Dislocations - Introduction

- Theoretical strength of perfect crystals
- History of dislocations
- Dislocations in continuum mechanics: Volterra construction
- Glide in crystals as motion of dislocations
- Dislocation line, Burgers vector, Burgers circuit
- Dislocation nodes and loops

References:
Hull and Bacon, Ch. 1.4
Kelly and Knowles, Ch. 8
Theoretical strength of perfect crystals

Dislocations play the key role in plastic deformation. The concept of dislocations in crystals was introduced by Taylor, Orowan and Polyani in 1934 to explain yield strength or real materials.

For small strain $\gamma = x/a$ Hooke’s law $\tau = G\gamma$ should be satisfied, i.e. $G = \left( \frac{d\tau}{d\gamma} \right)_{x=0}$.

$$\frac{d\tau}{dx} = \frac{d\tau}{d\gamma} \frac{d\gamma}{dx} \quad \Rightarrow \quad \left( \frac{d\tau}{dx} \right)_{x=0} = \frac{1}{a} \left( \frac{d\tau}{d\gamma} \right)_{x=0} \quad \Rightarrow \quad \tau = a \left( \frac{d\tau}{dx} \right)_{x=0} = \frac{2\pi a}{b} \tau_0 \quad \Rightarrow \quad \tau_0 = \frac{Gb}{2\pi a}$$
Theoretical strength of perfect crystals

thus, the theoretical strength of a perfect crystal is \( \tau_0 = \frac{Gb}{2\pi a} \)

since \( b \approx a \), the theoretical critical shear stress is \( \tau_0 \approx \frac{G}{6} \)

with more accurate calculations for real 3D crystals: \( \tau_0 \approx \frac{G}{30} \)

These values are much higher than the experimental yield strength of real materials.

Dislocations allow deformation at much lower stress than in a perfect crystal

<table>
<thead>
<tr>
<th>metal</th>
<th>( \tau_0=G/30 ) (GPa)</th>
<th>( \tau_{\text{exp}} ) (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>0.9</td>
<td>0.78</td>
</tr>
<tr>
<td>Cu</td>
<td>1.4</td>
<td>0.49</td>
</tr>
<tr>
<td>Ni</td>
<td>2.6</td>
<td>3.2</td>
</tr>
<tr>
<td>( \alpha )-Fe</td>
<td>2.6</td>
<td>27.5</td>
</tr>
</tbody>
</table>

2-3 orders of magnitude difference

bond rearrangement is localized in a small region along the dislocation → only a small fraction of the bonds are broken at any given time → this would require a much smaller force.
Theoretical strength of perfect crystals

(almost) defect-free crystals may approach the theoretical strength

- single-walled or multi-walled carbon nanotubes have an ideal strength of ~100 GPa
- near defect-free nanowhiskers
  - yield strength of 4 GPa in Pd nanowhiskers [PRL 109, 125503, 2012]
  - yield strength up to 7 GPa in Cu nanowhiskers [Nano Lett. 9, 3048, 2009]


**History of dislocations**

1901-1907: Weingarten, Timpe and Volterra introduced the concept of dislocation in the continuum elasticity theory

1926: Yakov Frenkel estimated the theoretical critical shear stress for perfect crystals

1927: Augustus Edward Hough Love introduced term dislocations for a certain type of distortions) in elastic medium

1934: Egon Orowan, Michael Polanyi and Sir Geoffrey Ingram Taylor postulated edge dislocations and suggested that they are responsible for the low stress deformation

1939: Jan Burgers postulated screw dislocations

1950: Charles Frank and Thornton Read suggested a mechanism of multiplication of dislocations

1956: Direct observation of dislocations in TEM by Hirsch, Horne, Whelan, and Bollmann

Dislocations:

- are the main sources of the elastic stresses in crystals
- can move with high velocities under external stresses
- dislocation density can increase due to the formation of new dislocations and dislocation multiplication and can reach high values and introduce large distortions of the crystal lattice

Linear elasticity is valid with accuracy of $\sim 10\%$ for elastic deformations up to $10\%$ ($\tau/G \leq 0.1$) → theory of elasticity is applicable for distances $r \geq 2a$ from the dislocation line, where $a$ is the lattice parameter → **dislocation = core ($r \leq 2a$) + stress field ($r \geq 2a$)**
Glide in crystals

At low $T$, crystals yield plastically by a process called glide or slip. Glide is the translation of one part of a crystal with respect to another without change in volume. The translation usually takes place upon a specific crystallographic plane and in particular direction in that plane.

When the resolved shear stress becomes sufficiently large, the crystal will start to yield - slip occurs along the most favorably oriented slip system. The onset of yielding corresponds to the yield stress, $\sigma_y$. The minimum shear stress required to initiate slip is termed the critical resolved shear stress.

University of Virginia, MSE 6020: Defects and Microstructure in Materials, Leonid Zhigilei
**Glide in crystals as motion of dislocations**

Consider an incomplete glide in a crystal along a slip plane. Dislocation is a line in the slip plane that separates the regions where slip has occurred from those where it has not.

- **screw dislocation** along SS’
  - displacement over PQSS’ area is $[010]a$
  - this displacement does not change as the dislocation moves through the crystal and it characterizes the dislocation: it is called **Burgers vector of the dislocation**

- **edge dislocation** along EE’
  - the same displacement vector as above, $[010]a$, but the dislocation line is normal to the displacement vector

- **mixed dislocation** along DD’
  - edge orientation at D’ and screw orientation at D, but the same displacement vector for the whole line
Dislocations in continuum mechanics: Volterra construction

Linear elastic discontinuities (or *distortions*) in the classical elastic medium (homogeneous isotropic body) were studied long before dislocations in crystals were considered.

Vito Volterra defined basic deformation cases of a continuum (distortions):

1. **Undistorted hollow cylinder**
2. **Screw and edge dislocations with Burgers vector $b$** equal to the translational displacement of the non-deformed surfaces of the cut bounded by a dislocation line.
3. **Wedge and twist disclination with Frank vector $\omega$** that defines the mutual rotation of the undeformed surfaces of the cut bounded by a disclination line.

Romanov and Kolesnikova, Progress in Materials Science **54**, 740, 2009
Dislocations in continuum mechanics: Volterra construction

Volterra construction for dislocations:

(1) make a cut using an imaginary “Volterra knife” (the cut area is outlined by the red line)

(2) Move the two parts of the crystal separated by the cut relative to each other by a translation vector $\mathbf{b}$, allowing elastic deformation of the lattice in the region around the dislocation line

(3) Fill in material or take some out, if needed (when $\mathbf{b}$ has a component perpendicular to the plane of the cut)

(4) Restore the crystal by "welding" together the surfaces of the cut

If $\mathbf{b}$ is chosen to be a translation vector of the lattice, the surfaces will fit perfectly together everywhere except of the region around the cut line - 1D defect is created.

http://www.tf.uni-kiel.de/
Dislocation line, Burgers vector, Burgers circuit

The Burgers vector of a dislocation can be found through the **Burgers circuit** construction - atom-by-atom path that forms a closed loop.

1. make a closed circuit that encloses the dislocation (any shape, can be 3D) - obtain closed chain of the base vectors which define the lattice.

2. apply the same chain of base vectors in a perfect reference lattice. It will not close. The vector needed for closing the circuit in the reference crystal is the **Burgers vector**.

Burgers vector is defined on a perfect lattice - does not include distortions of the lattice due to the elastic fields.

The direction of the Burgers vector depends on the direction of the circuit - have to use a **consistent convention** for defining the direction of the dislocation line \( l \) and Burgers vector \( b \).

- e.g. we can define the dislocation line direction to go into the page/screen plane, use clockwise circuit direction, and define Burgers vector as vector running from start to finish point of the reference circuit in the perfect crystal.
Dislocation line, Burgers vector, Burgers circuit

\[ \vec{b} = \vec{b}_1 + \vec{b}_2 \]

The vector to complete any Burgers circuit (the total Burgers vector) is equal to the sum of Burgers vectors of all dislocations that cross surface outlined by this circuit (the surface can be of arbitrary shape)

for both dislocations the line direction is assumed to go into the page/screen plane

if these two edge dislocations are parts of the same dislocation loop, however, it makes sense to keep the “sense of the line” continuous along the loop

In this case, the Burgers vectors of the two segments of the dislocation loop will have the same magnitude and direction

- **Burgers vector is conserved** along the dislocation line
- Dislocation line cannot end inside the crystal
- Dislocations either start at external or internal surfaces, interface, grain boundaries, form closed loops, or branch into other dislocations

University of Virginia, MSE 6020: Defects and Microstructure in Materials, Leonid Zhigilei
Dislocation line, Burgers vector, Burgers circuit

The Burgers vector of a *perfect* dislocation is a lattice translation vector.

In a screw dislocation $b$ is parallel to $l$ and the atomic planes perpendicular to $l$ are turned into a spiral ramp or single surface helicoid.

Left hand screw: $b$ and $l$ are in opposite directions, helix recedes one plane with clockwise circuit.

Right hand screw: $b$ and $l$ in same direction, helix advances one plane with clockwise circuit.

Dislocations with same line sense but opposite Burgers vectors, annihilate and restore perfect crystal if brought together.

$\bar{b} + \bar{l} = \text{perfect crystal}$
Dislocation line, Burgers vector, Burgers circuit

Dislocations are defined by two vectors, a unit vector directed along the dislocation line and changing its direction along the line (tangent to the dislocation line) $\mathbf{l}$ and Burgers vector $\mathbf{b}$ that remains constant along the dislocation line. $\mathbf{l} \perp \mathbf{b}$ for edge $\mathbf{l} \parallel \mathbf{b}$ for screw dislocations.

our view is limited to the blue region

Reversing the line sense reverses the direction of the Burgers vector

physically opposite dislocations (can annihilate) $\Rightarrow$ the same line sense but opposite Burgers vectors or the same Burgers vector but opposite line senses
**Dislocation nodes**

The Burgers vector found by the Burgers circuit procedure is equal to the sum of Burgers vectors of all dislocations that cross surface outlined by the circuit. The surface outlined by the Burgers circuit can be of any shape.

If dislocation with \( \mathbf{b}_1 \) branches into two dislocations with \( \mathbf{b}_2 \) and \( \mathbf{b}_3 \), then

\[
\mathbf{b}_1 = \mathbf{b}_2 + \mathbf{b}_3
\]

A point where three or more dislocations meet is called a dislocation node.

If the *directions of all dislocation lines are assumed to run from/to the node*, then the sum of the Burgers vectors of the dislocations is zero (similar to Kirchhoff’s law for electric current):

\[
\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 = 0
\]

\[
\sum_{i=1}^{n} \mathbf{b}_i = 0
\]
More on dislocation nodes

Let’s make two Volterra cuts *in the same plane*.

For the first cut we displace the two sides separated by the cut relative to each by displacement vector \( \mathbf{b}_1 \).

The second cut extends beyond the first one and is characterized by displacement vector \( \mathbf{b}_2 \).

We have three cut lines, with the black line being the superposition of the two cuts and characterized by the displacement vector \( \mathbf{b}_3 = \mathbf{b}_1 + \mathbf{b}_2 \).

Let’s make two Volterra cuts *in two different planes* and use the displacement vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) that are in the corresponding planes.

The dislocation produced at the intersection of the two cut planes may have Burgers vector \( \mathbf{b}_3 \) that is not parallel to any of the two (glide) planes and may be immobile.

\[ \mathbf{b}_3 = \mathbf{b}_1 + \mathbf{b}_2 \]
Summary

- theoretical strength of perfect crystals - in the absence of dislocations $\tau \approx \frac{G}{30}$
- plastic deformation = movement of dislocations through the crystal
- dislocation = core ($r \leq 2a$) + stress field ($r \geq 2a$)
- dislocation is defined by two vectors: line unit vector and Burgers vector
- Burgers vector = displacement (translation) vector in the Volterra procedure
- for a perfect dislocation, $b$ is always a translation vector of the lattice
- the angle between the line and Burgers vectors define the character or type of dislocation ($l \perp b$ - edge dislocation, $l \parallel b$ - screw dislocation)
- movement of dislocations occurs in a glide plane and shifts the parts separated by the glide plane with respect to each other
- the glide plane is defined by the dislocation line and Burgers vectors (any plane containing $l$ is a glide plane for a screw dislocation)