UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Exam: MEF 3000 / MEF 4000 – Functional materials
Day/time: Friday 9. December, kl. 14.30 – 17.30
Duration: 3 hours
The set is on: 9 pages including 4 appended papers (5 tasks)
Allowed aids: Calculator, colors, ruler and similar
Language: English

Candidate number:

Note:
Write your candidate number on page 1, and control that the set is complete before you begin to answer the tasks.

All tasks require only short answers. Remember therefore to answer shortly in order to be able to complete the set.

Task 1: Structure (30%).

Given the following structural data:

Imm2
a = 3.5024 Å, *b* = 5.3789 Å, *c* = 5.5209 Å

Na	2a		z = 0.58833
N	2a		z = 0.12277
O	4c	x = 0, y = 0.19646	

In the table for this space group the following information is given about the positions.

Positions

Multiplicity	Wyckoff letter	Site symmetry	Coordinates (0,0,0)+ (½, ½, ½)+			
8	e	1	x, y, z	-x, -y, z	x, -y, z	-x, y, z
4	d	m..	0, y, z	0, -y, z		
4	c	.m.	x, y, 0	-x, -y, 0		
2	b	mm2	0, ½, z			
2	a	mm2	0, 0, z			

a) What type of crystal system is this?

What is the Bravais lattice of this crystal system?

Give the corresponding point group for the given space group.

b) What is the chemical formula for this material?

How many formula units does the unit cell contain?

c) Make a stereographic projection of this point group and note how many times a general position is repeated.

d) Draw the structure as a projection on the **bc** plane. Draw in the N–O bonds. (Feel free to use one of the appended grids for your answer).

e) What is the distance between a N and one of the nearby O?

f) Can you from the stereographic projection and your structure drawing comment on whether this compound may be piezoelectric or not?

g) At higher temperature, a phase transition occurs that gives this compound the space group Immm. The structure can be visualized by adding the atoms:

Na	2a	z = 1-0.58833 = 0.41167
N	2a	z = 1-0.12277 = 0.87723

to the drawing that you did in b), do this.
In practice this is a mirroring of all the points along the c-axis.

Each atom that is mirrored will have an occupation number of 0.5. In this way there is a 50% chance to find an atom on that position or not. Also one avoids so close atomic positions that the operation otherwise would have given. Told in another way, the atoms are jumping back and forth between the two nearest positions in the structure.

h) Make a stereographic projection for the corresponding point group for the space group Immm. Note a general position and how this is being multiplied.

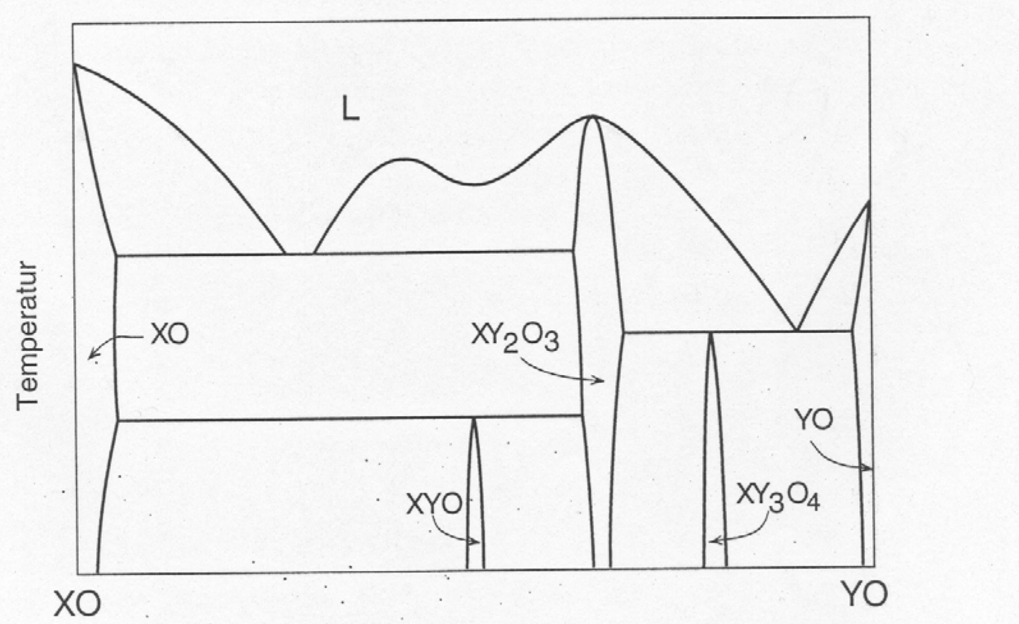
i) Can you on the basis of the new stereographic projection, and the new structure drawing comment on whether this compound may be piezoelectric at high temperatures or not?

Task 2: Phase diagrams (14%).

a) Draw schematic one or more phase diagrams that together contains at least one of each of the following reactions:

- Eutectic reaction
- Peritectic reaction
- Congruent melting
- Eutectoid reaction
- Peritectoid reaction

b) There are some errors in the phase diagram below (or rather special situations). Mark these on the figure and discuss these in the context of the phase rule. (Feel free to use one of the appended copies for your answer.)



Figur 3: Fasediagram med feil (eller usannsynlige faseforhold).

c) Consider a hypothetic binary oxide system $AO_2 – B_2O_3$ with one incongruently melting phase AB_2O_5. Assume that there is no solid solubility. Draw the phase diagram.

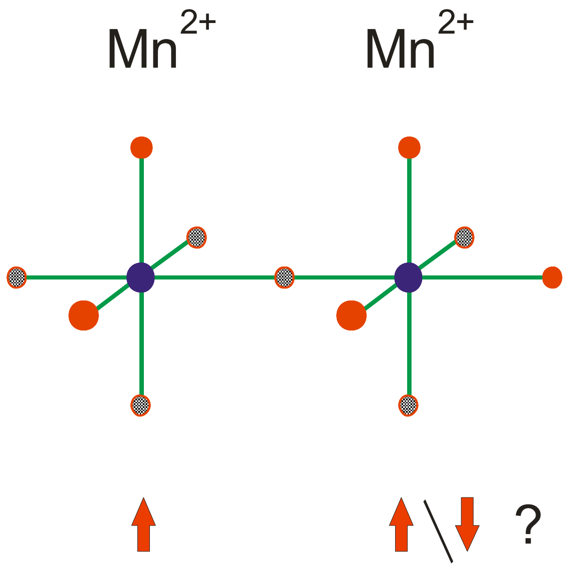
Task 3: Magnetism (13%).

a) What is magnetic susceptibility? Describe shortly.

b) Write the Curie and the Curie-Weiss relationship for ferromagnetic, paramagnetic and anti-ferromagnetic materials. Draw the $1/\chi$ versus temperature (χ is magnetic susceptibility) and explain how the constant θ varies between the different types of magnetism.

c) What are the characteristics of a hard and a soft magnet? Describe shortly.

d) Consider the structural elements below for two octahedrons of MnO_6 that are connected together in their corners. If the electron spin points up for the first manganese, what is the likely orientation of the electron spin at the other manganese?



How will a tilting / rotation of these octahedrons in relation to each other affect the magnetic exchange and transition temperature?

Task 4: Dielectric materials (13%).

a) How does one classify the isolating materials in subgroups?

b) What is the difference between a purely piezoelectric and a ferroelectric material? Describe shortly.

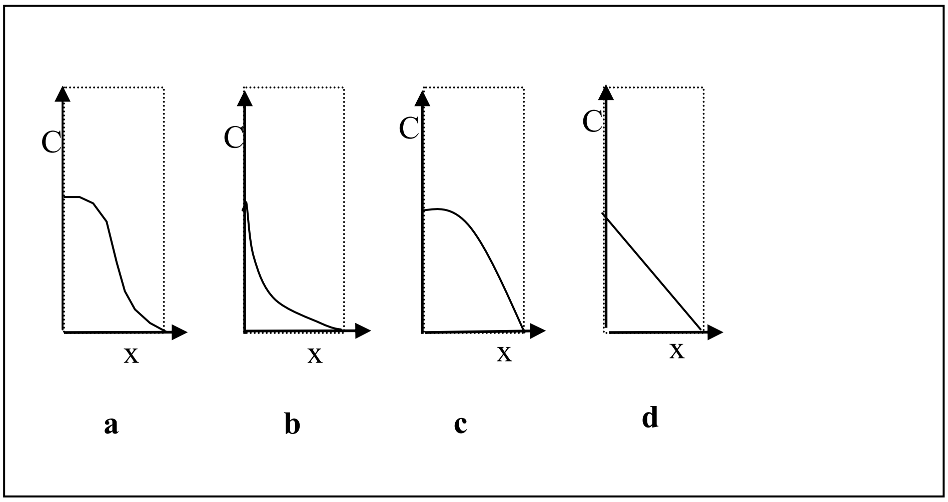
c) What types of mechanism / effects occurs in a dielectric material when an external electric field is applied? In other words, what is being polarized in the material? Mention shortly.

What is the relative importance of these effects as the frequency of the external field is varied? On other words, rate the effects to their response in time.

d) What is pooling of a material? Describe shortly.

Task 5: Diffusion, conduction and optical aspects (30%).

a) Hydrogen is diffusing through a Pd:Ag membrane at 400 °C. On one side of the membrane we have a gas mixture congaing H_2 at a constant pressure and composition. At the other side, H_2 is consumed by a motor running on hydrogen at constant speed, leaving the concentration on that side equal to zero. The system has been running for a long time. Below is a figure which shows four alternatives for how the concentration, C, varies through the thickness, x, of the membrane. (The stippled line indicates the extent of the membrane)



Pick the correct concentration profile and explain why you chose it.

b) A student wants to do an experiment with single photons to study the optical properties of a new type of material she has synthesized. She has a laser with a wavelength 435 nm and an output light power of 0.1 mW.
She first needs to adjust the intensity so that she can detect single photons. She has a very sensitive detector, giving an output pulse for every photon. In order that the signals don't overlap in time and can be counted, the counting rate has to be smaller than 10 kHz. She can adjust the counting rate by letting the laser beam go through a glass material with an absorption coefficient of 10^4 m^{-1}. How thick should the glass be?

Hint: You will need to use the physical constants of the table attached at the end of the problem set.

c) Describe briefly the geometric structure of amorphous silica (formulae SiO_2).

d) Which are the material(s) of an optical communication fibre?

Which material parameters relate to the signal attenuation in an optical fibre, and which physical and chemical processes are important?

e) Consider the semiconductor $Si_{0.9}Ge_{0.1}$. Draw schematically how the Fermi level will vary with temperature. Include the position of the conduction band and valence band in the diagram and comment on the low temperature and high temperature limits.

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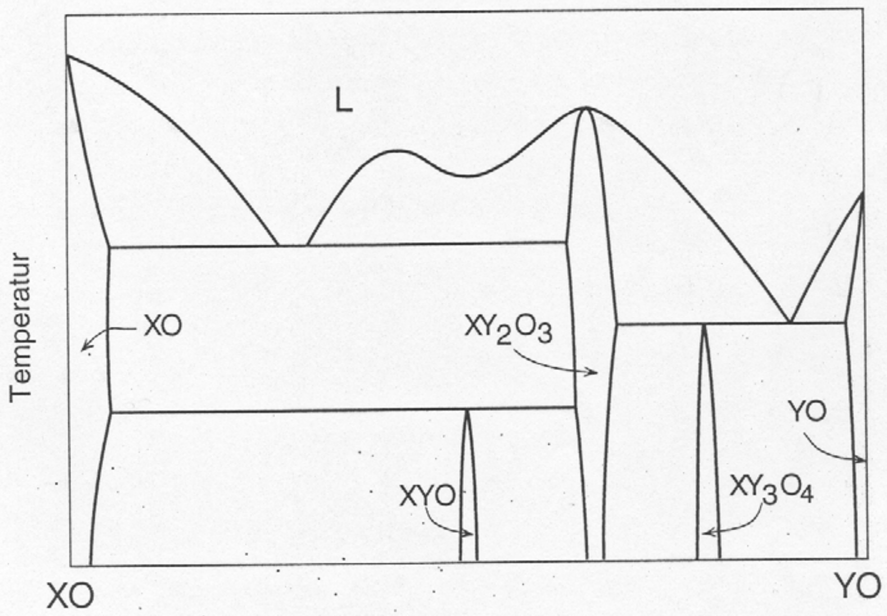
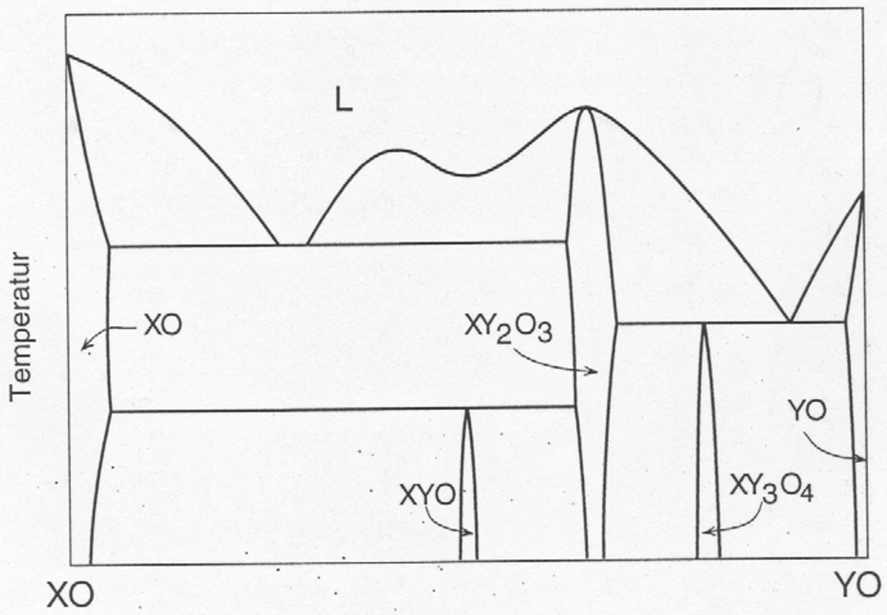


Figur 3: Fasediagram med feil (eller usannsynlige faseforhold).



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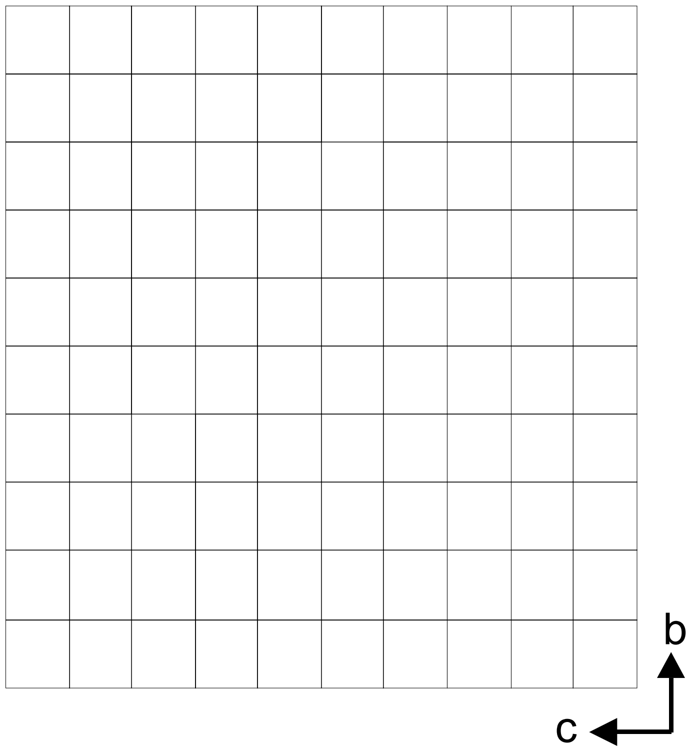

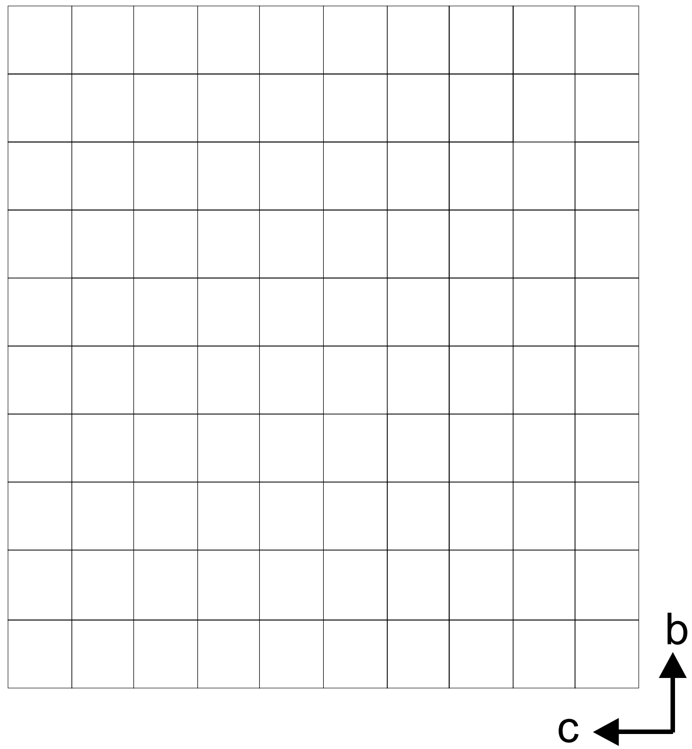

Period	Main groups		Transition metal groups										Main groups					
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
	1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A	8A
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110	111	112						

Lanthanides	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Conversion factors and other relationships

atmosphere (atm): 1(atm) = 101.325 kPa

electron volt (eV): 1(eV) = 96.485 kJ mol^{-1}

(eV) × 1.60218 × 10^{-19} ⟶ (J)

(J) × 6.24150 × 10^{18} ⟶ (eV)

atomic mass unit (u): 1(u) = 9.31494 × 10^{8} eV

electron mass = 5.48580 × 10^{-4} u

neutron mass = 1.00866 u

proton mass = 1.00728 u

calorie (cal): 1(cal) = 4.184 J

RT = 2.4790 kJ mol^{-1}

RT/F = 25.693 mV

hc = 1.98645 × 10^{-25} J m

Constants

Quantity	Symbol	Value	Units
atomic mass unit	$u = m[^{12}C]/12$	1.66054 × 10^{-27}	kg
Avogadro constant	N_A	6.02214 × 10^{23}	mol^{-1}
Bohr magneton	$\mu_B = eh/4\pi m_e$	9.27402 × 10^{-24}	J T^{-1}
Bohr radius	$a_0 = \varepsilon_0 h^2/\pi m_e e^2$	5.29177 × 10^{-11}	m
Boltzmann constant	k	1.38066 × 10^{-23}	J K^{-1}
elementary charge	e	1.60218 × 10^{-19}	C
electron mass	m_e	9.10939 × 10^{-31}	kg
Faraday constant	$F = N_A e$	9.6485 × 10^{4}	C mol^{-1}
gas constant	$R = N_A k$	8.31451	J K^{-1} mol^{-1}
neutron mass	m_n	1.67493 × 10^{-27}	kg
Planck constant	h	6.62608 × 10^{-34}	J s
	$\hbar = h/2\pi$	1.05457 × 10^{-34}	J s
proton mass	m_p	1.67262 × 10^{-27}	kg
Standard acceleration due to gravity	g	9.80665	m s^{-2}
vacuum permeability	μ_0	4π × 10^{-7}	H m^{-1}
vacuum permittivity	ε_0	8.85419 × 10^{-12}	F m^{-1}
velocity of light	c	2.99792 × 10^{8}	m s^{-1}