Dislocation theory

Subjects of interest

- Introduction/Objectives
- Observation of dislocation
- Burgers vector and the dislocation loop
- Dislocation in the FCC, HCP and BCC lattice
- Stress fields and energies of dislocations
- Forces on dislocations and between dislocations
Subjects of interest (continued)

- Dislocation climb
- Intersection of dislocations
- Jogs
- Dislocation sources
- Multiplication of dislocations
- Dislocation-point defect interactions
- Dislocation pile-ups
Objectives

• This chapter emphasises the understanding of the effects of dislocation behaviour on FCC, BCC and HCP crystal structures.

• This includes the interaction of dislocations such as climb, jogs, intersection and multiplication of dislocations and the roles of dislocations on plastic deformation of metals.
**Dislocations** introduce imperfection into the structure and therefore these could explain how real materials exhibit lower yield stress value than those observed in theory.

- Lower the yield stress from theoretical values.
- Produce plastic deformation (strain hardening).
- Effects mechanical properties of materials.
A variety of techniques have been used to observe dislocations in the past 20 years to aid the better understanding of dislocation behaviour.

Chemical (etch–pit) technique

- Using etchant which forms a pit at the point where a dislocation intersect the surface.
- Preferential sites for chemical attack are due to strain field around dislocation sites (anodic).
- Can be used in bulk samples but limited in low dislocation density crystal (10⁴ mm⁻²).

Note: Pits are 500 Å apart and with the dislocation density of 10⁸ mm⁻².
Decoration of dislocation technique

A small amount of impurity is added to form precipitates after suitable heat treatment to give internal structure of the dislocation lines.

- Hedges and Mitchell first used photolytic to decorate dislocation in AgBr.
- Rarely used in metals but in ionic crystals such as AgCl, NaCl, KCl and CaF₂.

Hexagonal network of dislocations in NaCl detected by a decoration technique.
Transmission electron microscope (TEM)

TEM is the most powerful technique used to study dislocations.

- A thin foil of 100 nm is prepared using electropolishing from a ~1 mm thick sheet.
- This thin foil is transparent to electrons in the electron microscope and this makes it possible to observed dislocation networks, stacking faults, dislocation pile-ups at grain boundaries.
- By using the kinematic and dynamic theories of electron diffraction it is possible to determine the dislocation number, Burgers vectors and slip planes.

Note: The sampling area is small therefore the properties observed cannot represent the whole materials.
**X-ray microscopy**

- Using an X-ray technique to detect dislocation structure.
- The most common techniques are the **Berg-Barret reflection method** and the **Lang topography method**.
- The resolution is limited to $10^3$ dislocations/mm$^2$. 
**Burgers vector and the dislocation loop**

*Burgers vector* is the most characteristic feature of a dislocation, which defines the magnitude and the direction of slip.

- Edge *Burgers vector* is \( \perp \) to the dislocation line.
- Screw *Burgers vector* is \( \parallel \) to the dislocation line.
- Both shear stress and final deformation are identical for both situations.

*Note:* Most dislocations found in crystalline materials are probably neither pure edge or pure screw but mixed.
Dislocations in single crystals are straight lines. But in general, dislocations appear in **curves or loops**, which in three dimensions form and interlocking dislocation network.

- Any small segments of the dislocation can be resolved into edge and screw components.

- **Ex:** pure screw at point A and pure edge at point B where along most of its length contains mixed edge and screw. But with the **same Burgers vector**.

**Dislocation loop lying in a slip plane.**
Burgers circuit is used to define the Burgers vector of dislocation.

If we trace a clockwise path from start to finish, the closure failure from finish to start is the Burgers vector \( \mathbf{b} \) of the dislocation, see fig (a).

A right-handed screw dislocation, fig (b), is obtained when traversing the circuit around the dislocation line and we then have the helix one atomic plane into the crystal.
Cross slip

In FCC cubic metals, the screw dislocations move in \{111\} type planes, but can switch from one \{111\} type plane to another if it contains the direction of \textbf{b}. This process is called \textit{cross-slip}.

- A screw dislocation at \textbf{S} is free to glide in either \{111\} or \{111\} closed-packed planes.
- \textbf{Double cross slip} is shown in \textit{(d)}.

Cross slip in a face-centred cubic crystal.

Cross slip on the polished surface of a single crystal of 3.25% Si iron.
**Dislocation dissociation**

*Dislocation dissociation* occurs when the strength of dislocation is more than unity. The system becomes unstable → dislocation therefore dissociate into two dislocation.

**Note:** Dislocation of unit strength is a dislocation with a Burgers vector equal to one lattice spacing.

The dissociation reaction $b_1 \rightarrow b_2 + b_3$ will occur when $b_1^2 > b_2^2 + b_3^2$.

- A dislocation of unit strength has a minimum energy when its **Burgers vector** is parallel to a direction of closest atomic packing.

- In close-packed lattices, dislocations with strength less than unity are possible. → therefore crystals always slip in the close-packed direction.
Dislocations in FCC lattice

- Slip occurs in the FCC lattice on the \{111\} plane in the \langle110\rangle direction and with a Burgers vector \((a/2)[110]\).

- The \{111\} planes are stacked on a close packed sequence ABCABC and vector \(b = (a_o/2)[101]\) defines one of the observed slip direction, which can favourably energetically decompose into two partial dislocations.

\[
b_1 \rightarrow b_2 + b_3
\]

\[
a_o \frac{[101]}{2} \rightarrow \frac{a_o}{6} [211] + \frac{a_o}{6} [112]
\]

**Shockley partials**

This **Shockley partials** creates a stacking fault ABCAC/ABC.

**Dissociation of a dislocation to two partial dislocations.**
**Dissociation of a dislocation into two partial dislocations**

- The combination of the two partials $AC$ and $AD$ is known as an **extended dislocation**.
- The region between them is a **stacking fault** which has undergone slip.
- The equilibrium of these partial dislocations depends on the stacking fault energy.

![Diagram of extended dislocation with stacking fault](image)

**Group of stacking fault in 302 stainless steel stopped at boundary**

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Stacking faults

The wider region between partial dislocation, the lower stacking fault energy

- **Characteristics of metals with low SPF:**
  1) Easy to strain harden
  2) Easy for twin annealing to occur
  3) Temperature dependent flow stress

- **Aluminium** – high stacking fault energy → more likely to cross slip.
- **Copper** – lower stacking fault energy → cross slip is not prevalent.

### Typical values of stacking fault energy

<table>
<thead>
<tr>
<th>Metal</th>
<th>Stacking fault energy (mJ m⁻²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brass</td>
<td>&lt;10</td>
</tr>
<tr>
<td>303 stainless steel</td>
<td>8</td>
</tr>
<tr>
<td>304 stainless steel</td>
<td>20</td>
</tr>
<tr>
<td>310 stainless steel</td>
<td>45</td>
</tr>
<tr>
<td>Silver</td>
<td>~25</td>
</tr>
<tr>
<td>Gold</td>
<td>~50</td>
</tr>
<tr>
<td>Copper</td>
<td>~80</td>
</tr>
<tr>
<td>Nickel</td>
<td>~150</td>
</tr>
<tr>
<td>Aluminium</td>
<td>~200</td>
</tr>
</tbody>
</table>
Frank partial dislocations are another type of partial dislocation in FCC lattice, which provide obstacles to the movement of other dislocations.

- A set of (111) plane (viewed from the edge) has a missing middle A plane with a Burgers vector \((a_0/3) [111]\) perpendicular to the central stacking fault.

- Unlike perfect dislocation, Frank partial dislocation cannot move by glide (sessile dislocation) but by diffusion of atom.
Intersection of \{111\} plane during duplex slip by glide of dislocations is called **Lomer-Cortrell barrier**.

**Ex:** consider two perfect dislocations lying in different \{111\} planes and both parallel to the line of intersection of the \{111\} plane.

\[
\frac{a_o}{2} [101] + \frac{a_o}{2} [\bar{1}10] \rightarrow \frac{a_o}{2} [011]
\]

**The new dislocation obtained has reduced energy.**
Dislocations in HCP lattice

• Slip occurs in the HCP lattice on the basal (0001) plane in the <1120> direction.

• The basal (0001) plane the close packed of a sequence ABABAB and a Burgers vector \( b = (a_o/3)[1120] \).

• Dislocations in the basal plane can reduce their energy by dissociating into Shockley partials according to the reaction.

\[
\frac{a_o}{3}[11\bar{2}0] \rightarrow \frac{a_o}{3}[10\bar{1}0] + \frac{a_o}{3}[01\bar{1}0]
\]

The stacking fault produced by this reaction lies in the basal plane, and the extended dislocation which forms it is confined to glide in this plane.
Dislocations in BCC cubic lattice

- Slip occurs in the BCC lattice on \{110\}, \{112\}, \{123\} planes in the \textbf{<111>} direction and a Burgers vector \( \mathbf{b} = (a_0/2)[111] \).

\textbf{Cottrell} has suggested a dislocation reaction which appears to cause \textbf{immobile dislocations}. \((a_0/2[001]\) in iron) → leading to a crack nucleus formation mechanism for brittle fracture.

\[
\frac{a_0}{2} [\overline{1} \overline{1} 1] + \frac{a_0}{2} [1 1 1] \rightarrow a_0 [001]
\]

the dislocation is \textbf{immobile} since the \textbf{(001)} is not a close-packed slip plane, the \textbf{(001)} plane is therefore the \textbf{cleavage plane} when brittle fracture occurs.

\textbf{Slip on intersecting (110) plane}.
A dislocation is surrounded by an elastic stress field that produces forces on other dislocations and results in interaction between dislocations and solute atoms.

- The cross section of an elastic cylindrical piece (dashed line) has been distorted after an edge dislocation running through point O parallel to the z axis (blue line).
- The strain is zero in the z axis and therefore can be treated in plane strain (x-y).
- The stresses vary inversely with distance from the dislocation line and become infinite at \( r = 0 \).

\[
\sigma_r = \sigma_\theta = -\frac{\tau_o b \sin \theta}{r}
\]

...Eq. 1

- The shear stress \( \tau_{xy} \) is a maximum in the slip plane, when \( y = 0 \).

\[
\tau_{xy} = \tau_o \frac{bx(x^2 - y^2)}{(x^2 + y^2)^2}
\]

...Eq. 2
Strain energies of dislocations

The strain energy involved in the formation of an edge dislocation can be estimated from the work involved in displacement the cut OA a distance $b$ along the slip plane.

\[ U = \frac{Gb^2}{4\pi(1-\nu)} \ln \frac{r_1}{r_o} \]  
...Eq. 3

The strain energy of a screw dislocation is given by

\[ U = \frac{Gb^2}{4\pi} \ln \frac{r_1}{r_o} \]  
...Eq. 4

Note: the total strain energy is the sum of elastic strain energy and the core energy of dislocation.

Deformation of a circle containing an edge dislocation.
Forces on dislocation

• A dislocation line moving in the direction of its **Burgers vector** under the influence of a uniform **shear stress** $\tau$.

• The force per unit length of dislocation $F$;

$$F = \frac{dW}{dl ds} = \tau b$$  \hspace{1cm} \text{...Eq. 6}

• This force is normal to the dislocation line at every point along its length and is directed toward the unslipped part of the glide plane.

• The Burgers vector is constant along the curved dislocation line.
Forces between dislocations

- Dislocations of **opposite sign** on the same slip plane will **attract** each other, run together, and annihilate each other.
- Dislocations of **alike sign** on the same slip plane will **repel** each other.

The **radial force** $F_r$ between two parallel **screw dislocations**

$$F_r = \tau \phi b = \frac{Gb^2}{2\pi r} \quad \text{...Eq. 7}$$

**Parallel screw (same sign) → +**

Aniparallel screw (opposite sign) → -

The **radial and tangential forces** between two parallel **edge dislocations**

$$F_r = \frac{Gb^2}{2\pi(1-\nu)} \frac{1}{r}, \quad F_\theta = \frac{Gb^2}{2\pi(1-\nu)} \frac{\sin 2\theta}{r}$$

**...Eq. 8**
**Dislocation climb**

*Dislocation climb* is a non conservative movement of dislocation where and edge dislocation can move out of the slip plane onto a parallel directly above or below the slip plane.

- **Climb** is *diffusion-controlled* (thermal activated) and occurs more readily at elevated temperature. \( \Rightarrow \) *important mechanism in creep.*

- **Positive direction of climb** \( \uparrow \) is when the edge dislocation moves upwards. Removing extra atom (or adding vacancy around \( \uparrow \)). *Compressive force produces + climb.*

- **Negative direction of climb** \( \downarrow \) is when the edge dislocation moves downwards. Atom is added to the extra plane. *Tensile forces to produce – climb.*

*Note:* Glide or slip of a dislocation is the direction parallel to its direction whereas climb of dislocation is in the *vertical* direction.
Intersection of dislocations

The intersection of two dislocations produces a sharp break (a few atom spacing in length) in dislocation line.

This break can be of two types:

- **Jog** is a sharp break in the dislocation moving it out of the slip plane.
- **Kink** is a sharp break in the dislocation line which remains in the slip plane.

*Note: Dislocation intersection mechanisms play an important role in the strain hardening process.*
**Jogs and Kinks**

**Jogs** are steps on the dislocation which move it from one atomic slip plane to another.

**Kinks** are steps which displace it on the same slip plane.

(a), (b) *Kinks in edge and screw dislocations*

(c), (d) *Jogs in edge and screw dislocations.*
1) Intersection of two dislocations with Burgers vectors at right angle to each other.

- An edge dislocation \( XY \) with Burgers vector \( b_1 \) is moving on plane \( P_{xy} \) and cuts through dislocation \( AB \) with Burgers vector \( b_2 \).
- The intersection causes jog \( PP' \) in dislocation \( AB \) parallel to \( b_1 \) and has Burgers vector \( b_2 \) and with the length of the jog \( = b_1 \).
- It can readily glide with the rest of dislocation.

Note: \( b_1 \) is normal to \( AB \) and jogs \( AB \), while \( b_2 \) is parallel to \( XY \) and no jog is formed.
**Intersection of two dislocations**

2) *Intersection of two dislocations with Burgers vectors parallel to each other*

- Both dislocations are jogged.
- The length of *jog PP’* is $b_1$ and the length of *jog QQ’* is $b_2$.
- The *jogs* both have a screw orientation and lie in the original slip plane. This is called *Kink*. → not stable.

*Intersection of edge dislocations with parallel Burgers vectors.*
Intersection of two dislocations

3) Intersection of edge and screw dislocations.

Intersection produces a *jog* with an edge orientation on the edge dislocation and a *kink* with an edge orientation on the screw dislocation.

4) Intersection of two screw dislocations.

The intersection produces *jogs* of edge orientation in both screw dislocations. → very important in *plastic deformation*.

*Note:* at temperature where climb cannot occur the movement of screw dislocation is impeded by jogs.
Jogs

- A stable jog \[\text{length of the dislocation line} \rightarrow \text{energy of the crystal}\]

(a) Many intersections occur when a screw dislocation encounter a forest of screw dislocations. \[\rightarrow \text{producing vacancy jogs and/or interstitial jogs}\.]

(b) Jogs act as pinning points and cause dislocations to bow out with the radius \[R\] when the shear stress \[\tau\] is applied.

(c) At some critical radius \[R_c\] the \[\tau\] required to further decrease \[R > \text{the stress needed for non-conservative climb}\. Then the dislocation will move forward leaving a trail of vacancies (interstitials) behind each jog.

Movement of jogged screw dislocation

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**Superjog** is a jog that has more than one atomic slip plane spacing high.

As the stress increases, the dislocation bows out between the superjogs, generating dislocation dipoles and later break into isolated loops.

- **Formation of dislocation loops from a dislocation dipole**
  - (a) Dislocation dipole.
  - (b) Elongated loop and jogged dislocation.
  - (c) Row of small loops.
Dislocation Sources

• All metals initially contain an appreciable number of dislocations produced from the growth of the crystal from the melt or vapour phase.

• Gradient of temperature and composition may affect dislocation arrangement.

• Irregular grain boundaries are believed to be responsible for emitting dislocations.

• Dislocation can be formed by aggregation and collapse of vacancies to form disk or prismatic loop.

• Heterogeneous nucleation of dislocations is possible from high local stresses at second-phase particles or as a result of phase transformation.
Frank & Read proposed that dislocations could be generated from existing dislocations.

- The **dislocation line** $AB$ bulges out ($A$ and $B$ are anchored by impurities) and produces **slip** as the shear stress $\tau$ is applied.
- The maximum $\tau$ for **semicircle** dislocation bulge, fig (b)
- Beyond this point, the **dislocation loop** continues to expand till parts $m$ and $n$ meet and **annihilate** each other to form a **large loop** and a **new dislocation**.

Note: Repeating of this process producing a dislocation loop, which produces slip of one Burgers vector along the slip plane.
Dislocation-point defect interactions

Point defect and dislocation will interact elastically and exert forces on each other.

**Negative** interaction energy → attraction

**Positive** interaction energy → repulsion

If the solute atom is larger than the solvent atom ($\varepsilon > 1$)

The atom will be repelled from the compressive side of a positive edge dislocation and will be attracted to the tension side.

If the solute atom is smaller than the solvent atom ($\varepsilon < 1$)

The atom will be attracted to the compression side.

- Vacancies will be attracted to regions of compression.
- Interstitials will be collected at regions of tension.
Dislocation pile-ups

Dislocations often pile up on slip planes at barriers i.e., grain boundaries or second phase particles.

High stress concentration on the leading dislocations in the pile-up.

If the pile-up stress > theoretical shear stress $\Rightarrow$ yielding

A pile-up of $n$ dislocations along a distance $L$ can be considered as a giant dislocation with a Burgers vector $nb$.

The breakdown of a barrier occur by
1) Slip on a new plane.
2) Climb of dislocation around the barrier.
3) Generation of high enough tensile stress to produce a crack.
References