PHY 481/581 - QUIZ 4

Name: Solutions

Date: 11/05/2018

1 Ordering in solids, reciprocal lattices, and wave scattering

Problem 1. Given the NaCl crystal shown in Fig. 1 below, determine the distance from a sodium atom to the nearest chlorine atom, assuming the lattice constant is a. Do the same for the nearest sodium atom.

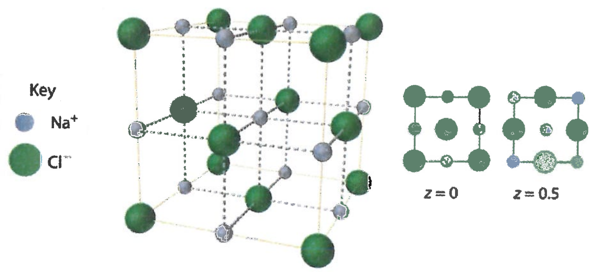

Figure 1: NaCl crystal structure.

Problem 2. Given a direct lattice vector $\vec{R}$, write down the single mathematical equation sufficient and necessary to prove $\vec{G}$ is a reciprocal lattice vector. Assuming $\vec{G}$ is a reciprocal lattice vector, determine the (real-space) spacing, d, between adjacent planes in a family of lattice planes.

Problem 3. Show that the reciprocal lattice of a face-centered cubic lattice is a body-centered cubic lattice, and determine the lattice constant. Recall the reciprocal lattice vector, $\vec{b}_1$, is related to direct lattice vectors $\vec{a}_2$ and $\vec{a}_3$ by

$$\vec{b}_1 = \frac{2\pi \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \tag{1}$$

with similar relations for the other two reciprocal lattice vectors.

Problem 4. From the table below, determine the entries of the empty column $\{\text{hkl}\}$. What kind of cubic crystal is this? See table of selection rules on page 2, if necessary.

2θ	$N = h^2 + k^2 + l^2$	$\{\text{hkl}\}$
22.7°	3	
26.3°	4	
37.7°	8	
44.3°	11	
46.2°	12	

Table 1: Results from a powder diffraction experiment using X-rays.

(1) Na → Cl distance $= a/2$

Na → Na distance $= a\sqrt{2}/2$

(2) $e^{i\vec{G}\cdot\vec{R}} = 1$ if & only if $\vec{G}$ is a reciprocal lattice vector

- distance between planes

$$d = \frac{2\pi}{|\vec{G}|}$$

(3) For the FCC

$$\vec{a}_1 = \tfrac{1}{2}a(\hat{y}+\hat{z}) \qquad \vec{b}_1 = \tfrac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$$

$$\vec{a}_2 = \tfrac{1}{2}a(\hat{x}+\hat{z}) \qquad \vec{b}_2 = \tfrac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$$

$$\vec{a}_3 = \tfrac{1}{2}a(\hat{x}+\hat{y}) \qquad \vec{b}_3 = \tfrac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$$

BCC with lattice const. $4\pi/a$

(4)

2θ	$N = h^2 + k^2 + l^2$	$\{hkl\}$
$22.7°$	3	1 1 1
$26.3°$	4	2 0 0
$37.7°$	8	2 2 0
$44.3°$	11	3 1 1
$46.2°$	12	2 2 2

- this is an FCC crystal

Bonus $\rho(r) = \sum_n \delta(r - an)$

- take the Fourier transform

$$\mathcal{F}[\rho(r)] = \int dr\, e^{ikr} \rho(r) = \sum_n \int dr\, e^{ikr} \delta(r-an)$$

$$= \sum_n e^{ikan}$$

$$= \frac{2\pi}{|a|} \sum_m \delta(k - 2\pi m/a)$$