

Phys 771

Condensed Matter Physics

Problem Set # 3

Dr. Gassem Alzoubi

The Hashemite University Department of Physics, Zarqa, Jordan

1. Marder 3.1
2. (a) Show that the volume of the reciprocal lattice primitive cell is given by $V_R = (2\pi)^3/V_c$, where V_c is the volume of a primitive cell of the direct lattice
 (b) Show that the reciprocal lattice vector \vec{G}_{hkl} is perpendicular to direct lattice plane (hkl)
 (c) Determine the Miller indices for the planes A and B shown in **Figure 1**

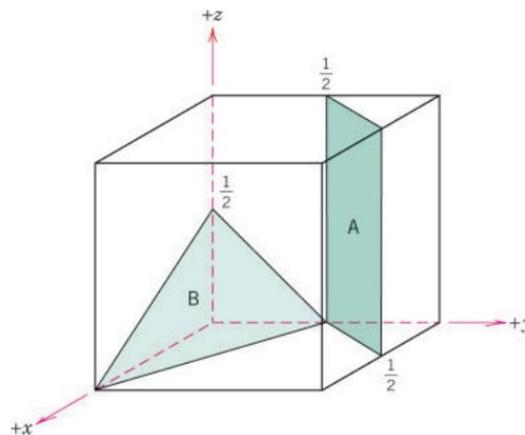
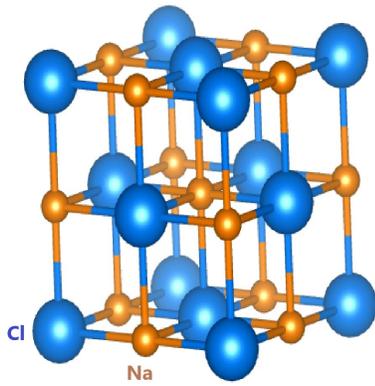


Figure 1:

3. Consider the two planes $x + y = 1$ and $x - y = 0$
 - (a) Plot the two planes, write down the Miller indices and the normal vector for each plane (Hint: to visualize the two planes, use <https://technology.cpm.org/general/3dgraph/>)
 - (b) Find the angle between the two planes
 - (c) Find parametric equations for the line of intersection between the two planes (Hint: to check your answer use <https://www.geogebra.org/m/sSfqfEuz>)
4. Marder 3.2
5. Marder 3.3



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Title      NaCl
Lattice type  F
Space group name  F m -3 m
Space group number  225
Setting number  1
Lattice parameters

a  b  c  alpha  beta  gamma
5.62000  5.62000  5.62000  90.0000  90.0000  90.0000

Unit-cell volume = 177.504317 Å^3
Structure parameters

      x  y  z  Occ.  U  Site  Sym.
1 Cl  Cl1  0.00000  0.00000  0.00000  1.000  0.000  4a  m-3m
2 Na  Na1  0.50000  0.50000  0.50000  1.000  0.000  4b  m-3m
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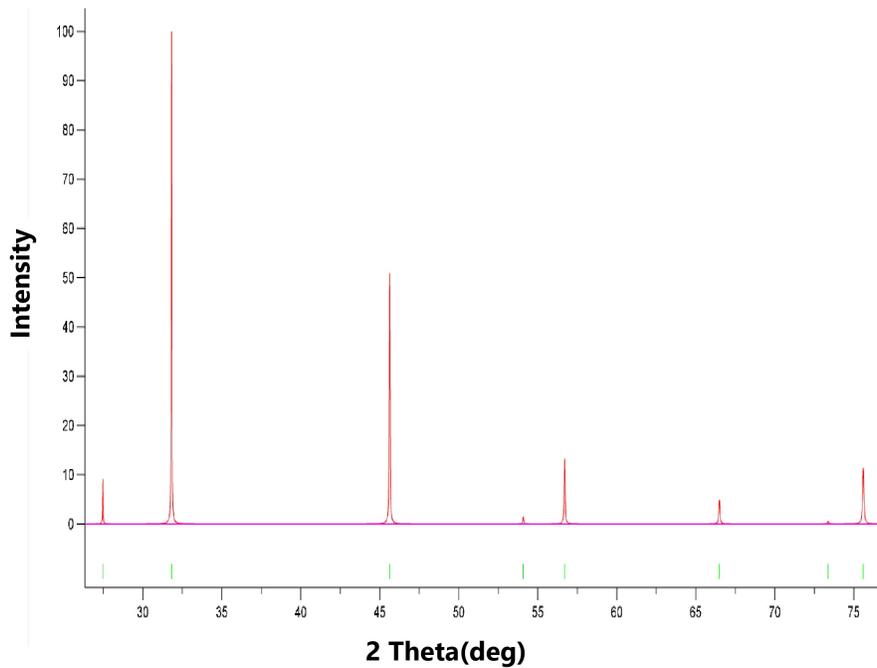


Figure 2:

6. **Figure 2** shows the NaCl unit cell, along with some structural details and a simulated XRD pattern generated by the VESTA software. Calculate the structure and modulation factors of the NaCl lattice, assuming it is an fcc with 4 Na^+ and 4 Cl^- ions per unit cell. Based on your structural factor finding, index all peaks shown in the XRD simulated spectrum.
7. Write a simple code to generate figure 3.3 in textbook for the case $N=30$. For simplicity take the lattice constant $a = 1$