

# Introduction to Solid State Physics

## Problems N°1

### **Ex1: Atomic planes and Miller indices**

Bravais lattice of Lithium is a centered cubic of cell parameter  $a = 3.48 \text{ \AA}$

1. Assuming that the atoms are in contact along the rows  $[111]$ , represent the distribution of these atoms following the crystallographic orientations  $(100)$ ,  $(110)$ ,  $(111)$ , and  $(201)$ .
2. For each of the 2D representations, specify the direction and modulus of the basis vectors  $\vec{a}_1$  and  $\vec{a}_2$  of the primary unit cell, and the value of the angle  $\gamma$ .
3. Give the numerical value of the atomic concentration and the mass density of the lithium.

### **Ex2: Properties of the reciprocal lattice**

1. Show that all vectors of the reciprocal lattice  $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$  is orthogonal to the planes of Miller indices  $(h, k, l)$  within the direct lattice.
2. Show that the distance  $d_{hkl}$  between two consecutive planes  $(h, k, l)$  is proportional to the inverse of  $\|\vec{G}\|$ .
3. Deduce the expression of  $d_{hkl}$  for simple cubic and orthorhombic systems ( $a \neq b \neq c$ ,  $\alpha = \beta = \gamma = \frac{\pi}{2}$ ).

### **Ex3: Angle between reticular planes**

In a cubic lattice, give the expression of the angle  $\Phi$  between planes  $(h_1, k_1, l_1)$  and  $(h_2, k_2, l_2)$ . Check this result with  $(100)$  and  $(110)$ .

### **Ex4: 2D Bravais lattice**

Graphite is a lamellar crystal in which the carbon atoms are distributed to the tops of regular hexagons (of side  $d$ ) that fit into one another in each layer to form a honeycomb structure.

1. Characterize this structure by its Bravais lattice and motif.
2. Graph the corresponding reciprocal lattice and plot the first Brillouin zone.

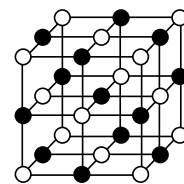
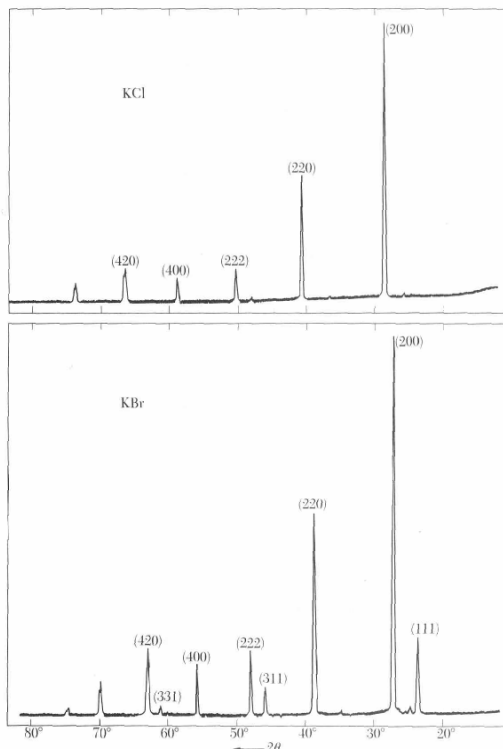
3. Give the literal expression of the structure factor  $F(h, k)$  and specify the different values taken by this factor.

**Ex5: Structure factor**

1. Give the expression of the structure factor for the following crystal modes: centered cubic (cc), face centered cubic (fcc), and simple cubic (sc).
2. Indicate for each case the planes of indices (h k l) that do not give rise to the presence of diffraction peaks. The table on the following page may be completed.

Indices (hkl)	Simple cubic (sc)	Centered cubic (cc)	Face centered cubic (fcc)
100			
110			
111			
200			
210			
211			
220			
221 et 300			
310			
311			
222			
320			
321			
400			
410 et 322			
411 et 330			
331			
420			
421			
332			
422			

**Ex6:** How to explain the difference in X-Rays diffraction pattern between KCl and KBr. Could you propose an interpretation of this experimental result if both KCl and KBr exhibit a “Sodium Chloride” type of arrangement?



Sodium chloride structure

**Ex7: Lennard-Jones potential**

The attractive part of the potential energy between two noble gas atoms (van der Waals interactions), at a distance  $r$ , is represented by a  $A/r^6$  term whereas repulsive part due to overlap of electronic orbitals is of type  $B/r^{12}$ . The Lennard-Jones potential energy model is usually expressed as:

$$U(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

1. Write A and B as a function of  $\epsilon$  and  $\sigma$ .
2. Give the distance  $r_{eq}$  separating two atoms at equilibrium as a function of  $\sigma$ , and conclude on the physical meaning of parameters  $\epsilon$  and  $\sigma$ .

The Bravais lattice of noble gas crystals is centered cubic and the cell parameters are respectively:  $a = 4,46 \text{ \AA}$  (Ne) ;  $a = 5.31 \text{ \AA}$  (Ar) ;  $a = 5.64 \text{ \AA}$  (Kr) ;  $a = 6.13 \text{ \AA}$  (Xe) . Furthermore, cohesive energies of these noble gas crystals are respectively: 20 meV/atom (Ne), 80 meV/atom (Ar), 116 meV/atom (Kr), 170 meV/atom (Xe).

3. Deduce the numerical values of  $\epsilon$  and  $\sigma$  for each element.