CHAPTER 7
DISLOCATIONS AND STRENGTHENING MECHANISMS
ISSUES TO ADDRESS...

• PLASTIC DEFORMATION and DISLOCATIONS
  * Dislocation motion
  * Slip in:
    - single crystals
    - polycrystalline materials
  * Dislocation motion and strength

• HOW TO INCREASE MATERIALS STRENGTH?
  * Grain size reduction
  * Solid-solution strengthening
  * Strain hardening

• HEATING and STRENGTH
  * Recovery
  * Recrystallization
  * Grain Growth
The Strength of Perfect Crystal

\[ \sigma = E \varepsilon \]

\[ 2\sigma = E (1.25r_o - r_o) / r_o \]

\[ \sigma = E / (8 - 15) \]

All metals have yield strength far below predicted perfect crystal values!!!
The Concept

- Why plastic deformation occurs at stresses that are much smaller than the theoretical strength of perfect crystals?

- Why metals could be plastically deformed?

- Why the plastic deformation properties could be changed to a very large degree, for example by forging, without changing the chemical composition?

- These questions can be answered based on the idea proposed in 1934 by Taylor, Orowan and Polyani:

   Plastic deformation is due to the motion of a large number of dislocations
Reminder: Edge-Dislocation

Extra half-plane of atoms!!

If we applied shear stress:

Edge dislocation line

Burgers vector
How does Edge Dislocation Move?

Only the atoms bonds at the center of dislocation break and restore to allow the dislocation to move.

Introduction of the dislocation into a crystal, its migration (slip) through its volume and expulsion at the crystal surface lead to material plastic deformation.

The lower half of the crystal slips by a distance \( b \) under the upper part.
Thus in both cases slip leads to the material plastic deformation, e.g. permanent step formation on the crystal surface.
Dislocations are the elementary carriers of plastic flow thus they define material mechanical properties.

Dislocations allow deformation at much lower stress than in a perfect crystal because slip does not require all bonds across the slip line to break simultaneously, but only small fraction of the bonds are broken at any given time.
Some theory: Schmidt’s Law

- In order for a dislocation to move in its slip system, a shear force, so-called, **resolved stress**, acting in the *slip direction* must be produced by the applied force.
SLIP IN SINGLE CRYSTAL: Resolved Shear Stress

- Crystals slip in particular direction on particular plane due to a **resolved shear stress**, \( \tau_R \), i.e. shear stress applied along these plane and direction.

**Applied tensile stress:** \( \sigma = \frac{F}{A} \)

**Resolved shear stress:** \( \tau_R = \frac{F_s}{A_s} \)

**Relation between \( \sigma \) and \( \tau_R \):**

\[
\tau_R = \sigma \left( \cos \lambda \cos \phi \right)
\]

Schmidt’s factor
• Crystal orientation can make it easy or hard to move dislocations

\[ \tau_R = \sigma / 2 \quad \lambda = 45^\circ \quad \phi = 45^\circ \]

\[ \tau_R = 0 \quad \lambda = 90^\circ \quad \phi = 90^\circ \]

In general, one slip system is oriented to produce largest \( \tau_R = \tau_R^{\text{max}} = \sigma (\cos \phi \cos \lambda)^{\text{max}} \)

- Condition for dislocation motion:
  \[ \tau_R^{\text{max}} > \tau_R^{\text{critical}} \]

  typically
  \[ 10^{-4}G \text{ to } 10^{-2}G \]

Thus the yield, \( \sigma_y \), strength is:

\[ \sigma_y = \frac{\tau_R^{\text{critical}}}{(\cos \phi \cdot \cos \lambda)^{\text{max}}} \]

Compare with \[ \sigma = E/(8 - 15) \]
In this space we operate with crystallographic directions. Typically, we need to calculate the angle between crystallographic directions, \([u \, v \, w]\) and \([u^* \, v^* \, w^*]\), within a certain crystal. By using full expressions of these vectors, namely, \(r = ua_1 + va_2 + wa_3\) and \(r^* = u^*a_1 + v^*a_2 + w^*a_3\), we find:

\[
\cos \varphi = \frac{r \cdot r^*}{|r| \cdot |r^*|} = \frac{(ua_1 + va_2 + wa_3)(u^*a_1 + v^*a_2 + w^*a_3)}{\sqrt{(ua_1 + va_2 + wa_3)(ua_1 + va_2 + wa_3)} \sqrt{(u^*a_1 + v^*a_2 + w^*a_3)(u^*a_1 + v^*a_2 + w^*a_3)}}
\]

e.g. between [010] and [-111] in BCC: \(\cos \lambda = \frac{1}{\sqrt{3}}\)

Or between [110] and [010] in BCC: \(\cos \phi = \frac{1}{\sqrt{2}}\)
Typical Problem

- A single crystal of BCC iron. Tensile stress (52MPa) is applied along [010] direction. Compute the resolved shear stress along (110) plane and [-111] direction.
- For the same slip system and direction of the applied tensile stress, calculate the magnitude of the applied tensile stress necessary to initiate yielding if critical resolved shear stress known to be equal to 30MPa

\[
\tau_R = \sigma \left( \cos \lambda \cos \phi \right)
\]

\[
\tau_R = 52 \left(\frac{1}{\sqrt{2}}\right) \left(\frac{1}{\sqrt{3}}\right) = 21.2 \text{ MPa}
\]

\[
\sigma_y = \frac{\tau_{R\text{critical}}}{(\cos \phi \cdot \cos \lambda)_{\text{max}}}
\]

\[
\sigma_y = 30/[(\cos 45^\circ)1/\sqrt{3}] = 73.4 \text{ MPa}
\]
Polycrystalline materials involve numerous number of *randomly* oriented crystals (grains).

Thus slip planes & directions, as well as $t_R$ *change* from one grain to another.

The crystal with the largest $\tau_R$ yields first, other (less favorably oriented) crystals yield later.

As a result polycrystalline metals are typically *stronger* than single crystals.
• It is important that deformation of grains is constrained by grain boundaries, which maintain their integrity and coherency (i.e. typically do not come apart and open during deformation). Thus even though a single grain may be favorable oriented for slip, it cannot deform until the less favorable adjacent grains are also capable to slip. adjacent (and less favorably oriented) grains are capable of slip also. For large deformation the shape of the individual crystals changes but the grain boundaries do not come apart.

Result could be anisotropy in $\sigma_y$. Initially equi-axed grains elongated in direction of the applied shear stress.
Conclusion: Material Strength & Dislocations Movement

- Thus dislocations are *imperfections* in the crystal lattice, which are mobile and *can move* through the lattice when stress is applied.

- They have extremely *important effects* on the materials *properties*.

- In particular, on the *mechanical strength*, since they are the mechanism by which materials yield and plastically deform.

- Metals are *strengthened* by making it more *difficult to move* dislocations.
STRATEGIES FOR MATERIALS STRENGTHENING

1: REDUCTION of GRAIN SIZE – increase surface of grain boundary which acts a barrier for the dislocation motion

2: SOLID SOLUTION STRENGTHENING – impurity atoms, imposing additional lattice strain, may hinder dislocation movement

3: STRAIN HARDENING – e.g. by cold working (i.e. material deformation at room temperature) increase dislocations density that leads to resistance of dislocation motion by other dislocations
Grain boundaries are **barriers** to slip:

- Owing to *misalignment* of the slip planes in adjacent grains, a dislocation passing the grain boundary have to change its direction and thus lose its energy.
- A single grain may be favorably oriented for slip, but cannot deform until the adjacent grains (less favorable) are also capable to slip;
- **Low angle boundaries** are less effective in blocking than high angle ones.

- Small grain size: **higher structural disorder**
- Smaller grain size: **more barriers for slip**
- More barrier for slip: **higher material strength**
**Strengthening by Reduction of Grain Size**

The *Hall-Petch equation* describes dependence of yield strength, $\sigma_y$, as a function of average grain diameter, $d$:  

$$\sigma_y = \sigma_0 + k_y d^{-0.5}$$

The $\sigma_0$ is the Peierls (frictional) stress and is the minimum stress needed to induce dislocation glide in a single crystal and $k_y$ is the Hall–Petch slope.

- **Example:**
  70wt%Cu-30wt%Zn brass alloy

- **Graph:**
  - Grain size, $d$ (mm)
  - Yield strength (MPa)

- **Points:**
  - 0.75mm

- **Observation:**
  - Grain size can be changed for example by plastic deformation or heat-treatment

- **Remark:**
  - Valid for many materials but not for nano-structures!!
2: Solid Solution Strengthening (1)

• Alloys of a particular metal are usually stronger than the pure metal.

• Interstitial or substitutional impurities in a solution cause lattice strain. As a result, these impurities interact with dislocation strain fields and hinder dislocation motion.

• Impurities tend to diffuse and segregate around the dislocation core to find atomic sites more suited to their radii. This reduces the overall strain energy and “anchor” or “pin” the dislocation.

• The total lattice strain will increase if dislocation movement is initiated since the dislocation core moves to a region with larger local lattice strain (not compensated by impurity).

• Greater applied stress is required to initiate and continue plastic deformation than without the impurity.

• Requires diffusion of solute atoms and hence T dependent. At high T, interstitial atoms can catch up to dislocations and re-pin them.
2: Solid Solution Strengthening (2)

- Interstitial or substitutional impurity atoms distort the lattice, generating additional stress that interacting with dislocation strain field may produce a barrier to dislocation motion.

- Smaller substitutional impurity

  Impurity generates local shear at A and B that opposes dislocation motion to the right.

- Larger substitutional impurity

  Impurity generates local shear at C and D that opposes dislocation motion to the right.
Example: Solid Solution Strengthening in Copper

- Tensile strength & yield strength increase with increase of C, which is wt.% of Ni.

Empirical relation: \( \sigma_y \sim C^{1/2} \)

- In general alloying increases strength and hardness
3: Strain Hardening

- Strain hardening or cold working is the phenomenon of increasing hardness and strength of a ductile material as a result of plastic deformation at temperatures far below its melting point.

- Indeed, plastic deformation leads to the multiplication of dislocations, which strain fields start to interact more "closely", hindering the dislocations motion.

Dislocation tangles produced by plastic deformation in Iron

“Initial”  “Intermediate”  “Final”
Dislocations generate stress.
This traps other dislocations.

Red dislocation generates shear at points A and B that opposes motion of green dislocation from left to right.
Cold work being rolled into copper alloy strip.

Cold Work
In all cases cold work (CW) results in changing of sample cross section (A). Thus percent of cold work can be defined as follows:

$$\%CW = \frac{A_o - A_d}{A_o} \times 100$$
**Result of Cold Work**

- **Dislocation density**, $\rho_d$, goes up:
  - Carefully prepared sample: $\rho_d \sim 10^3$ mm/mm$^3$
  - Heavily deformed sample: $\rho_d \sim 10^{10}$ mm/mm$^3$

- Ways of measuring dislocation density:

  - Using volume, $V$:
    \[
    \rho_d = \frac{l_1 + l_2 + l_3}{V}
    \]
  - Using area, $A$:
    \[
    \rho_d = \frac{N}{A}
    \]

  ![Diagram of dislocation density measurement](image)
Impact of Cold Work

- **Yield strength** $(\sigma_y)$ **increases.**
- **Ductility** (% EL or %AR) **decreases.**

**Example:** The influence of cold work on the stress-strain behavior of low-carbon steel

![Graph showing the impact of cold work on stress-strain behavior](image.png)

- Initial wire
- 1st drawn wire
- 3rd drawn wire
Cold Work Analysis

- What is the tensile strength & ductility after cold working?

\[
\%\text{CW} = \frac{\pi r_0^2 - \pi r_d^2}{\pi r_0^2} \times 100 = 35.6\%
\]

% Cold Work

- Yield strength: \( \sigma_y = 300\text{MPa} \)
- Tensile strength: \( \text{TS} = 340\text{MPa} \)
- Ductility: \( \%\text{EL} = 7\% \)

\( D_0 = 15.2\text{mm} \quad D_d = 12.2\text{mm} \)
**S-S Behavior vs Temperature**

- **EXAMPLE:** polycrystalline iron

- $\sigma_y$ and TS decrease with increasing test temperature.
- % EL increases with increasing test temperature.

- **Why?**
Because the density of **vacancies** increases with temperature and they help dislocations **past obstacles**.

2. **vacancies replace atoms on the disl. half plane**
3. **disl. glides past obstacle**

1. **disl. trapped by obstacle**
Cold Work and **Annealing**

- Thus plastic deformation during cold work leads to the microstructural changes in crystal lattice, (e.g. dislocation density, grain size distribution, etc,) that lead to the changing of material properties (e.g. strength, hardness)
- **Question**: How can one restore these properties back to the pre-cold-worked states?
- **Answer**: It can be done by special material heat treatment, i.e. **annealing**, which involves several processes: **recovery, recrystallization and grain growth**
Recovery, Recrystallization, Grain Growth

- **Plastic deformation** introduces massive changes into the crystal lattice, including **increased dislocation density** (single and polycrystalline materials) and **changed grain size** distributions (polycrystalline materials).

- This results in **stored strain energy** in the system (dislocation strain fields and grain distortions). When the applied external stress is removed - most of the dislocation, grain distortion and associated strain energy are retained.

- Restoration to the state prior to cold-work can be accomplished by **heat treatment** and involves two processes: **recovery and recrystallization**, which may be followed by **grain growth**.
Effect of Heat-treatment after Cold Work

- 1 hour treatment at $T_{\text{anneal}}$ decreases TS and increases % EL.
- Effects of cold work are reversed!

- Three annealing stages to be discussed:
  - Recovery
  - Recrystallization
  - Grain Growth
Heating $\rightarrow$ increased diffusion $\rightarrow$ enhanced dislocation motion $\rightarrow$ decrease in dislocation density by annihilation, formation of low-energy dislocation configurations $\rightarrow$ relief of the internal strain energy.

- The enhanced atomic diffusion leads to "healing" of defects.
- The defects can either be annihilated or form lower-energy defect structures (e.g. polygonization).

Low angle boundary
Recovery (2)

Different ways to reduce of dislocation density through annihilations

• Scenario 1

extra half-plane of atoms

atoms diffuse to regions of tension

extra half-plane of atoms

Dislocations annihilate and form a perfect atomic plane.

The enhanced atomic diffusion at higher temperatures leads to the “healing” of the defects

• One of healing mechanisms is defects annihilation

• Another is the formation of the lower-energy structures (e.g. low-angle boundaries)

• Scenario 2

1. dislocation blocked and cannot move to the right
2. gray atoms left by vacancy diffusion allowing dislocation to “climb”
3. “Climbed” dislocation can now move on new slip plane
Recrystallization

- After recovery is completed, the grains are still in **high strain state**.
- During the next annealing stage, i.e. **recrystallization**, formation of new grains occurs.
  - The driving force of the process is **difference** in **internal energy** between the strained and unstrained grains.
  - Recrystallization occurs through formation of **fine nuclei** and their growth by short-range **diffusion** mechanism until they completely consume the parent material.
- Structure and properties of the final material depend on the **temperature – time schedule** of the annealing process.
- As a result the material mechanical properties that were changed during cold working can **be tuned up** or restored.
Different Recrystallization Stages

Brass 33% CW

Nuclei formation:
3s 580 C

Partial replacement of CW grains:
4s 580 C

Complete recrystal.:
8s 580 C

Grain growth:
15 min 580 C

Grain growth:
10 min 700 C
Recrystallization Temperature

- $T_{\text{recryst.}}$ is the temperature at which recrystallization is completed in 1 hour.
- Typically $T_{\text{recryst.}}$ is between $1/3$ and $1/2$ of material melting point, $T_m$.

- Recrystallization temperature depends on impurity and prior CW:
  - $T_{\text{recryst.}}$ is lower for pure metal than in alloys (can be as high as $0.7 \ T_m$);
  - below a critical limit of CW (2-20%) it is impossible to initiate recrystallization (not sufficient driving force).
Grain Growth

- At longer times, larger grains consume smaller ones.
- Why? Grain boundary area (and thus surface energy) is reduced.

Kinetics of Grain Growth (empirical relation):

\[ d^n - d_o^n = Kt \]

where \( d \) – grain diameter
and \( K \) – coefficient dependent on material and \( T \).
SUMMARY

- Dislocations are observed primarily in metals and alloys.
- Strength is increased by making dislocation motion difficult.
- Specific means of increasing material strength include: decreasing grain size, solid solution strengthening, cold working, and precipitate strengthening.
- Heating (annealing) can reduce dislocation density and increase grain size, allowing tune up the material’s properties.