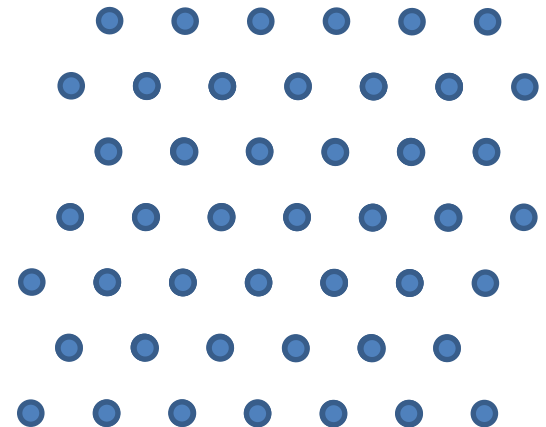
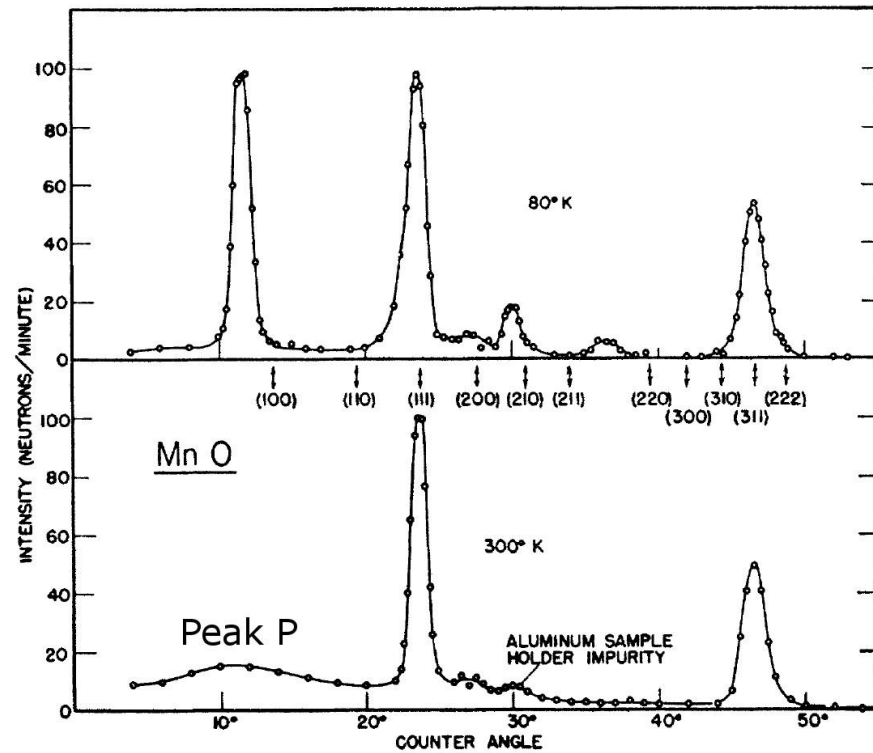


Exercise Chapter 1 and 2:

- 1) You want to study the structure of a crystal and use for that purpose x-rays, electrons, and neutrons. What is the Energy of the particles, if you want to have a wavelength of $\lambda = 1 \text{ \AA}$.
- 2) The right figure shows the 2-dimensional plane of a 3-dimensional crystal.
 - Please indicate in the figure a primitive unit cell!
 - Please indicate the conventional unit cell !
 - please indicate in the figure the Wigner-Seitz cell !
 - What is the definition of the Wigner-Seitz cell ?
 - Which 3-dimensional crystal has a 2-dimensional plane with an hexagonal arrangement of atoms ?





3) The left Fig. shows data from neutron scattering experiments on MnO. MnO grows as a fcc crystal with three equal sides and a two atomic base. 左圖是MnO的中子散射實驗。MnO是兩種原子基底的三等邊面心立方晶體

Starting with the room temperature data, two peaks (at 23.6 and 46.5 degree) representing scattering at the 111 and 311 plane are identified. The neutron wavelength is $\lambda = 0.205$ nm. 從室溫的資料開始，在23.6度和46.5度的兩個峰值，代表111表面和311表面的散射。

a) calculate the plane separation d_{111} . 計算面間距 d_{111} .

b) prepare a sketch to schematically illustrate the 111 and 311 plane in a fcc structure.

請用圖表示面心立方結構的111和311晶面

c) calculate the size 'a' of the conventional unit cell!
計算 conventional unit cell 'a' 值長度

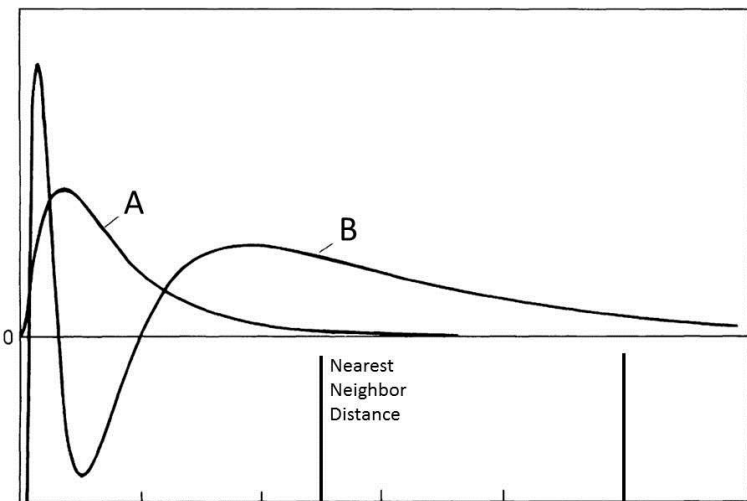
e) why do we not find for all crystal planes a scattering peak ? 為什麼我們沒有找到所有的晶面的散射峰值？

f) X-Ray data for the same system do not show a change in the crystal structure at different temperatures. Which physical properties can be studied by neutron scattering but not by x-ray scattering: 同樣系統的X-Ray 晶體結構散射資料在不同溫度下並沒有改變。那些物理性質是中子散射可以探測但是X-ray 散射做不到的嗎？

g) at 80 K a new peak appears in the neutron data at 11.2 degree. What do you think is the origin of this peak ? Can you give a physical interpretation ? 80K時 中子散射資料 12度出現了一個新的峰值，你覺得這個峰值的來源是什麼？請給出一個物理的解釋？

h) for room temperature data, a very broad and weak peak can also be observed at the same energy. Based on the result of f) – can you make a suggestion for the weak and broad peak ?

室溫下的資料，可以在同樣能量下看見一個比較寬和小的峰值，從f)所提到的結果來看，你可以解釋這個峰值的產生嗎？



4a) What are the 5 mechanisms of bonding in condensed matter systems (atoms, molecules, crystals)? 請問在凝態系統(原子、分子、晶體)裡有五種鍵結方法分別為哪些?

1:
3:
5:

2:
4:

4b) The graph shows the electron wave function versus distance from the atomic center for two cases (A,B). 下圖分別為兩種不同情形 (A,B) 鍵結電子的波函數與距離的關係，原點為原子中心。

Which kind of bonding do you expect for case (A) and (B) in a crystal? 請問你期待在晶體結構裡，(A,B)分別為哪種鍵結?

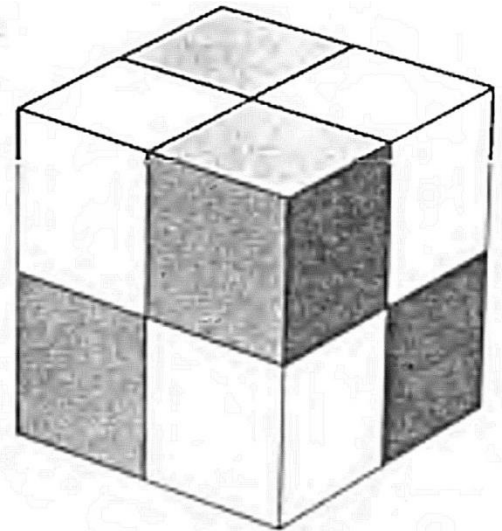
(A)

(B)

5a) Which symmetry operations exist? 請問對稱系統有哪些?

1:
2:
3:
4:

5b) Please indicate for the square on the left all symmetry operations (axes and planes)! 請指出左圖的全部的對稱性 (包含軸與平面)



6) You have a crystal and the following translational vectors:

$$\mathbf{T}_1 = \begin{pmatrix} a \\ -a \\ a \end{pmatrix} \quad \mathbf{T}_2 = \begin{pmatrix} a \\ a \\ -a \end{pmatrix} \quad \mathbf{T}_3 = \begin{pmatrix} -a \\ a \\ a \end{pmatrix}$$

Calculate the Reciprocal Lattice Vectors: $\mathbf{T}_1^*$, $\mathbf{T}_2^*$, $\mathbf{T}_3^*$