Homework Sheet No. 1

<u>Issued 18 Sept. 2017 and **due 2 October 2017**</u>

1. Derive the *c/a* ratio for an ideal hexagonal close-packed structure (two spheres per unit cell). If *c/a* is significantly larger than this value, the crystal structure may be thought of as composed of planes of closely packed atoms, the planes being loosely stacked.

2. What is the Bravais lattice formed by all points with Cartesian coordinates (n_1, n_2, n_3) if
(a) The n_i are either all even or all odd?
(b) The sum of the n_i is required to be even?

3. Derive the expression for primitive reciprocal lattice in three dimension given by

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|},\ \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|},\ \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|}.$$

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4. Consider a graphene (honeycomb) lattice in which each atom has three nearest neighbors. Give primitive translation vectors, basis vectors for the atoms in the unit cell, and the reciprocal lattice primitive vectors. Show that the Brillouin zone is hexagonal.

5. Determine the coordinates of the points on the boundary of the Brillouin zone in fcc (X, W, K, U) and bcc (H, N, P).

6. Prepare the POSCARs and use the VESTA to draw the crystal structures of the following materials. Include the POSCARs and one picture for each structure in your answer sheet.
(a) GaAs in zincblende structure; (b) NaCl in fcc structure; (c) SrTiO3 in simple cubic structure; (d) 2H MoS_2.

7. Effect of weak periodic potential at places in k-space where Bragg planes meet. Consider the point W ($\mathbf{k}_W = (2\pi/a)(1,1/2,0)$ in the Brillouin zone of the fcc structure. Here three Bragg planes ((200), (111), (11-1) meet, and accordingly the free electron energies

$$\varepsilon_1^0 = \frac{\hbar^2}{2m}k^2, \qquad \varepsilon_2^0 = \frac{\hbar^2}{2m}\left[\mathbf{k} - \frac{2\pi}{a}(1,1,1)\right]^2,$$

$$\varepsilon_3^0 = \frac{\hbar^2}{2m}\left[\mathbf{k} - \frac{2\pi}{a}(1,1,\bar{1})\right]^2, \varepsilon_4^0 = \frac{\hbar^2}{2m}\left[\mathbf{k} - \frac{2\pi}{a}(2,0,0)\right]^2$$

are degenerate when $\mathbf{k} = \mathbf{k}_W$, and equal to $\varepsilon_W = \hbar^2 \mathbf{k}_W^{\ 2}/2m$.
(a) Show that in a region of **k**-space near W, the first-order energies are given by solutions to

$$\begin{vmatrix} \varepsilon_1^0-\varepsilon & U_1 & U_1 & U_2 \\ U_1 & \varepsilon_2^0-\varepsilon & U_2 & U_1 \\ U_1 & U_2 & \varepsilon_3^0-\varepsilon & U_1 \\ U_2 & U_1 & U_1 & \varepsilon_4^0-\varepsilon \end{vmatrix} = 0$$

where $U_2 = U_{200}$, $U_1 = U_{111} = U_{11\text{-}1}$, and that at W the roots are
$\varepsilon = \varepsilon_W - U_2$ (twice), $\varepsilon = \varepsilon_W + U_2 \pm 2U_1$.
(b) Using a similar method, show that the energies at the point U ($\mathbf{k}_U = (2\pi/a)(1,1/4,1/4)$ are

$\varepsilon = \varepsilon_U - U_2$, $\varepsilon = \varepsilon_U + (1/2)U_2 \pm (1/2)(U_2^2 + 8\, U_1^2)^{1/2}$,

where $\varepsilon_W = \hbar^2 \mathbf{k}_U{}^2 /2m$.
(See also Ashcroft + Mermin, Ch. 9, p. 171-172.)

8. Prove that Wannier functions centered on different lattice sites are orthogonal

$\int \phi_n^*(\mathbf{r}-\mathbf{R})\phi_{n'}(\mathbf{r}-\mathbf{R}')d\mathbf{r} \propto \delta_{n,n'}\delta_{\mathbf{R},\mathbf{R}'}$,

by appealing to the orthonormality of the Bloch functions and the identity $\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} = N\delta_{\mathbf{R},\mathbf{0}}$.

Show also that $\int |\phi_n(\mathbf{r})|^2 \, d\mathbf{r} = 1$ if the integral of the $|\phi_n(\mathbf{r})|^2$ over a primitive cell is normalized to unity.
(See also Ashcroft + Mermin, Ch. 10, p. 190.)

9. Calculate the density of states for electrons that are
(a) confined in a channel of rectangular shape, so that $\Psi(x,y,z) = 0$ for $|x| > a$ and $|y| > b$;
(b) confined in a slab, so that $\Psi(x,y,z) = 0$ for $|x| > a$.