Deformation of single crystals

NFPL135: Physics of Materials I

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Elastic and plastic deformation

Elastic deformation

▶ stretching of interatomic bonds
▶ no dislocation motion occurs
▶ deformation is completely recovered when applied stress is removed
▶ linear relationship between stress $\sigma$ and strain $\varepsilon$ – Hooke’s law:

$$\sigma = E\varepsilon,$$

where $E$ is the Young’s modulus (elastic modulus)

Plastic deformation

▶ irreversible deformation when the applied stress is removed
▶ can begin abruptly – well defined yield stress; or the transition between elastic and plastic regions can be gradual – stress required to start macroscopic plastic flow known as flow stress
▶ mechanisms of plastic deformation:
  ▶ slip (dislocation motion)
  ▶ twinning
Schematic interpretation of (a) dislocation glide and (b) twinning during deformation. (a) does not show individual dislocations but the resulting changes after passage of a large number of dislocations [link].
Critical resolved shear stress

- **critical resolved shear stress** (CRSS) – stress that will cause a sufficiently large number of dislocations to move – measurable strain
- materials are not usually tested in shear, but in tension or compression (shear test difficult – introduction of bending moments where the sample is gripped)
- relation between the applied tensile stress and the shear stress resolved on the slip plane (resolved shear stress)
- assume a tilted slip plane $A_{sp}$ with normal $p$ and slip direction $d$
- the angle between the slip plane normal and the stress axis is $\theta$
- the angle between the slip direction and the stress axis is $\phi$
- specimen cross-section $A_n$ to $A_{sp}$

\[
\frac{A_n}{A_{sp}} = \cos \theta
\]

Determination of resolved shear stress \[1\]
Critical resolved shear stress

- stress on the slip plane $\sigma_A$ in the direction of the force $f_n$

$$\sigma_A = \frac{f_n}{A_{sp}} = \frac{f_n}{A_n} \cos \theta$$

- we need a component of $\sigma_A$ acting in the slip direction $d$ → resolved shear stress $\tau$

$$\tau = \sigma_A \cos \phi = \frac{f_n}{A_n} \cos \theta \cos \phi$$

- since normal stress $\sigma = \frac{f_n}{A_n}$

$$\tau = \sigma \cos \theta \cos \phi$$

... Schmid's law, $\cos \theta \cos \phi = m$ ... Schmid factor

- tensile axis $\perp$ to the slip plane $\rightarrow \phi = 90^\circ \rightarrow \tau = 0$
- stress axis $\parallel$ to the slip plane $\rightarrow \theta = 90^\circ \rightarrow \tau = 0$
- not possible to produce strain on slip planes either parallel or perpendicular to the tensile stress axis
- maximum $\tau \leftrightarrow \theta = \phi = 45^\circ$ ($\tau = 0.5\sigma$)
Critical resolved shear stress

- Critical resolved shear stress – independent of the crystal orientation – the stress at which the material yields is constant.

- Tensile stress vs. \( \cos \theta \cos \phi \) for high purity Mg single crystals: smooth curve – constant yield stress (0.43 MPa), points – measured data.

- Sensitive to chemical composition – purer metals \( \rightarrow \) lower yield stress.

- E.g. Ag – decreasing the purity from 99.999 to 99.93 increases the critical resolved shear stress by a factor of \( \sim 3 \).

- CRSS is a function of temperature (FCC – weak dependence, other symmetries – more sensitive) – yield stress increases with decreasing temperature.

- Slip occurs preferentially on the slip systems with the highest resolved shear stress.
Plastic deformation by slip – FCC

- FCC – octahedral \{111\} planes, each 3 close-packed direction → 12 slip systems

\(a:\) tensile axis close to \(\langle 100 \rangle\) → several slip systems have nearly equal RSS → plastic deformation by slip on several slip planes → steep slope from the beginning of deformation (strain hardening due to interaction of dislocations)

Typical stress-strain curves of FCC crystals; \(a\) – deformation by multiple glide from start of deformation, \(b\) – single slip (easy glide) followed by multiple glide [1]
Plastic deformation by slip – FCC

- FCC – *octahedral* \{111\} planes, each 3 close-packed direction → 12 slip systems

\[ b: \] one slip plane more stressed at the beginning of deformation → other slip planes are inactive at the beginning of deformation

Typical stress-strain curves of FCC crystals; \( a \) – deformation by multiple glide from start of deformation, \( b \) – single slip (easy glide) followed by multiple glide [1]
Plastic deformation by slip – FCC

Region 1
- *easy glide* – slip on a single slip plane
- small slope – small strain hardening

Region 2
- *multiple glide* on intersecting slip planes
- dislocation density grows with increasing strain, Lomer-Cottrell
- nearly independent of temperature
- heterogeneous distribution of dislocations (regions of small/high $\rho$)
- correlation of resolved shear stress $\tau$ with $\rho$:

$$\tau = \tau_0 + \alpha G b \sqrt{\rho}$$

where $\tau_0$ is the shear stress needed to move an isolated dislocation
- metals with a high stacking fault energy (e.g. Al) – very small stage 2 region (easy cross slip)

Region 3
- *dynamical recovery* – decrease of strain hardening rate – dislocation multiplication diminished
- dislocations escape barriers by cross slip
- strong temperature dependence (beginning of the stage, flow stress)
## Critical resolved shear stresses for selected FCC metals [1]

<table>
<thead>
<tr>
<th>Metal</th>
<th>Purity</th>
<th>Slip System</th>
<th>Critical Resolved Shear Stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu*</td>
<td>99.999</td>
<td>{111} ⟨110⟩</td>
<td>0.63</td>
</tr>
<tr>
<td>Ag†</td>
<td>99.999</td>
<td>{111} ⟨110⟩</td>
<td>0.37</td>
</tr>
<tr>
<td>Au‡</td>
<td>99.99</td>
<td>{111} ⟨110⟩</td>
<td>0.91</td>
</tr>
<tr>
<td>Al§</td>
<td>99.996</td>
<td>{111} ⟨110⟩</td>
<td>1.02</td>
</tr>
</tbody>
</table>

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Temperature, strain rate and impurity concentration dependence of flow curve parameters (FCC)

- $\tau_0$, $\tau_{III}$, $\gamma_{II}$ are the most temperature sensitive
- $\vartheta_I$ weak dependence on $T$
- $\vartheta_{II}$ does not depend on $T$
- qualitatively opposite dependence on $\dot{\gamma}$ and $T$

Schematic true stress - true strain curve (flow curve) for FCC crystal
Temperature, strain rate and impurity concentration dependence of flow curve parameters (FCC)

Temperature dependence of $\tau_0$ for a) Ag, b) Al

Strain rate dependence of $\tau_0$ for Ag ($\dot{\alpha} = \dot{\gamma}$)

$$\tau_0 \approx \ln \dot{\gamma}$$
Temperature, strain rate and impurity concentration dependence of flow curve parameters (FCC)

Logarithmic dependence of $\tau_{III}$ for a) Cu, b) Au on temperature

$\ln \tau_{III} = c_1 + c_2 \ln \dot{\alpha}$

$\tau_{III}$ as a function of temperature and strain rate for a) Cu and b) Ag
Temperature, strain rate and impurity concentration dependence of flow curve parameters (FCC)

Temperature and strain rate dependence of $\gamma_{II} = a_{II}$ for Cu

Temperature and impurity concentration dependence of $\tau_0$ for Ag-In solid solution

Dependence on impurity concentration $c_{imp}$

- $\tau_0$ increases with increasing $c_{imp}$
- slopes of stages I and II roughly independent on $c_{imp}$
- $\gamma_{II}$ usually increases with increasing $c_{imp}$
Plastic deformation by slip – HCP

basal planes (0001) have the same arrangement of atoms as \{111\} in FCC → easy glide should be observed – true for only some HCP metals (Zn, Mg, Cd)

Critical resolved shear stress for selected HCP metals with basal slip [1]

<table>
<thead>
<tr>
<th>Metal</th>
<th>Purity</th>
<th>Slip Plane</th>
<th>Slip Direction</th>
<th>Critical Resolved Shear Stress MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zinc*</td>
<td>99.999</td>
<td>(0001)</td>
<td>\langle 1120 \rangle</td>
<td>0.18</td>
</tr>
<tr>
<td>Cadmium†</td>
<td>99.996</td>
<td>(0001)</td>
<td>\langle 1120 \rangle</td>
<td>0.57</td>
</tr>
<tr>
<td>Magnesium‡</td>
<td>99.95</td>
<td>(0001)</td>
<td>\langle 1120 \rangle</td>
<td>0.43</td>
</tr>
</tbody>
</table>


basal slip – strain hardening much smaller than in FCC metals (basal planes do not intersect) → large plasticity of single crystals when the basal plane is favourably oriented (e.g. Mg single crystals)
Critical resolved shear stresses for HCP

- Ti, Be, Zr – critical resolved shear stress for basal slip is very high (e.g. \(~110\) MPa for Ti), CRSS on prism \{1\overline{1}0\} planes lower (e.g. \(~50\) MPa for Ti) → *prismatic slip* on \{1\overline{1}0\}⟨1\overline{1}20⟩ slip system
- possible explanation: \(c/a\) ratio (ideal \(c/a = \sqrt{8/3} \approx 1.633\))

- Zn, Cd – unique slip system when basal slip unfavourable: \{1\overline{1}22\}⟨1\overline{1}23⟩ → *second order pyramidal slip* (note that the slip direction is not the most densely packed)

<table>
<thead>
<tr>
<th>Metal</th>
<th>(c/a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd</td>
<td>1.886</td>
</tr>
<tr>
<td>Zn</td>
<td>1.856</td>
</tr>
<tr>
<td>Mg</td>
<td>1.624</td>
</tr>
<tr>
<td>Zr</td>
<td>1.590</td>
</tr>
<tr>
<td>Ti</td>
<td>1.588</td>
</tr>
<tr>
<td>Be</td>
<td>1.586</td>
</tr>
</tbody>
</table>

\(c/a\) ratio for selected *hcp* metals [1]
Temperature, strain rate and impurity concentration dependence of flow curve parameters (HCP)

- the same qualitative dependence of $\tau_0, \tau_C$ as for FCC
- difference from FCC: strain hardening rates $\vartheta_A, \vartheta_B$ strongly depend on $T$
Temperature, strain rate and impurity concentration dependence of flow curve parameters (HCP)

Temperature dependence of $\tau_0$ for Zn

Strain rate and temperature dependence of $\tau_0$ for Zn

$\tau_0 \approx \ln \dot{\gamma}$
Temperature, strain rate and impurity concentration dependence of flow curve parameters (HCP)

Dependence of stress-strain curve parameters on $T$ for Cd

Temperature and strain rate dependence of $\tau_C$ for Zn
Temperature, strain rate and impurity concentration dependence of flow curve parameters (HCP)

Temperature dependence of the strain hardening coefficient \( \vartheta_A \) for Cd

Temperature dependence of the strain hardening coefficient \( \vartheta_B \) for Cd
Temperature, strain rate and impurity concentration dependence of flow curve parameters (HCP)

Temperature and impurity concentration dependence of $\tau_0$ for Mg-Zn solid solution

$\tau_0$ for Cd-Zn at low temperatures
Temperature, strain rate and impurity concentration dependence of flow curve parameters (BCC)

- Many possible slip systems → multiple slip from the beginning of deformation
- Similar to FCC, very short transition between stages 2 and 3
- Strong dependence on $T$
Temperature, strain rate and impurity concentration dependence of flow curve parameters (BCC)
Temperature and strain rate dependence of flow curve parameters (crystals with ionic and covalent bonds)

- ionic crystals – dislocation mobility is very low → brittle
- covalent crystals – ductile only at high temperatures, $T > 2/3 T_m$
- 3 stages of flow curve similar to FCC, parameters of the flow curve depend on $T$ and $\dot{\gamma}$
Temperature and strain rate dependence of flow curve parameters (crystals with ionic and covalent bonds)

Strain rate dependence of critical shear stress for a) Ge, b) InSb

Ionic crystal (NaCl)

Covalent crystal (InSb)
Temperature and strain rate dependence of flow curve parameters (crystals with ionic and covalent bonds)

- The length of region I ($\gamma_I$) decreases with increasing $T$.
- $\tau_0$ increases with increasing content of impurity atoms.

Ionic crystal (NaCl)

Covalent crystal (InSb)
Taylor’s equation

1934 – Taylor proposed a theoretical relationship between flow stress and dislocation density (equivalent to experimentally observed parabolic relationship)

assumptions: parallel dislocations move on parallel slip planes, regularly spaced

the average distance between dislocations is then $\propto \rho^{-1/2}$

stress field of a dislocation: $\tau \approx \frac{G b}{r}$, where $G$ is the shear modulus, $r$ the distance from the dislocation

the flow shear stress is then

$$\tau = \alpha G b \sqrt{\rho}$$

material with obstacles hindering dislocation motion – additional stress $\tau_0$ added

$$\tau = \tau_0 + \alpha G b \sqrt{\rho}$$

the relation has been found to be valid for FCC as well as HCP and BCC materials
Orowan equation

- relationship between dislocation velocity and applied strain rate
- edge dislocation: the shear displacement produced by dislocation glide is $b \frac{\Delta A}{A}$, where $A$ is the area of the slip plane and $\Delta A$ is the fraction of the slip plane passed over by the dislocation
- shear strain $\gamma$ given by shear displacement divided by crystal height $z$
  \[
  \Delta \gamma = \frac{b \Delta A}{Az} = \frac{b \Delta A}{V},
  \]
  \[
  V = Az \text{ is the volume of the crystal}
  \]
- when $n$ edge dislocations of length $l$ move over an average distance $\Delta \bar{x}$
  \[
  \Delta \gamma = \frac{bnl \Delta \bar{x}}{V} = \rho b \Delta \bar{x}
  \]
- dislocations move over $\Delta \bar{x}$ in a time interval $\Delta t$
  \[
  \frac{\Delta \gamma}{\Delta t} = \dot{\gamma} = \rho b \bar{v}
  \]
  where $\bar{v}$ is the average dislocation velocity
Strain hardening of single crystals

- Plastic deformation of metals – shear stress required to produce slip continually increases with increasing shear strain → work (strain) hardening

- Dislocations interact with each other or with obstacles

- Multiplication of dislocations with increasing strain (Frank-Read sources, cross slip, emission from high-angle grain boundaries)

**Back stress**

- Due to dislocation pile-up at barriers (sessile dislocations, foreign atoms, precipitates)

- Opposes the resolved shear stress on the slip plane

- When the stress is reversed, the yield stress is lower – dislocation pile-ups aid the reversed slip; dislocation sources can produce dislocations of opposite sign → annihilation → lattice softening

- *Bauschinger effect*
Strain hardening of single crystals

Intersection of dislocations

- dislocation forest – dislocations intersecting the active slip plane (lying on other slip planes)
- formation of jogs – dislocation intersections or cross slip – especially jogs at screw dislocations
Crystal structure rotation during slip

- in a tensile/compressive test, the ends of the crystal are not free to move “sideways” → central part of the crystal changes orientation
- tension: slip plane and slip direction tend to align parallel to the tensile axis
- compression: slip plane tends to be perpendicular to the stress axis
- stereographic projection: can be represented by rotation of the stress axis relative to the crystal

a), b) slip in an unconstrained single crystal; c) rotation and bending of deformed single crystal gripped at its ends [2]
The lattice rotation in tension is equivalent to a rotation of the stress axis $a$ toward the slip direction

- stereographic projection for an FCC crystal
- each of the unit triangles in the stereographic projection defines a region in which a particular slip system operates
- the active slip direction is the closest $\langle 110 \rangle$ direction that can be reached by crossing a boundary of the stereographic triangle that contains the stress axis (general rule for FCC crystals)
- angles $\phi$ and $\theta$ – found along great circles through $10\overline{1} - a - 111$
Crystal structure rotation during slip

In compression, the crystal rotates so that the slip plane tends to become perpendicular to the stress axis.

The lattice rotation in compression is equivalent to a rotation of the stress axis $a$ toward the pole of the active slip plane [1].
Crystal structure rotation during slip

- **primary slip system** – favoured – the highest resolved shear stress, i.e. the highest Schmid factor (e.g. \((111)[10\bar{1}]\) for \(a_1\))

- **cross-slip system** – the other slip plane containing \([10\bar{1}]\) direction, i.e. \((1\bar{1}1)\)

- **conjugate slip system** – becomes the preferred one when the stress axis moves out of its original stereographic triangle \((a_4)\) → the resolved shear stress greater on \((1\bar{1}1)[110]\) system → stress axis moves to \([110]\) direction

- oscillation between the two slip systems → stress axis reaches \([211]\) direction, which lies on the same great circle as the primary and conjugate slip directions (stable orientation of the crystal with respect to the stress axis)

- the fourth \(\{111\}\) plane (here \((1\bar{1}1)\)) – **critical plane**
Orientation dependence of the Schmid factor

- The highest value of Schmid factor – stress axis on the great circle between slip direction and slip plane normal, $\theta = \phi = 45^\circ$

Orientation of the stress axis with the highest Schmid factor for FCC crystals [3]

Contours of constant Schmid factor for FCC crystals [3]
in BCC metals, slip direction always \(\langle 111\rangle\), various slip planes \(\{110\}, \{112\}, \{123\}\)

- pencil glide – slip can occur on any plane that contains a \(\langle 111\rangle\) direction

- the orientation triangle for pencil glide (uniaxial tension) is divided into two regions with different \(\langle 111\rangle\) slip directions

Orientation dependence of Schmid factors for \(\langle 111\rangle\)-pencil glide in BCC crystals [3]
Plastic deformation by twinning

- a portion of the crystal adopts an orientation that is a mirror image of the parent crystal
- **twin plane (boundary)** – the plane of symmetry between the twinned and parent regions
- cooperative movement of atoms by a fraction of the interatomic distance

Twinning as a result of an applied shear stress. Twin is visible on a polished surface because a step is produced. If the surface was levelled by polishing, twins would be visible after etching [4]
Plastic deformation by twinning

▶ *deformation (mechanical) twins* – produced in BCC or HCP metals during shock loading (low temperatures); FCC metals do not usually twin (some exceptions, e.g. shock loading Cu at 4 K)

▶ *annealing twins* – formed during annealing following plastic deformation, typical for FCC metals with a low to intermediate stacking fault energy (<100 mJ/m²)

▶ twinning occurs in a specific direction and plane depending on the crystal structure

### Twin planes and directions

<table>
<thead>
<tr>
<th>Crystal structure</th>
<th>Examples</th>
<th>Twin plane</th>
<th>Twin direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>BCC</td>
<td>$\alpha$-Fe, Ta</td>
<td>(112)</td>
<td>[111]</td>
</tr>
<tr>
<td>FCC</td>
<td>Ag, Au, Cu</td>
<td>(111)</td>
<td>[112]</td>
</tr>
<tr>
<td>HCP (tension)</td>
<td>Co, Mg, Zr, Ti, Be</td>
<td>(1012)</td>
<td>[1011]</td>
</tr>
<tr>
<td>HCP (tension)</td>
<td>Co, Re, Zr</td>
<td>(1121)</td>
<td>[1126]</td>
</tr>
<tr>
<td>HCP (compression)</td>
<td>Mg</td>
<td>(1011)</td>
<td>[1012]</td>
</tr>
<tr>
<td>HCP (compression)</td>
<td>Ti, Zr</td>
<td>(1122)</td>
<td>[1123]</td>
</tr>
</tbody>
</table>
Deformation and annealing twins

Deformation twins in cold-rolled Zn (University of Cambridge; www.doitpoms.ac.uk)

Annealing twins in Cu-30%Zn (G. V. Voort; vacaero.com)
Plastic deformation by twinning

(a) Slip systems
- (0001) Basal Slip
- {10-10} Prismatic Slip
- {10-11} First-Order Pyramidal Slip
- {11-22} Second-Order Pyramidal Slip

(b) Twinning systems
- \( b_t = \langle 10-11 \rangle \)
- \( b_t = \langle 11-26 \rangle / 3 \)
- \( b_t = \langle 10-12 \rangle \)
- \( b_t = \langle 11-23 \rangle / 3 \)

{10-12} Tension Twin (TT₁)
{11-21} Tension Twin (TT₂)
{10-11} Compression Twin (CT₁)
{11-22} Compression Twin (CT₂)

Plastic deformation by twinning

- twinning not a dominant mechanism for metals with many slip systems
- twinning occurs when slip systems are restricted (e.g. low temperatures, high strain rates)
- deformation produced by twinning is small, e.g. Zn crystal converted into a twin on a \{10\overline{1}2\} plane extends only by \( \sim 7.4\% \) → the important role of twinning is not the produced strain, but it may place new slip systems into orientations favourable for slip → twinning important in metals with a low number of slip systems
Plastic deformation by twinning

<table>
<thead>
<tr>
<th>twin</th>
<th>martensite</th>
</tr>
</thead>
<tbody>
<tr>
<td>the same crystal structure</td>
<td>different crystal structure</td>
</tr>
<tr>
<td>driving force: shear stress</td>
<td>driving force: free energy difference between martensite and parent crystal</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>twinning</th>
<th>slip</th>
</tr>
</thead>
<tbody>
<tr>
<td>mirror orientation with respect to twin plane</td>
<td>the same crystal orientation above and below the slip plane</td>
</tr>
<tr>
<td>displacement of atoms only fractions of atomic spacing</td>
<td>slip in discrete multiples of interatomic distances</td>
</tr>
<tr>
<td>every atomic plane involved in the deformation</td>
<td>slip on relatively widely spread planes</td>
</tr>
<tr>
<td>formation $\sim \mu$s – sometimes can be heard</td>
<td>slip band $\sim$ ms</td>
</tr>
</tbody>
</table>
Twinning vs. martensitic reaction

- Twinning – e.g. Zn – both the twinned region and the parent crystal have an hcp structure, only different orientations
- Martensitic transformation – e.g. steel during rapid cooling to RT – high temperature fcc $\rightarrow$ martensitic plates of body-centred orthorhombic phase

Deformation twins in polycrystalline Zr [1]
Martensite plates in Fe-1.5C-5.1Ni steel [1]
Twinning, slip and martensitic transformation

Schematic comparison of twinning and slip, (a) initial crystal, (b) deformed crystal after multiple dislocation slip, (c) twinned crystal

Stress induced martensitic transformation, part of the crystal changes into a different phase with different crystal lattice (but the same chemical composition)
Twin propagation

Schematics of twinning in a BCC crystal. a) Untwinned material in [110] projection showing stacking sequence of (112) planes. b) Twinning dislocations $\vec{b} = \frac{1}{6}[\overline{1}11]$ glide to the right under applied shear stress [5].

Deformation twin grows (or shrinks) by glide of steps along twin boundary plane – dislocation character of steps (*twinning dislocations*).
Questions

1. When making hardness measurements, what will be the effect of making an indentation very close to a previous indentation? Why?

2. Would you expect a crystalline ceramic material to strain harden at room temperature?
References


