Exam Materials Science and Engineering

November 6 2015, 9:00-12:00

- *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.*
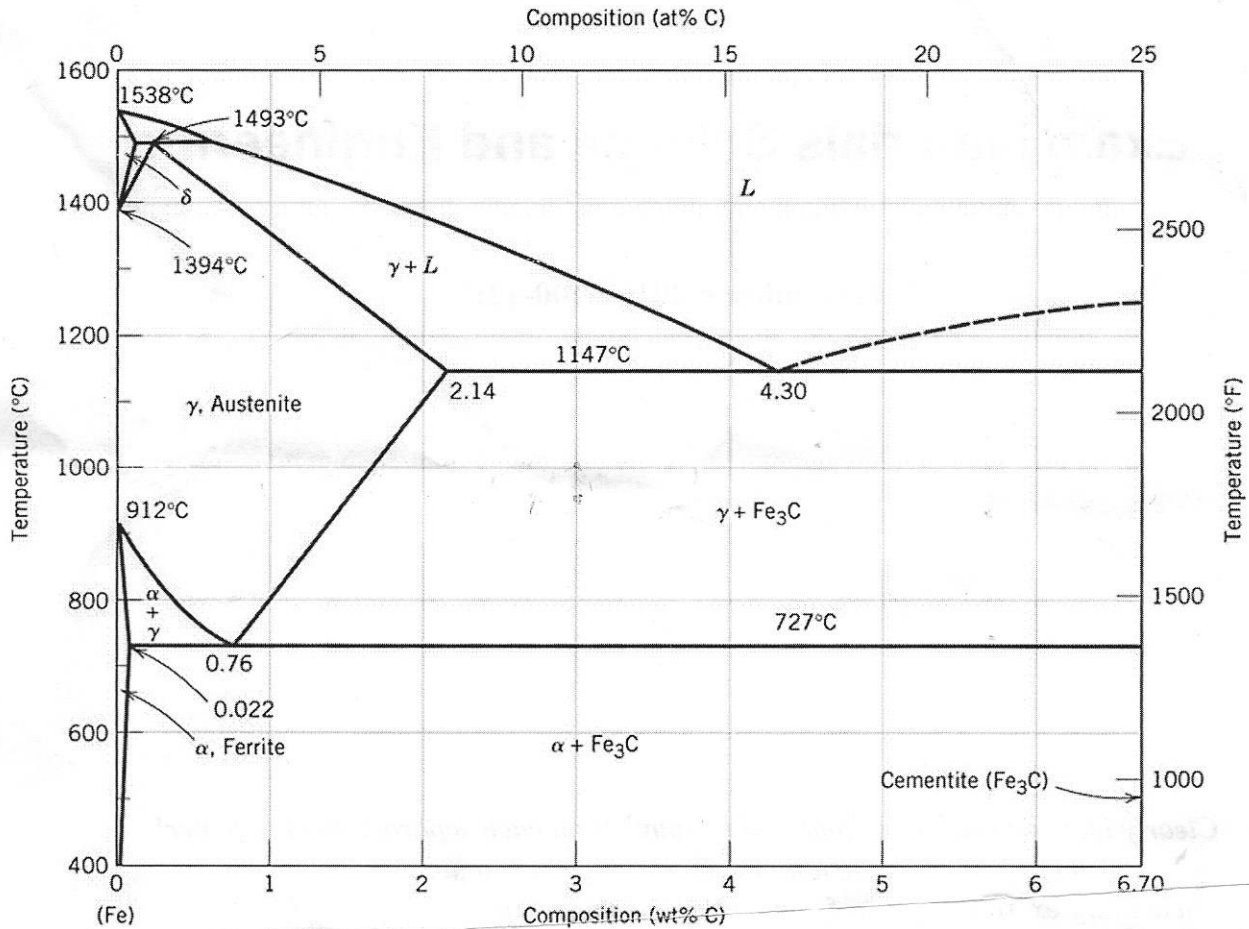- *Make every exercise (of 1 to 5) on a different sheet of paper.*

Mark for the exam = 1 + 9*((sum of total points scored)/66)

Suggestions:
- *Answer concisely: For all questions it is possible to write down the answers in not more than a few sentences.*
- *When you have difficulty to find an answer and to formulate it, do not keep on thinking 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).*

Exercise 1 (16 points)

The Fe-C phase diagram is the base of steel.

Composition (at% C)

Temperature (°C)

Temperature (°F)

1538°C
1493°C
δ
1394°C
γ + L
L
1147°C
2.14
4.30
γ, Austenite
912°C
γ + Fe₃C
α + γ
727°C
0.76
0.022
α, Ferrite
α + Fe₃C
Cementite (Fe₃C)

(Fe)
Composition (wt% C)

a) We have an Fe-C alloy with 1 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) of this solid. (2 pt)

b) At what temperature does the last liquid drop disappear in this 1 wt.% C alloy upon cooling? What is the composition (value) of this last liquid? (2 pt)

c) Suppose a Fe-C alloy with a certain amount of C is cooled down to 728 °C. Austenite and cementite phases are observed, and the weight fraction of austenite is measured to be 0.95. What is the concentration of C in the alloy? Show how you compute your answer. (2 pt)

d) What phases with which fractions are present in the steel with 1 wt.% C at 1200 °C and 726 °C? Show how you calculate your answers. (3 pt)

e) At what temperature will the eutectoid pearlite be formed from austenite? Compute the fractions of the phases present in pearlite. (3 pt)

f) Cold rolling and after annealing can be used to strengthen low C steel. Explain how cold rolling can strengthen the steel (1 pt). Why can it be necessary to anneal cold rolled steel? (2 pt) Still, also after various cycles of cold-rolling and recrystallizing the steel can be strengthened compared to the original material. Explain how this is possible. (1 pt)

Exercise 2 (12 points)

We have a crane whose vertical arm has a cross-sectional area of $5x5 \ cm^2$, and a length of $5 \ m$. This arm is loaded parallel to its length. We know that it behaves according to linear elasticity for the regime we are working. The manufacturer told us that this behavior will stop when the load exceeds $100000 \ kg$, i.e. 100 tons. This load will produce an elongation of the arm of the crane of $1 \ cm$.
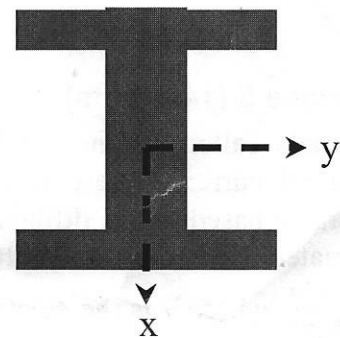
a) Calculate the yield strength of the material. (3 pt)
b) Calculate the yield strain of the material. (1 pt)
c) Calculate the Young's modulus of the material. (1 pt)
d) If the Poisson ratio is 0.3, calculate in terms of percentage the reduction in cross-sectional area due to a loading of $100000\ kg$. (3 pt)
e) What happens both on a macroscopic and an atomic scale in the metal when the load exceeds $100000\ kg$? Each of the two answers is possible in one sentence. (2 pt)
f) Would it make a difference for the mechanical behaviour of the arm whether the material has a crystalline or an amorphous structure? Motivate your answer. (2 pt)

Exercise 3 (14 points)

a) When comparing ceramics and metals, ceramics have several potentially favourable properties. Mention three (3) such properties. (3 pt)
b) However, the fracture toughness of ceramics is in general very unfavourable, i.e. much lower than that of metals. Explain why this is the case. (3 pt)
c) Cis 1,4 poly-isoprene is natural rubber and trans 1,4 poly-isoprene is the much harder gutta percha (with much less favourable properties than natural rubber). Apparently a relative small change in chain configuration can have a large influence on the properties. Explain what the difference is between the cis and trans configurations (i.e. how we can represent their structures in general). (2 pt)
d) We have a thermoplastic polymer near its glass transition temperature Tg. Explain what happens with the stiffness of this polymer around Tg (1 pt). Such a polymer then also exhibits strain-rate sensitive behavior. Describe qualitatively what the difference in mechanical (stress-strain) behavior is of this polymer when loading is very slow or very fast. (2 pt)
e) We have a polymer that consists of a mixture of 4 types of molecules with molecular weights corresponding to 200, 400, 600 and 800 times the monomer weight. The *weight fractions* for these 4 types, are 0.2, 0.3, 0.3 and 0.2, respectively. Calculate the weight average molecular weight and the number average molecular weight in terms of monomer weight. (3 pt)

Exercise 4 (10 points)

a) An I shaped column, with its cross-section shown on the right, is subjected to compressive loading along the z-axis. Its limiting factor is buckling. Will this buckling occur by bending (curvature in the column with displacement) towards the x or y axis? Motivate your answer. (2 pt)
b) We want to select a material for the column that minimizes its weight. In case of buckling and for a design that is constrained by (a sufficiently high) stiffness, materials with the highest possible value for $E^{0.5}/\rho$ are most suitable. E is the Young's modulus of the material and ρ its density. Note that for any designer also price and process-ability is an issue. When you are the designer, which material based on the graph below (on the next page) would you choose? To do this, compare and describe several (at least 3) potential relevant materials in different material classes/families and motivate your final material selection. (4 pt)
c) Suppose the same I shaped column is now only loaded in tension. Which material would you choose now? Motivate your answer. (2 pt)
d) Coming back to the compressively loaded column that fails because of buckling in questions a and b. Can you design (actually sketch!) for this case a cross-sectional shape that is optimized, i.e. with shape factor clearly higher than the one of the I shape? (2 pt)

1. MODULUS-DENSITY
YOUNGS MODULUS E
($G \approx 3E/8$; $K \approx E$.)

MFA:88-91

Axis label (y): YOUNGS MODULUS, E (GPa)
Axis label (x): DENSITY, ρ (Mg/m³)

Exercise 5 (14 points)

Materials called thermoelectrics use a temperature difference to obtain energy in the form of electrical current. These materials have a high Seebeck coefficient: $S = V/\Delta T$. A voltage V is generated based on the difference in temperature ΔT between 2 contacts. Current will flow through the material based on this voltage and the material properties. Performance is characterized by the $Z = \frac{S^2 \sigma}{\kappa}$ where σ is the electrical conductivity, and κ the thermal conductivity. High-performance (High Z value) thermoelectric materials are usually semiconductors. Silicon compounds for instance, although by far not the best performing, are cheap and easily incorporated in modern technology.

a) Why are metals bad thermoelectric materials? (1 pt)

b) Why are (electrical) insulators bad thermoelectric materials? (1 pt)

c) By which two mechanisms is heat conducted in solid materials? (2 pt)

d) Most thermoelectrics operate better at high temperatures (for identical ΔT). This can be explained based on the electrical conductivity vs temperature behavior of a doped semiconductor. Sketch this behavior and denote the various regimes. (4 pt)

e) One of the most effective thermoelectrics is lead telluride (PbTe). Its performance can be increased by doping with, for instance, iodine (I). What kind of semiconductor does this form, and why does this improve the performance Z? (3 pt)

Extrinsic Silicon doped with Gallium has a conductivity of 3.6 $(\Omega m)^{-1}$ at room temperature, which is in the pure extrinsic regime. At room temperature, the electron mobility in Si is μ_e=0.19 m2/(Vs), the hole mobility μ_h=0.045 m^2/(Vs). The unit charge e = 0.16 10^{-18} C, Avogadro's number N_{Av} = 6 10^{23} (mole)$^{-1}$ and Boltzmann's constant k = 8.617 10^{-5} eV/K.

f) Calculate the relevant numbers of conduction electrons and holes per cubic micrometer. (3 pt)

IUPAC Periodic Table of the Elements

Equations Materials Science

Mechanical properties:

$$\sigma = \frac{F}{A_0}, \quad \varepsilon = \frac{l - l_0}{l_0}$$

stress σ is force F divided by area A, strain is relative length change

normal stress (σ) $F \perp A$, shear stress (τ) $F /\!/ A$

$$\varepsilon_{/\!/} = \frac{\sigma}{E}, \quad \varepsilon_\perp = -v\frac{\sigma}{E},$$

E : Young's modulus (*elasticiteitsmodulus*),

v : Poisson's ratio (*dwarscontractie*)

shear: $\gamma = \tan\alpha = \frac{\tau}{G}$, with $G = \frac{E}{2(1+v)}$

Work/Energy U: (toughness)

$$U = \int F ds = V_0 \int \sigma d\varepsilon$$

Area below stress-strain curve = energy uptake in the material per unit volume

elastic: $U_e = \frac{V_0}{2}\sigma\varepsilon = \frac{V_0}{2}\frac{\sigma^2}{E}$

For shear stress on glide system it holds:

$$\tau_R = \sigma\cos\phi\cos\lambda$$

Phase diagrams:

Lever rule: in a 2-phase area the fractions of both phases can be computed with the lever rule.

Example: in the 2-phase area $\alpha + L$ with an average x_B^0 (with $x_B^\alpha > x_B^L$) it holds:

$$\text{Fraction } \alpha = \frac{x_B^0 - x_B^L}{x_B^\alpha - x_B^L}$$

$$\text{Fraction } L = \frac{x_B^\alpha - x_B^0}{x_B^\alpha - x_B^L}$$

Polymers:

Number average molecular weight: $\quad \overline{M}_n = \sum x_i M_i \left(= P_n M_0\right)$

Weight average molecular weight: $\quad \overline{M}_w = \sum w_i M_i \left(= P_w M_0\right)$

viscoelasticity:

with small strains: solid state = elastic, liquid = viscous

polymers in their rubber state, $T_g < T < T_m$, combine elastic and viscous properties.

elastic (Hooke) $\varepsilon = \frac{\sigma}{E}$

(instantaneous response of strain on stress, no further strain as a function of time and full recovery of strain by removal of stress)

viscous (Newton) $\quad \frac{d\varepsilon}{dt} = \frac{\sigma}{\eta}$

(no direct response of strain on stress, strain increases with constant load proportionally with time and no (zero) recovery of strain by removal of stress)

viscoelastic: $\varepsilon = \sigma\left[\frac{1}{E_1} + \frac{1}{E_2}\left(1 - e^{-t/\tau}\right) + \frac{t}{\eta}\right]$

(instantaneous elastic strain + time-dependent elastic deformation (reversible creep) with time constant τ + viscous flow (irreversible creep)).

Electrical properties:

Ohm's Law: $V = IR$ (voltage = current times resistance)

Resistivity: $\rho = \dfrac{RA}{l}$ (with A cross-section area and l length of wire)

Conductivity: $\sigma = \dfrac{1}{\rho}$

Electron conductance: $\sigma = n|e|\mu_e$

with n number of free (conduction) electrons per unit volume, $|e|$ the absolute charge of an electron and μ_e the electron mobility

Resistivity of metals:

$$\rho_{Total} = \rho_{Thermal} + \rho_{Im\,purity} + \rho_{Deformation}$$

$$\rho_{Thermal} \approx aT + b$$

For pure undeformed metals: b=0 (!!!): $\rho_{Total} \approx aT$

with a and b constants. At high temperatures atoms will vibrate more heavily and therefore electrons will be scattered more severely (electron-phonon interaction) and and therefore the resistivity increases more or less proportional with temperature.

Semiconductors:

An electron that can escape from the valence band to the conduction band leaves a hole behind in the valence band. For the conduction it holds:

$$\sigma = n|e|\mu_e + p|e|\mu_h$$

with p the number of holes and μ_h the mobility of the holes ($\mu_h < \mu_e$)

intrinsic semiconductor: n=p

$$\sigma \approx C_1 n = C_1 p = C_2 \exp\left(-\frac{E_g}{2kT}\right)$$ with E_g the bandgap energy

extrinsic semiconductor: doping with foreign atom in intrinsic semiconductor

n-type: n>>p by doping with +1 element, e.g. As or P in Si, whereby +1 element acts as electron donor to conduction band:

$$\sigma \approx C_a n = C_b \exp\left(-\frac{E_g - E_d}{kT}\right)$$

with E_d the energy of the donor level in the bandgap.

p-type: p>>n by doping with -1 element, e.g. B or Al in Si, whereby -1 element acts as electron acceptor from valence band:

$$\sigma \approx C_c p = C_d \exp\left(-\frac{E_a}{kT}\right)$$

with E_a the energy of the acceptor level in the bandgap.

Thermal properties:

Linear expansion coefficient α_l leads to:

$$\frac{\Delta l}{l_0} = \int \alpha_l dT$$

With a thin film on a substrate and assuming isotropic elasticity the plane stress in the film will be:

$$\sigma_{//} = \frac{E}{1-v} \int (\alpha_{substrate} - \alpha_{film}) dT$$