Physics 140A Winter 2011

Homework 4 due Wednesday February 2

1. Using the Lennard-Jones potential, show that the ratio of the cohesive energies of neon in the bcc and fcc stuctures is 0.956. The lattice sums for the bcc structure are:

$$\sum_j{}' p_{ij}^{-12} = 9.11418 \tag{1}$$

and

$$\sum_j{}' p_{ij}^{-6} = 12.2533. \tag{2}$$

Based on your result, what structure do you expect solid neon to assume?

2. Consider a line of $2N$ atoms of alternating charge $\pm q$ with a repulsive potential energy A/R^n between nearest neighbors.

(a) Show that at the equilibrium separation:

$$U(R_0) = -\frac{2Nq^2 \ln 2}{R_0}(1 - \frac{1}{n}). \tag{3}$$

(b) Let the crystal be compressed so that $R_0 \to R_0(1-\delta)$. Show that the work done in compressing the crystal has the leading term $\frac{1}{2}C\delta^2$, where:

$$C = \frac{(n-1)q^2 \ln 2}{R_0}. \tag{4}$$

Note that you should not expect to obtain this result from the expression for $U(R_0)$, but must use the complete expression for $U(R)$.

3. A common way to measure crystal structures is to use powder x-ray diffraction, in which a powder of an unknown sample is exposed to a beam of x-rays, and the reflections are recorded as a function of scattering angle. (See Figure below). Powder samples of three different monatomic cubic crystals are analyzed in this fashion. It is know that one sample is fcc, one is bcc, and the other has the diamond stucture. The approximate position of the first four reflections are:

A	B	C
$\phi = 42.2°$	28.8°	42.8°
49.2°	41.0°	73.2°
72.0°	50.8°	89.0°
87.3°	59.6°	115.0°

(a) Identify the crystal structure of A, B, and C.

(b) If the wavelength of the incident X-ray beam is 1.5Å, what is the length of the side of the conventional cubic cell in each case?

HW 4 Solutions.

Note Title 1/29/2010

(1) cohesive energy $U = 2N\epsilon\left[\underbrace{\left(\sum_j{}' p_{ij}^{-12}\right)}_{\equiv S_1}\left(\frac{\sigma}{R}\right)^{12} - \underbrace{\left(\sum_j{}' p_{ij}^{-6}\right)}_{\equiv S_2}\left(\frac{\sigma}{R}\right)^{6}\right]$

25 pts

to find R_{bcc}, R_{fcc}, need to minimize:

$$\frac{dU}{dR} = 2N\epsilon\left[-12S_1\frac{\sigma^{12}}{R^{13}} + 6S_2\frac{\sigma^6}{R^7}\right] = 0$$

$$\Rightarrow \quad 12S_1\left(\frac{\sigma}{R_0}\right)^{12} = 6S_2\left(\frac{\sigma}{R_0}\right)^6$$

$$\frac{2S_1}{S_2} = \left(\frac{R_0}{\sigma}\right)^6$$

$$\Rightarrow \quad \frac{R_0}{\sigma} = \left(\frac{2S_1}{S_2}\right)^{1/6}$$

we then find: $U = 2N\epsilon\left[S_1\left(\frac{S_2}{2S_1}\right)^2 - S_2\left(\frac{S_2}{2S_1}\right)\right]$

$$U_{coh} = 2N\epsilon\left[\frac{S_2^2}{4S_1} - \frac{S_2^2}{2S_1}\right]$$

$$= -N\epsilon\left(\frac{S_2^2}{2S_1}\right)$$

substituting, we find:

	bcc	fcc
S_1	9.11418	12.13188
S_2	12.2533	14.45392
$\frac{U_{coh}}{N\epsilon}$	-8.2368	-8.6102

ratio : $\frac{U_{coh}(bcc)}{U_{coh}(fcc)} = 0.95663$

We expect the fcc structure because this one has the lowest energy. (greatest cohesive energy.)

(2) $- \oplus - \ominus - \underbrace{\oplus - \ominus}_{R} - \oplus - \ominus - \oplus \cdots\cdots$

25 pts

$$U(r_{ij}) = \begin{cases} \frac{A}{R^n} - \frac{q^2}{R} & nn \\ \frac{q^2}{R}\left(\frac{\pm 1}{p_{ij}}\right) & \text{otherwise} \end{cases}$$

$$\Rightarrow \quad U = N\left\{ \frac{A}{R^n} - \frac{q^2}{R} + {\sum_j}' \left(\frac{q^2}{R}\right)\left(\frac{\pm 1}{p_{ij}}\right) \right\}$$

$$= N\left\{ \frac{A}{R^n} - \frac{\alpha q^2}{R} \right\}$$

for the linear chain, $\alpha = 2\ln 2$

at equilibrium, $\dfrac{dU}{dR} = N\left\{ -nAR^{-(n+1)} + \dfrac{2q^2\ln 2}{R^2} \right\} = 0$

$$\Rightarrow \quad \frac{nA}{R_0^{n+1}} = \frac{2q^2\ln 2}{R_0^2}$$

$$\Rightarrow \quad R_0^{n+1-2} = \frac{nA}{2q^2\ln 2} = R_0^{n-1}$$

$$\Rightarrow \quad \frac{1}{R_0^{n-1}} = \frac{2q^2\ln 2}{nA}$$

$$\Rightarrow \quad U_0 = \frac{N}{R_0}\left\{ \frac{A}{R_0^{n-1}} - 2q^2\ln 2 \right\}$$

$$= \frac{N}{R_0}\left(\frac{2q^2\ln 2}{n} - 2q^2\ln 2 \right)$$

$$= \frac{2Nq^2\ln 2}{R_0}\left(\frac{1}{n} - 1\right)$$

or $\boxed{U_0 = \frac{-2Nq^2\ln 2}{R_0}\left(1-\frac{1}{n}\right)}$

(b) work $W = U(R_0(1-\delta)) - U(R_0)$ (because electrostatic forces are conservative)

$$\Rightarrow \quad U = N\left(\frac{A}{R^n} - \frac{2q^2\ln 2}{R}\right)$$

$$W = N\left(\frac{A}{R_0^n(1-\delta)^n} - \frac{2q^2\ln 2}{R_0(1-\delta)} - \frac{A}{R_0^n} + \frac{2q^2\ln 2}{R_0}\right)$$

expanding $(1-\delta)^{-1} = 1+\delta+\delta^2+\cdots$

$$(1-\delta)^{-n} = 1 + n\delta + \frac{n(n+1)}{2}\delta^2 + \cdots$$

but we know that $\frac{A}{R_0^n} = \frac{2q^2\ln 2}{nR_0}$ (see part (a))

so we get

$$W = N\frac{2q^2\ln 2}{nR_0}\left\{\frac{1}{n}\left(1+n\delta+\frac{n(n+1)}{2}\delta^2 - 1\right) + \left(1+\delta+\delta^2-1\right) + \cdots\right\}$$

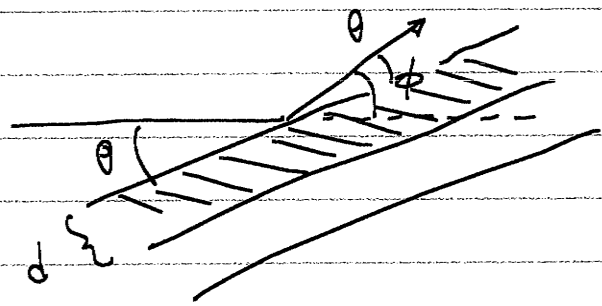
$$\Rightarrow W = N\frac{2q^2\ln 2}{R_0}\left[\delta + \frac{n+1}{2}\delta^2 - \delta - \delta^2 + \dots\right]$$

$$= N\frac{2q^2\ln 2}{R_0}\left[\frac{n-1}{2}\delta^2 + \dots\right]$$

$$= \frac{1}{2}C\delta^2 + \dots$$

where $\boxed{C = \frac{2Nq^2\ln 2}{R_0}(n-1)}$

(3) note that the Bragg angle $\theta = \frac{1}{2}\phi$:



35 pts

and for a sc lattice we have

$$2d\sin\theta = n\lambda \quad (\text{Bragg law})$$

$$\frac{a}{\sqrt{h^2+k^2+l^2}} = d$$

$$\Rightarrow \sqrt{h^2+k^2+l^2} = \frac{a}{d} = \frac{2a\sin\theta}{n\lambda}$$

$$= \left(\frac{2a}{n\lambda}\right) \sin\theta$$

$$\left(\sin\theta = \sin\left(\frac{\phi}{2}\right)\right)$$

note that $\sin^2\theta = \left(\frac{n\lambda}{2a}\right)^2 (h^2+k^2+l^2)$

so...

	A	ratio^2	B	ratio	C	ratio
$\sin\theta =$	0.36	1.0	0.248	1	0.369	1
	0.416	$1.33 = \frac{4}{3}$	0.35	2	0.596	$2.67 = \frac{8}{3}$
	0.588	$2.66 = \frac{8}{3}$	0.43	3	0.701	$3.69 = \frac{11}{3}$
	0.690	$3.67 = \frac{11}{3}$	0.497	4	0.843	$5.34 = \frac{16}{3}$

so to get those ratios, must find h,k,l s.t. $h^2+k^2+l^2 =$ ratio:

A (3 : 4 : 8 : 11)

$1.0 \Rightarrow 1^2+1^2+1^2$ (111)

$\frac{4}{3} \Rightarrow 2^2+0^2+0^2$ (200)

$\frac{8}{3} \Rightarrow 2^2+2^2+0^2$ (220)

$\frac{11}{3} \Rightarrow 3^2+1^2+1^2$ (311)

B $(1:2:3:4)$

$1.0 \Rightarrow 1^2+0^2+0^2 \quad (100)$

$2.0 \Rightarrow 1^2+1^2+0^2 \quad (110)$

$3.0 \Rightarrow 1^2+1^2+1^2 \quad (111)$

$4.0 \Rightarrow 2^2+0^2+0^2 \quad (200)$

C $(3:8:11:16)$

$1.0^2 \Rightarrow 1^2+1^2+1^2 \quad (111)$

$8 \Rightarrow 2^2+2^2+0^2 \quad (220)$

$11 \Rightarrow 3^2+1^2+1^2 \quad (311)$

$16 \Rightarrow 4^2+0^2+0^2 \quad (400)$

rules for bcc: $h+k+l$ = odd $\Rightarrow$ no reflections

$h+k+l$ = even $\Rightarrow$ reflections

fcc: hkl all odd or all even $\Rightarrow$ reflections

otherwise $\Rightarrow$ no reflections

Note that for A; we have either all odd or all even.

$\Rightarrow$ $\boxed{\text{A must be fcc}}$

for B, we could also have the ratio: $2:4:6:8)$

with $hkl = (110) \Rightarrow 2$

$(200) \Rightarrow 4$

$(211) \Rightarrow 6$

$(220) \Rightarrow 8$

so $\boxed{\text{B could be bcc with indices } (110), (200), (211) \text{ \& } (220)}$

(note that $h+k+l =$ even)

now, for C, it must be diamond, but consider the rule:

$\{h+k+l = 4n$ (n integer) & h,k,l all even$\}$ or $\{$all odd$\}$

this is satisfied by the assignments above:

(hkl)	
111	all odd ✓
311	all odd ✓
(220)	all even & $h+k+l=4$ ✓
(400)	all even & $h+k+l=4$ ✓

so $\boxed{\text{C is diamond}}$

(b) if $\lambda = 1.5$ Å, we have for the lowest order reflection in each case:

15 pts

$$\sin^2\theta = \left(\frac{n\lambda}{2a}\right)^2 (h^2+k^2+l^2)$$

so for $n=1$,

$$a = \frac{\lambda}{2\sin\theta}\sqrt{(h^2+k^2+l^2)}$$

$\Rightarrow$ A: $a = \dfrac{1.5\,\text{Å}}{2\sin(\phi/2)}\sqrt{3} = \boxed{3.6\,\text{Å},\ \text{fcc}}$

B: $a = \dfrac{1.5\,\text{Å}}{2\sin(\phi/2)}\sqrt{2} = \boxed{4.26\,\text{Å},\ \text{bcc}}$

C: $a = \dfrac{1.5\,\text{Å}}{2\sin(\phi/2)}\sqrt{3} = \boxed{3.56\,\text{Å},\ \text{diamond}}$