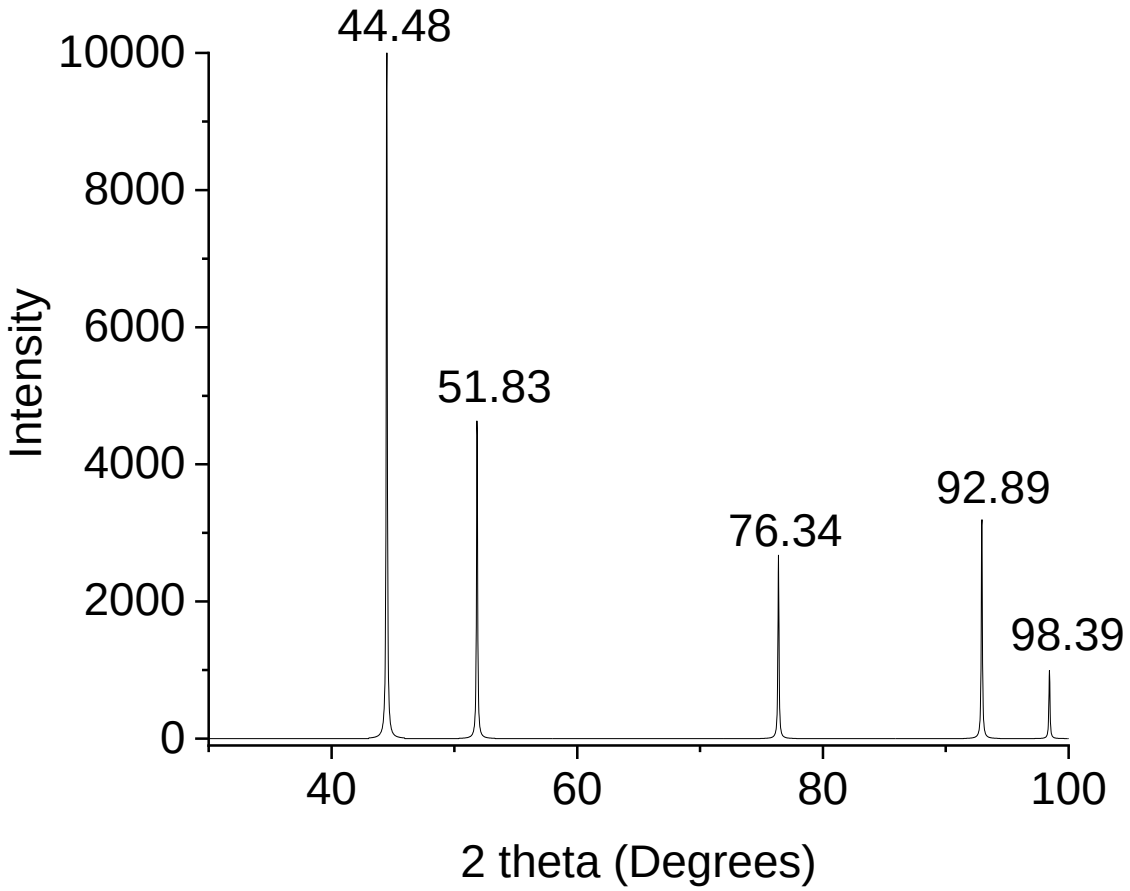
1. **Accumulate 100 points (out of 140).**

2. **If you submit more than 100 points, the grade will be calculated as a ration between “applied” and “earned”.**

Submission date: 18/05/2021

Q1(20 points)

From the following XRD pattern (λ=1.54 Å) of element in a cubic structure, please determine the crystal structure (SC, BCC, FCC or Diamond) of the element and calculate its lattice parameter.



Q2 (20 points)

a) Calculate the Madelung energy of two ionic crystals, PbS and CeO_2, using Haber-Born cycle (the relevant values can be found in the lecture).

b) Estimate the fractional ionic character of the bonds in each of the above materials from the Madelung energies.

c) Compare the fractional ionic character of the bonds you got to the one calculated from electronegativity. What it is tell you about the electronegativity?

Material	Gibbs energy of formation, KJ/mol
PbS	- 98.7
CeO_2	-1024.6

Madelung Constants

Crystal Structure	Madelung Constant
Cesium chloride	1.763
Fluorite	2.519
Rock salt	1.748
Sphalerite	1.638
Wurtzite	1.641

Q3 (20 points)

Estimate the enthalpy of vacancy formation for Ni, Mg and Mo and explain the results

Q4 (20 points)

Consider a crystal of sylvinite (NaCl)(KCl) (usually nice pinkish crystals). Canadian sylvinite is ≈25 mol% of KCl and it is a random alloy. Please calculate the lattice parameter of Canadian sylvinite.

Q5 (20 points)

a) Determine if the following dislocations are edge dislocation, screw dislocation or mixed dislocation (edge and screw together). Calculate for each dislocation the slip plane (the plane that contain both Burgers, $\vec{b}$, vector and Line vector, $\vec{t}$).

I) $b_1 = a/2[001]$ $t_1 = [010]$

II) $b_2 = a/2[011]$ $t_2 = [011]$

III) $b_1 = a/2[100]$ $t_1 = [122]$

Q6 (20 points)

For an unknown metal the following data have been obtained: density ρ =2.7 g/cm^3 structure =FCC; d(101)=2.86 x10^{-10} m. (d(101) is the spacing between (101) planes in the crystal lattice). What is the atomic weight of this metal?

Q7 (20 points)

Calculate the lattice parameter and the crystallographic density of Li_2O (the relevant values can be found in the lecture).