

UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Exam MENA1000 – Materials, energy and nanotechnology

Day: 6 December 2007

Duration: 3 hours

The set counts 6 pages (12 questions)

Attachments: None

Allowed aids: Calculator without communication or stored information

Language: English

Note:

Control that the set of questions is complete, before you start answering questions.

All questions 1, 2, 3 etc. count equal.

Chemical reaction equations shall be balanced unless otherwise stated.

Standard conditions shall be assumed unless otherwise stated.

Question 1

By help of diffraction we can determine the distance between atomic planes in crystals. For this we need radiation with a wave length of a similar order of magnitude as the plane distances in the crystal, i.e. distances between atoms. If we use electromagnetic radiation, what is roughly the wave length domain we need, and what range of frequencies and energies does this correspond to?

Question 2

Three plates are put flat on top of each other on horizontal ground. The bottom and top plates are metal plates, while the middle is a light, elastic plate. All plates measure 0,1 m x 0,1 m x 0,01 m each. The metal plates weigh 1 kg each.

a) What is the gravitational force that the top plate acts on the middle plate? What is the force that the middle plate acts on the top plate?

b) What is the normal stress that the middle plate is subjected to? The middle plate has stiffness (E-modulus, Young's modulus) of 0.1 GPa. How much is it compressed under the weight of the top plate?

Question 3

a) The inner energy U of a crystal has many contributions. Mention the most important ones.

b) The inner energy U can be approximated by the enthalpy, H . This can, in turn, be split into Gibbs energy G and TS , where S is entropy. What do we know (or don't we know) about H , G , and S for a perfect crystal of a pure compound at $T = 0$ K?

Question 4

Lanthanum cuprate, La_2CuO_4 , was among the first oxides to be investigated with respect to high temperature superconductivity

- a) Assign formal oxidation states for the elements in lanthanum cuprate, La_2CuO_4 .
- b) What is a probable electron configuration in the ground state of copper ions in this compound?
- c) Every copper ion has six oxide ion neighbours in this oxide. Consider whether the compound can be coloured and whether it can be paramagnetic in view of crystal field considerations for the copper ions in an octahedral field.

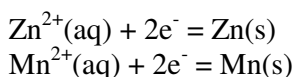
Question 5

Graphite consists of only carbon atoms, forming layers 0.335 nm apart. In the layers the atoms are found in six-rings with bond lengths of 0.142 nm.

- a) Draw a Lewis structure (using dots or simply lines to show bonds) for a small part of a graphite layer so as to show the essentials of the electron structure and bonds in the material. Ensure that all valence electrons are included.
- b) Explain why diamond is an isolator and a very hard material while graphite conducts electrical current and is soft enough to be used as lubricant and in pencils.
- c) Name at last one other element that takes on the diamond structure. If you do not know the answer, make a guess, and explain your choice.
- d) If one could “cut out” an elongated rectangle of a graphite layer, roll it up, and bond the carbon atoms along the two long edges to each other, a single walled carbon nanotube would result. Explain what kind of functional and mechanical properties we may expect that such a nanotube gets. What can such nanotubes be used for?

Question 6

We shall make a zinc-manganese battery. We make two half-cells: In one we put a zinc bar in a 1 M aqueous solution of ZnSO_4 , in the other we put a manganese bar in a 1 M aqueous solution of MnSO_4 . In both half-cells we have $\text{pH} = 0$. The two half-cells are connected with a salt-bridge, and the two metal bars are connected with a resistor (load). Standard reduction potential for the half-cells are:



$$\begin{aligned}E^0 &= -0.76 \text{ V} \\ E^0 &= -1.18 \text{ V}\end{aligned}$$

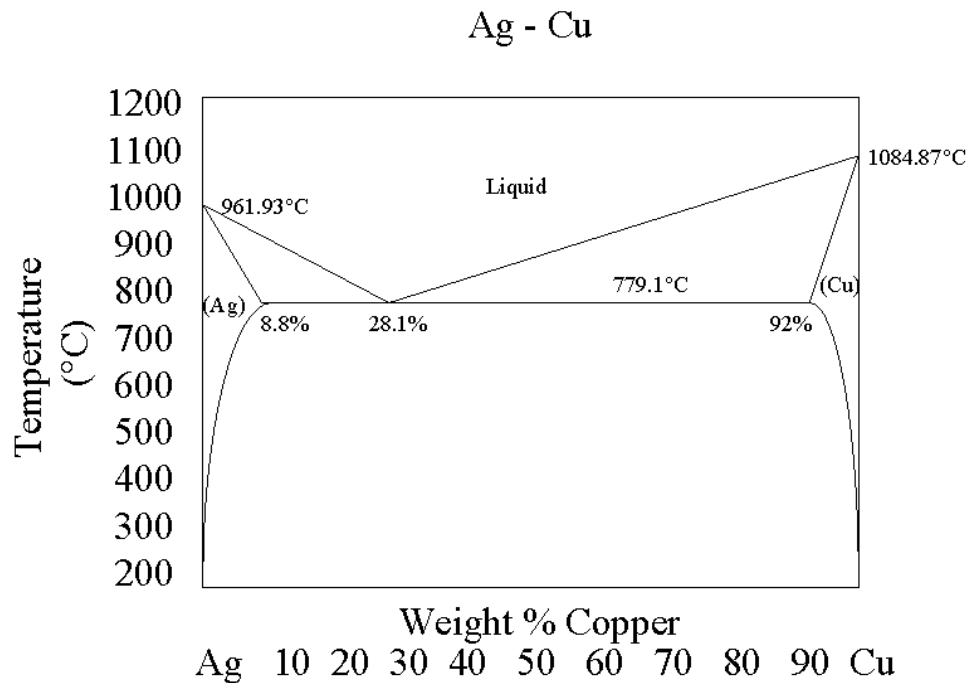
- a) Draw the setup of the cell. Mark cathode and anode, positive and negative electrode, and direction of flow of electrons when the cell delivers current.
- b) Write a total cell reaction. What is the standard cell voltage?
- c) Under neutral or basic conditions divalent zinc can be precipitated as zinc hydroxide with solubility product $K_{sp} = 3 \cdot 10^{-17}$. What is the concentration of $Zn^{2+}(aq)$ in a saturated solution of zinc hydroxide at $pH = 7$?

Question 7

Zirconium oxide, ZrO_2 has a monoclinic unit cell when undoped. When we substitute in yttrium, Y, we get defects and as a result of this, structures with higher symmetry. Y-substituted ZrO_2 has several areas of applications which are based on particular mechanical or functional properties. Describe one such area of application and how the material's essential property is obtained and utilised.

Question 8

Below is given the phase diagram for silver (Ag) – copper (Cu) alloys. We have an alloy of silver with 4 weight-% Cu in a crucible and heat this to $1000^\circ C$. Describe the alloy at this temperature. We cool to $800^\circ C$ and equilibrate. What do we have now? We cool slowly further to room temperature. The alloy has become harder and stronger than the metal. Give an explanation of this.



Question 9

- a) Super-pure germanium, Ge, is an intrinsic semiconductor, in which electrons and holes are formed by thermal excitation over the band gap. Write a reaction equation for this process.
- b) A super-pure (undoped) intrinsic semiconductor can be mainly an n-type or a p-type conductor. Give an explanation based on what you know about the conductivity for a charge carrier. How can we measure whether the material is n- or p-type conducting.?
- c) What can Ge be doped with to make it i) a good n-type conductor and ii) a good p-type conductor?
- d) How does a diode work? (Use a drawing if you like.)

Question 10

- a) Methanol, CH_3OH , is a possible fuel and energy carrier today and in the future. It can be produced from fossil or biological sources. Explain the production route for at least one of these.
- b) Write the reaction equation for complete combustion of methanol with oxygen.
- c) What is the standard cell voltage for a fuel cell at 25 °C that runs on methanol dissolved in water and oxygen gas, from the following thermodynamic data?

	$\text{O}_2(\text{g})$	$\text{CO}_2(\text{g})$	$\text{H}_2\text{O}(\text{l})$	$\text{CH}_3\text{OH}(\text{aq})$
$\Delta_f H^\circ$, kJ/mol	0	-394	-286	-246
S° , J/molK	205	214	70	133

Question 11

A possible energy carrier for cars and other vehicles in the future is hydrogen. Describe briefly three different ways of storing hydrogen onboard, and point out what challenges each of them face, especially regarding materials.

Question 12

- a) Describe briefly two of today's technologies for digital data storage or processing within what we may call microtechnology.
- b) Describe two areas where nanotechnology can bring data storage and/or processing further with respect to data density and speed. If you think that pointing out such an area is dependent on a definition of nanotechnology, you may also include the definition.

Formulae and tables

$$E = \frac{1}{2}mv^2 \quad E = mc^2$$

$$F = \frac{\gamma m_1 m_2}{r^2} \quad F = gm$$

$$F = \frac{k_e q_1 q_2}{r^2} = \frac{q_1 q_2}{4\pi\epsilon_0 r^2}$$

$$E_p = \frac{k_e Qq}{r}$$

$$F = qvB \quad \mathcal{E} = lvB$$

$$\frac{U_s}{U_p} = \frac{N_s}{N_p}$$

$$\lambda_m = \frac{a}{T} \quad M_e = \sigma T^4$$

$$E_k = hf - W \quad \lambda = \frac{h}{mv}$$

Lukket system: $\Delta U = q + w$

Bare volumarbeid, konstant trykk: $w = -P\Delta V$.

Entalpiendring $\Delta H = q_p$

$$\Delta H = n \int_{T_1}^{T_2} C_p dT$$

$$\Delta H = n \overline{C_p} \Delta T$$

Konstanter

Tyngdeakselerasjonen	g	9,80665	m/s ²
Atomær masseenhet	u	1,6605*10 ⁻²⁷	kg
Elektronets masse	m _e	9,110*10 ⁻³¹	kg
Elementærladningen	e	1,602*10 ⁻¹⁹	C
Elektronvolt	eV	1,602*10 ⁻¹⁹	J
Protonets masse	m _p	1,673*10 ⁻²⁷	kg
Nøytronets masse	m _n	1,675*10 ⁻²⁷	kg
Lyshastigheten i vakuum	c	2,99792*10 ⁸	m/s
Boltzmanns konstant	k	1,381*10 ⁻²³	J/K
		8,6174*10 ⁻⁵	eV/K
Plancks konstant	h	6,626*10 ⁻³⁴	Js
Rydberg-konstanten	\mathcal{R}	1,097*10 ⁷	m ⁻¹
Bohrs konstant	B	2,18*10 ⁻¹⁸	J
Avogadros tall	N _A	6,022*10 ²³	mol ⁻¹
Gasskonstanten	R	8,31451	J/molK
		0,0820578	Latm/molK
Faradaykonstanten	F	96485	C/mol
Gravitasjonskonstanten	γ	6,672*10 ⁻¹¹	Nm ² /kg ²
Permeabiliteten for vakuum	μ_0	1,257*10 ⁻¹²	H/m
Permittiviteten for vakuum	ϵ_0	8,854*10 ⁻¹²	F/m
Elektrisk konstant $= (4\pi\epsilon_0)^{-1}$	k _e	9,0*10 ⁹	Nm ² /C ²
Magnetisk konstant	k _m	2*10 ⁻⁷	N/A ²
Stefan-Boltzmannkonstanten	σ	5,67*10 ⁻⁸	W/m ² K ⁴
Wiens konstant	a	2,90*10 ⁻³	mK
Volum av 1 mol ideell gass	V _{m,298K}	24,4651	L

$$S = k \ln W \quad \Delta S = \int_1^2 \frac{dq_{rev}}{T} \approx \frac{\Delta q_{rev}}{T} \stackrel{\text{Konst. trykk}}{=} \frac{\Delta H}{T}$$

$$\Delta U = q_{rev} + w_{rev} = q_{irrev} + w_{irrev} \quad PV = nRT$$

Gibbs energi: $G = H - TS$ Frivillig prosess: $\Delta G = \Delta H - T\Delta S < 0$

$$\Delta_r G = \Delta_r G^0 + RT \ln Q \stackrel{\text{eksempel}}{=} \Delta_r G^0 + RT \ln \frac{a_C^c a_D^d}{a_A^a a_B^b}$$

$$w_{el} = \Delta G = -nFE$$

$$\Delta G^0 = -nFE^0$$

$$\text{Nernst: } E = E^0 - \frac{RT}{nF} \ln Q$$

$$\text{Likevekt: } \Delta_r G^0 = -RT \ln Q_{\text{likevekt}} = -RT \ln K \quad E^0 = \frac{RT}{nF} \ln Q_{\text{likevekt}} = \frac{RT}{nF} \ln K$$

$$\Delta_r H^0 = \sum_{\text{produkter}} \Delta_f H^0 - \sum_{\text{reaktanter}} \Delta_f H^0 \quad \Delta_r S^0 = \sum_{\text{produkter}} S^0 - \sum_{\text{reaktanter}} S^0 \quad \Delta_r G = \sum_{\text{produkter}} G - \sum_{\text{reaktanter}} G$$

$$pH = -\log[H^+]$$

$$pK_a = -\log K_a$$

$$\text{Buffer: } pH = pK_a + \log \frac{[B]}{[A]}$$

Gitterenergi $E_L = N_A k_e e^2 \frac{z_C z_A}{d_{eq}} \left(1 - \frac{d^*}{d_{eq}} \right) A$ Hydratisering: $E_{hyd} = - \left(K_C \frac{z_C^2}{r_C} + K_A \frac{z_A^2}{r_A} \right)$

Vektarmregelen: $m_1(q - a_1) = m_2(a_2 - q)$

Gibbs faseregell: $F + P = C + 2$

Bragg: $n\lambda = 2d \sin\theta$ $d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

Selvdifusjon: $D_r = D_r^0 e^{-Q_D/RT}$, $d_{r,total} = \frac{6D_r t}{d}$, $r_{r,radiell} = \sqrt{6D_r t}$, $r_x = \sqrt{2D_r t}$

$D_{r,defekt} [defekt] = D_{r,s} [s]$

$\vec{v} = B\vec{F}$, $D_r = kTB$, $u = zeB$, $\sigma = zecu$

$\sigma_s = z_s e c_s u_s = \frac{(z_s e)^2 c_s D_{r,s}}{kT} = \sigma_{s,defekt} = z_s e c_{s,defekt} u_{s,defekt} = \frac{(z_s e)^2 c_{s,defekt} D_{r,s,defekt}}{kT}$

Netto fluks: $\vec{j} = c\vec{v} = cB\vec{F} = \frac{cD_r}{kT} \vec{F}$ Kraft i elektrokjemisk felt: $F = - \left(\frac{d\mu}{dx} + ze \frac{d\phi}{dx} \right) = - \frac{d\eta}{dx}$

Elektriske egenskaper: $G = \sigma \frac{a}{d}$ $G = \frac{1}{R}$ $i = \sigma E$ $I = \frac{U}{R}$ Effekt: $P = UI$

Virkningsgrad: $\eta_{total} = \eta_{Gibbs} \eta_{Faraday} = \eta_{Gibbs} u_{fuel} = \frac{P_e}{P_{in}}$

Mekanisk: $\vec{\sigma} = \frac{\vec{F}}{A}$ $\varepsilon = \frac{\Delta l}{l}$ $\sigma = E\varepsilon$ Polymer: $\sigma_B \approx \sigma_{B,max} - \frac{A}{M}$ Lyd: $v = \sqrt{\frac{E}{\rho}}$

Snell: $\frac{\sin i}{\sin r} = \frac{v_i}{v_r}$ Magnetisk: $\vec{B} = \mu \vec{H} = \mu_0 \vec{H} + \mu_0 \vec{M} = \mu_0 (\vec{H} + \vec{M}) = \mu_0 \vec{H} (1 + \chi)$

PERIODIC CHART OF THE ELEMENTS

IA	IIA	IIIB	IVB	VB	VIB	VII B	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	INERT GASES	
1 H 1.00797																1 H 1.00797	2 He 4.0026	
3 Li 6.939	4 Be 9.0122											5 B 10.811	6 C 12.0112	7 N 14.0067	8 O 15.9994	9 F 18.9984	10 Ne 20.183	
11 Na 22.9898	12 Mg 24.312											13 Al 26.9815	14 Si 28.086	15 P 30.9738	16 S 32.064	17 Cl 35.453	18 Ar 39.948	
19 K 39.102	20 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.942	24 Cr 51.996	25 Mn 54.9380	26 Fe 55.847	27 Co 58.9332	28 Ni 58.71	29 Cu 63.54	30 Zn 65.37	31 Ga 69.72	32 Ge 72.59	33 As 74.9216	34 Se 78.96	35 Br 79.909	36 Kr 83.80	
37 Rb 85.47	38 Sr 87.62	39 Y 88.905	40 Zr 91.22	41 Nb 92.906	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.905	46 Pd 106.4	47 Ag 107.870	48 Cd 112.40	49 In 114.82	50 Sn 118.69	51 Sb 121.75	52 Te 127.60	53 I 126.904	54 Xe 131.30	
55 Cs 132.905	56 Ba 137.34	*57 La 138.91	72 Hf 178.49	73 Ta 180.948	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.09	79 Au 196.967	80 Hg 200.59	81 Tl 204.37	82 Pb 207.19	83 Bi 208.980	84 Po (210)	85 At (210)	86 Rn (222)	
87 Fr [223]	88 Ra [226]	†89 Ac [227]	104 Rf [261]	105 Db [261]	106 Sg [266]	107 Bh [262]	108 Hs [265]	109 Mt [266]	110 ? [271]	111 ? [272]	112 ? [277]							

Numbers in parenthesis are mass numbers of most stable or most common isotope.

Atomic weights corrected to conform to the 1963 values of the Commission on Atomic Weights.

The group designations used here are the former Chemical Abstract Service numbers.

* Lanthanide Series

58 Ce 140.12	59 Pr 140.907	60 Nd 144.24	61 Pm [147]	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.924	66 Dy 162.50	67 Ho 164.930	68 Er 167.26	69 Tm 168.934	70 Yb 173.04	71 Lu 174.97
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† Actinide Series

90 Th 232.038	91 Pa [231]	92 U 238.03	93 Np [237]	94 Pu [242]	95 Am [243]	96 Cm [247]	97 Bk [247]	98 Cf [249]	99 Es [254]	100 Fm [253]	101 Md [256]	102 No [256]	103 Lr [257]
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