Lecture #9:
- Physical basis of metal plasticity
- Rate-dependent metal plasticity models

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Physical Basis of Metal Plasticity
Crystal Structures

In metals, the atoms are arranged in periodic crystal structures. The most frequent crystal structures are the FCC, BCC and HCP configurations:

- **Face centered cubic (FCC) crystal structure**
Crystal Structures

- Body centered cubic (BCC) crystal structure
Crystal Structures

- Hexagonally closed packed (HCP) crystal structure
## Crystal Structures

<table>
<thead>
<tr>
<th>Metal</th>
<th>Crystal Structure</th>
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<tbody>
<tr>
<td>Iron</td>
<td>BCC</td>
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<tr>
<td>Tungsten</td>
<td>BCC</td>
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<tr>
<td>Copper</td>
<td>FCC</td>
</tr>
<tr>
<td>Lead</td>
<td>FCC</td>
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<tr>
<td>Aluminum</td>
<td>FCC</td>
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<tr>
<td>Titanium</td>
<td>HCP</td>
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<tr>
<td>Zinc</td>
<td>HCP</td>
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</table>
Polycrystalline Microstructure

When a melted (liquid) metal begins to solidify, multiple crystals “grow” simultaneously. Each crystal continues to grow until it impinges upon a neighboring crystal. The result is a **polycrystalline microstructure**.

In metals, crystals are also often referred to as **grains**. The main difference between neighboring grains is the orientation of the crystal lattice. **The size of the grains can be influenced through the temperature history during cooling.** Rapid cooling usually results in fine grain structures, while large grains are often the result of slow cooling.
Polycrystalline Microstructure

The orientation of crystal lattices can be conveniently measured using diffraction techniques such as the EBSD (Electron Back Scatter Diffraction) module of a Scanning Electron Microscope.

www.ebsd.info
Steel Crystal Structures

• **Steel Phases**

  **Ferrite**
  - Pure iron with BCC crystal structure
  - Soft & ductile

  **Cementite**
  - Hard & brittle ceramic (nonmetallic solid)
  - Chemical compound of Fe3C (6.7%C, 93.3Fe)
  - Orthorhombic crystal structure

  **Austenite**
  - Pure iron with FCC crystal structure
  - Exists above eutectic temperature
  - Soft, moderate strength

  **Martensite**
  - BCT crystal structure supersaturated with carbon
  - Non-equilibrium phase formed at very high cooling rates
  - Hard & brittle

• **Two-phase microstructures**

  **Pearlite**
  - Fine lamellar structure of ferrite (88wt%) and cementite (12 wt%)

  **Bainite**
  - Fine non-lamellar structure of ferrite and cementite

Graph showing the phase diagram of carbon content and temperature.
Dual Phase Steels

Dual Phase (DP) steels feature a soft ferrite matrix with strong martensite islands. The carbon content of dual phase steels varies from 0.06 to 0.15 wt%. DP steels belong to the family of so-called **Advanced High Strength Steels (AHSS)** which are widely used in automotive engineering.
Polycrystalline Microstructure

The **interatomic distance** in metals is of the **order of 0.1nm** at room temperature. From metal to metal, it varies from about 0.1nm to 0.3nm. The grain size in widely used engineering materials varies typically from 1 to 100 $\mu$m.

In other words, even in small grains there are **more than 10’000 atoms along the grain width**.
Strength of Metals

The **real strength of metals is much lower than the ideal strength** associated with the bond between atoms!

This significant difference is attributed to dislocations. **Dislocations are crystallographic defects** that can move in the crystal structure upon mechanical loading, thereby causing plastic deformation at stresses well below the theoretical strength.

Defect-free lattice

Lattice with edge dislocation
Dislocation Motion

The motion of dislocations is primarily driven by shear stresses.

\[ \tau \]

\[ \tau \]

\[ \tau \]
Dislocation Motion - kinematics

- Consider dislocation movement as the only agent for plastic deformation
- Magnitude of Burgers vector (offset caused by dislocation): \( b \)
- Mobile dislocation density: \( \rho_m \)
- Average velocity of mobile dislocations: \( \bar{v} \)
- Average plastic strain rate: \( \dot{\gamma} \)

Orowan (1940) relation

\[
\dot{\gamma} = \rho_m b \bar{v}
\]
Average dislocation velocity

- Orowan relation
  \[ \dot{\gamma} = \rho_m b \bar{v} \]

- Constitutive function
  \[ \bar{v} = \bar{v}[\tau, \theta, s] \]

Critical slip resistance
Resolved shear stress
Temperature

Johnston and Gilman (1957)

\[ \text{VELLOCITY OF (1\bar{1}0) (1\bar{1}0) SHEAR WAVES = 3.6 \times 10^5 \text{ cm/sec}} \]

Dislocation velocity [m/s]

Applied shear stress [MPa]

10 100 1000
The “slip” (motion) of a dislocation usually takes place on closely packed atomic planes, i.e. hypothetical planes in a crystal that feature the highest planar density of atoms. Such planes are called **slip planes**. On a slip plane, dislocation motion is preferred along the directions of highest linear density which are called **slip directions**. The ensemble of slip plane and slip direction is referred to as **slip system**.

- **FCC crystal**
  - 4 slip planes
  - 3 slip directions per plane
  
  \[= 12 \text{ slip systems}\]

An BCC crystal features 48 potential slip systems.
Effect of temperature on slip resistance

Temperature effect #1 (modulus)

- Critical slip resistance is governed by elastic interaction on the atomic scale of mobile dislocation segments with microstructural state
- Increase in temperature results in decrease of slip resistance due to decrease of elastic moduli

Temperature effect #2 (short-range obstacles)

- With increasing temperature, the local energy barriers to dislocation motion due to short-range obstacles can be overcome at a lower applied stress with the help of thermal fluctuations

Key reference: Kocks, Argon and Ashby (1975), Thermodynamics and kinetics of slips
Simple model

\[ s = s_a \text{(microstructural state)} + s_{th} \text{(microstructural state)} \]

- Resistance due to athermal obstacles (mostly long-range)
- Resistance due to thermally activatable obstacles (mostly short-range)

Temperature and rate-dependency
Athermal barriers to slip

- Dislocation groups
- Large incoherent precipitates
- Inclusions
- Grain boundaries
Thermally activated short-range barriers to slip

An increase in temperature corresponds to an increase of the vibration of atoms. As a result, a lower shear stress is required to overcome short-range barriers to dislocation motion such as

- Forest dislocations (dominant effect in FCC and HCP) interactions with other non-coplanar dislocations intersecting the slip plane
- Peierls-Nabarro forces (dominant in BCC) The force needed to move a dislocation is related to the shear modulus and the atomic bond strength which both decrease as a function of temperature
- Solute atoms
Activation free enthalpy as function of stress

- “Thermal shear stress”: Resolved shear stress in excess of athermal resistance

\[ \tau_{th} = |\tau| - S_a \]

- Required activation free enthalpy as function of “thermal shear stress”

\[ \Delta G = \Delta F \left[ 1 - \left( \frac{\tau_{th}}{S_{th}} \right)^p \right]^q \]
Statistical mechanics argument

- Probability that a thermal fluctuation at temperature $\theta$ can supply the energy $\Delta G$ required for a shear increment is

$$p_B = \exp\left(-\frac{\Delta G}{k_B \theta}\right)$$

- Rate at which dislocations overcome these obstacles is

$$f_0 \exp\left(-\frac{\Delta G}{k_B \theta}\right)$$

$f_0$ is a characteristic frequency of the order of $10^{12} \text{s}^{-1}$

- Average advance of a mobile dislocation segment: $\bar{l}$

- Average velocity of mobile dislocations

$$\bar{v} = \bar{l} f_0 \exp\left(-\frac{\Delta G}{k_B \theta}\right)$$
Thermally activatable short-range barriers to slip

- Average plastic shearing strain rate

\[ \dot{\gamma} = \dot{\gamma}_0 \exp \left( -\frac{\Delta G}{k_B \theta} \right) \quad \text{with} \quad \dot{\gamma}_0 = \rho_m b \bar{f}_0 \]

\[ \Delta G = k_B \theta \ln \left( \frac{\dot{\gamma}_0}{\dot{\gamma}} \right) \]

- Recall

\[ \Delta G = \Delta F \left[ 1 - \left( \frac{\tau_{th}}{S_{th}} \right)^p \right]^q \]

- Temperature and rate sensitivity of the thermal shear stress

\[ \left( \frac{\tau_{th}}{S_{th}} \right)^p = 1 - \left[ \frac{k_B \theta}{\Delta F} \ln \left( \frac{\dot{\gamma}_0}{\dot{\gamma}} \right) \right]^{1/q} \]
Temperature and strain rate dependence of resolved shear stress

\[ |\tau| = \tau_{th} + S_a \]

with

\[ \left( \frac{\tau_{th}}{S_{th}} \right)^p = 1 - \left[ \frac{k_B \theta}{\Delta F} \ln \left( \frac{\dot{\gamma}_0}{\dot{\gamma}} \right) \right]^{1/q} \]

- \( |\tau| \) increases with strain rate
- \( |\tau| \) decreases with temperature
Summary

• Thermally activated obstacles to dislocation motion are responsible for the effect of strain-rate and temperature on the flow stress in metals

• Short range obstacles mostly fall into the category of thermally activated barriers, while long range obstacles are mostly athermal

• The Peierls-Nabarro stress is the rate-controlling mechanism in BCC metals (e.g. steel with high ferrite content)

• Forest dislocations control the rate sensitivity in FCC metals (e.g. aluminum)

• Basic statistical mechanics arguments suggest that the flow stresses increases as a function of strain rate and decreases as a function of the temperature
Rate-dependent metal plasticity models
MODELING FRAMEWORKS

1. Mechanism-based polycrystal plasticity models, e.g.
   - Balasubramanian-Anand model

2. Mechanism-inspired macroscopic models, e.g.
   - Zerilli-Armstrong model
   - Rusinek-Klepaczko model

3. Empirical models, e.g.
   - Cowper-Symonds model
   - Johnson-Cook model
   - Roth-Mohr model
Polycrystal Plasticity

In polycrystal plasticity, the material response is evaluated at two length scales. At the microscopic level, the heterogeneous polycrystalline microstructure is taken into account and the stress-strain response of each slip system is computed.

At the macroscopic level, the material is considered as a homogeneous solid. The special feature of polycrystal plasticity models is that the macroscopic material response is estimated based on the analysis of a representative volume of the polycrystalline microstructure.

This estimation requires not only an accurate mechanical models of individual crystal, but also micro-macro relationships (homogenization models) that relate the macroscopic stress and strain tensor to their counterparts at the microscopic level.
Balasubramanian and Anand (2002) make use of a Taylor model, i.e. they assume that the stress field is uniform at the microscopic level and equal to the applied macroscopic stress.

Their representative microstructure model includes 400 grains of distinct orientations which are distributed in a spatially isotropic manner.
Polycrystal Plasticity
Model by Balasubramanian & Anand (2002)

- Kinematics
  \[ F = F^e F^p \]

- Constitutive equation for stress
  \[ \sigma = C : (E^e - A(\theta - \theta_0)) \]

- Flow rule
  \[ L^p = \sum_{\alpha} \dot{\gamma}^p_{\alpha} m_{\alpha} \otimes n_{\alpha} \]
POLYCRYSTAL PLASTICITY

- Resolved shear stress for slip system $\alpha$
  \[ \tau_\alpha = \sigma : (m_\alpha \otimes n_\alpha) \]

- Constitutive function for slip system $\alpha$
  \[ \dot{\gamma}^p_\alpha = \dot{\gamma}^p_\alpha [\tau_\alpha, \theta, s_\alpha] \]

- Evolution of slip system resistances (self-hardening & latent-hardening)
  \[ \dot{s}_\alpha = \sum_\beta h^{\alpha\beta} \dot{\gamma}^p_\beta \]
• Variation of elastic lattice moduli for pure Al (FCC crystal) over temperature

Simmons and Wang (1971)
POLYCRYSTAL PLASTICITY

- FCC structure with twelve slip systems (per grain)

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$[\mathbf{n}_0^z]_c$</th>
<th>$[\mathbf{m}_0^z]_c$</th>
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<td>0 1 $\bar{1}$</td>
<td>B5</td>
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</table>
• Selected results

![Graph showing stress-strain curves for different temperatures with experimental data from Senseny et al. (1978).]

\[
\begin{align*}
\varepsilon_1 &= 1.155 \times 10^{-4} \text{ sec}^{-1} \\
\varepsilon_2 &= 173.2 \text{ sec}^{-1}
\end{align*}
\]
- Strain-rate jump tests on Al 1100-O

---

![Graphs showing stress-strain relationship for different temperatures and strain rates.](image)

Experimental data from Senseny et al. (1978)

Simulations by Balasubramanian & Anand (2002)
MODELING FRAMEWORKS

• Mechanism-based polycrystal plasticity models, e.g.
  • Balasubramanian-Anand model
• Mechanism-inspired macroscopic models, e.g.
  • Zerilli-Armstrong model
  • Rusinek-Klepaczko model
• Empirical models, e.g.
  • Cowper-Symonds model
  • Johnson-Cook model
  • Roth-Mohr model
MECHANISM-INSPIRED CONSTITUTIVE MODELS

Recall the stress/strain rate/temperature relationship for a single slip system:

$$|\tau| = \tau_{th} + s_a$$

with

$$\left( \frac{\tau_{th}}{s_{th}} \right)^p = 1 - \left[ \frac{k_B \theta}{\Delta F} \ln \left( \frac{\dot{\gamma}_0}{\dot{\gamma}} \right) \right]^{1/q}$$

In mechanism-inspired models, the expressions for the resolved shear stress and plastic shearing rate in the single crystal model are substituted by equivalent stress and strain measure:

$$\tau = \sqrt{\frac{1}{2} \mathbf{s} : \mathbf{s}}$$

$$\dot{\gamma} = \sqrt{2 \dot{\mathbf{e}}^p : \dot{\mathbf{e}}^p}$$

$$\dot{\mathbf{e}}^p = \dot{\gamma} \frac{\partial \mathbf{\sigma}}{\partial \mathbf{\sigma}}$$

Examples for mechanism-inspired models are:

- Zerilli-Armstrong model (1990)
MODELING FRAMEWORKS

- Mechanism-based polycrystal plasticity models, e.g.
  - Balasubramanian-Anand model
- Mechanism-inspired macroscopic models, e.g.
  - Zerilli-Armstrong model
  - Rusinek-Klepaczko model
- Empirical models, e.g.
  - Johnson-Cook model
  - Roth-Mohr model
EMIRICAL CONSTITUTIVE MODELS

- Elasticity
  \[ \sigma = \mathbf{C} : \left( (\varepsilon - \varepsilon^p) - \mathbf{A}(\theta - \theta_0) \right) \]

- Yield condition
  \[ f = \bar{\sigma} - k = 0 \]
  with
  \[ k = f[\varepsilon_p, \theta]g[\dot{\varepsilon}_p]h[\theta] \]

- Flow rule
  \[ \dot{\varepsilon}^p = \dot{\varepsilon}_p \frac{\partial \bar{\sigma}}{\partial \sigma} \]

  + loading/unloading conditions
EMIRICAL CONSTITUTIVE MODELS

Multiplicative decomposition of the yield stress

\[ k = f[\overline{\varepsilon}_p]g[\dot{\varepsilon}_p]h[\theta] \]

- strain hardening
- temperature sensitivity
- strain rate sensitivity

Examples:
- Johnson and Cook model (1983)
- Klopp-Clifton-Shawki model (1985)
- Roth-Mohr model (2014)
JOHNSON-COOK MODEL

\[ k = f[\bar{\varepsilon}_p]g[\dot{\varepsilon}_p]h[\theta] \]

- Strain hardening: \[ f[\bar{\varepsilon}_p] = \sigma_0 + B\bar{\varepsilon}_p^n \]
- Strain rate sensitivity: \[ g[\dot{\varepsilon}_p] = 1 + C \ln\left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right) \]
- Temperature sensitivity: \[ h[\theta] = 1 - \left(\frac{\theta - \theta_r}{\theta_m - \theta_r}\right)^m \]
JOHNSON-COOK MODEL

- Hopkinson bar test results
TAYLOR IMPACT TEST

- Model validation based on Taylor impact test

v=190 m/s

Chung and Taejon

Zerilli and Armstrong (1987)
Roth-Mohr Plasticity Model

\[ k = f[\bar{\varepsilon}_p]g[\dot{\varepsilon}_p]h[\theta] \]

- Strain hardening:
  \[ f[\bar{\varepsilon}_p] = \alpha \left( A(\bar{\varepsilon}^{pl} + \varepsilon_0)^n \right) + (1 - \alpha) \left( k_0 + Q \left( 1 - e^{-\beta \bar{\varepsilon}^{pl}} \right) \right) \]
  Combined Swift-Voce

- Strain rate sensitivity:
  \[ g[\dot{\varepsilon}_p] = 1 + C \ln \left( \frac{\dot{\varepsilon}^{pl}}{\dot{\varepsilon}_0} \right) \]
  same as Johnson-Cook

- Temperature sensitivity:
  \[ h[\theta] = 1 - \left( \frac{\theta - \theta_r}{\theta_m - \theta_r} \right)^m \]

- Non-associated flow rule (only associated flow considered in class)
Roth-Mohr Plasticity Model

- Explicit temperature-displacement analysis
- Temperature is treated as internal state variable!

\[
dT = \frac{\eta_k}{\rho C_v} \bar{\sigma} \, d\bar{\varepsilon}_p
\]

\[
\omega[\hat{\varepsilon}_p] = \begin{cases} 
0 & \text{for } \hat{\varepsilon}_p < \hat{\varepsilon}_{it} \\
\left(\frac{\hat{\varepsilon}_p - \hat{\varepsilon}_{it}}{\hat{\varepsilon}_a - \hat{\varepsilon}_{it}}\right)^2 \left(3 \hat{\varepsilon}_a - 2 \hat{\varepsilon}_p - \hat{\varepsilon}_{it}\right) \left(\hat{\varepsilon}_a - \hat{\varepsilon}_{it}\right)^3 & \text{for } \hat{\varepsilon}_{it} \leq \hat{\varepsilon}_p \leq \hat{\varepsilon}_a \\
1 & \text{for } \hat{\varepsilon}_a < \hat{\varepsilon}_p
\end{cases}
\]

- For ease of model calibration
  \[
  \hat{\varepsilon}_{it} = \hat{\varepsilon}_0
\]
  \[\rightarrow\] Explicit analysis with temperature softening capability
Roth-Mohr Plasticity Model

- Illustration of material response for different $\omega$ at different strain rates
  
  $\omega = 0$ (isothermal)  
  $\omega = \omega[\varepsilon_{pl}]$  
  $\omega = 1$ (adiabatic)

![Graphs illustrating material response](image)
Calibration experiment

- Notched Tension R=20mm (NT20)

![Graph showing calibration experiment results with displacement, force, and strain data for different speeds.](image-url)
Roth-Mohr Plasticity Model

- Notched Tensile R=20 - model calibration

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Hosford-Coulomb Ductile Fracture Model
(recall from Lecture #7)

- **General form**

  von Mises equivalent plastic strain to fracture

  \[
  \varepsilon_f = \varepsilon_{HC}[\eta, \bar{\theta}, a, b, c]
  \]

- **Detailed expressions**

 \[
  \varepsilon_{HC} = b \left( \frac{1 + c}{g_{HC}[\eta, \bar{\theta}]} \right)^{\frac{1}{n}}
  \]

  \[
  g_{HC} = \left( \frac{1}{2} | f_I - f_{II} |^a + \frac{1}{2} | f_{II} - f_{III} |^a + \frac{1}{2} | f_I - f_{III} |^a \right)^{\frac{1}{a}} + c(2\eta + f_I + f_{III})
  \]

  \[
  f_I[\bar{\theta}] = \frac{2}{3} \cos \left( \frac{\pi}{6} (1 - \bar{\theta}) \right) \quad f_{II}[\bar{\theta}] = \frac{2}{3} \cos \left( \frac{\pi}{6} (3 + \bar{\theta}) \right) \quad f_{III}[\bar{\theta}] = -\frac{2}{3} \cos \left( \frac{\pi}{6} (1 + \bar{\theta}) \right)
  \]
Incorporation of the effect of strain rate

The effect of strain rate and temperature on ductile fracture is still an ongoing research topic today. In the absence of new results, it is recommended to follow the Johnson-Cook approach by multiplying the strain to fracture for isothermal static loading with strain rate and temperature dependent functions:

\[ \bar{\varepsilon}_f = \bar{\varepsilon}_{HC} [\eta, \bar{\Theta}] g[\dot{\varepsilon}] h[\Theta] \]

\[ g = \begin{cases} 
1 & \text{for } \dot{\varepsilon}_p < \dot{\varepsilon}_0 \\
1 + \gamma \ln \left[ \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0} \right] & \text{for } \dot{\varepsilon}_p \geq \dot{\varepsilon}_0 
\end{cases} \]

with \( \dot{\varepsilon}_0 \) taken from the plasticity model.
Rate-dependent Fracture Model

The resulting rate-dependent Hosford-Coulomb model (Mohr and Roth, 2014) then predicts an increase in ductility as a function of the strain rate.
Reading Materials for Lecture #9

- Kocks, Argon and Ashby (1975), Thermodynamics and kinetics of slips
- M.A. Meyers, Dynamic behavior of Materials