Exercise for the Lecture on Materials Science

Prof. Peter Müller-Buschbaum, Lea Westphal, Ziyan Zhang, Doan Duy Ky Le

Exercise Sheet 1

Solutions

Task 1 – Material Classes

Property	**Metals**	**Glasses**	**Ceramics**	**Polymers**	**Elastomers**	**Hybrid Materials**
Elastic Modulus	high	low	high	low	low	variable
Strength	high	/	high	high	variable	variable
Impact Toughness	high	low	high	variable	high	variable
Formability	good	with T	poor	good	good	poor
Hardness	variable	high	high	low	low	variable
Thermal Conductivity	high	variable	variable	low	low	variable
Electrical Conductivity	high	no	low	low	low	variable
Corrosion Resistance	poor	good	good	good	good	variable
Brittleness	no	yes	yes	variable	temperature dependent	variable
Optical Properties	shiny	transparent	opaque	variable	variable	variable

Task 2 – Suitable Material Properties

a) **Material for Excavator Teeth:**

- Extremely high mechanical stress due to cutting, digging, and crushing rock and soil.
- Important: high hardness H for wear resistance.
- Additionally: high fracture toughness K_{1c} to prevent breakage.
- Corrosion resistance is beneficial for use in water, mud, etc.
- Material costs are secondary – avoiding downtime is crucial.

b) **Material for an Energy-Efficient Cooking Pot:**

- Good heat transfer and distribution required → high thermal conductivity λ.
- Corrosion resistance against:
  * saltwater,
  * acids (e.g., vinegar),
  * alkalis (e.g., baking soda).
- Typical materials: aluminum or copper core, possibly with stainless steel coating.

c) **Material for Environmentally Friendly Disposable Water Bottles:**

- **Essential Requirements:**
  * Non-toxic – no contamination of the water.
  * Free from processing residues.
  * Cost-effective to produce – for mass use.

- **Desirable Properties:**
  - Recyclable or biodegradable.
  - Mechanically robust – not brittle, easy to handle.
  - Lightweight and preferably transparent.

Task 3 – Crystal Structures and Density

a) Ratio $c/a = 1.633$ for hcp:

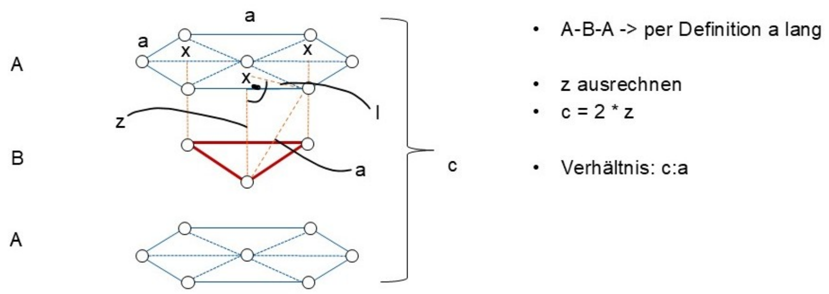

Figure 1: Schematic layered construction of hcp structure

- The hcp structure consists of three close-packed layers in ABA stacking.
- In the A-layer, three atoms form an equilateral triangle with side length a.
- The B-layer atom is positioned directly above the triangle's center.
- Distance from the center to a corner atom: $l = \frac{a}{\sqrt{3}}$.
- Vertical spacing between A and B layers: $z = \sqrt{a^2 - l^2} = \sqrt{\frac{2}{3}}a$.
- Cell height: $c = 2z = \sqrt{\frac{8}{3}}a$.
- Result: $\frac{c}{a} = \sqrt{\frac{8}{3}} \approx 1.633$.

b) Density of Lithium (bcc):

- Structure: body-centered cubic (bcc), 2 atoms per unit cell.
- Given: atomic radius $r = 0.152\,\text{nm}$, atomic mass $M = 6.94\,\text{g/mol}$.
- Lattice parameter: $a = \frac{4r}{\sqrt{3}} = \frac{4 \cdot 0.152}{\sqrt{3}} \approx 0.351\,\text{nm}$.
- Cell volume: $V = a^3 = (0.351 \cdot 10^{-7}\,\text{cm})^3 \approx 4.33 \cdot 10^{-23}\,\text{cm}^3$.
- Density formula: $\rho = \frac{n \cdot M}{N_A \cdot V}$, with $n = 2$, $N_A = 6.022 \cdot 10^{23}$.
- Inserted:
$$\rho = \frac{2 \cdot 6.94}{6.022 \cdot 10^{23} \cdot 4.33 \cdot 10^{-23}} \approx 0.534\,\text{g/cm}^3.$$
- Result matches literature value.

Task 4 – Ionic Radius Ratio and Packing Density

a) Radius ratio $R_k/R_a \geq 0.732$ for coordination number 8:

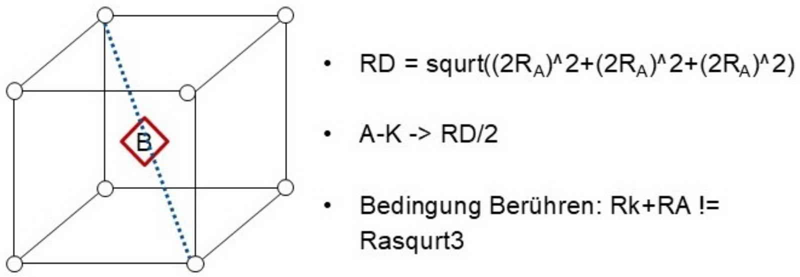

Figure 2: Schematic ion crystal

- In ionic crystals with CN = 8, the cation is centered in a cube with anions at the corners.
- The body diagonal of the cube is $d = \sqrt{3}a = 2(R_k + R_a)$.
- Cube edge: $a = 2R_a \Rightarrow R_k = \left(\frac{\sqrt{3}-1}{2}\right) a$.
- Thus:

$$\frac{R_k}{R_a} = \sqrt{3} - 1 \approx 0.732.$$

b) Packing densities for fcc and bcc:

- Packing density: $\eta = \frac{V_{\text{atoms}}}{V_{\text{cell}}}$.
- **fcc structure:**
  * 4 atoms per unit cell.
  * Spheres touch along face diagonal: $a = 2\sqrt{2}r$.
  * Cell volume: $V = a^3 = (2\sqrt{2}r)^3 = 16\sqrt{2}r^3$.
  * Atomic volume: $4 \cdot \frac{4}{3}\pi r^3 = \frac{16}{3}\pi r^3$.
  * Packing density:

$$\eta_{\text{fcc}} = \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} \approx 0.74.$$

- **bcc structure:**
  * 2 atoms per unit cell.
  * Spheres touch along body diagonal: $a = \frac{4r}{\sqrt{3}}$.
  * Cell volume: $V = \left(\frac{4r}{\sqrt{3}}\right)^3 = \frac{64}{3\sqrt{3}}r^3$.
  * Atomic volume: $2 \cdot \frac{4}{3}\pi r^3 = \frac{8}{3}\pi r^3$.
  * Packing density:

$$\eta_{\text{bcc}} = \frac{\frac{8}{3}\pi r^3}{\frac{64}{3\sqrt{3}}r^3} = \frac{\pi\sqrt{3}}{8} \approx 0.68.$$

Task 5 – Polymer Calculation

a) Repeat unit and molar mass of PVAL:

- Repeat unit: $-[CH_2CH(OH)]-$.
- Atomic masses:
  * C: 12.01 g/mol,
  * H: 1.008 g/mol,
  * O: 16.00 g/mol.
- Calculation:

$$M_0 = 2 \cdot 12.01 + 4 \cdot 1.008 + 16.00 = 44.05\,\text{g/mol}.$$

b) Number of repeat units N:

- Given: $M = 10\,\text{kg/mol} = 10\,000\,\text{g/mol}$.
- Formula: $N = \frac{M}{M_0}$.
- Inserted:

$$N = \frac{10\,000}{44.05} \approx 227.$$

- Thus, one PVAL molecule consists of approx. 227 repeat units.