Re-Exam Materials Science

April 9, 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 course and pose your question in the chat. An instructor is almost continuously available during the exam to answer your questions.*

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

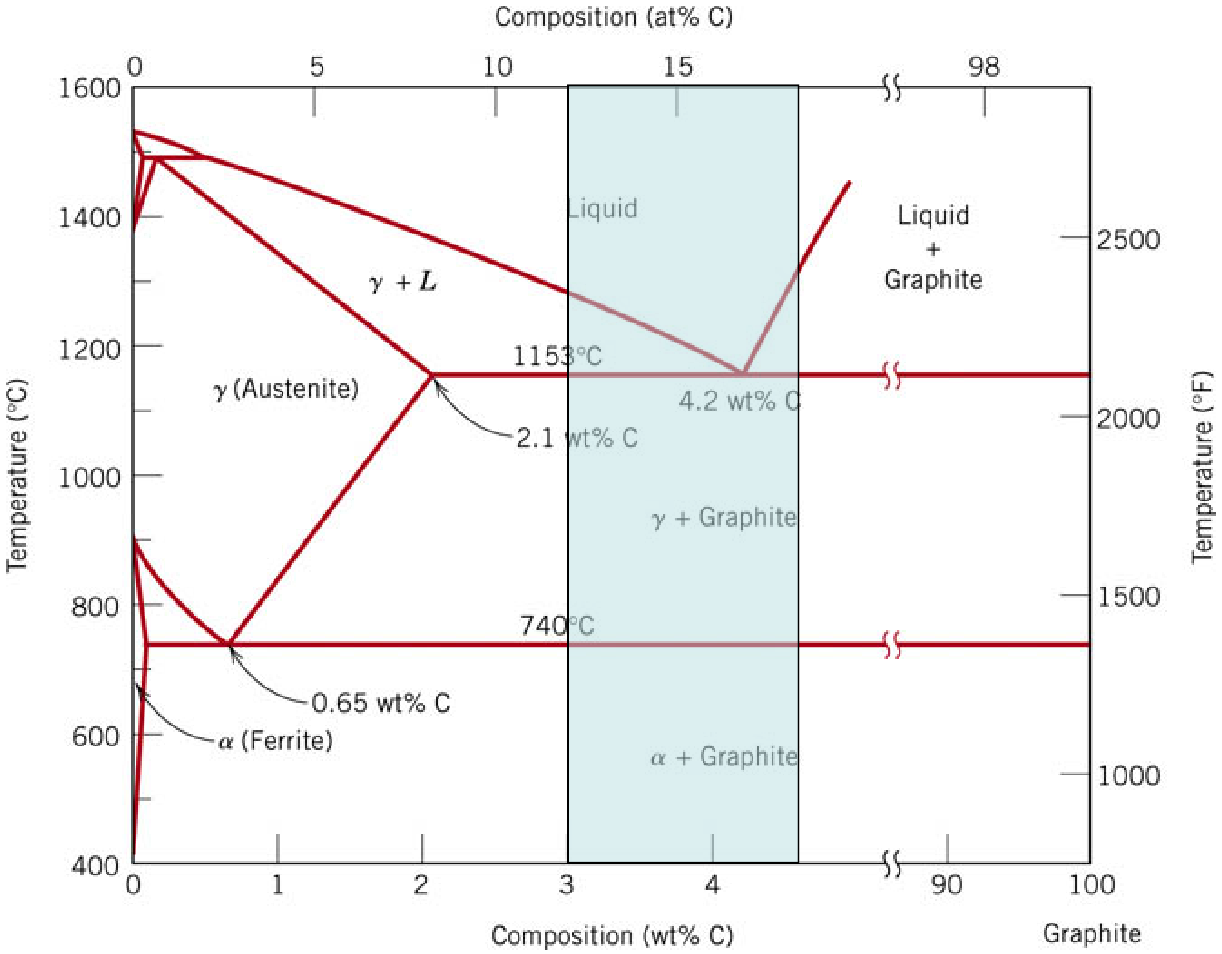
Suggestions:

- *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 (14 points)

In the figure below you see the Iron-Graphite equilibrium phase diagram. This is the relevant diagram for cast iron (and not for steel). The light blue area indicates the relevant composition range of cast iron. Although it is a binary phase diagram, it is required to add (at least) a third element in order to stabilize the graphite phase, for which generally Silicon with about 2 wt.% is used.



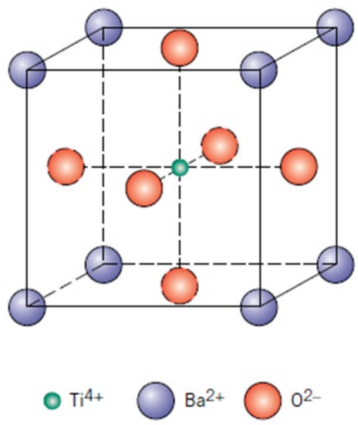
a) We have an Fe-C alloy with 3 wt.% C slowly cooling down from 1600 °C to room temperature. At what temperature does the first (tiny amount of) solid form? Give the composition (value in wt.% C) of this solid. (2 p)
b) At what temperature does the last liquid drop disappear in this 3 wt.% C alloy upon cooling? What is the composition (value) of this last liquid? (2 p)
c) What phases with which fractions are present in the steel with 3 wt.% C at 1152 °C and 739 °C? Show how you calculate your answers. (4 p)
d) When cooling down the steel with 3 wt.% C a eutectic reaction occurs. What fraction of the steel will be subjected to this eutectic (not eutectoid!) reaction? Show your calculation. (2 p)
e) Explain why for cast iron the indicated blue composition range is used in practice. (2 p)
f) Explain why for cast iron it is important that graphite is stabilized, i.e. that measures are taken to avoid cementite (Fe_3C) which is instead present in steel (2 p).

Exercise 2 (18 points)

Bulk metallic glasses (BMG) are solid metallic materials that have significantly higher yield strength compared to normal metals. One of the methods to produce BMGs is to cool the molten metal extremely rapidly. For pure elements this cooling rate cannot be achieved in practice for large volumes. A workable approach is to make an alloy of several elements that requires a lower cooling rate, which is done in the case of the commercial Liquidmetal (an alloy of zirconium, copper, nickel, titanium and beryllium). A result of this production process is that the BMG have a structure similar to glass. Liquidmetal has a yield strength of 1800 MPa and a Young's modulus of 95 GPa. Whereas a similar high strength normal metal (alloy of titanium, aluminium and vanadium) has a yield strength of 900 MPa and a Young's modulus of 110 GPa.

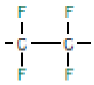
a) Describe the main difference in atomic structure of a normal metal and a BMG. (2 p)
b) What is the atomic scale mechanism that allows normal metals to deform plastically? How does this compare to the deformation mechanisms of BMGs, and what are the implications for its mechanical properties, in particular fracture toughness? Include the role played by stress concentrations in your answer. (4 p)
c) Suppose we have a wire of Liquidmetal with a diameter of 3 mm. What is the maximum load in kilograms this wire can carry just before it starts to yield? (3 p)
d) Suppose we have wires of both materials with a length of one (1) meter. Calculate the maximum elastic elongation of the BMG and of the normal metal. (3 p)
e) Calculate the maximum stored elastic energy per unit volume for the BMG and for the normal metal. (3 p)
f) BMGs were used to make golf clubs and baseball bats and were initially highly rated by users. Explain why BMGs are initially very attractive for these applications, but in the end are abandoned. (3 p)

Exercise 3 (16 points)



a) The figure on the right shows schematically the unit cell of the so-called perovskite crystal structure containing Titanium, Barium and Oxygen atoms, arranged in a cubic lattice. Write the chemical formula of this compound! (1 p)
b) What are the coordination numbers of the cations and anions in the perovskite structure you can derive from the schematic? (3 p)
c) A large number of 950 ceramic cylinders (1 cm high) have been subjected to a tensile test, each up to the stress σ_{max}. The tests show that overall 19 samples failed. Apply the weakest link model (frequently assumed for brittle ceramic materials) and estimate (on the base of result of aforementioned tests) what will be the probability that a 20 cm long ceramic cylinder with the same diameter and material will fail in the same tensile test! (3 p)
d) Why are ceramics so brittle? Include the types of chemical bonds and dislocations in your answer. (3 p)

e) Polytetrafluoroethylene (PTFE) polymer, more well-known as Teflon, is for the present case formed by an assembly of the same number of four different lengths of molecules, containing 2 000 and 4 000, 6 000 and 8 000 units of



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Calculate the number-average molecule length of this polymer expressed in number of structural units and also in g/mol. Use molar mass of Carbon and Fluorine 12 and 19 g/mol, respectively. Calculate also the weight-average molecule length of this polymer assembly expressed in number of structural units. (3 p)

f) The total extended chain length L of a linear polymer molecule depends on the bond length between chain atoms d, the total number of bonds in the molecule N and the angle between neighbouring backbone chain atoms θ, as follows:

$$L = Nd \sin(\theta/2).$$

However, the real end-to-end distance r for a randomly zigzagged linear polymer molecule is:

$$r = d\sqrt{N} .$$

The same type polymer as in the previous exercise e) has the number-average molecule weight of 250 000 g/mol. Compute average values of L and r for this polymer, using the bonding length between Carbon atoms $d = 0.154$ nm and the angle $\theta = 109°$. (3 p)

Exercise 4 (12 points)

a) Explain why *the selection* of materials in mechanically loaded constructions can be affected by material's *shape*. Explain this by comparing specifically steel and wood. (3 p)

b) 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. When we take a fully dense large plate with a constant thickness over its entire area as reference, explain how the plate can be reshaped to increase its stiffness for loading in bending, but without increasing its weight? (Note that this cannot be an I-profile, because this shape is very good for a long beam, but not for a large area plate. Note that several good solutions are possible for the plate.) (3 p)

The theoretical strength of solids is sometimes approximated as: $\sigma_{th} \approx \frac{E}{10}$, with E the Young`s modulus of the solid. Obviously, such a simple estimation cannot be precise and generally valid. The Ashby map (see figure below) that plots the Young`s modulus against the fracture strength of many materials can be used to explore how the real strength of different materials deviates from the above approximation. Please answer the following questions:

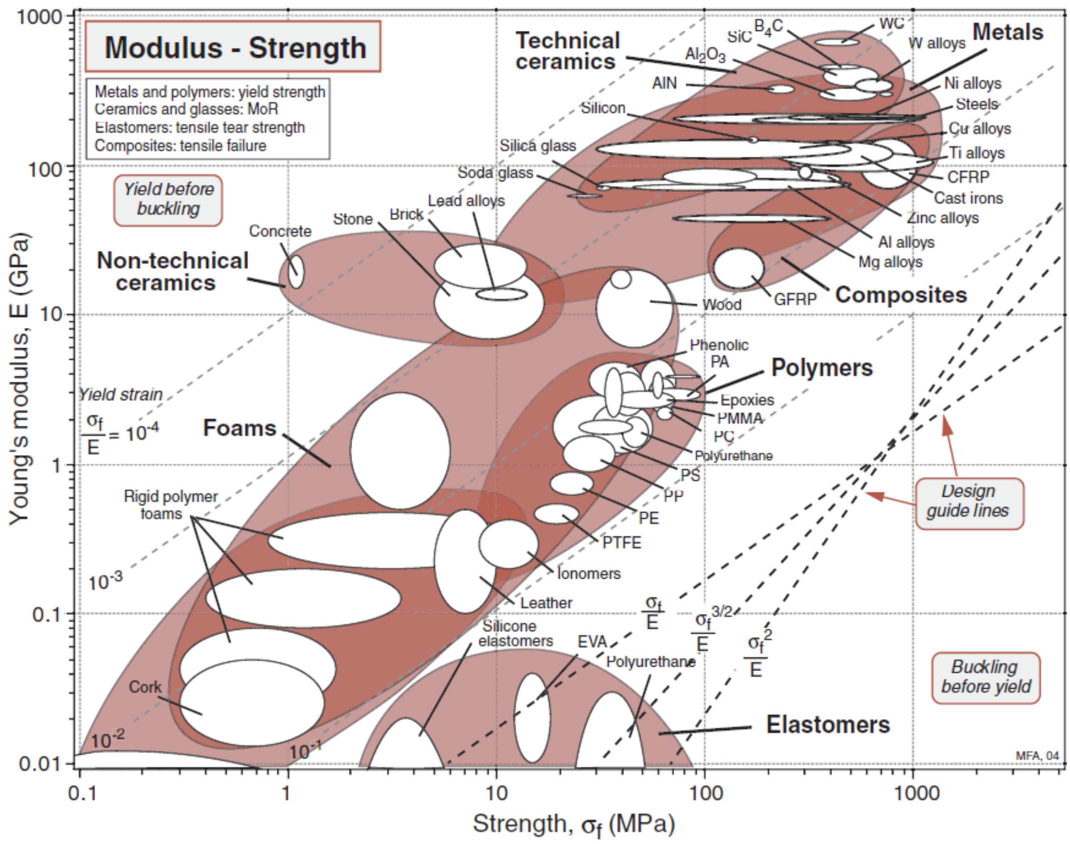
c) When looking at this Ashby map in general, is the above mentioned theoretical strength mostly an overestimation or an underestimation of the real strength? Motivate your answer. Be careful with the units. (2 p)

d) Which group of materials approaches the theoretical strength most closely? (1 p)

e) Which material deviates from the above mentioned estimation the most? (1 p)

f) Which group of materials group shows real strengths even higher than their corresponding theoretical estimations are? (1 p)

g) What is the ratio between the theoretical and the real strength of Concrete (1 p)



Exercise 5 (16 points)

a) Explain why solid materials in general expand upon heating. Hint: Use the potential energy versus interatomic distance curve for solids. (2 p)

b) Explain the difference in room temperature electrical conductivity between copper and silicon from an atomic bonding model perspective. (4 p)

c) Schematically draw the electronic band structures for (i) silicon doped with gallium and (ii) silicon doped with nitrogen. Clearly indicate the different bands, the band gap and the donor or acceptor level. (3 p)

d) Pure silicon at room temperature has a density of 2.33 g/cm^3, electrical conductivity of $4\text{x}10^{-4}$ $(\Omega m)^{-1}$, electron mobility of 0.14 m^2/(Vs), and hole mobility of 0.05 m^2/(Vs). The atomic weight of silicon is 28.09 g/mol, Avogardo's number is $6.02\text{x}10^{23}$ mol^{-1} and the electron charge is $1.61\text{x}10^{-19}$ C. Calculate the average number of conduction electrons per atom in this material at room temperature. (4 p)

e) In your own words, explain why the free charge carrier concentration remains constant over a large temperature range in the extrinsic regime in the case of an extrinsic semiconductor. (3 p)