Exam Materials Science

January 26, 2021, 15:00-18:00

- *Clearly indicate your name and student number on each separate sheet of paper!*
- *Indicate on the first sheet the total number of papers you hand in.*
- *Take a photo of each paper you want to hand in, save them in a well readable format (preferably pdf and preferably single file).*
- *Then upload the file via the Assignment tool in the Nestor Exam page of this course.*
- *In case the previous step creates problems then find another solution to send your well-readable results in time, e.g. by email to b.j.kooi@rug.nl.*
- *If you have a(n urgent) question when making the exam, then join the Class Room in Blackboard Collaborate Ultra available in the Nestor page of this exam (not the one used during the course!) and pose your question in the chat. An instructor is continuously available during the exam to answer your questions.*

Mark for the exam = 1 + 9*((sum of total points scored)/(max. number of point (76)))

Suggestions:

- *Work fast and write down answers concisely.*
- *When you have difficulty to find an answer and to formulate it, do not keep on thinking (and looking for (internet) sources) for a long time, but move to the next question. Then, come back to this (skipped and unanswered) question later when you still have time.*

Five (5) exercises in total.

Exercise 1 (19 points)

In the figure below you see the Al-Mg equilibrium phase diagram. Pure solid Aluminium has a face centred cubic (FCC) structure with lattice constant at room temperature: $= 0.404\ nm$. Pure Magnesium crystallizes in a hexagonal close packed (HCP) structure with lattice parameters: $a = 0.320\ nm$ and $c = 0.520\ nm$. Mg atom is 12 % larger than Al atom.
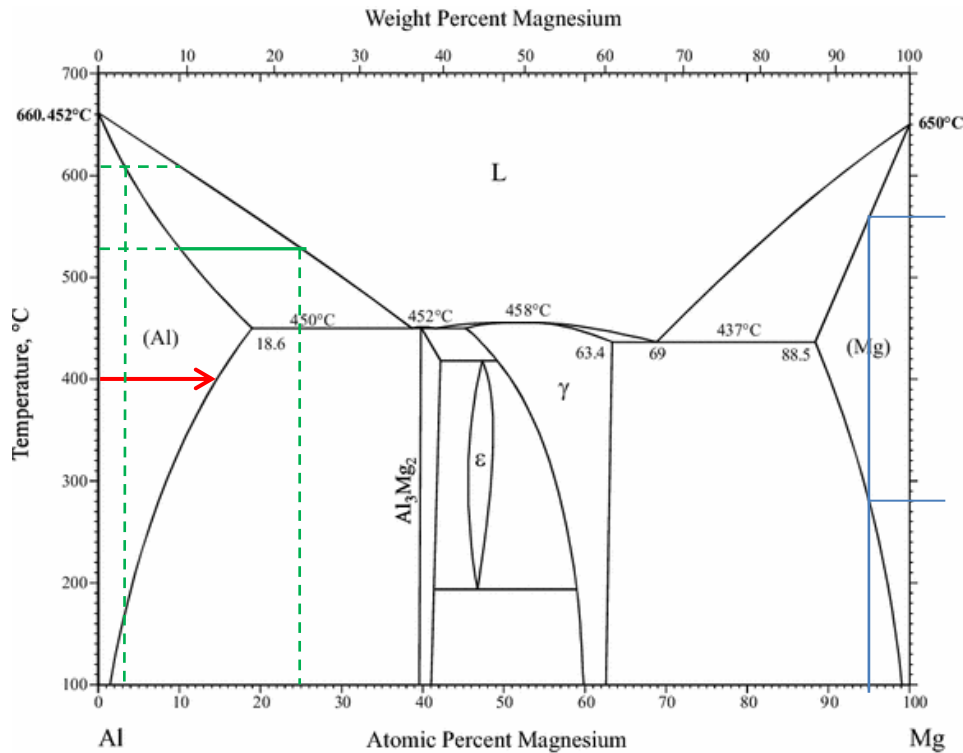
a) The red arrow in the phase diagram crosses different compositions (from 0 to 14.5 at% Mg) at the same temperature 400 °C. How would you characterize phase(s) present at this temperature, covering the whole composition range from the left to the right of this arrow? Please, give its (their) crystal structure(s) and determine if lattice parameter(s) will vary (increase, decrease, no change) with the composition change along the arrow. (3 pt)
   The whole red arrow is inside the single-phase area of a solid solution of Mg in Al. This phase has FCC crystal structure (as pure Al) with Mg atoms randomly occupying lattice sites. Due to fact that Mg atom is larger than Al atom, lattice parameter will gradually increase with the amount of dissolved Mg atoms.

b) Determine a temperature range of solid solubility of Al-Mg alloy with 5 at% of Al. How does this temperature range change with a further increase of Al amount in this alloy? Up to which composition and temperature can we increase the amount of Al and still observe only an equilibrium solid solution of Al in Mg phase? What will be the crystal structure of this phase? (3 pt)
   Vertical line at 5 at% of Al and its intersections with solidus and solvus lines determine the temperature range of solubility. Reading from the blue lines in the above figure we see that this temperature range at 5 at% of Al is from 280 to 560 °C. With increased amount of Al this temperature range will be smaller and smaller, with increasing bottom and decreasing

top temperatures. Maximum solubility of Al in Mg is at 11.5 at% of Al at temperature 437 ℃. Solid solution of Al in Mg has hcp crystal structure, the same as pure Mg.

c) We have Al-Mg alloy with 10 at% of Mg, very slowly cooled down from liquid to room temperature. From the binary diagram determine:

i) at which temperature liquid starts to solidify and what is the composition of this first solid phase; (2 pt)

ii) at which temperature the last drop of liquid is present and what is the composition of this liquid; (2 pt)

iii) which phases and in which proportion are present at a temperature of 100 ℃? (2 pt)

Drawing a vertical line at 10 at% of Mg, and tie lines at its intersection with Liquidus and Solidus line (green lines in phase diagram) we may directly read:

i) Solidification will start at 610 ℃ and composition of first solid phase will be 3 at% Mg;

ii) Last drop of liquid is present at 530 ℃ with composition of about 25 at% of Mg.

iii) At 100 ℃ two phases are in equilibrium: solid solution of 1.5 at% of Mg in Al and Al_3Mg_2 phase. Amounts of these phases should be calculated by the lever rule along a tie line at temperature 100 ℃. This tie line ranges from 1.5 at% till 39.5 at% of Mg, and is split into two parts at composition of 10 at%. Amount of the solid solution phase is:

$$SS = \frac{39.5 - 10}{39.5 - 1.5} = \frac{29.5}{38} = 77.6 \, \% \, .$$

Amount of Al_3Mg_2 phase is:

$$Al_3Mg_2 = \frac{10 - 1.5}{39.5 - 1.5} = \frac{8.5}{38} = 22.4 \, \% \, .$$

d) We would like to maximize the strength of this material via thermal treatment. Propose such treatment consisting of three steps: Isothermal Heating 1, Cooling and Isothermal Heating 2. Propose temperatures and suggest times for both heating steps and specify if cooling between them should be slow or fast. (3 pt)

Describe by your own words the expected difference in microstructure of this alloy before and after thermal treatment. (2 pt)

Do you recommend a long time use of the strength of this material at temperatures around 200 ℃? Why? (2 pt)

This type of alloys could be strengthened by so called precipitation hardening. In the first heating step all equilibrium coarse precipitates of Al_3Mg_2 phase has to be dissolved in Al-Mg solid solution. This heating should be performed at temperatures higher than 330 ℃, to be higher than Solvus line at this composition. To minimize time of this heating step, the temperature could be even higher (say ~450 ℃) to increase diffusion rate. After this first heating, a rapid cooling must be performed to create an unstable oversaturated solid solution of 10 at% of Mg in Al. The last step of thermal processing should be a precipitation heating at a temperature clearly lower than 330 ℃, (typically 150-180 ℃). The cooling rate after this final step is not so relevant (does not have to be controlled well). (3 pt).

Initial equilibrium microstructure contains relatively large Al_3Mg_2 precipitates in almost pure aluminium. After precipitation hardening a metastable microstructure containing randomly dispersed small precipitates of new phase inside oversaturated Al-Mg solid solution is formed. (2 pt)

Temperature of 200 ℃ is probably too high for long-time use of this material, as it is too close to the temperature of precipitation hardening. Due to microstructural meta-

Exercise 2 (15 points)

You are asked to design the core of bungee jumping rope made from **natural rubber** with Young's modulus E = 1.5 MPa, UTS = 28 MPa and being elastic until elongation of 600 %. Jumps will be performed from a bridge, which is 55 meters above the ground level. Jumps are considered to be save, when during a jump:
i) the heaviest allowed jumper's head down (mass 100 kg, height 2 m, with rope fixed on his ankles) will not approach the ground closer than 8 m and
ii) the rubber rope will not be strained more than 200 %.

(For simplicity we assume linear elasticity, which is not accurate for these large strains in the rubber and we also neglect the weight of the rubber rope, which in practice readily can be_15 kg.)
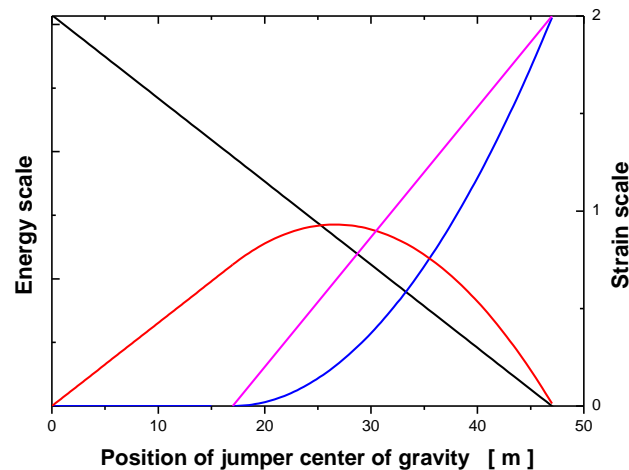
a) Let the zero of the coordinate system be located at the initial position of jumper gravity centre (56 m above the ground level) and jump length is measured from this point downwards the ground along the horizontal axis. In the above sketch there is a graph of four important physical quantities, calculated for the heaviest jumper from the moment of jump start until the moment of reaching the lowest jump point. These four quantities are:
- jumper potential **energy** U_p
- **strain** of the rubber rope ε
- elastic **energy** U_e accumulated in the rubber rope
- jumper kinetic **energy** U_k.
Associate the colour of each line within the graph with its appropriate quantity! (2 pt)
U_p – **black**: linearly decreasing potential energy of jumper from the highest to the lowest position point given by: $\Delta U_p(x) = -mgx$;
ε – **magenta**: the strain of the rubber rope, being zero until the point, when it starts to be

elastically (linearly) stretched until the lowest jumper position;

U_e – **blue**: elastic energy accumulated in the rope. It can be expressed as: $U_e = c_1\sigma\varepsilon = c_2\,\varepsilon^2$, which means a parabolic dependence on x. It is zero until a point, where the rope starts to be stretched and equal to the overall loss of potential energy: $-\Delta U_p$ at the lowest jump point;

U_k – **red**: jumper kinetic energy, being during the whole jump given by a loss of potential energy reduced by elastic energy accumulated in the rope. It is zero at the beginning, then linearly increasing until a point when rope starts to be strained and again equal zero at the lowest jump point. (0.5 pt for each correct couple)

b) Using the fact that the maximum allowed strain is 200% for approaching the ground not closer than 8 m, calculate the idle (initial) length l_o of the rope. (2 pt)

The lowest point of jumper head is allowed 8 m over the ground, that means the maximal length of the stretched rope should be: $55 - 8 - 2 = 45$ m. From the allowed rope strain 200 % and the final length of the strained rope (45 m) we may calculate the idle (initial) length l_0:

$\frac{\Delta l}{l_0} = 2$, $l_0 + \Delta l = 45\,m$ => $l_0 = 15\,m$.

c) This bungee jumping is a dynamic problem and therefore a bit difficult. However, when the 100 kg two meter tall person is hanging upside down in equilibrium (static) on the rope, his head is 28.5 m above the ground. Calculate the initial cross-sectional area A_0 of the rope core. (3 pt)

28.5 m above ground means that $l_0 + \Delta l + 2\,m = 55 - 28.5\,m$. With $l_0 = 15\,m$ this means $\Delta l = 9.5\,m$. Then the strain is $\varepsilon = \frac{\Delta l}{l_o} = \frac{9.5}{15} = 0.06\overline{3}$. Then the stress is $\sigma = E\varepsilon = 1.5\ 10^6\frac{9.5}{15} = 0.95\,MPa$. Since it holds $\sigma = \frac{F}{A} = \frac{mg}{A}$, we can derive $A = \frac{mg}{\sigma} = \frac{100\ 9.81}{0.95\ 10^6} = 1.033\ x10^{-3}m^2 = 1033\,mm^2$

The initial effective cross section of the rope should thus be 1033 mm².

d) Natural rubber is available as a wire having a diameter of 4.4 mm. How many of these wires together are required to make the overall rope? What total length of rubber wire is required for making the rope? If you were not able to calculate l_o and A_o in previous questions, use values of 13 m and 1000 mm², respectively. (2 pt)

The cross-section area of individual wires is $A = \pi r^2 = \pi 2.2^2\,mm^2 = 15.2\,mm^2$. For the total rope it is 1033 mm². So, at least $\frac{1033}{15.2} \doteq 68$ wires have to be brought together in the rope. Since each with the length of 15 m, we have to order 68 x 15 = 1 020 m of rubber wire.

e) On the Internet and in the literature a bungee jump rope it often characterized by its spring constant: k [N/m], that characterize force required to elongate a particular rope by 1 m. Calculate the spring constant for the just designed rope (2 pt) and derive how spring constant k depends in general on rope geometry (A_o, l_o) and Young modulus E. (2 pt)

Spring constant tells us which load should be applied to elongate the rope 1 m. Strain of the rope with initial length of 15 m elongated by 1 m is: $\varepsilon = \frac{\Delta l}{l_o} = \frac{1}{15} = 0.0\overline{6}$. The load F required for this strain should be calculated from Hook's law: $\sigma = \frac{F}{A_o} = E\,\varepsilon$ =>

$F = A_o E\,\varepsilon = 103.3\,N$. Spring constant of the rope is 103.3 N/m. (1 pt)

Substitution of $\varepsilon = \frac{\Delta l}{l_o}$ into the previous equation results in: $F = \frac{A_o E}{l_o}\Delta l$, that clearly defines: $k = \frac{A_o E}{l_o}$. (1 pt)

f) Estimate the safety coefficient comparing the maximal elastic stress (based on maximum strain of 200%) acting during the extremal jump with the UTS of the material used. (2 pt)
Safety coefficient is given by the ratio of UTS and the maximal allowed stress: $S = UTS/\sigma_{max}$. Maximal stress in the rope acts at its maximal elongation, when $\varepsilon = 2$. From the Hook's law and Young's modulus E it follows that $\sigma_{max} = 3\ MPa$. Therefore: $S = \frac{28}{3} = 9.\bar{3}$.

Exercise 3 (16 points)

One of the existing iron oxides is FeO, which has an FCC crystal structure with the rock salt symmetry, see the schematic on the right. The density of FeO is 5.74 g/cm³. The molar mass of iron is 55.85 g/mol, the molar mass of oxygen is 16.0 g/mol and Avogadro's constant is 6.022x10²³ 1/mol.

O^{2-}
Fe^{2+}
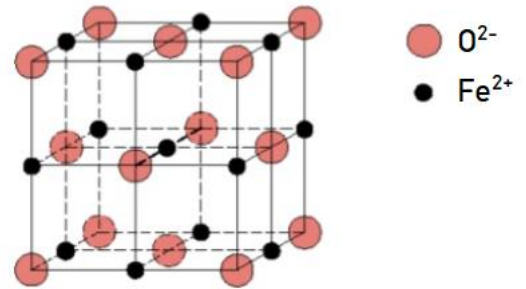
a) What is the ratio of Fe to O ions in FeO? Why? (1pt)
The ratio of Fe^{2+} cations to O^{2-} anions is 1:1 (as already clear from FeO), because then charge neutrality is maintained. (1pt)
b) What is the coordination number and coordination geometry of FeO? (1pt)
In the case of the rock salt unit cell, the coordination number for both cations and anions is 6 and the coordination geometry is octahedral. (1pt)
c) Calculate the lattice parameter (unit cell edge length) of FeO. (3pt)
First the volume of the unit cell has to be found using the density of FeO and the total mass of the unit cell. Then from the unit cell volume the lattice parameter can be found. Note that both Fe and O ions are present 4 times in the FCC rock salt unit cell. (1pt)

$$V = \frac{n \cdot A_{Fe} + n \cdot A_O}{\rho \cdot N_A} = \frac{4 \cdot 55.85\frac{g}{mol} + 4 \cdot 16.0\frac{g}{mol}}{5.74\frac{g}{cm^3} \cdot 6.022 \cdot 10^{23}\frac{1}{mol}} = \frac{287.4\frac{g}{mol}}{3.46 \cdot 10^{24}\frac{g}{mol \cdot cm^3}}$$
$$= 8.31 \cdot 10^{-23}\ cm^3 = 8.3110^{-2}\ nm^3$$

$a = V^{1/3} = 0.436\ nm\ (2pt)$

d) What are the theoretical stable extreme values (minimum and maximum) for the radii of the Fe^{2+} and O^{2-} ions? Use 0.430 nm as lattice parameter for FeO in case you did not find the solution to (c). (3pt)
The Fe^{2+} cations are octahedrally coordinated with six O^{2-} anions. With six-fold coordination the minimum r_C/r_A value occurs when all ions are touching. And the maximum r_C/r_A value for six-fold coordination is the minimum for 8-fold coordination when all ions are touching (1pt).

$Minimum\ (using\ face\ diagonal): 2 \cdot (r_C + r_A) = \sqrt{2} \cdot 2r_A \Rightarrow \frac{r_C}{r_A} = \sqrt{2} - 1 \approx 0.414$

$Maximum\ (using\ body\ diagonal): 2 \cdot (r_C + r_A) = \sqrt{3} \cdot 2r_A \Rightarrow \frac{r_C}{r_A} = \sqrt{3} - 1 \approx 0.732$

The lattice parameter of FeO is equal to twice the radius of the cation and anion.

$$a = 2 \cdot (r_C + r_A) \; and \; r_C = c \cdot r_A \; (with \; c \; the \; \frac{r_C}{r_A} \; ratio)$$

$$r_A = \frac{a}{2 \cdot (1 + c)} \; and \; r_C = c \cdot r_A$$

$$r_A = \frac{0.436 \; nm}{2 \cdot (1 + 0.414)} = 0.154 \; nm \; and \; r_C = 0.414 \cdot 0.154 \; nm = 0.064 \; nm$$

$$r_A = \frac{0.436 \; nm}{2 \cdot (1 + 0.732)} = 0.126 \; nm \; and \; r_C = 0.732 \cdot 0.126 \; nm = 0.092 \; nm \; (2pt)$$

e) We have a polymer that consists of a mixture of four types of molecules with molecular weights corresponding to 200, 400, 600, 800 times the monomer weight. The number fractions for the *first* two types are 0.40 and 0.30, respectively. The number average molecular weight is 400 (in terms of monomer weight). Calculate the number fractions for the *last* two types. (2 pt)
0.40 + 0.30 + X + Y = 1 and thus Y = 0.3-X.
0.4 x 200 + 0.3 x 400 + X x 600 + (0.3-X)x800 = 400 and thus -200X = 400-80-120-240, i.e. -200X = -40 and thus X = 0.2 and thus Y = 0.3-0.2 = 0.1.

f) Now calculate the weight average molecular weight (in terms of monomer weight). (2 pt)
We have the number fractions but not clear weight fractions. These can be readily determined from the answer in e. Therefore the weight average molecular weight is:
(80/400)x200 + (120/400)x400 + (120/400)x600 + (80/400)x800 = 40 + 120 + 180 + 160 = 500.

g) We have two (cylindrical) bars of natural rubber (poly-isoprene) with a length of 10 cm. One is vulcanized the other not. We load at room temperature both pieces parallel to their length for a few minutes to a total strain of 400% (which is about 80% of their fracture strain) and then take away the load. Estimate what length in centimeters both pieces have after the load is taken away. (2 pt)
The vulcanized one (normal rubber) is fully elastic and thus recovers its original length and thus remains 10 cm (1 pt). The one not vulcanized is a viscous liquid and thus flows upload load to a total permanent strain of 400%, which is the relative increase in length. Its final length will thus be 50 cm (the other point).

h) What happens if the whole experiment in the previous exercise is performed with the same loads below the glass transition temperature of the rubber? (2 pt)
Below the glass transition the same load results in very little strain, because the stiffness of both types of rubber increases orders of magnitude. The behaviour of both materials is now elastic, because below the glass transition temperature the molecules are completely rigid and cannot slide with respect to each other. So, they recover their initial length. Both will keep their initial lengths of 10 cm (2 pts, 1 point when 10 cm is given as answer for each type of material with a reasonable motivation).
Note that in this case the answer can also be that both pieces fracture. This is only correct when it is explicitly written that the load is then not applied gently, but rather suddenly. Upon impact load the materials indeed might fracture, but not when load is applied gently.

Exercise 4 (10 points)

a) Explain why *the selection* of materials in mechanically loaded constructions can be affected by the shape of the materials. (3 pts)

The selection of materials is affected by shape since it is not possible to shape all materials in similar optimized forms. For instance, metals like steel and aluminium can be shaped easily (cheaply) into hollow tubes or I-profiles, whereas this is not possible for e.g., wood. Comparing materials in bulk form, wood is often much more advantageous than steel and would be selected for applications. However, when the steel shape is optimized, then steel can become a better choice and is selected for applications.

b) Explain why in constructions that are loaded in bending and torsion materials should be shaped into *hollow rectangular* cross-sections for bending and *hollow circular* cross-sections for torsion. (3 pts)

In constructions we want to use the minimum amount of material that allows the proper and safe use of the constructions (i.e. the construction still satisfies the requirements set to it). A construction can better resist bending or torsion when the material is brought far away from the bending axis or rotation centre, respectively. So, instead of a dense material it is much more efficient to use a hollow cross-section where the materials is moved far from the bending axis or rotation centre. With less material we can still bear the same bending or torsional loading or with the same amount of material we can bear much more bending or torsional loading.

In case of bending, we have a bending axis, which is a line in the cross-section. Bringing material far out of the line implies that we get a rectangular section with a larger height than width. In case of torsion, we have a rotation centre in the cross-section. Bringing material far out of this point implies that we get a circular section around this point. (In the bending case we have to make the integral $y^2 dA$ as large as possible with y the distance to the bending axis and dA infinitesimal pieces of the total area A. In the torsion case we have to make the integral $r^2 dA$ as large as possible with r the distance to the rotation centre. Making y as large as possible for given A implies rectangular shape with a larger height than width. Making r as large as possible for given A implies circular shape.)

c) The shape factor for bending is defined as $\phi_B^e = 4\pi I_{xx}/A^2$ with $I_{xx} = \int y^2 dA$ with y the distance to the bending axis. We have a long beam with as cross section a H or an I profile (with identical cross-sectional areas); see figure below. The bending axis is horizontal in the center of the profiles. Explain by proper qualitative reasoning which one of the two profiles has a larger shape factor and thus performs better in case of bending. For the I profile shown on the left write down (without solving it!!!) the appropriate integral I_{xx} $= \int y^2 dA$ with dA and the proper integration intervals in terms of the a, b, c and d dimensions as indicated in the figure. (4 pt.)

The I profile (on the left) provides more resistance to bending than the H-profile (on the right), because in the formula for the second moment of area and thereby in the shape factor, infinitesimal pieces of area contribute to the integral after multiplication by the distance to the bending axis squared. In the I profile it is clear that much more cross-sectional area is at larger distance from the bending axis than for the H profile and this integral will yield a much larger I_{xx} and thus shape factor (first 2 points).

I profile: $I_{xx} = \int_{d-c/2}^{-d+c/2} by^2 \delta y + 2\int_{-d+c/2}^{c/2} ay^2 \delta y = 2\left[\int_{0}^{-d+c/2} by^2 \delta y + \int_{-d+c/2}^{c/2} ay^2 \delta y\right]$ (2 pts)
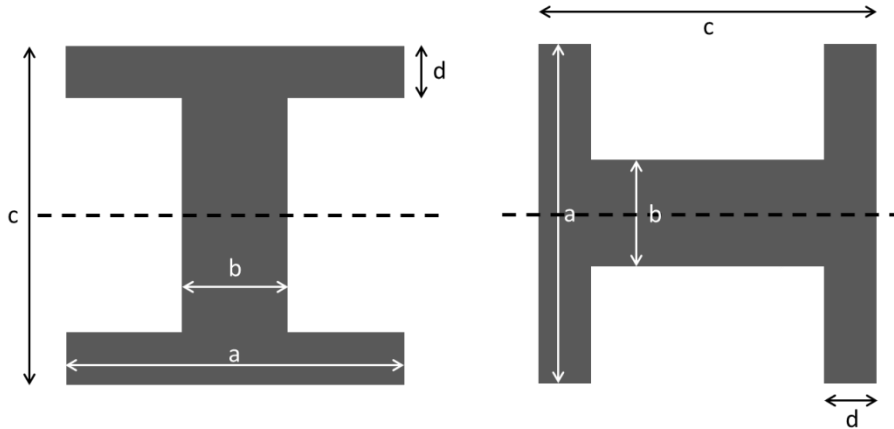
Exercise 5 (16 points)

a) Diamond has a very high Young's modulus of around 1050 GPa. Do you expect diamond to be a good or a poor thermal conductor? Motivate your answer in 1-2 sentences. (2 pt)
Diamond is a good thermal conductor, because the high Young's modulus is an effect of the very strong and stiff bonds between the (carbon) atoms in the diamond. These stiff bonds rapidly transport the lattice vibrations (heat) at one side of the material to the other side of the material (when it would be colder and heats up the entire material rapidly). So, diamond is a very good thermal conduction based on phonon conduction.

b) Lead has a low Young's modulus of around 14 GPa. Do you expect lead to be a good or a poor thermal conductor? Motivate your answer in 1-2 sentences. (2 pt)
Lead is a good thermal conductor, because it is a metal and all metals transport heat well by their free (delocalized) electrons. Lead is likely a poor thermal conduction based on phonon conduction, but this is not relevant, because the electron conduction is dominant.

c) The resistivity of a pure copper wire at 20 °C is 1.7 10^{-8} Ωm and of one containing 1 at.% nickel (and thus 99 at.% Cu) is 2.7 10^{-8} Ωm. When we increase the temperature from 20 °C to about 310 °C what resistivity value you expect for each of the two wires? Show how you determine the values. (3 pt)
When going from 20 °C to 310 °C, the absolute temperature increases from 290 K to 580 K and thus doubles. For pure copper it means that the resistivity doubles, i.e., becomes 3.4 10^{-8} Ωm. For the wire containing 1 at.% nickel the increase in resistivity is the same, but it starts already 1.0 10^{-8} Ωm higher. Its final resistance thus becomes 4.4 10^{-8} Ωm.

d) When we shine visible light on a semiconductor its electrical resistivity can significantly change. This can be nicely used in sensors. Explain if the resistivity increases or decreases and explain why it changes. (2 pt)
The resistivity decreases, because when the light has an energy larger than the band gap of the semiconductor it promotes electrons from the valence band across the band gap into the

conduction band. Therefore, the charge carrier density increases and the semiconductor becomes a better conductor.

e) Would you expect a difference in resistivity when we shine either blue (close to UV) or red (close to IR) light on the semiconductor? Explain your answer. (2 pt)

In general yes. Blue light has more energy than the red light (e.g. 3 eV versus 1 eV) and thus can more easily promote electrons from the valence into the conduction band. Particularly, when the band gap has an energy in-between the ones of the blue and red light, which happens for many semiconductors, then the difference in resistivity is huge. Then the red light cannot promote electrons across the band gap, whereas the blue light can do this very effectively.

f) We have two samples of indium phosphide (InP, which belongs to the class of III-V semiconductors). Sample 1 is produced with perfect crystal structure and in sample 2 on average for each 10^7 crystal unit cells (lattice parameter of the cell a_{InP}=0.586 nm) 1 In atom is replaced by 1 P atom. What type of semiconductor is sample 1 and what type is sample 2? Explain your answer (2 pt.)

Sample 1 is an intrinsic semiconductor (with n=p) and sample 2 is an n-type (extrinsic) semiconductor since the P atoms contain 2 more electrons than the In atoms and thus create excess electrons which can become relatively easily free electrons.

g) The mobility of electrons μ_e=0.50 m²/(Vs) and of holes μ_g=0.015 m²/(Vs). The unit charge = 0.16 10^{-18} C. Compute the resistivity of sample 2 when it is in the extrinsic (exhaustion) regime. (3 pt.)

Note that each replacement provides in this regime 2 free electrons. The main problem is to find the right value for n: $n = \dfrac{2}{10^7(0.585\ 10^{-9})^3} = 1.00\ 10^{21}\ m^{-3}$

$$\sigma = n|e|\mu_e = 1.00\ 10^{21}\ 1.6\ 10^{-19}\ 0.50 = 80\ (\Omega m)^{-1}$$
$$\rho = 1/\sigma = 0.0125\ \Omega m$$