Mechanical properties of solid bulk materials and thin films

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1.1. Importance of mechanical properties

Mechanical properties are important in many respects:

a) This is trivial for “mechanical applications”, such as
   - in case of tools,
   - for reduction of friction,
   - for protection against wear, etc..

   ⇒ materials shall be hard, stiff, tough,...

b) For other applications (electrical, optical, etc.): mechanical properties...
   - may be important in addition, cf. durability of optical films on glasses,
   - may be connected with the “main property”, e.g. low-k dielectrics have high porosity → low dielectric constant, but
     → breaks during CMP process,
   - may cause interactions which eventually influence the “main property”:

   Example: formation of dislocations during LOCOS (local oxidation) process in silicon IC technology AND dislocations cause leakage current (so called beards beak structure, figure taken from [A]):

   ⇒ optimum mechanical properties depending on special case needed.
1.2. Empirical: Stress-strain curves / Hooke's law

uniaxial tensile test [B]:

Fig. 1-4. A schematic drawing of a testing machine. The specimen is held by grips and a load is applied to the movable crosshead. This load is transmitted to the specimen and causes elongation. The specimen is in tension for this arrangement. Reversing the direction of the load subjects the specimen to compressive stress.

typical stress-strain curves [B]:

stress: psi = pound / square inch
strain: inch/inch = m/m = %....

> linear behaviour (Hooke's law)
> (upper) yield point = yield strength $\sigma_0$, marks onset of permanent deformation
> ultimate stress $\sigma_u$
> fracture strain
Comment: Mild steel is a typical example for the occurrence of a sharp drop after the upper yield point towards a lower yield point. Since the former may be sensitive to loading rate, the latter is considered to be a trustworthy value similar to the 0.2% offset value below.

In case of poorly defined yield point, the **yield strength at 0.2% offset** is used:

**MgO ceramics** exhibits brittle fracture rather than plasticity:

Stress-strain curves depend on many factors including:
- strain rate ($\Delta\varepsilon/\Delta t$),
- temperature,
- modification of structure (dislocations, grain boundaries, phase transformation,...)

Trivial influence: formation of a *necked* region

(picture from [B])
engineering stress/strain is based on the original cross section. It is useful for small deformations.

True stress/strain is based on the current (true) cross section due to necking. Note that strain gets inhomogeneous after necking begins! Increase in true strain corresponds to reduced cross-section (constant volume assumed). (picture from [C])

1.3. Hardness

...is probably the most well known mechanical property. We discriminate scratch hardness and indentation hardness.

**Scratch hardness:** Describes the ability of one material to scratch another one.

**Hardness Scale for minerals after Karl F. C. Mohs (1820):**

<table>
<thead>
<tr>
<th>Material</th>
<th>MOHS Hardness</th>
<th>Indentation Hardness¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>Talkum (Talc)</td>
<td>1</td>
<td>0.02</td>
</tr>
<tr>
<td>Gips (Gypsum)</td>
<td>2</td>
<td>0.4</td>
</tr>
<tr>
<td>Kalkspat (Calcite)</td>
<td>3</td>
<td>1.1</td>
</tr>
<tr>
<td>Flussspät (Fluorite)</td>
<td>4</td>
<td>1.9</td>
</tr>
<tr>
<td>Apatit (Apatite)</td>
<td>5</td>
<td>5.4</td>
</tr>
<tr>
<td>Kalifeldspät (Orthoclase (Feldspar))</td>
<td>6</td>
<td>8.0</td>
</tr>
<tr>
<td>Quarz (Quartz)</td>
<td>7</td>
<td>11.2</td>
</tr>
<tr>
<td>Topas (Topaz)</td>
<td>8</td>
<td>14.3</td>
</tr>
<tr>
<td>Korund (Corundum)</td>
<td>9</td>
<td>20.6</td>
</tr>
<tr>
<td>Diamant (Diamond)</td>
<td>10</td>
<td>(100)</td>
</tr>
</tbody>
</table>

¹ after ISO 14577
**Indentation hardness:** (since about 1900) defines “resistance of a body against permanent deformation” (A. Martens, 1912)

- Indenter of very hard material (diamond, WC),
- pressed into the sample with load F,
- Area A of the permanent impression measured:

→ general hardness definition: \( H = \frac{F}{A} \)

<table>
<thead>
<tr>
<th>Test</th>
<th>Indenter</th>
<th>Shape of Indentation</th>
<th>Load</th>
<th>Formula for hardness number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brinell</td>
<td>10-mm sphere of</td>
<td></td>
<td></td>
<td>BHN = ( \frac{2P}{\pi(D - \sqrt{D^2 - d^2})} )</td>
</tr>
<tr>
<td></td>
<td>steel or tungsten</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>carbide</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vickers</td>
<td>Diamond pyramid</td>
<td></td>
<td></td>
<td>VHN = 1.72P/d_1^2</td>
</tr>
<tr>
<td>Knoop</td>
<td>Diamond pyramid</td>
<td></td>
<td></td>
<td>KHN = 14.2P/t_a</td>
</tr>
<tr>
<td>microhardness</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rockwell</td>
<td>Diamond cone</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>1/16-in. diameter</td>
<td></td>
<td>60 kg</td>
<td>( R_A = )</td>
</tr>
<tr>
<td>C</td>
<td>steel sphere</td>
<td></td>
<td>150 kg</td>
<td>( R_C = )</td>
</tr>
<tr>
<td>D</td>
<td></td>
<td></td>
<td>100 kg</td>
<td>( R_D = )</td>
</tr>
<tr>
<td>H</td>
<td>1/32-in. diameter</td>
<td></td>
<td>100 kg</td>
<td>( R_H = )</td>
</tr>
<tr>
<td>F</td>
<td>steel sphere</td>
<td></td>
<td>60 kg</td>
<td>( R_F = )</td>
</tr>
<tr>
<td>G</td>
<td></td>
<td></td>
<td>150 kg</td>
<td>( R_G = )</td>
</tr>
<tr>
<td>E</td>
<td></td>
<td></td>
<td>100 kg</td>
<td>( R_E = )</td>
</tr>
</tbody>
</table>

**Dimension of hardness:** \([H] = \text{force/area} \rightarrow \text{Newton/m}^2 = \text{Pascal, Pa}\)

typical values for hard materials: 1 – 100 GPa

At present usually 3-sided pyramid (Berkovich indenter) used, fig. from [D]:

**Present-day hardness measurement:**

small indentation depth (< 100 nm),
small dimensions of the permanent impression (< 1 μm),
⇒ optical measurement becomes impossible!

**How to solve this problem?**

Fortunately it proves that

area of permanent impression..... \(A_{\text{perm}} \approx A_{\text{load}} \) ....area under load

AND: \(A_{\text{load}}\) can be determined from \(h_{\text{max}}\) and the shape of the indenter

⇒ **Instrumented indentation** (*registrierende Härtemessung*)
Important restriction: **Hardness is not a universal quantity!** The very value of the hardness of a material depends
- on the method of measurement (e.g. VICKERS hardness, HV), and
- on the applied load (e.g. HV 100).

Hardness only considers the area of the impression. From the viewpoint of hardness, the following impressions are identical (pictures courtesy of T. Chudoba):

![Impressions](image)

Therefore, we aim at the use of universal mechanical properties like
- YOUNG’s modulus,
- POISSON’s ratio,
- yield strength, etc.,

which can be measured with different methods for comparison and which can in principle be used for modelling of the mechanical situation → cf. further chapters!

**Addendum: The renaissance of scratch hardness**

It is obvious that indentation hardness becomes questionable for materials whose hardness is comparable to that of diamond → **superhard materials (H > 40 GPa)**:

- c-BN (cubic boron nitride)
- ta-C (tetrahedral amorphous carbon)
- U-C60 (ultrahard C60 fullerite)
Fullerenes are large molecules composed of carbon atoms, e.g. C60:

(fig.: Dr. F Huisken, Jena) (figures taken from www.wikipedia.org)

V. BLANK et al.: Fullerite formed by sintering of C60 molecules @ 9.5 - 13.5 GPa; 600 - 1800 K.

Fullerite appears to be harder than diamond! Hardness measurement by novel scratch hardness method (NanoScan):

<table>
<thead>
<tr>
<th>Material</th>
<th>Vickers hardness.</th>
<th>SEM hardness.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Gpa</td>
<td>Gpa</td>
</tr>
<tr>
<td>Quartz</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Topaz</td>
<td>17</td>
<td>19</td>
</tr>
<tr>
<td>Garnet</td>
<td>19</td>
<td>19</td>
</tr>
<tr>
<td>Sapphire</td>
<td>23</td>
<td>23</td>
</tr>
<tr>
<td>Cubic ZrO₂</td>
<td>24</td>
<td>27</td>
</tr>
<tr>
<td>Cubic BN</td>
<td>...</td>
<td>60</td>
</tr>
<tr>
<td>Type Ila diamond (100)</td>
<td>...</td>
<td>137</td>
</tr>
<tr>
<td>Type Ila diamond (111)</td>
<td>...</td>
<td>167</td>
</tr>
<tr>
<td>Ultrahard fullerite</td>
<td>...</td>
<td>310</td>
</tr>
</tbody>
</table>

The results of the hardness tests
2. Elastic Behaviour

2.1. Stress, strain and elastic moduli

The following derivation is valid for isotropic solids!

2.1.1. Elongation and compression

A body (length $l$, width $b$, cross section $A$) is expanded by $\Delta l$ due to a force $F$. $F$ is oriented perpendicular to $A$.

For sufficiently small elongation, $\Delta l$ is proportional to $l \cdot F/A$:

$$\Delta l = \frac{l \cdot F}{A} \quad (1)$$

with $E$ being the material specific Young’s modulus. We rewrite eq.(1) and get the normal strain $\varepsilon$ corresponding to

$$\varepsilon \equiv \frac{\Delta l}{l} = \frac{1}{E} \cdot \frac{F}{A} \quad (2)$$

By introducing the normal stress $\sigma = \text{force/area}$ we get

$$\varepsilon = \frac{1}{E} \cdot \sigma \quad \text{and} \quad \varepsilon \cdot E = \sigma, \text{ resp.} \quad (3)$$
So we have: **strain ∝ stress** (Hooke’s law) which proves for all materials within certain limits.

Two views: A particular (given) stress induces a certain strain, OR

a particular (given) strain is connected with a certain (inner) stress.

unit: \[ [E] = \frac{N}{m^2} \equiv \text{Pa} \ldots \text{Pascal} \]

E has the dimension force/area, i.e. the same as stress or pressure.

**Convention:**
- tensile: \( \sigma > 0, \varepsilon > 0 \)
- compressive: \( \sigma < 0, \varepsilon < 0 \)

The stretched body tries to keep its volume constant, i.e. stretching in one direction yields contraction in lateral directions (\( b \rightarrow b - \Delta b \)) ⇒ **Poisson’s ratio, \( \nu \)**

\[
\nu \equiv \frac{\Delta b}{b} \left( \frac{\Delta l}{l} \right)
\]

The relative volume change is given by

\[
\frac{\Delta V}{V} = \frac{\sigma}{E} (1 - 2\nu).
\]

From eq. (5) we can draw the following conclusions:

i) for tensile strain (\( \sigma > 0 \)) the volume change should be \( \Delta V \geq 0 \). Therefore we get

\[
0 \leq \nu \leq 0.5.
\]

ii) extreme values are:

- \( \nu = 0.5 \) → \( \Delta V = 0 \)
- \( \nu = 0 \) → \( \Delta V \) maximal (no transversal deformation).

Typical solids have \( \nu \) between 0.25 and 0.35.

**Hydrostatic pressure (tension):**

Each of the three dimensions contributes a \( \frac{\Delta V}{V} \) corresponding to eq. (5), yielding

\[
\left| \frac{\Delta V}{V} \right| = \frac{3 \cdot \Delta p}{E} (1 - 2\nu)
\]
Remark: We use $\Delta p$ for the hydrostatic pressure in order to make clear that this pressure is usually in addition to the atmospheric pressure.

Convention: Hydrostatic pressure is defined to be $\Delta p > 0$, hence

$$\frac{\Delta V}{V} = -\frac{3 \cdot \Delta p}{E} (1 - 2\nu) \quad (6)$$

We write

$$\frac{\Delta V}{V} = -\frac{\Delta p}{K} \quad (7)$$

with: $K \equiv \frac{E}{3(1-2\nu)}$ ... Bulk modulus

We see that $\frac{\Delta V}{V}$ depends on $E$ and $\nu$!

2.1.2. Shear deformation

In contrast to the case shown above, the force vector now lies in the area $A$:

Apart from that, in complete analogy to eq. (1) we get:

$$\Delta l = \frac{1}{G} \cdot \frac{1}{A} \cdot F \quad (8)$$

with $G$ being the material specific shear modulus. Introducing

$$\frac{F}{A} = \tau \ldots \text{Shear stress}$$

it follows from eq. (8) that

$$\frac{\Delta l}{l} = \frac{1}{G} \cdot \tau$$

Taking into consideration that $\frac{\Delta l}{l} = \tan \alpha = \gamma$ we finally get

$$\gamma = \frac{1}{G} \cdot \tau \quad \text{and} \quad G \cdot \gamma = \tau, \text{ resp.}, \quad (9)$$

with $\gamma$ being the shear strain.
Similarly as $K$ depends on $E$ and $\mu$ (cf. eq. (7)) it can be shown that

$$G \equiv \frac{E}{2(1+\nu)}.$$  \hspace{1cm} (10)

This is a consequence of the fact that **an isotropic material has only two independent elastic constants**. Accordingly, the elastic moduli $E$, $G$ and $K$ as well as Poisson’s ratio $\nu$ are connected to each other by equations like (7) and (10). This issue will be more accentuated in section 2.3.

### 2.2. Interatomic forces and mechanical properties

Mechanical properties of solids are determined by the interatomic or chemical bond forces. An atom in a chemical bond experiences attractive and repulsive forces with the net force being zero in a certain equilibrium distance $r_0$. For this distance, the potential energy resulting from the bonding forces is minimal (picture from [B]):

- Slope of the net bonding force at $r = r_0$ determines Young’s modulus.
- Maximum value of net bonding force determines theoretical strength.
Ionic crystal (NaCl type) as an example:
main facts\(^2\):

Force \( f \) between two ions = attractive (COULOMB) force AND repulsive force:

\[
f = \frac{-Z_1 Z_2 e^2}{r^2} - \frac{nb}{r^{n+1}}
\]

The potential energy \( V \) of the bond is obtained as:

\[
V = \int_{-\infty}^{r} (f_{\text{attractive}} + f_{\text{repulsive}}) \, dr = \int_{-\infty}^{r} \left[ -\frac{Z_1 Z_2 e^2}{r^2} - \frac{nb}{r^{n+1}} \right] \, dr = \frac{Z_1 Z_2 e^2}{r} + \frac{b}{r^n}
\]

Force component \( f_x \) (in x direction) between one ion at \( x = r \) and all ions in a half space defined by \( x \leq 0 \):

\[
f_x = \frac{0.29Z_C Z_A e^2}{r^2} - \frac{0.29Z_C Z_A e^2 r_0^{n-1}}{r^{n+1}} = \frac{0.29Z_C Z_A e^2}{r^2} \left[ 1 - \left( \frac{r_0}{r} \right)^{n-1} \right]
\]

Summing up the forces \( f_x \) for all ions occupying a macroscopic plane \( \perp x \) direction delivers YOUNG’s modulus \( E \) in terms of the atomic parameters \( Z_C, Z_A, \) and \( r_0 \):

\[
\frac{\sigma_x}{\varepsilon_x} = E = \frac{0.29Z_C Z_A e^2 \left( \frac{n-1}{r_0^{n}} \right)}{1 - 2\mu} (14)
\]

Comment: \( E \) is proportional to the bond force (here: Coulomb force) AND to an additional factor \( r_0^{-2} \). Hence: Short and strong bonds yield high YOUNG’s modulus.

From eq. (14) we see that

\[
E \propto \frac{1}{r_0^4} \quad (15)
\]

Because of eq. (10) the same applies to the shear modulus, \( G \):

\[
G \propto \frac{1}{r_0^4} \quad (16)
\]

\(^2\) Note: Complete derivation is given at the blackboard as well as in provisional form in Appendix 1.
The $r_0^{-4}$ behaviour is indeed confirmed by measurements. Shear modulus of ionic (left), metallic (middle) and covalent materials (right) in dependence on the interatomic distance (figures taken from [B]):

**Theoretical shear strength:**

Now, we give a simple estimation of the theoretical shear strength, i.e. the maximum shear strength value which can be expected under ideal conditions:

Moving two crystal planes against each other [through states (a) → (b) → (c) → (d)] is connected with a period change of the shear stress corresponding to the crystal structure (picture taken from [B]):
The shear stress \( \tau \) in dependence on the displacement \( x \) can be approximated by

\[
\tau = \tau_0 \sin \frac{2\pi x}{b}.
\]  

(17)

For small displacements \( x \) the deviation of this function corresponds to the shear modulus:

\[
G = \frac{d\tau}{d\gamma} \bigg|_{x=0} = h \frac{d\tau}{dx} \bigg|_{x=0}.
\]  

(18)

Obtaining \( d\tau/dx \) from eq. (17) and putting into (18) one gets

\[
\tau_0 = \frac{Gb}{2\pi h}.
\]  

(19)

Since in many crystal lattices (think of a closed packed lattice!) \( h \approx b \), we finally get for the maximum bearable shear stress

\[
\tau_b = \frac{G}{2\pi} \approx 0.16G.
\]  

(20)

**Comment:** Experimentally it is found that perfect whisker crystals can approach the theoretical values at least by a factor of 2 to 5 while usual polycrystalline materials show ultimate shear stress values much below the theoretical ones (table from [B]):

<table>
<thead>
<tr>
<th>Material</th>
<th>Shear modulus (psi)</th>
<th>Observed ultimate shear strength (polycrystalline) (psi)</th>
<th>Calculated ultimate shear strength (psi)</th>
<th>Observed ultimate shear strength (whisker) (psi)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copper</td>
<td>( 7.0 \times 10^6 )</td>
<td>32,000</td>
<td>1,120,000</td>
<td>302,000</td>
</tr>
<tr>
<td>Iron</td>
<td>( 11.6 \times 10^6 )</td>
<td>42,000</td>
<td>1,805,000</td>
<td>1,380,000</td>
</tr>
<tr>
<td>Nickel</td>
<td>( 11.0 \times 10^6 )</td>
<td>69,000</td>
<td>1,750,000</td>
<td>395,000</td>
</tr>
<tr>
<td>Al(_2)O(_3)</td>
<td>( 24.7 \times 10^6 )</td>
<td>3,950,000</td>
<td>2,120,000</td>
<td>2,120,000</td>
</tr>
<tr>
<td>BeO</td>
<td>( 19.7 \times 10^6 )</td>
<td>40,000 (tension)</td>
<td>3,150,000</td>
<td>1,340,000</td>
</tr>
<tr>
<td>SiC</td>
<td>( 29.3 \times 10^6 )</td>
<td>25,000 (tension)</td>
<td>4,690,000</td>
<td>2,120,000</td>
</tr>
</tbody>
</table>

As we will see later, shear strength is strongly correlated to tensile strength (cf. section 3.4.). Hence, also the tensile strength is much reduced in comparison to the theoretical values.

This reduction is due to the fact that the movement of atoms of one plane against those of another does not occur at once but successively (movement of single dislocations, cf. section 3.5.1.)
**Influence of Temperature**

Thermal expansion can be explained by the asymmetry of the potential energy minimum of the interatomic force (cf. section 2.2.):

Having an energy of oscillation $\epsilon'$, the atom moves between $r_a$ and $r_b$ with a mean position $r_c$. Since $r_0 - r_a < r_c - r_0$, $r_c$ is bigger than $r_0$ corresponding to an expansion

Moreover, since the said asymmetry increases with temperature, the linear thermal expansion coefficient increases with temperature:

Comment: The ordinate axis is divided in units of $10^{-6}$

Due to the increase of the interatomic distance ($r_0 \rightarrow r_c$), also the slope of the force curve changes with temperature:

---

3 All figures in this section taken from [B]
Due to the decrease of the slope at average position, YOUNG’s modulus is reduced with increasing temperature:

Interrelation of thermal expansion coefficient and Young’s modulus
This figure (from M. F. Ashby, Engineering Department, Cambridge University, U.K.) shows a general rule for Young’s modulus and linear thermal expansion coefficient (both at room temperature): The larger Young’s modulus the smaller the linear thermal expansion coefficient. In other words: Materials with short and strong bonds are stable against both deformation and thermal influence.

2.3. Anisotropy of elastic behaviour

Introduction:

The argumentation presented so far was based on the assumption that the considered material be isotropic, i.e. has the same mechanical behaviour in all directions.

For instance, if we measure Young’s modulus by tensile tests in different directions and visualise it by a surface in the 3D space (with the distance of the surface from the origin of the coordinate system representing the modulus in a certain direction) we get a sphere (picture courtesy of M.H. [E]):

Fortunately, many important materials are isotropic (for instance amorphous substances like glasses, which have no preferred directions) or behave approximately isotropic since they are polycrystalline with an arbitrary orientation of the crystal grains. In the latter case, the varying elastic properties in different directions are “averaged out” provided that the size of the sample under consideration is much bigger than the single grains.

However, many important materials have at least one preferred direction which has particular elastic properties. This case is called transverse isotropy. An important example are most thin films where the growth direction is preferred. - Not to speak about single crystals which might have a quite complex dependence of elastic properties on the crystal symmetry.
Elongated grains (columnar growth) with preferred (111) orientation along the growth direction in a diamond layer deposited by PE-CVD (plasma enhanced chemical vapour deposition):

In the following, a short and simplified overview of the elasticity of anisotropic materials will be given. Subsequently, the important cases of cubic crystals and transverse isotropic materials will be treated.

**Main facts about anisotropy**

- The concept of stresses (figure taken from [F]):

---

4 Note: Complete derivation is given at the blackboard as well as in provisional form in Appendix 2.
- Stress in a point described by the stress tensor (figure from [F]):

If axes of the co-ordinate system identical to the principal axes → diagonal form of stress tensor:
Only (normal) principal stresses, no shear stresses

The relation between the stress and strain tensor (both of rank 2) is given by a tensor of rank 4, the tensor of elasticity:

\[ \sigma_{ij} = c_{ijkl} \cdot \varepsilon_{kl} \]

In general, each component of the stress tensor influences each component of the strain tensor and vice versa, for example:

\[ \sigma_{11} = c_{1111} \cdot \varepsilon_{11} + c_{1112} \cdot \varepsilon_{12} + c_{1113} \cdot \varepsilon_{13} + c_{1121} \cdot \varepsilon_{21} + c_{1122} \cdot \varepsilon_{22} + c_{1123} \cdot \sigma_{23} + c_{1131} \cdot \varepsilon_{31} + c_{1132} \cdot \varepsilon_{32} + c_{1133} \cdot \varepsilon_{33}, \]
This would formally give \( 9^2 = 81 \) components for the tensor of elasticity. However, for reasons of symmetry \( \sigma_{ij} = \sigma_{ji} \), therefore the stress tensor has only 6 independent components. The same is true for the strain tensor.

Moreover, the existence of a thermodynamic potential called \textit{strain energy density} finally reduces the number of independent components from \( 6^2 = 36 \) to 21.

These 21 components are valid for the most asymmetric case in nature, the triclinic lattice:

\[
\alpha, \beta, \gamma \neq 90^\circ \\
a \neq b \neq c
\]

Some important cases have a much higher symmetry which will be discussed in the following.

**Cubic crystals:**

The matrix of coefficients of the tensor of elasticity for a cubic material includes three independent constants \( C_{11}, C_{12} \) and \( C_{44} \). It has the following structure:

\[
(C_{ij}) = \begin{pmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{pmatrix}
\]

(Note: The matrix for the isotropic material looks very similar with the only difference that \( C_{44} \) is a function of \( C_{11} \) and \( C_{12} \))

In contrast to isotropic materials, cubic crystals may be very diverse with respect to their elastic behaviour. Just a few examples [E]:
### Examples of elastic stiffness values:

<table>
<thead>
<tr>
<th></th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>165.7</td>
<td>63.9</td>
<td>79.6</td>
</tr>
<tr>
<td>Al</td>
<td>107.3</td>
<td>60.9</td>
<td>28.3</td>
</tr>
<tr>
<td>Cu</td>
<td>168.3</td>
<td>122.1</td>
<td>75.7</td>
</tr>
<tr>
<td>Li</td>
<td>13.50</td>
<td>11.44</td>
<td>8.78</td>
</tr>
</tbody>
</table>

### Graphs

- **Si**
- **Al**
- **Cu**
- **Li**
Depending on the said constants and their relative magnitudes the cubic material may be nearly isotropic (Al) or very anisotropic (Li).

The same is true for other parameters like POISSON’s ratio which also can be more or less anisotropic.

This is shown by an example from\textsuperscript{5} WORTMAN and EVANS:

\begin{equation}
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\
c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{(c_{11} - c_{12})}{2}
\end{bmatrix}
\end{equation}

\textbf{Transverse isotropy:}

This material has five independent constants: $C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$ and $C_{44}$. The stiffness matrix looks like follows:

Examples (from [E]): Elastic stiffness parameters for transverse symmetry:

<table>
<thead>
<tr>
<th></th>
<th>C_{11}</th>
<th>C_{12}</th>
<th>C_{33}</th>
<th>C_{13}</th>
<th>C_{44}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg</td>
<td>59.50</td>
<td>26.12</td>
<td>61.55</td>
<td>21.80</td>
<td>16.35</td>
</tr>
<tr>
<td>Zn</td>
<td>163.68</td>
<td>36.40</td>
<td>63.47</td>
<td>53.00</td>
<td>38.79</td>
</tr>
<tr>
<td>Ice</td>
<td>14.10</td>
<td>6.60</td>
<td>15.15</td>
<td>6.24</td>
<td>2.88</td>
</tr>
<tr>
<td>Low-k</td>
<td>6.80</td>
<td>1.46</td>
<td>2.17</td>
<td>0.54</td>
<td>2.30</td>
</tr>
</tbody>
</table>

Mg

Zn

hexagonal Ice (Ih)

porous low-k dielectric film
References


[H] Cd from http://www.doitpoms.ac.uk/tlplib/miller_indices/images/cadmium%20slip.jpg
   Al from http://www.univie.ac.at/hochleistungsmaterialien/mikrokrist/characterization.htm

[I] Cu from http://www.tms.org/Meetings/Annual-08/images/AM08educ_clip_image002.jpg
   Au from http://www.imechanica.org/node/679


Appendix 1: Complete derivation from section 2.2.

\[ f = f_{\text{attract}} + f_{\text{repel}}, \quad \text{with} \]

\[ f_{\text{attract}} = -\frac{t_1 t_2 e^l}{r^2}, \quad \text{(1a)} \]

and

\[ f_{\text{repel}} = \frac{n b}{r^{n+1}}, \quad \text{(1b)} \]

Typical in values are \( t_1 > t_2 > n \).

\[ (1a), (1b) \rightarrow \]

\[ f = -\frac{t_1 t_2 e^l}{r^2} - \frac{n b}{r^{n+1}}, \quad \text{(2)} \]

Potential energy \( V \):

\[ V = \int \left( f_{\text{attract}} + f_{\text{repel}} \right) \, dr = \frac{t_1 t_2 e^l}{r^2} + \frac{n b}{r^{n+1}} \]

\[ \leq 0 \quad \text{!} \]

Determination of \( b \) from

\[ f(r = r_0) = 0 \quad \text{(1.1)} \]
\[ b = -\frac{n}{m} \left[ \frac{b_0}{r_0} \right] \]  

Bond energy is obtained from (1) for \( r = r_0 \) and using \( b \) from (1):

\[ BE = V(r = r_0) = \frac{Ze^2}{r_0} - \frac{1}{2} n^2 \left[ \frac{Ze^2}{r_0} \right] \]

\[ BE = \frac{Ze^2}{r_0} \left[ 1 - \frac{2n^2}{Z} \right] \]  

Comment:
- \( BE < 0 \) because of opposite sign of \( b_a \) and \( b_c \).
- This is the bond energy between two ions. As it is different to the bond energy in a 3D solid?

Hooke’s law in a grid:

This is done by D. P. B. (article). Formation for properties of uranium.

Van Nostrand, Princeton, N.J., 1964, etc. Consider: 1. 2. 3. 4. 5.

Considering a certain compound \( x \), the \( x \) component of this space acting on a given ion are summed up.

\[ x \cdot a \]

\[ x \cdot b \]

\[ x \cdot c \]

(5) (4) (3) (2) (1) (1)

* Called after Frisch, p. 100
The total force on the considered ion (as discussed) is from all self-motion and repulsive "potential forces":

\[ F = \frac{d}{10} \frac{t_{e} e^{2}}{r_{0}} \left[ 1 - \left( \frac{r}{r_{0}} \right)^{n-1} \right] \quad (b) \]

Even though this is the net force, it is not for \( r = r_{0} \)!

Induced charge, \( q \), \( \rightarrow \) mean atomic stress:

\[ F_{x} \rightarrow G_{x} \cdot A \]

\[ G_{x} = \frac{F_{x}}{A} = \frac{f_{x}}{r_{0}^{2}} \quad (c) \]

Showing:

\[ \varepsilon_{x} = \frac{T - r_{0}}{r_{0}} \quad \Rightarrow \quad \varepsilon_{x} - r_{0} = r - r_{0} \quad (d) \]

Now, we would like to express \( F_{x} \) [eq. (b)] as a function of \( (r - r_{0}) \) rather than \( r \). This can be done by expanding eq. (b) in a Taylor series about \( r_{0} \).
\[ f_x(r) = f_x(r_o) + \frac{d f_x}{d x} \bigg|_{x=r_o} \frac{r-r_o}{r_o^2} + \frac{d^2 f_x}{d r^2} \bigg|_{r=r_o} \frac{(r-r_o)^2}{2!} r_o \]  

\[ f_x(r) = \left[ 0.2 \cdot \frac{b}{a} \cdot \frac{k}{e} \cdot \frac{1}{r_o^2} \left( \frac{n-1}{r_o^2} \right) \right] \cdot (r-r_o) \]  

\[ f_x(r) = r_o \cdot \varepsilon_x \]  

(1)  

(2)  

(3)  

(4)  

\[ \varepsilon_x = \varepsilon_0 = \left[ 0.2 \cdot \frac{b}{a} \cdot \frac{k}{e} \cdot \frac{1}{r_o^2} \left( \frac{n-1}{r_o^2} \right) \right] \cdot r_o \]  

Which can be rearranged to give

\[ \frac{\varepsilon_x}{\varepsilon_k} = \frac{0.2 \cdot \frac{b}{a} \cdot \frac{k}{e} \cdot \frac{1}{r_o^2} \left( \frac{n-1}{r_o^2} \right)}{0.2 \cdot \frac{b}{a} \cdot \frac{k}{e} \cdot \frac{1}{r_o^2} \left( \frac{n-1}{r_o^2} \right)} = 1 \]  

Hence, we have neglected the transmission depolarisation in our derivation!
The completely correct definition is

\[ E = 0.25 \cdot t_\alpha \cdot t_\omega \cdot e \cdot \frac{n - 8}{s} \cdot \left( \frac{n - 8}{s} \right) \]  \hspace{1cm} (14) \]

Discussion:

\[ E \sim \frac{t_\alpha \cdot t_\omega}{\sigma^2} \left( \frac{r_s}{r} \right)^2 \]

\[ F_{coulomb} \equiv \mathcal{F}_{B = 0} \]

From Eq. (14) we see that

\[ E \propto \frac{n}{r_0} \]  \hspace{1cm} (15) \]

Because of Eq. (14 - 16) the same applies to the shear modulus \( G \):

\[ G \propto \frac{n}{r_0^3} \]  \hspace{1cm} (16) \]
Appendix 2: Complete derivation from section 2.3:

We consider an elastic continuum which is divided by an area $A$ into two volumes $V_1$ and $V_2$. Let $\Delta A$ be a small part of $A$, having the normal vector $\mathbf{n}$:

Volume $V_1$ acts on $\Delta A$ in form of a small force $\Delta \mathbf{F}$ and a small torque $\Delta \mathbf{M}$. The limit is:

For $\Delta A \to 0$ we get the following limits:

$$\lim_{\Delta A \to 0} \frac{\Delta \mathbf{F}}{\Delta A} = \frac{\mathbf{F}}{A} = \mathbf{f}$$  \hspace{1cm} (I)

$$\lim_{\Delta A \to 0} \frac{\Delta \mathbf{M}}{\Delta A} = 0$$  \hspace{1cm} (II)

$\mathbf{f}$ is the force vector acting at a small $\Delta A$ having the normal vector $\mathbf{n}$. Since the body is in equilibrium, the following equation is fulfilled:

$$\mathbf{n} \times \mathbf{f} = \mathbf{0}$$  \hspace{1cm} (III)

Eq. (III) is an expression of Newton's 3rd Basic Postulate. \hspace{1cm}$\blacksquare$
From above:

- \( \mathbf{A} \) is normal to the plane of \( \theta \) in the component normal (\( \mathbf{n} \)), nonparallel (\( \mathbf{v} \)).

Following Duhem in 1924,

\[
\left( \frac{\partial}{\partial x} \frac{\partial}{\partial y} \right) = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}
\]

To find the strain in a point closer than with respect to a lattice DA in consists a volume element and introduces minor elastin co-ordinates \( n, l, m \) (\( x, y, z \)):

\[
\begin{align*}
\frac{\partial}{\partial x} &= \frac{\partial}{\partial n} n_x + \frac{\partial}{\partial l} l_x + \frac{\partial}{\partial m} m_x = \frac{\partial}{\partial n} n_x + \frac{\partial}{\partial l} l_x + \frac{\partial}{\partial m} m_x \\
\frac{\partial}{\partial y} &= \frac{\partial}{\partial n} n_y + \frac{\partial}{\partial l} l_y + \frac{\partial}{\partial m} m_y = \frac{\partial}{\partial n} n_y + \frac{\partial}{\partial l} l_y + \frac{\partial}{\partial m} m_y \\
\frac{\partial}{\partial z} &= \frac{\partial}{\partial n} n_z + \frac{\partial}{\partial l} l_z + \frac{\partial}{\partial m} m_z = \frac{\partial}{\partial n} n_z + \frac{\partial}{\partial l} l_z + \frac{\partial}{\partial m} m_z
\end{align*}
\]
In conclusion, the vector at point \( p \) which is characterized by the three vectors \( \vec{e}_1, \vec{e}_2, \vec{e}_3 \) which are related to the co-ordinate system with the basic vector \( \vec{v}_1, \vec{v}_2, \vec{v}_3 \), may also be described by nine scalar components.

\[
\begin{bmatrix}
| \vec{e}_1 | \\
| \vec{e}_2 | \\
| \vec{e}_3 |
\end{bmatrix}
\]

which forms the \text{main frame}. \hspace{1cm} (6)

\[ A_{ij} \] \text{(the matrix of components)}

What do the components of this force represent? Example:

a) \( \vec{F}_m \) belongs to \( \vec{F}_m \parallel \vec{v}_n \). i.e. the \( \vec{v}_n \) component of \( \vec{F} \).

This means it is directed in such a form \( \vec{F}_m \parallel \vec{v}_n \) acting at \( \vec{A} \perp \vec{v}_n \).

\[ \Rightarrow \text{Normal force} \parallel \vec{v}_n \]

b) \( \vec{g}_1 \) belongs to \( \vec{g}_1 \parallel \vec{v}_n \), i.e. the \( \vec{v}_n \) component of \( \vec{g} \).

This means direction of \( \vec{g}_1 \parallel \vec{v}_n \) acting at \( \vec{A} \perp \vec{v}_n \).

Finally: \( \vec{F}_m, \vec{g}_1, \vec{g}_2 \) or \( \vec{g}_1, \vec{g}_2, \vec{g}_3 \) are normal vectors components.
and \( i,j \) with \( i \neq j \) (see VI.) are similar than components.

Transformation of the components of the new vector:

Depending on the choice of some vectors \( \vec{v}_1, \vec{v}_2, \vec{v}_3 \) of the coordinate system the matrix here very different. However, it is one and the same then there!

With a special choice of the \( \vec{v}_i \) the matrix looks like that:

\[
\begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\]  (diagonal matrix). (7)

In this case it was happened that the coordinate axes are oriented parallel to the direction of the principal axes (principal directions). For this special choice of the co-ordinate system the above

\[
\text{choose}\; \vec{v}_i = \frac{\text{max}}{\text{length}}
\]


\[
\text{thus yield} \; \vec{a} = \vec{a}_1 \vec{v}_1 + \vec{a}_2 \vec{v}_2 + \vec{a}_3 \vec{v}_3
\]

\[
\text{where yield} \; \vec{a} (7)
\]

\[
\vec{a} = \vec{a}_1 \vec{v}_1 + \vec{a}_2 \vec{v}_2
\]

Comment:

- As in the case of the vector the principal coordinate system

  change is general from point to point.
Theorem: Several considerations:

We know:
- Tensor of 1st order (scalar), e.g., temperature
- Tensor of 2nd order (vector), e.g., velocity, force
- Tensor of 3rd order:

Such tensors can be considered as the combination of two vectors. It is a linear operation which moves from one order to another order.

The stress tensor can perhaps be visualized as a combination of the force $F$ and the orientation of the interacting area (as defined by $A$).

The strain is an organized tensor for the stress tensor.

Young's modulus and Poisson's ratio are related to each other.

By the nature of elasticity, this is a tensor of 4th order (rank 4). Consider that the relation of stress and strain tensor is difficult for intuition. The principal directions of the stress tensor are in general different to those of the strain tensor! A direction of stress = direction of weak strain? (depending only for isotropic materials)


The nature of elasticity:

- The stress tensor is 3D and points in six basic directions.
- Each component of the stress tensor depends on the stress component of the other, not in principle.

\[ \sigma_{ij} = \epsilon_{ij} + C_{ijkl} \sigma_{kl} + \epsilon_{ijkl} \sigma_{kl} \]

The stress tensor should have 18 components.

However, since \( \epsilon_{ij} = \epsilon_{ji} \), so we have only 9 stress tensor components, so the stress tensor can be expressed as:

\[ \sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \]

or more compactly:

\[ \sigma = \begin{bmatrix} \sigma_{x} & \sigma_{y} & \sigma_{z} \\ \tau_{xy} & \tau_{yz} & \tau_{zx} \end{bmatrix} \]

Normal shear stresses:

- The same is true for the strain tensor, so we have only 18 components:

\[ \epsilon_{ij} = \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{bmatrix} \]

in the standard basis.
The stress and strain appear in the forms:

As $C$-Matrix

\[ C_{ij} = C_{ijk} \epsilon_{kij} \]

(Also called stiffness matrix), and as $S$-Matrix

\[ E_{ij} = S_{ijk} \epsilon_{kij} \]

(called compliance matrix).
However, the components are not independent of each other.

Illustration: during deformation, material units must overlap itself and must remain connected:

\[ \Rightarrow \text{out} \Rightarrow \text{are not allowed!} \]

The \( C_{ij} \) matrix is symmetric (which simply is \( (10) \))

\[ \Rightarrow \text{uncoupled is an independent parameter.} \]

This is the most complex elastic behavior existing in nature (e.g., \( Pi \) is mechanics!)

It corresponds to a kinematic couple:

\[ a \neq b + c \]

\[ d \neq f + y \]

Which is the most asymmetric of the 19 Bravais lattices

1) More correct: Geršgorin (1893–1944) showed that this criterion

As the existence of a thermodynamic potential called strain entropy
denoting (which depends on the state only, inside volume of the path)

\[ \Rightarrow \text{out} \Rightarrow \text{are not allowed!} \]