UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Midterm exam: MEF 3000 / MEF 4000 – Functional materials
Day/time/place: Tuesday 10. October, kl. 13.30 – 14.30,
Gymsal 4 Idrettsbygget
Duration: 1 hour
The set of tasks is on: 3 pages (3 tasks)
Appendix: None
Allowed aids: Calculator
Language: English

Candidate number:

Note:
Fill in the candidate number on page 1 and controll that the task set is complete before you answer the questions.

Useful constants:

Avogadros number: $N_A = 6.022 \times 10^{23}$
Atomic mass for Po = 209 u $\rightarrow$ 209 g·mol^{-1}
Volume of a sphere with radi r is given by the formula: $V = (4/3)\ \pi\ r^3$
$\pi \approx 3.1416$

Task 1 (50%)

Polonium metal (Po) forms among others crystals that adopt the spacegroup Pm-3m.

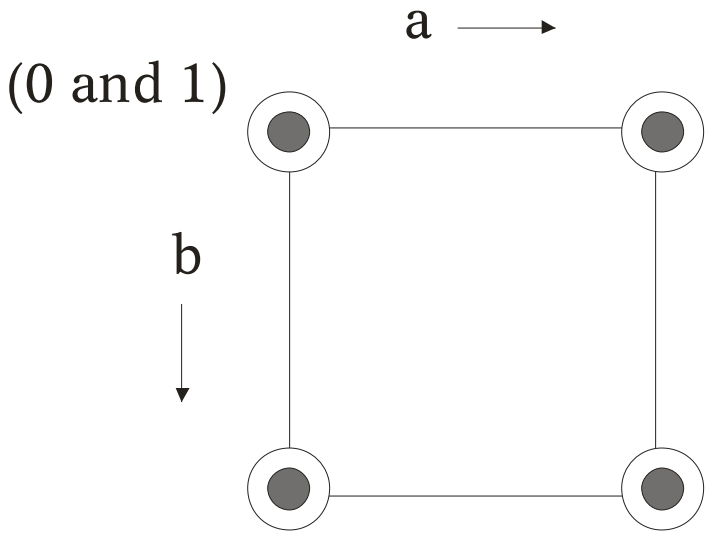
For this crystal structure, the following are given:

Spacegroup: Pm-3m,
Unitcell. a = b = c = 3.359 Å, $\alpha = \beta = \gamma = 90°$
Po in 1 (a) position with x = 0, y = 0, z = 0.

a) Explain the symbols in the spacegroup Pm-3m.

P = Primitive Bravais lattice
m = mirrorplane
-3 = threefold rotoinversonaxis

b) How many formula units are there in the cell? 1
c) Sketch the unit cell in the a-b plane.



(remember to note the axes and the height of the atoms)

d) What is the radius of a Po atom? r = a/2 = 1.680
e) Calculate the x-ray density for Po.
X-ray density is the same as the physical density of the material calculated with basis in the weight and volume of one unitcell = $1*209*10^{-3}$ kg/mol / $((3.359*10^{-10}m)^3 * 6.022*10^{23})$ = 9157470 kg/m^3 = 9.16 g/ml
f) What type of sphere packing is this? Primitive cubic
g) What is the coordination for Po? 6
h) What is the density of packing for this type of sphere packing?
Packing density is occupied volume divided by total volume =
$1*4/3*\pi*(1.608Å)^3/(3.359^3Å)$ = 46%
i) What type of structure do you obtain if a new Po atom is inserted into the position (½, ½, ½)? Body centered cubic, bcc
j) What type of structure do you obtain if a different type of atom is inserted into the position (½, ½, ½)? CsCl-type

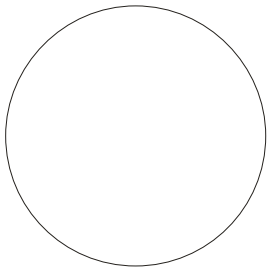
Task 2 (25%)

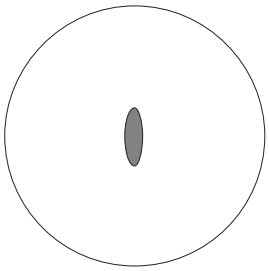
a) Give the point group symbol for the stereographic projections below.
Chose from the list: 1, 2, 2/m, mmm, 222, 3, 4/mmm, 6mm, 6/mmm,

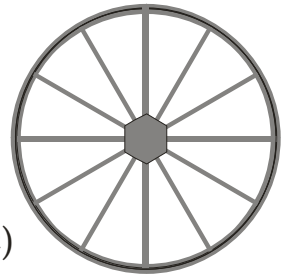
a = 1, b = 2, c = 6/mmm, d = mmm, e = 4/mmm, f = 3, g = 222, h = 2/m, j = 6mm

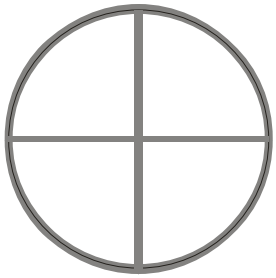
b) Tell which of the point groups in the list that are centrosymetric.

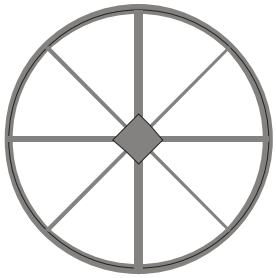
6/mmm, mmm, 4/mmm, 2/m

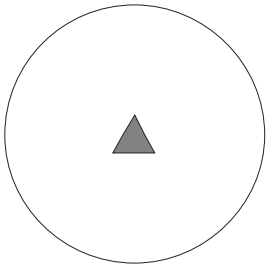
a) 

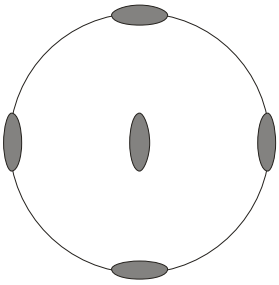
b) 

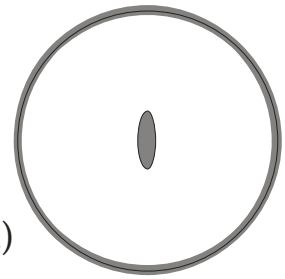
c) 

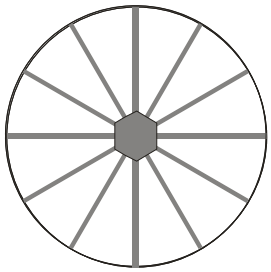
d) 

e) 

f) 

g) 

h) 

i) 

Task 3 (25%)

a) What type of holes exists in a cubic close packed structure, and how many holes are there pr. packing sphere.

1 octahedra hole pr packing sphere
2 tetrahedra holes pr packing sphere

b) What type of holes exists in a hexagonal close packed structure, and how many holes are there pr. packing sphere.

1 octahedra hole pr packing sphere
2 tetrahedra holes pr packing sphere
1 trigonal bipyramidal hole pr packing sphere

c) Name the different structure types for the different cases of hole fillings below. Chose names from the list: NaCl, NiAs, Cu, Mg, CaF_2, ZnS (blende), ZnS (würtsitt), $MgAl_2O_4$

Number	**Basis structure**	**Filling degree for octaedra holes**	**Filling degree for octaedra holes**	
1)	hcp	0	0	Mg
2)	hcp	1	0	NiAs
3)	hcp	0	½	ZnS (würtsitt)
4)	ccp/fcc	0	0	Cu
5)	ccp/fcc	1	0	NaCl
6)	ccp/fcc	0	½	ZnS (blende)
7)	ccp/fcc	0	1	CaF_2
8)	ccp/fcc	½	¼	$MgAl_2O_4$