Homework 1, due January 15, 1999

Problem 1. Ashcroft-Mermin 4.1

For all three parts it is clear that the points on the corners of the original simple cubic lattice have the same environment. We need to compare the corner points with the new points.

(a) New points have same environment. Always surrounded by four atoms in a square in the horizontal plane and two atoms in the vertical direction. It is a Bravais lattice. Primitive vectors: $\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}-\hat{y})$, $\vec{a}_3 = a\hat{z}$. Tetragonal lattice.

(b) Different environment. Nearest neighbors of corner points are new points. Each corner point has 8 nearest neighbors and they form a tetragonal block. The new points also have 8 nearest neighbors (four old corner points and four new points), but they form a tetragonal block that is rotated from the other one. Difference in direction. Simple cubic with basis: $\vec{d_1} = \vec{0}$, $\vec{d_2} = \frac{a}{2}(\hat{x}+\hat{z})$, $\vec{d_3} = \frac{a}{2}(\hat{y}+\hat{z})$.

(c) Corner atoms have 6 nearest neighbors, but new atoms only have two. Not a Bravais lattice. Simple cubic with a basis: $\vec{d_1} = \vec{0}$, $\vec{d_2} = \frac{a}{2}\hat{x}$, $\vec{d_3} = \frac{a}{2}\hat{y}$, $\vec{d_4} = \frac{a}{2}\hat{z}$.

Problem 2. Ashcroft-Mermin 4.3

Use Figure 4.18 with a=1. Central atom E at $\vec{E} = \frac{1}{4}(\hat{x}+\hat{y}+\hat{z})$. Nearest neighbors at $\vec{A} = \vec{0}$, $\vec{B} = \frac{1}{2}(\hat{x}+\hat{y})$, $\vec{C} = \frac{1}{2}(\hat{y}+\hat{z})$, $\vec{D} = \frac{1}{2}(\hat{z}+\hat{x})$.

Distance AD $= |\vec{D}| = \frac{1}{2}\sqrt{2}$.
Distance AE $= |\vec{E}| = \frac{1}{4}\sqrt{3}$.
Distance DE = Distance AE by symmetry.
Cosine rule:
$AD^2 = AE^2 + ED^2 - 2AEDE\cos(\alpha)$
gives
$\cos(\alpha) = -\frac{1}{3}$

Problem 3. Ashcroft-Mermin 4.4

(a) By construction, for every vector in the Bravais lattice the inverse vector is also in the Bravais lattice. Following the construction of the Wigner-Seitz cell using bysecting lines we find that for every side of the Wigner-Seitz cell there is another that is the inverse of this. The number of sides of the Wigner-Seitz cell is even. Two is not possible, hence the number of sides is four (rectangle), six(hexagon), or more.

Take one Bravais lattice point as origin O. The nearest BL point is A. There is a second point at -A. Take the closest point to O not on the line OA. Call this B. Construct the line normal to OA through O. Assume B is on the left of this line. There is a BL point C on the line through B parallel to OA and on the right of this line with BC=OA. Any other BL point on BC will not contribute a side to the Wigner-Seitz cell, since it has to be further out than A,B,C, and -A. SImilarly, on the other side of OA we find the points -B, -C. The Wigner-Seitz cell is a hexagon, unless B is on the normal line constructed before, in which case the cell is a rectangle.

(b) One diagonal connects $\frac{a}{2}(1,1,0)$ and $\frac{a}{2}(1,0,1)$. Length $\frac{a}{2}\sqrt{2}$. The other diagonal connects $\frac{a}{4}(1,1,1)$ and $\frac{a}{4}(1,1,3)$, length $\frac{a}{2}$ (half the cube!). Ratio $\sqrt{2}:1$.

(d) We do (d) first. Look at Figure 4.15 in the book.Take the central point as the origin. It looks as if the hexagon faces could have sides of two different lengths, but opposite sides of the haxagon must have the same length since they are in contact when we add a second Wigner-Seitz cell centered on a corner point.

(c) The corners of the square on top are given by $(\pm b, 0, \frac{a}{2})$ and $(0, \pm b, \frac{a}{2})$ The length of this side is $b\sqrt{2}$. Points on the square on the right face are given by $(\pm b, -\frac{a}{2}, 0)$ and $(0, -\frac{a}{2}, \pm b)$. The distance between a point on the top and side square is teh distance between $(0, -b, \frac{a}{2})$ and $(0, -\frac{a}{2}, b)$. This is $(\frac{a}{2} - b)\sqrt{2}$. Therefore $b = (\frac{a}{2} - b)$ and $b = \frac{a}{4}$ and the length is $\frac{a}{4}\sqrt{2}$.

Problem 4. Ashcroft-Mermin 4.5

(a) Look at figure 4.20 and use spheres of radius R. We get $a = |\vec{a}_1| = 2R$, $|\frac{1}{3}(\vec{a}_1 + \vec{a}_2) + \frac{1}{2}\vec{a}_3| = 2R$, $c = |\vec{a}_3|$. The second equation gives $|\frac{1}{3}(\vec{a}_1 + \vec{a}_2)|^2 + \frac{1}{4}c^2 = 4R^2$ and since the angle between the first two primitive vectors is sixty degrees we have $|\vec{a}_1 + \vec{a}_2| = a\sqrt{3}$ or $\frac{1}{3}a^2 + \frac{1}{4}c^2 = 4R^2$ with $a = 2R$ we get $\frac{1}{4}c^2 = \frac{2}{3}a^2$ which gives the required result.

(b) In the bcc cubic phase $V^C_{WS} = \frac{1}{2}a^3_C$, while in the hcp phase $V^H_{WS} = \frac{\sqrt{3}}{4}a^2_H c_H$. Using the ideal c/a ratio we find $V^H_{WS} = \frac{\sqrt{2}}{2}a^3_H$. If these volumes are the same: $\frac{1}{2}a^3_C = \frac{\sqrt{2}}{2}a^3_H$ or $a_H = 2^{-\frac{1}{6}}a_C$. This gives $a_H = 3.77 Ang$.

Problem 5. Ashcroft-Mermin 4.7

Write the points in the form (l,m,n) where all values are allowed for simple cubic, where l,m,n are all even or odd for bcc, and where l+m+n is even for fcc. The number of vectors is the number of different permutations, including sign changes, we can make out of (l,m,n). Ordered by length we have

vector	N	sc	bcc	fcc
0,0,0	1	X	X	X
1,0,0	6	X		
1,1,0	12	X		X
1,1,1	8	X	X	
2,0,0	6	X	X	X
2,1,0	24	X		
2,1,1	24	X		X
2,2,0	12	X	X	X
2,2,1	24	X		
3,0,0	6	X		
3,1,0	24	X		X
3,1,1	24	X	X	
2,2,2	8	X	X	X
3,2,0	24	X		
3,2,1	48	X		X
4,0,0	6	X	X	X

From this we find easily (note we give R-squared)

	N sc	R2 sc	N bcc	R2 bcc	N fcc	R2 fcc
1	6	1	8	3	12	2
2	12	2	6	4	6	4
3	8	3	12	8	24	6
4	6	4	24	11	12	8
5	24	5	8	12	24	10
6	24	6	6	16	8	12