1 Decorated cubic lattices

Base-centered cubic is a Bravais lattice generated by $\{a\hat{\mathbf{x}}, a(\hat{\mathbf{x}}+\hat{\mathbf{y}})/2, \hat{\mathbf{z}}\}$.

Side-centered cubic is not a Bravais lattice since it contains the vectors $a(\hat{\mathbf{x}}+\hat{\mathbf{z}})/2$ and $a(\hat{\mathbf{y}}+\hat{\mathbf{z}})/2$ but not the sum $a(\hat{\mathbf{x}}/2+\hat{\mathbf{y}}/2+\hat{\mathbf{z}})$. It is generated by a simple cubic lattice with basis $\{0, a(\hat{\mathbf{x}}+\hat{\mathbf{z}})/2, a(\hat{\mathbf{y}}+\hat{\mathbf{z}})/2\}$.

Edge-centered cubic is not a Bravais lattice since it contains the vectors $a\hat{\mathbf{x}}/2$ and $a\hat{\mathbf{y}}/2$ but not the sum $a(\hat{\mathbf{x}}+\hat{\mathbf{y}})/2$. It is generated by a simple cubic lattice with basis $\{0, a\hat{\mathbf{x}}/2, a\hat{\mathbf{y}}/2, a\hat{\mathbf{z}}/2\}$.

2 Skipping alternate lattice points

n_i are all even. Displacements in the lattice are generated by $\{2\hat{\mathbf{x}}, 2\hat{\mathbf{y}}, 2\hat{\mathbf{z}}\}$. This is a simple cubic lattice with side 2 containing the origin.

n_i are all odd. This is a simple cubic lattice with side 2 containing the point (1,1,1).

$\sum_i n_i$ is even. For a given lattice point, either all three coordinates are even, or exactly 1 coordinate is even, with the other two odd. Points of the first type form a simple cubic lattice with side 2. Points of the second type lie in the face centers of this lattice, forming an FCC lattice with side 2.

$\sum_i n_i$ is odd. Either all three coordinates are odd, or exactly one coordinate is odd, with the other two even. Points of the first type form a SC of side two, and together with the second set this is again an FCC with side 2.

3 Optimal tavern problem

(See pg. 74 of A&M for WS cells of BCC, FCC). The point with maximal distance x to the nearest lattice point is a vertex of the Wigner-Seitz (WS) cell. This means it is also equidistant from the four nearest lattice points.

BCC. From the illustration note that all vertices of the WS cell are equivalent. A given vertex lies on some face of the conventional cell (of side a) and is equidistant from four points: two corners of the cell face, the body center, and the body center of a neighboring cell. Denote the maximal distance as d. One vertex of the WS cell is $(a\hat{\mathbf{x}}/2+y\hat{\mathbf{y}})$ which is equidistant from 0, $a\hat{\mathbf{x}}$, $a(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/2$, and $a(\hat{\mathbf{x}}+\hat{\mathbf{y}}-\hat{\mathbf{z}})/2$.

$$d = |(a\hat{\mathbf{x}}/2+y\hat{\mathbf{y}}) - 0| = |(a\hat{\mathbf{x}}/2+y\hat{\mathbf{y}}) - a(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})/2|$$

The solution is $y = a/4$, $d = a\sqrt{5/16}$. Since the volume per lattice site is $v = a^3/2$, the BCC lattice has $d = (5^{1/2}2^{1/3}/4)\, v^{1/3} \approx 0.704\, v^{1/3}$.

FCC. The illustration (note that cell of Figure 4.16 is not the conventional cell) shows that the WS cell has two types of vertices, one at which four faces of the WS cell meet and another at which only 3 faces meet. Those of the first type bisect edges of the conventional cell (side a) and are equidistant from two corners and two face centers, giving $d = a/2$. Those of the second type lie on the interior of the conventional cell, and are equidistant from one corner and three face centers. For example, the point $\alpha(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})$ is equidistant from 0, $a(\hat{\mathbf{x}}+\hat{\mathbf{y}})/2$, $a(\hat{\mathbf{y}}+\hat{\mathbf{z}})/2$, and $a(\hat{\mathbf{z}}+\hat{\mathbf{x}})/2$ when

$$d = |\alpha(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}) - 0| = |\alpha(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}) - a(\hat{\mathbf{x}}+\hat{\mathbf{y}})/2|$$

which occurs for $\alpha = a/4$ giving $d = a\sqrt{3}/4$. Since $a\sqrt{3}/4 < a/2$ we take the maximal distance as $a/2$. The volume per lattice site is $v = a^3/4$ leading to $d = (4^{1/3}/2)\,v^{1/3} \approx 0.794\,v^{1/3}$. The BCC lattice has the lesser maximal distance.

4 Morphs in reciprocal space

Given R in the direct lattice and K in the reciprocal lattice, $R \cdot K = 2\pi N(R,K)$ where N is an integer function of R and K. Given a continuous transformation (such as rotation or dilation), $N(R,K)$ must vary continuously as R and K are changed. However, since N must be an integer, then $N(R,K)$ and thus $R \cdot K$ remain constant under the transformation. If the direct lattice undergoes a rotation $\mathbf{M}$, the only way to keep $R \cdot K$ constant for all pairs (R,K) is if the reciprocal lattice undergoes the same rotation: $(\mathbf{M}R)\cdot(\mathbf{M}K) = R^{\mathrm{T}}\mathbf{M}^{\mathrm{T}}\mathbf{M}K = R^{\mathrm{T}}K = R \cdot K$. If the direct lattice is squeezed by a factor λ in the vertical direction, then the reciprocal lattice is dilated by λ in the vertical direction to maintain $R \cdot K$: $R_z K_z = (R_z/\lambda)(K_z \lambda)$

5 Density of points in a lattice plane

If ρ_a is the density of lattice points in the plane, d is the interplane separation, and v is the volume per lattice site, then $\rho_a = d/v$. Fixing v, the family of planes with the highest ρ_a must have the highest d. For this family, the shortest reciprocal lattice vector whose direction is perpendicular to all the planes has magnitude $2\pi/d$. It suffices, then, to find the shortest reciprocal lattice vector(s).

FCC. An FCC lattice generated by $(a/2)\{(\hat{\mathbf{x}}+\hat{\mathbf{y}}), (\hat{\mathbf{y}}+\hat{\mathbf{z}}), (\hat{\mathbf{z}}+\hat{\mathbf{x}})\}$ has a reciprocal lattice generated by $(2\pi/a)\{(\hat{\mathbf{x}}+\hat{\mathbf{y}}-\hat{\mathbf{z}}), (\hat{\mathbf{y}}+\hat{\mathbf{z}}-\hat{\mathbf{x}}), (\hat{\mathbf{z}}+\hat{\mathbf{x}}-\hat{\mathbf{y}})$. The shortest reciprocal lattice vectors have length $(2\pi/a)\sqrt{3}$, an example being $(2\pi/a)(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}})$. Since lattice planes of FCC and BCC lattices coincide with those of the SC, it is conventional to use the conventional cubic cell to define the Miller indices. The desired planes are denoted $\{111\}$, which includes eight families: (111), $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$, $(\bar{1}\bar{1}1)$, $(\bar{1}1\bar{1})$, $(1\bar{1}\bar{1})$, $(\bar{1}\bar{1}\bar{1})$.

BCC. A BCC lattice generated by $(a/2)\{(\hat{\mathbf{x}}+\hat{\mathbf{y}}-\hat{\mathbf{z}}), (\hat{\mathbf{y}}+\hat{\mathbf{z}}-\hat{\mathbf{x}}), (\hat{\mathbf{z}}+\hat{\mathbf{x}}-\hat{\mathbf{y}})$ has a reciprocal lattice generated by $(2\pi/a)\{(\hat{\mathbf{x}}+\hat{\mathbf{y}}), (\hat{\mathbf{y}}+\hat{\mathbf{z}}), (\hat{\mathbf{z}}+\hat{\mathbf{x}})\}$. The shortest reciprocal lattice vectors have length $(2\pi/a)\sqrt{2}$, an example being $(2\pi/a)(\hat{\mathbf{x}}+\hat{\mathbf{y}})$. The corresponding planes have Miller indices $\{110\}$, which includes 12 families: (110), (101), (011), $(\bar{1}\bar{1}0)$, $(\bar{1}0\bar{1})$, $(\bar{1}\bar{1}0)$, $(1\bar{1}0)$, $(10\bar{1})$, $(\bar{1}10)$, $(\bar{1}01)$, $(01\bar{1})$, $(0\bar{1}1)$.