First Principle 2017-Fall Homework 1 Solution

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1. The hcp structure is shown as following :

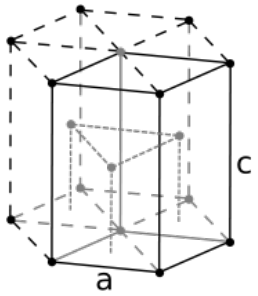

FIG. 1. hcp structure

we can calculate the c/a ratio as :

$$x \equiv \frac{c}{2}$$
$$x = \sqrt{a^2 - (\frac{a}{\sqrt{3}})^2} = a \cdot \sqrt{\frac{2}{3}}$$
$$c/a = 2\sqrt{\frac{2}{3}}_{\#}$$

2. (a) for all $n_i \in$ even with primitive vectors $(2\hat{x}, 2\hat{y}, 2\hat{z})$, the lattice is a simple cubic lattice with side length 2 origin at $(0\hat{x}, 0\hat{y}, 0\hat{z})$

   for all $n_i \in$ odd with primitive vectors $(2\hat{x}, 2\hat{y}, 2\hat{z})$, the lattice is also a simple cubic lattice with side length 2 include point $(0\hat{x}, 0\hat{y}, 0\hat{z})$

   (b) In the case where $\sum_i n_i$ is even, this is a simple cubic lattice with side length $\sqrt{3}$ (which can be thought as a $\sqrt{3}$ scaled + 45^o rotated version of sc.)

3. Let's defined the primitive reciprocal lattice is formed by $\langle G_1, G_2, G_3 \rangle$. Which defined as :

$$G_i \cdot b_j = 2\pi\delta_{ij} \tag{1}$$

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With the known relation:

$$\begin{aligned} b_i &\equiv \frac{2\pi(a_j \times a_k)}{|a_1 \cdot (a_2 \times a_3)|} \\ a_i \cdot b_j &= 2\pi\delta_{ij} \end{aligned} \tag{2}$$

we can see :

$$G_i = a_{i\#} \tag{3}$$

4. The honeycomb lattice is formed by primitive vectors as the same as parallelogram, with basis contain 2-sites. In which the reciprocal vectors also forms parallelogram. Since the Brillouin zone is just the Wigner-Seitz cell in reciprocal space. The Wigner-Seitz cell formed from parallelogram is hexagonal structure.

5. The first Brilluion zone is the Wigner-Seitz cell in k-space. Which we can represent the boundary point (H,N,P) in terms of reciprocal vector $\vec{b_i}$:

$$\vec{k} = \alpha\vec{b_1} + \beta\vec{b_2} + \gamma\vec{b_3} \tag{4}$$

For Brilluion zone in bcc lattice, the reciprocal lattice is fcc structure with reciprocal vectors:

$$\begin{aligned} \vec{b_1} &= \frac{2\pi}{a}(\hat{x} + \hat{z}) \\ \vec{b_2} &= \frac{2\pi}{a}(\hat{y} + \hat{z}) \\ \vec{b_3} &= \frac{2\pi}{a}(\hat{y} + \hat{z}) \end{aligned}$$

The boundary point (H,N,P) thus can be represent in basis of reciprocal vector$\langle\alpha, \beta, \gamma\rangle$:

$$\begin{aligned} H &: \langle -0.5, 0.5, 0.5\rangle \\ N &: \langle 0, 0.5, 0\rangle \\ P &: \langle 0.25, 0.25, 0.25\rangle \end{aligned}$$

For Brilluion zone in fcc lattice, the reciprocal lattice is bcc structure with reciprocal vectors:

$$\begin{aligned} \vec{b_1} &= \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}) \\ \vec{b_2} &= \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z}) \\ \vec{b_3} &= \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}) \end{aligned}$$

The boundary point (X,W,K,U) thus can be represent in basis of reciprocal vector$\langle\alpha,\beta,\gamma\rangle$:

$$X : \langle 0, 0.5, 0.5\rangle$$
$$W : \langle 0.25, 0.75, 0.5\rangle$$
$$K : \langle 0.25, 0.25, 0.25\rangle$$
$$U : \langle 0.375, 0.75, 0.375\rangle$$

6. (a) $GaAs$

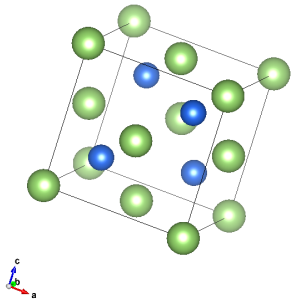

FIG. 2. GaAs zinc-blende structure

POSCAR :

```
GaAs
5.653
1.000000000   0.000000000   0.000000000
0.000000000   1.000000000   0.000000000
0.000000000   0.000000000   1.000000000
Ga     As
4      4
Direct
0.000000000   0.000000000   0.000000000
0.000000000   0.500000000   0.500000000
0.500000000   0.500000000   0.000000000
0.500000000   0.000000000   0.500000000
0.750000000   0.250000000   0.750000000
0.250000000   0.250000000   0.250000000
0.250000000   0.750000000   0.750000000
0.750000000   0.750000000   0.250000000
```

(b) $NaCl$

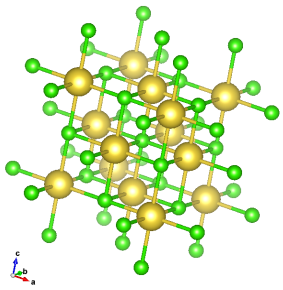

FIG. 3. NaCl fcc structure

POSCAR :

```
NaCl
5.64
1.000000000   0.000000000   0.000000000
0.000000000   1.000000000   0.000000000
0.000000000   0.000000000   1.000000000
Na    Cl
4     4
Direct
0.000000000   0.000000000   0.000000000
0.000000000   0.500000000   0.500000000
0.500000000   0.000000000   0.500000000
0.500000000   0.500000000   0.000000000
0.500000000   0.500000000   0.500000000
0.500000000   0.000000000   0.000000000
0.000000000   0.500000000   0.000000000
0.000000000   0.000000000   0.500000000
```

(c) $SrTiO_3$

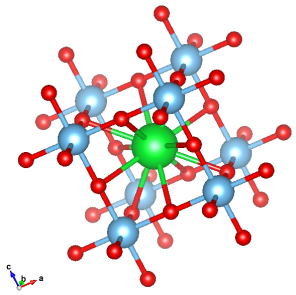

FIG. 4. SrTiO3 sc structure

POSCAR :

```
SrTiO3
3.98805
1.000000000   0.000000000   0.000000000
0.000000000   1.000000000   0.000000000
0.000000000   0.000000000   1.000000000
Sr    Ti    O
1     1     3
Direct
0.500000000   0.500000000   0.500000000
0.000000000   0.000000000   0.000000000
0.500000000   0.000000000   0.000000000
0.000000000   0.500000000   0.000000000
0.000000000   0.000000000   0.500000000
```

(d) $2HMoS_2$

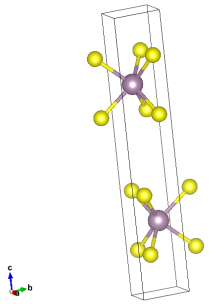

FIG. 5. MoS2-2H

POSCAR :

```
2H–MoS2
3.19
  1.000000000   0.000000000   0.000000000
 −0.500000000   0.866025403   0.000000000
  0.000000000   0.000000000   4.664263323
Mo  S
2  4
Direct
0.3333333333   0.666666667   0.250000000
0.6666666666   0.333333333   0.750000000
0.3333333333   0.666666667   0.855174000
0.3333333333   0.666666667   0.644826000
0.6666666666   0.333333333   0.355174000
0.6666666666   0.333333333   0.144826000
```

7.

8. Considering the block wave function $\psi_{n,\vec{k}}(r)$ with band index n, and wave vector$\vec{k}$. The Wannier functions center at lattice position $\vec{R}$ can be written in terms of inverse Fourier transform with constant κ :

$$\phi_n(\vec{r}-\vec{R}) = \kappa \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}} \psi_{n,\vec{k}}(\vec{r}) \tag{5}$$

Thus :

$$
\begin{aligned}
&\int \phi_n(\vec{r}-\vec{R})\phi_{n'}(\vec{r}-\vec{R}')d^D\vec{r} \\
&= \kappa^2 \sum_{\vec{k},\vec{h}} e^{i\vec{k}\cdot\vec{R}} e^{-i\vec{h}\cdot\vec{R}'} \int \psi^*_{n,\vec{k}}(\vec{r})\psi_{n',\vec{h}}(\vec{r})d^D\vec{r} \\
&= \kappa^2 \sum_{\vec{k},\vec{h}} e^{i\vec{k}\cdot\vec{R}} e^{-i\vec{h}\cdot\vec{R}'} \delta_{n,n'}\delta_{\vec{k},\vec{h}'} \\
&= \kappa^2 \delta_{n,n'} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}-\vec{R}')} \\
&= \kappa^2 N \delta_{n,n'}\delta_{\vec{R},\vec{R}'} \\
&\propto \delta_{n,n'}\delta_{\vec{R},\vec{R}'} \#
\end{aligned}
\tag{6}
$$

The constant κ can be derived by the normalization:

$$
\begin{aligned}
&\int \phi_n(\vec{r}-\vec{R})\phi_{n'}(\vec{r}-\vec{R}')d^D\vec{r} = \delta_{n,n'}\delta_{\vec{R},\vec{R}'} \\
&\kappa^2 N = 1 \\
&\kappa = \frac{1}{\sqrt{N}} \#
\end{aligned}
$$