Solution

First Exam Physics 555
Introduction to Solid State Physics
You may use your textbook, calculator and ruler during the exam

Name: Zhiling Dun SSN: , Feb-1-2013, 1:25 PM till 2:15 PM

Note: Show all steps and identify all symbols that you use. Write in ink on both sides of this paper and extra papers if necessary. You can choose any two of the three problems. However, if you do all three, you will obtain extra credit that will be counted into your total grade (compensate for future lower exam grades).

1. Consider a lattice for which the primitive cell vectors ***a***, ***b***, and ***c*** have different lengths and for which the cell angles are not 90 degrees. Consider two successive (*hkl*) planes, which are a distance *d* apart. If we denote a unit vector in the direction perpendicular to an (*hkl*) plane as **n**, show without resorting to a reciprocal lattice formulation that

$$d = \frac{\vec{a}\cdot\hat{n}}{h} = \frac{\vec{b}\cdot\hat{n}}{k} = \frac{\vec{c}\cdot\hat{n}}{l} \quad \text{(15 points)}$$

$\vec{b}_1 = 2\pi\frac{\vec{b}\times\vec{c}}{\vec{a}\times\vec{b}\cdot\vec{c}}$

$\vec{b}_2 = 2\pi\frac{\vec{c}\times\vec{a}}{\vec{a}\times\vec{b}\cdot\vec{c}}$

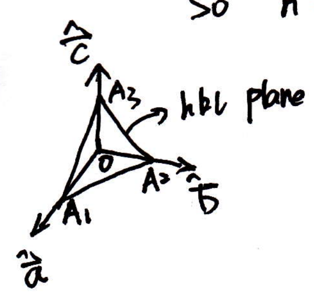
$\vec{b}_3 = 2\pi\frac{\vec{a}\times\vec{b}}{\vec{a}\times\vec{b}\cdot\vec{c}}$

$\vec{b}_1 \cdot \vec{b}_2\ \vec{b}_3$ are recepical lattice vector

Demonstrating that this produces $d = a/\sqrt{h^2+k^2+l^2}$ for a cubic lattice in which $|a|=|b|=|c|$ and $\vec{a}\cdot\vec{b} = \vec{a}\cdot\vec{c} = \vec{b}\cdot\vec{c} = 0$. (15 points)

a) the vector $\vec{G}$ that is perpendicular to (hkl) is $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

So $\hat{n} = t(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)$ where $t = \frac{1}{|\vec{G}|}$ $\left(\hat{n} = \frac{\vec{G}}{|\vec{G}|}\right)$



$\vec{a} = h\vec{OA_1}$

$\vec{b} = k\vec{OA_2}$

$\vec{c} = l\vec{OA_3}$

in solid geometry, if $\hat{n}$ is the unit vector perpendicular to plane $A_1A_2A_3$, then the distance from o to $A_1A_2A_3$ is $\vec{OA_1}\cdot\hat{n}$ $(= \vec{OA_2}\cdot\hat{n} = \vec{OA_3}\cdot\hat{n})$

So
$$\begin{aligned} d &= \vec{OA_1}\cdot\hat{n} = \frac{\vec{a}}{h}\cdot\hat{n} \\ &= \vec{OA_2}\cdot\hat{n} = \frac{\vec{b}\cdot\hat{n}}{k} \\ &= \vec{OA_3}\cdot\hat{n} = \frac{\vec{c}\cdot\hat{n}}{l} \end{aligned}$$

b) $|\vec{G}| = \sqrt{\vec{G}\cdot\vec{G}} = \sqrt{(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)}$

$\because \vec{a}\cdot\vec{b} = \vec{a}\cdot\vec{c} = \vec{b}\cdot\vec{c} = 0$ $\therefore \vec{b}_1\cdot\vec{b}_2 = \vec{b}_2\cdot\vec{b}_3 = \vec{b}_3\cdot\vec{b}_1 = 0$ $|b_1| = |b_2| = |b_3| = \frac{2\pi}{a}$

$|\vec{a}| = |\vec{b}| = |\vec{c}|$

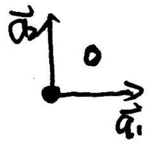
$\therefore |\vec{G}| = \sqrt{h^2+k^2+l^2}\cdot\frac{2\pi}{a}$

$$d = \frac{\vec{a}\cdot\hat{n}}{h} = \frac{\vec{a}\cdot(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)}{h\cdot\frac{2\pi}{a}\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{k^2+h^2+l^2}}$$

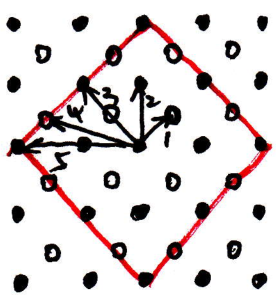
2.

Madelung constant (30 points).

Consider a hypothetical, two-dimensional square lattice consisting of an equal amount of positive and negative ions. Arrange the ions such that the Madelung energy is maximum. Find the Madelung constant by considering pair interactions up to the fifth nearest neighbor (Note that the series has not yet converged).

unit cell 

two atoms per unit cell $\quad |\vec{a}_1| = |\vec{a}_2| = R$



	1st	2nd	3rd	4th	5th
# of atom	4	4	4	8	4
distance	$\frac{\sqrt{2}}{2}R$	R	$\sqrt{2}R$	$\frac{\sqrt{10}}{2}R$	2
Charge	−	+	+	−	+

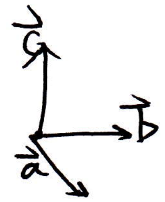
$$U = e^2\left(-\frac{4}{\frac{\sqrt{2}}{2}R} + \frac{4}{R} + \frac{4}{\sqrt{2}R} - \frac{8}{\sqrt{10}/2 \cdot R} + \frac{4}{2R}\right)$$

$$= -\frac{e^2}{R}\left(+\frac{8}{\sqrt{2}} - 4 - \frac{4}{\sqrt{2}} + \frac{16}{\sqrt{10}} - 2\right)$$

$$= -1.89\frac{e^2}{R}$$

$$\therefore \ \alpha = 1.89$$

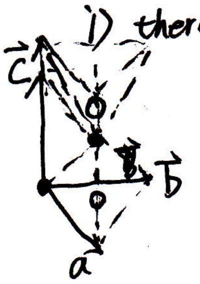
$|\vec{a}| = |\vec{b}|$ $\frac{|\vec{C}|}{|\vec{a}|} = \sqrt{\frac{8}{3}}$



3.

CrTe is a binary compound consisting of a 1:1 ratio of Chromium (Cr) and Tellurium (Te) atoms. The CrTe structure can be viewed as an hexagonal close-packed arrangement of Te atoms with the much smaller Cr atoms filling the octahedral holes. Let's talk about X-ray diffraction:

i) Find the structure factor for CrTe.
ii) What can you say about the intensity of the (001) reflection?
iii) Find a (*hkl*) reflection for which the Cr and Te atoms scatter in phase.
iv) What is the difference between the CrTe structure and the NaCl structure?
v) Suppose we have $Cr^{2+}Te^{2-}$. Can you give a hand waving argument why the NaCl structure would be a more favorable arrangement for the Cr^{2+} and Te^{2-} ions (from an electrostatic point of view) ?



i) there are 4 atoms per unit cell

Cr at $(\frac{1}{3}, \frac{2}{3}, \frac{1}{8})$ $(\frac{1}{3}, \frac{2}{3}, \frac{7}{8})$

Te at $(0, 0, 0)$ $(\frac{1}{3}, \frac{2}{3}, \frac{1}{2})$

$$F = \sum_j f_i \exp(i\, \vec{G} \cdot \vec{r}_i)$$

With $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

$$F = f_1 + f_1 e^{2\pi i(\frac{h}{3} + \frac{2}{3}k + \frac{1}{2}l)} + f_2 e^{2\pi i(\frac{h}{3} + \frac{2}{3}k + \frac{1}{8}l)} + f_2 e^{2\pi i(\frac{h}{3} + \frac{2}{3}k + \frac{7}{8}l)}$$

ii) for (001) $G = \vec{b}_3$ $h=k=0$ $l=1$

$$F = f_1 + f_1 e^{\pi i} + f_2 e^{i\frac{\pi}{4}} + f_2 e^{i\frac{7}{4}\pi} = f_1 - f_1 + 2f_2 \cos\frac{\pi}{4} = \sqrt{2} f_2$$

$\therefore I = |F|^2 = 2f_2^2$

iii) for example: (008) plane

$F(hkl) = F(008) = 2(f_1 + f_2)$ in phase

iv)	NaCl	CrTe
type	cubic	hexagonal
# per cell	2 atom/cell	4 atom/cell
nearest neighbor	$\frac{\sqrt{2}}{2}R$	$\frac{\sqrt{3}}{3}R$

v) If we calculate Modelung constant we will find that α in Nacl structure is larger than that of hexagonal structure.

That means Nacl structure has a smaller energy, more stable.