8.511 Theory of Solids I **Problem Set 2** **Due September 28, 2004**

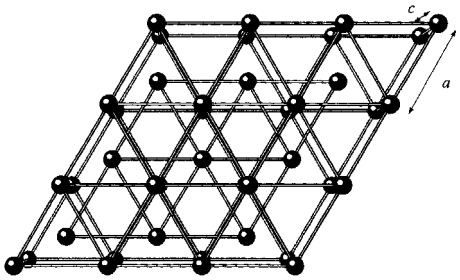

Figure 2.19. Top view of an hcp lattice.

1. *Problem 2.5(b) from page 38 of Marder.*

   (a) The hcp also has a glide plane, which is parallel to a plane containing both the **a** and **c** axes. Describe where this plane may be located, so that translation along **c**/2 followed by reflection about the plane leaves the lattice invariant.

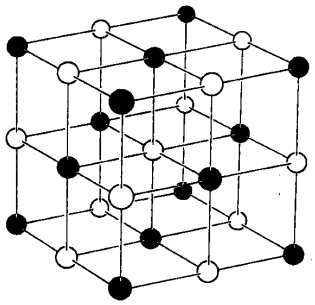

Figure 4.24
The sodium chloride structure. One type of ion is represented by black balls, the other type by white. The black and white balls form interpenetrating fcc lattices.

   (b) *Problem 5 from page 109 of Ashcroft & Mermin.*

      i. The sodium chloride structure (Figure 4.24) can be regarded as an fcc Bravais lattice of cube side a, with a basis consisting of a positively charged ion at the origin and a negatively charged ion at $(a/2)\hat{\mathbf{x}}$. The reciprocal lattice is body-centered cubic, and the general reciprocal lattice vector has the form (6.19)

$$\mathbf{K} = \frac{4\pi}{a}(\nu_1\hat{\mathbf{x}} + \nu_2\hat{\mathbf{y}} + \nu_3\hat{\mathbf{z}}), \tag{1}$$

      with all the coefficients ν_i either integers or integers $+\frac{1}{2}$. If the atomic form factors for the two ions are f_+ and f_-, show that the structure factor is $S_K = f_+ + f_-$, if the ν_i are integers, and $f_+ - f_-$, if the ν_i are integers $+\frac{1}{2}$. (Why does S vanish in the latter case when $f_+ = f_-$?)

      ii. The zincblende structure (Figure 4.18) is also a face-centered cubic Bravais lattice of cube side a, with a basis consisting of a positively charged ion at the origin and a negatively charged ion at $(a/4)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$. Show that the structure factor $S_{\mathbf{K}}$ is $f_+ \pm if_-$ if the ν_i are integers $+\frac{1}{2}$, $f_+ + f_-$ if the ν_i are integers, and $\Sigma\nu_i$ is even, and $F_+ - f_-$ if ν_i are integers and $\Sigma\nu_i$ is odd.

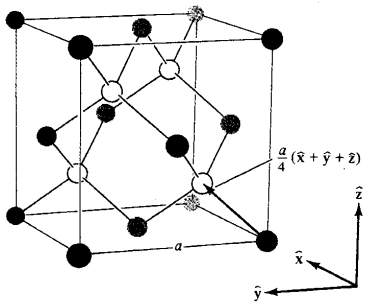

Figure 4.18
Conventional cubic cell of the diamond lattice. For clarity, sites corresponding to one of the two interpenetrating face-centered cubic lattices are unshaded. (In the zincblende structure the shaded sites are occupied by one kind of ion, and the unshaded by another.) Nearest-neighbor bonds have been drawn in. The four nearest neighbors of each point form the vertices of a regular tetrahedron.

iii. Suppose that a cubic crystal is known to be composed of closed-shell (and hence spherically symmetric) ions, so that $f_{\pm}(\mathbf{K})$ depends only on the magnitude of $\mathbf{K}$. The positions of the Bragg peaks reveal that the Bravais lattice is face-centered cubic. Discuss how one might determine, from the structure factors associated with the Bragg peaks, whether the crystal structure was likely to be of the sodium chloride or zincblende type.

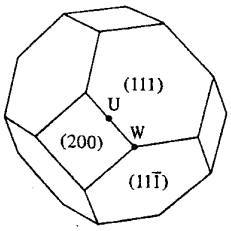

Figure 9.14
First Brillouin zone for a face-centered cubic crystal.

2. *Problem 3 from page 171 of Ashcroft & Mermin.* **Effect of Weak Periodic Potential at Places in *k*-Space where Bragg Planes Meet.** Consider the point W($\mathbf{k}_{\rm w} = (2\pi/a)(1, \frac{1}{2}, 0)$) in the Brillouin zone of the fcc structure shown (see Fig. 9.14). Here three Bragg planes ($(200), (111), (11\bar{1})$) meet, and accordingly the free electron energies

$$\begin{aligned}
\varepsilon_1^0 &= \frac{\hbar^2}{2m}k^2, \\
\varepsilon_2^0 &= \frac{\hbar^2}{2m}\left(\mathbf{k} - \frac{2\pi}{a}(1,1,1)\right)^2, \\
\varepsilon_3^0 &= \frac{\hbar^2}{2m}\left(\mathbf{k} - \frac{2\pi}{a}(1,1,\bar{1})\right)^2, \\
\varepsilon_4^0 &= \frac{\hbar^2}{2m}\left(\mathbf{k} - \frac{2\pi}{a}(2,0,0)\right)^2,
\end{aligned} \tag{2}$$

are degenerate when $\mathbf{k} = \mathbf{k}_{\rm w}$, and equal to $\varepsilon_{\rm w} = \hbar^2\mathbf{k}_{\rm w}^2/2m$.

(a) Show that in a region of k space near W, the first-order energies are given by solutions

to [1]

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

where $U_2 = U_{200}$, $U_1 = U_{111} = U11\bar{1}$, and that at W the roots are

$$\varepsilon = \varepsilon_{\rm w} - U_2 \ \ \text{(twice)}, \ \ \varepsilon = \varepsilon_{\rm w} + {\rm U}_2 \pm 2{\rm U}_1. \tag{3}$$

(b) Using a similar method, show that the energies at the point $U(\mathbf{k}_{\rm U} = (2\pi/a)(1, \frac{1}{4}, \frac{1}{4}))$ are

$$\varepsilon = \varepsilon_{\rm U} - U_2, \varepsilon = \varepsilon_{\rm U} + \frac{1}{2}U_2 \pm (U_2^2 + 8U_1^2)^{1/2} \tag{4}$$

where $\varepsilon_{\rm U} = \hbar^2 \mathbf{k}_{\rm U}^2 / 2m$.

---

[1] Assume that the periodic potential U has inversion symmetry so that the $U_{\mathbf{k}}$ are real.