$\sigma_{ij} = \iint_{(\delta A)} d\sigma_{ij} \qquad (2.13)$$

- $\left.\begin{array}{l}\text{Displacements}\\ \text{Stresses}\end{array}\right\}$ do not depend on the shape.

  only depend on the area of the loop.

3. Stress field and energy of finite loop.

- $\underline{\underline{\sigma}}$; can be derived in different ways.
  - ex) from (2.13)
  - very complicated.
  - ref [10] [35] [19].
    - pure prismatic circular loop
    - slip circular loop
    - angular dislocations.
  - in the neighbourhood of the dislocation line of the loop
    - $\sigma \sim 1/\rho$
  - at a large distance
    - $\sigma \sim 1/\rho^3$
  - Stresses of an infinitesimal loop gives a very good approximation for the stresses of finite loop not only at large distances but also not very far away from the loop $(\sim \rho > 2R)$

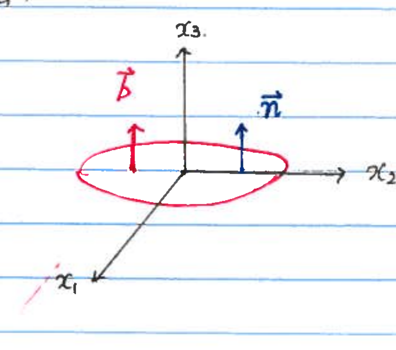
- The elastic energy E of the loop.
  - Volume integral of the strain energy density
  - Core of dislocation (ε) must be left out.
  - $\varepsilon \sim b$

$$E = \frac{1}{2} \iint_{(SA')} n_i \sigma_{ij} b_j \, dA$$

(SA' : area of the loop from which the neighbourhood of dislocation line is left out)

For a plane Volterra loop (n_i, b_i ; constant)

$$E = \frac{1}{2} n_i b_j \iint_{(SA')} \sigma_{ij} \, dA$$



example) Pure prismatic loop

$$E = \frac{1}{2} b \iint_{(SA')} \sigma_{33} \, dA$$

$$E = \frac{\mu}{2(1-\nu)} b^2 R \left(\ln \frac{8R}{\varepsilon} - 1\right)$$ (pure prismatic circular loop)

$$E = \frac{\mu(2-\nu)}{4(1-\nu)} b^2 R \left(\ln \frac{8R}{\varepsilon} - 1\right)$$ (slip circular loop)

$$E_E = \frac{\mu b^2}{4\pi(1-\nu)} \ln \frac{r_1}{\varepsilon} \quad ; \ E/\text{length}$$ (straight edge dislocation)

$$E_S = \frac{\mu b^2}{4\pi} \ln \frac{r_1}{\varepsilon} \quad , \ E/\text{length}$$ (" screw ")

(r_1 ; dimension of the crystal ~ 1cm)

[Note] $E/\text{length}\big|_{\text{loop}} < E/\text{length}\big|_{\text{straight}}$

- The total loop energy = elastic energy + core energy.
  - Peierls - Nabarro model : $E_{core}/\text{length} = \dfrac{\mu b^2}{4\pi(1-\nu)}$ (edge)

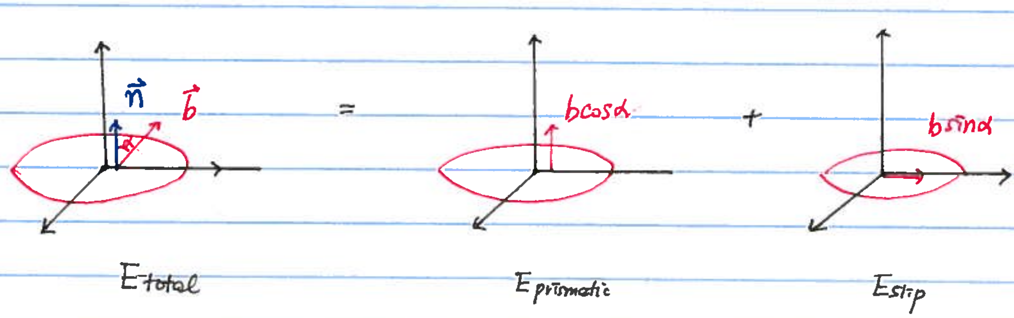
    $\dfrac{\mu b^2}{4\pi}$ (screw)

- Rough approximation $E_{total} \simeq E_{elastic}$ (if $\varepsilon \ll 1$)

- The energy of a general prismatic loop.

  = energies of pure prismatic loop with $\vec{b} = b\cos\alpha\,\vec{n}$

  + energies of a slip loop with $\vec{b} = b\sin\alpha$.



(interaction E of these loops = "0")

$$E \cong \frac{\mu b^2}{4\pi(1-\nu)} \underset{\uparrow\, 2\pi R}{L} \left(\cos^2\alpha + \frac{1-\nu}{2}\sin^2\alpha\right) \ln \frac{R}{\varepsilon}$$

4. Interaction of loops with other lattice defects.

- only elastic interaction.
- Consider σ_{ij}' (from external force or another defect on finite plane loop)
- E_{int} (work necessary to form the loop in the stress σ_{ij}')

$$E_{int} = n_i b_j \iint_{(SA')} \sigma_{ij}' \, dA$$

- dF' (force on the element of dislocation line ds due to σ_{ij}'

$$dF_i' = \epsilon_{ijk} \sigma_{jl}' b_l dS_k$$

- F (total force)

$$F_i = \oint_{(S)} \epsilon_{ijk} \sigma_{jl}' b_l dS_k$$

- For a homogeneous stress field σ_{ij}'

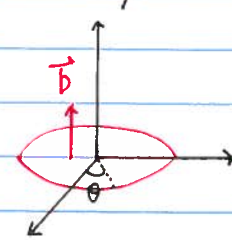
$$\begin{cases} F = 0 \\ E = \text{constant} \end{cases}$$

Only the resultant of the force dF_i' is zero, but the force dF_i' try to expand or contract the loop.

- Ex) Pure prismatic loop.

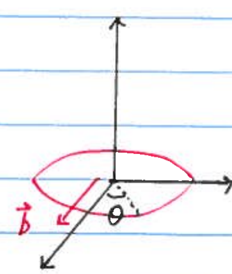
f_i' ; force on unit element of circular loop.

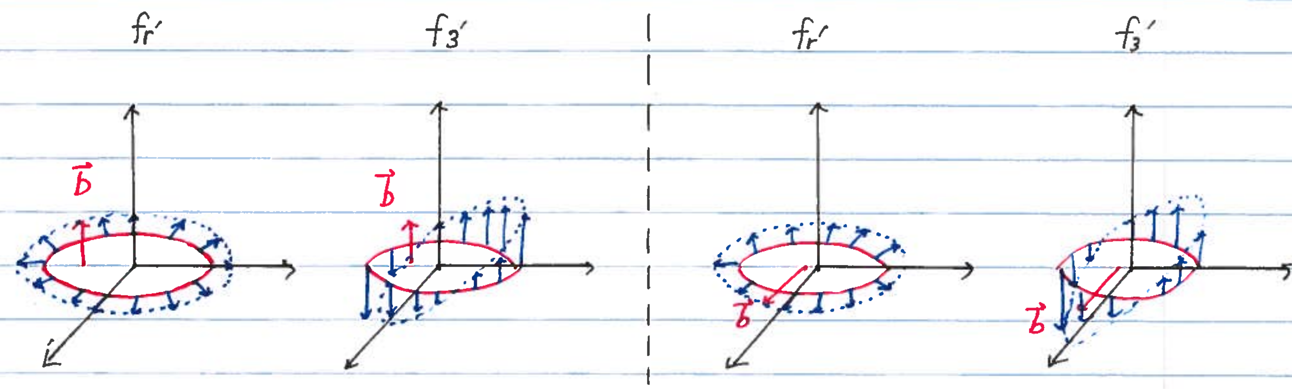
$$\begin{cases} f_1' = -\sigma_{33}' b_3 \cos\theta \\ f_2' = -\sigma_{33}' b_3 \sin\theta \\ f_3' = (\sigma_{13}' \cos\theta + \sigma_{23}' \sin\theta) b_3 \end{cases} \quad \Big) \; f_r' = -\sigma_{33}' b_3$$



Ex2) Slip loop.

$$f_1' = -\sigma_{13}' b_1 \cos\theta$$
$$f_2' = -\sigma_{13}' b_1 \sin\theta \quad \Big) \; f_r' = -\sigma_{13}' b_1$$
$$f_3' = (\sigma_{11}' \cos\theta + \sigma_{12}' \sin\theta) b_1$$





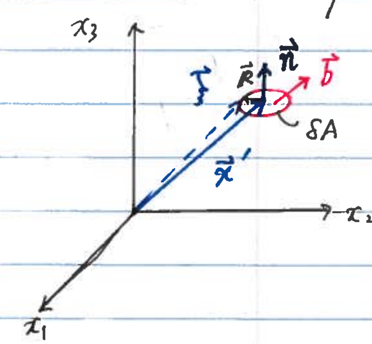
[pure prismatic loop] [slip loop]

f_r' ; expand the loop by climb (for prismatic loop)
by glide (for slip loop)

f_3' ; rotate the loop

- In a non-homogeneous σ_{ij}' → non-zero resultant
→ translate the loop

- The influence of σ_{ij}' on an infinitesimal dislocation loop.



- The interaction energy

$$E_{int} = n_i \sigma_{ij}' b_j \delta A$$

- The total force

$$F_k = -\frac{\partial E_{int}}{\partial x_k'} = -n_i \sigma_{ij,k}' b_j \delta A$$

- The "induced surface tension"

$$\sim E_{int} / \text{unit Area}$$

$$p' = n_i \sigma_{ij}' b_j$$

if $p' > 0$; acts inwards ~ contract the loop
$p' < 0$; acts outwards ~ expand the loop

- The moment of forces.

$$M_i' = \oint e_{ijk} \xi_i \, dF_k'$$

$$\xi_j = x_j' + R_j$$

$$M_i' = M_{F_i} + F_{C_i}'$$

$$= \underbrace{\oint \epsilon_{ijk} x_j' dF_k'}_{} + \oint \epsilon_{ijk} R_j dF_k'$$

$= \epsilon_{ijk} x_j' \oint dF_k'$

$= \epsilon_{ijk} x_j' F_k$ ~ moment of the total force on the loop with respect to the origin of coordinate sys.

For infinitesimal loop.

$$M_{F_i} = -\epsilon_{ijk} x_j' n_l \sigma_{lm,k}' b_m \, \delta A$$

- M_F depends on the choice of the coordinate system
  - not interesting from the physical point of view.
- M_C' ~ physically important.
  ~ moment of the forces on the loop w.r.t its center.

$$M_{C_i}' = -\epsilon_{ijk} n_j b_l \sigma_{lk}' \, \delta A$$

- E_{int}, P', M_{C_i}' ~ σ_{ij}'
  ~ non-zero in the homogeneous σ_{ij}'
  (cf) F_k, $M_{F_i} = 0$)
- E_{int}, P', F_k, M_{F_i}, M_{C_i}'
  ~ do not depend on the shape of the infinitesimal lo
- Self-energy of small loop depends on its shape
- Self-force try to contract the loop.
- The total self-force = "0"