Problem 1. BCC and FCC lattices Show that the reciprocal lattice of a body-centered cubic lattice (BCC) of spacing a is a face-centered cubic (FCC) lattice of spacing $4\pi/a$, and that the reciprocal lattice of a FCC lattice of spacing a is a BCC lattice of spacing $4\pi/a$.

Solution. A set of primitive unit vectors for the BCC lattice of lattice spacing a is given by Ashcroft & Mermin (4.4),

$$\mathbf{a}_1^{\mathrm{BCC}} = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), \qquad \mathbf{a}_2^{\mathrm{BCC}} = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), \qquad \mathbf{a}_3^{\mathrm{BCC}} = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}). \tag{1}$$

A set of primitive unit vectors for the FCC lattice of lattice spacing a is given by their (4.5),

$$\mathbf{a}_1^{\mathrm{FCC}} = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \qquad \mathbf{a}_2^{\mathrm{FCC}} = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \qquad \mathbf{a}_3^{\mathrm{FCC}} = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \tag{2}$$

According to their (5.3), the reciprocal lattice of a direct lattice with primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ has the primitive vectors

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \qquad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \qquad \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}. \tag{3}$$

We begin by finding the lattice reciprocal to the BCC lattice. For the denominator of Eq. (3), note that

$$\begin{aligned}
\mathbf{a}_2^{\mathrm{BCC}} \times \mathbf{a}_3^{\mathrm{BCC}} &= \frac{a^2}{4}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}) \times (\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \\
&= \frac{a^2}{4}(\hat{\mathbf{z}} \times \hat{\mathbf{x}} + \hat{\mathbf{z}} \times \hat{\mathbf{y}} + \hat{\mathbf{x}} \times \hat{\mathbf{y}} - \hat{\mathbf{x}} \times \hat{\mathbf{z}} - \hat{\mathbf{y}} \times \hat{\mathbf{x}} + \hat{\mathbf{y}} \times \hat{\mathbf{z}}) \\
&= \frac{a^2}{2}(\hat{\mathbf{z}} \times \hat{\mathbf{x}} + \hat{\mathbf{x}} \times \hat{\mathbf{y}}) \\
&= \frac{a^2}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}),
\end{aligned}$$

so

$$\mathbf{a}_1^{\mathrm{BCC}} \cdot (\mathbf{a}_2^{\mathrm{BCC}} \times \mathbf{a}_3^{\mathrm{BCC}}) = \frac{a^3}{4}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}) \cdot (\hat{\mathbf{y}} + \hat{\mathbf{z}}) = \frac{a^3}{4}(\hat{\mathbf{y}} \cdot \hat{\mathbf{y}} + \hat{\mathbf{z}} \cdot \hat{\mathbf{z}}) = \frac{a^3}{2}.$$

For the numerators,

$$\begin{aligned}
\mathbf{a}_3^{\mathrm{BCC}} \times \mathbf{a}_1^{\mathrm{BCC}} &= \frac{a^2}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \times (\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}) \\
&= \frac{a^2}{4}(\hat{\mathbf{x}} \times \hat{\mathbf{y}} + \hat{\mathbf{x}} \times \hat{\mathbf{z}} + \hat{\mathbf{y}} \times \hat{\mathbf{z}} - \hat{\mathbf{y}} \times \hat{\mathbf{x}} - \hat{\mathbf{z}} \times \hat{\mathbf{y}} + \hat{\mathbf{z}} \times \hat{\mathbf{x}}) \\
&= \frac{a^2}{2}(\hat{\mathbf{x}} \times \hat{\mathbf{y}} + \hat{\mathbf{y}} \times \hat{\mathbf{z}}) \\
&= \frac{a^2}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}),
\end{aligned}$$

$$\begin{aligned}
\mathbf{a}_1^{\mathrm{BCC}} \times \mathbf{a}_2^{\mathrm{BCC}} &= \frac{a^2}{4}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}) \times (\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}) \\
&= \frac{a^2}{4}(\hat{\mathbf{y}} \times \hat{\mathbf{z}} + \hat{\mathbf{y}} \times \hat{\mathbf{x}} + \hat{\mathbf{z}} \times \hat{\mathbf{x}} - \hat{\mathbf{z}} \times \hat{\mathbf{y}} - \hat{\mathbf{x}} \times \hat{\mathbf{z}} + \hat{\mathbf{x}} \times \hat{\mathbf{y}}) \\
&= \frac{a^2}{2}(\hat{\mathbf{y}} \times \hat{\mathbf{z}} + \hat{\mathbf{z}} \times \hat{\mathbf{x}}) \\
&= \frac{a^2}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}).
\end{aligned}$$

So the reciprocal lattice of the BCC lattice has the primitive vectors

$$\mathbf{b}_1^{\mathrm{BCC}} = 2\pi \frac{a^2}{2} \frac{\hat{\mathbf{y}} + \hat{\mathbf{z}}}{a^3/2} = \frac{2\pi}{a}(\hat{\mathbf{y}} + \hat{\mathbf{z}}),$$
$$\mathbf{b}_2^{\mathrm{BCC}} = 2\pi \frac{a^2}{2} \frac{\hat{\mathbf{z}} + \hat{\mathbf{x}}}{a^3/2} = \frac{2\pi}{a}(\hat{\mathbf{z}} + \hat{\mathbf{x}}),$$
$$\mathbf{b}_3^{\mathrm{BCC}} = 2\pi \frac{a^2}{2} \frac{\hat{\mathbf{x}} + \hat{\mathbf{y}}}{a^3/2} = \frac{2\pi}{a}(\hat{\mathbf{x}} + \hat{\mathbf{y}}),$$

which are the primitive unit vectors of Eq. (2) with $a \to 4\pi/a$. So we have shown that the BCC reciprocal lattice is the FCC lattice with spacing $4\pi/a$. □

Next we find the lattice reciprocal to the FCC lattice. Proceeding similarly as before, note that

$$\mathbf{a}_2^{\mathrm{FCC}} \times \mathbf{a}_3^{\mathrm{FCC}} = \frac{a^2}{4}(\hat{\mathbf{z}} + \hat{\mathbf{x}}) \times (\hat{\mathbf{x}} + \hat{\mathbf{y}}) = \frac{a^2}{4}(\hat{\mathbf{z}} \times \hat{\mathbf{x}} + \hat{\mathbf{z}} \times \hat{\mathbf{y}} + \hat{\mathbf{x}} \times \hat{\mathbf{y}}) = \frac{a^2}{4}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}),$$
$$\mathbf{a}_3^{\mathrm{FCC}} \times \mathbf{a}_1^{\mathrm{FCC}} = \frac{a^2}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \times (\hat{\mathbf{y}} + \hat{\mathbf{z}}) = \frac{a^2}{4}(\hat{\mathbf{x}} \times \hat{\mathbf{y}} + \hat{\mathbf{x}} \times \hat{\mathbf{z}} + \hat{\mathbf{y}} \times \hat{\mathbf{z}}) = \frac{a^2}{4}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}),$$
$$\mathbf{a}_1^{\mathrm{FCC}} \times \mathbf{a}_2^{\mathrm{FCC}} = \frac{a^2}{4}(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \times (\hat{\mathbf{z}} + \hat{\mathbf{x}}) = \frac{a^2}{4}(\hat{\mathbf{y}} \times \hat{\mathbf{z}} + \hat{\mathbf{y}} \times \hat{\mathbf{x}} + \hat{\mathbf{z}} \times \hat{\mathbf{x}}) = \frac{a^2}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}),$$

and that

$$\mathbf{a}_1^{\mathrm{FCC}} \cdot (\mathbf{a}_2^{\mathrm{FCC}} \times \mathbf{a}_3^{\mathrm{FCC}}) = \frac{a^3}{8}(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \cdot (\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}) = \frac{a^3}{8}(\hat{\mathbf{y}} \cdot \hat{\mathbf{y}} + \hat{\mathbf{z}} \cdot \hat{\mathbf{z}}) = \frac{a^3}{4}.$$

Then the reciprocal lattice of the FCC lattice has the primitive vectors

$$\mathbf{b}_1^{\mathrm{FCC}} = 2\pi \frac{a^2}{4} \frac{\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}}{a^3/4} = \frac{2\pi}{a}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}),$$
$$\mathbf{b}_2^{\mathrm{FCC}} = 2\pi \frac{a^2}{4} \frac{\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}}{a^3/4} = \frac{2\pi}{a}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}),$$
$$\mathbf{b}_3^{\mathrm{FCC}} = 2\pi \frac{a^2}{4} \frac{\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}}{a^3/4} = \frac{2\pi}{a}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}),$$

which are the primitive unit vectors of Eq. (1) with $a \to 4\pi/a$. So we have shown that the FCC reciprocal lattice is the BCC lattice with spacing $4\pi/a$. □

Problem 2. Reciprocal lattice cell volume Show that the volume of the primitive unit cell of the reciprocal lattice is $(2\pi)^3/\Omega_{\mathrm{cell}}$, where Ω_{cell} is the volume of the primitive unit cell of the crystal.

Solution. Let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ be the primitive unit vectors of the crystal and $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ those of the reciprocal lattice. From Ashcroft & Mermin (5.15),

$$\Omega_{\mathrm{cell}} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3).$$

We want to find $\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)$. We will use the vector identity [1]

$$(\mathbf{A} \times \mathbf{B}) \cdot (\mathbf{C} \times \mathbf{D}) = (\mathbf{A} \cdot \mathbf{C})(\mathbf{B} \cdot \mathbf{D}) - (\mathbf{A} \cdot \mathbf{D})(\mathbf{B} \cdot \mathbf{C}),$$

and Ashcroft & Mermin (5.4) [2, p. 93],

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}. \tag{4}$$

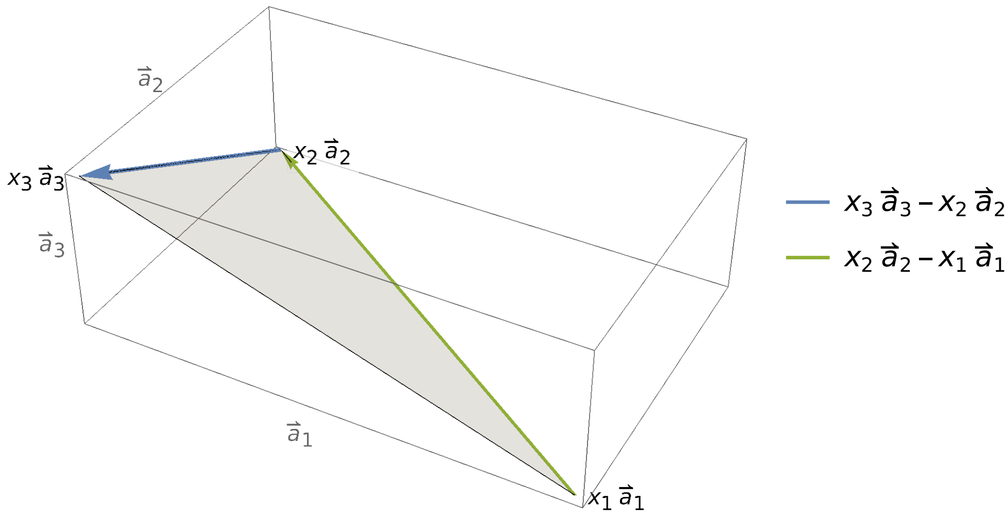

Figure 1: An illustration of the (hkl) plane. The gray shaded region is a portion of the (hkl) plane, in which the vectors $x_3\mathbf{a}_3 - x_2\mathbf{a}_2$ (blue) and $x_2\mathbf{a}_2 - x_1\mathbf{a}_1$ (green) lie. The Miller indices are inversely proportional to the x_i [2, p. 92].

Then, applying Eq. (3),

$$\begin{aligned}
\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) &= 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \cdot (\mathbf{b}_2 \times \mathbf{b}_3) \\
&= \frac{2\pi}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} [(\mathbf{a}_2 \cdot \mathbf{b}_2)(\mathbf{a}_3 \cdot \mathbf{b}_3) - (\mathbf{a}_2 \cdot \mathbf{b}_3)(\mathbf{a}_3 \times \mathbf{b}_2)] \\
&= \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\
&= \frac{(2\pi)^3}{\Omega_{\text{cell}}},
\end{aligned}$$

as we wanted to show. □

Problem 3. Bragg's law

3(a) Show that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to the (hkl) plane of the crystal lattice.

Solution. As shown in Fig. 1, the (hkl) plane intersects the $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ axes at the points $x_1\mathbf{a}_1$, $x_2\mathbf{a}_2$, and $x_3\mathbf{a}_3$. Let $\mathbf{R} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$. Then, by (3.10) in the lecture notes,

$$\mathbf{G} \cdot \mathbf{R} = 2\pi m, \tag{5}$$

where m is an integer. Then, adapting Ashcroft & Mermin (5.13),

$$x_1 = \frac{m}{h}, \qquad x_2 = \frac{m}{k}, \qquad x_3 = \frac{m}{l}. \tag{6}$$

The vectors $x_3\mathbf{a}_3 - x_2\mathbf{a}_2$ and $x_2\mathbf{a}_2 - x_1\mathbf{a}_1$ lie in the (hkl) plane, as shown in Fig. 1. The cross product of these vectors is therefore perpendicular to the (hkl) plane. We have

$$\begin{aligned}(x_3\mathbf{a}_3 - x_2\mathbf{a}_2) \times (x_2\mathbf{a}_2 - x_1\mathbf{a}_1) &= x_2x_3\mathbf{a}_3 \times \mathbf{a}_2 - x_1x_3\mathbf{a}_3 \times \mathbf{a}_1 + x_1x_2\mathbf{a}_2 \times \mathbf{a}_1 \\ &= -m^2\left(\frac{\mathbf{a}_2 \times \mathbf{a}_3}{kl} + \frac{\mathbf{a}_3 \times \mathbf{a}_1}{hl} + \frac{\mathbf{a}_1 \times \mathbf{a}_2}{hk}\right) \\ &= -\frac{m^2}{hkl}(h\mathbf{a}_2 \times \mathbf{a}_3 + k\mathbf{a}_3 \times \mathbf{a}_1 + l\mathbf{a}_1 \times \mathbf{a}_2) \\ &= -\frac{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}{2\pi}\frac{m^2}{hkl}(h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) \\ &\propto \mathbf{G},\end{aligned}$$

where we have used Eq. (3). We have shown that $\mathbf{G}$ is a scalar multiple of a vector perpendicular to the (hkl) plane; therefore, $\mathbf{G}$ itself is perpendicular to the (hkl) plane. □

3(b) Show that the distance between two adjacent (hkl) planes is $2\pi/|\mathbf{G}|$.

Solution. Let $\mathbf{R}_i$ and $\mathbf{R}_{i+1}$ be vectors in two adjacent (hkl) planes. With n an arbitrary integer, we can write

$$\mathbf{R}_i = \frac{n}{h}\mathbf{a}_1 + \frac{n}{k}\mathbf{a}_2 + \frac{n}{l}\mathbf{a}_3, \qquad \mathbf{R}_{i+1} = \frac{n+1}{h}\mathbf{a}_1 + \frac{n+1}{k}\mathbf{a}_2 + \frac{n+1}{l}\mathbf{a}_3,$$

where we have consulted Eqs. (5) and (6). Then

$$\Delta\mathbf{R} = \mathbf{R}_{i+1} - \mathbf{R}_i = \frac{1}{h}\mathbf{a}_1 + \frac{1}{k}\mathbf{a}_2 + \frac{1}{l}\mathbf{a}_3$$

is a vector pointing from one adjacent plane to the other. Note that $\Delta\mathbf{R}$ satisfies Eq. (5) with $m = 1$ via Eq. (6). That is,

$$\mathbf{G} \cdot \Delta\mathbf{R} = 2\pi.$$

The projection of $\Delta\mathbf{R}$ vector onto any vector perpendicular to one of the planes is the distance between the planes [3]. We know that $\mathbf{G}$ is normal to any (hkl) plane. So the distance is

$$d = \frac{|\mathbf{G} \cdot \Delta\mathbf{R}|}{|\mathbf{G}|} = \frac{2\pi}{|\mathbf{G}|},$$

as we wanted to show. □

3(c) Show that the condition Eq. (3.12) may be written as

$$\frac{2\pi}{\lambda}\sin\theta = \frac{\pi}{d},$$

where $\lambda = 2\pi/k$ and θ is the angle between the incident beam and the crystal plane.

Solution. Equation (3.12) is

$$\mathbf{k} \cdot \frac{\mathbf{G}}{2} = \left(\frac{G}{2}\right)^2.$$

Since $\mathbf{G}$ is perpendicular to the crystal plane and $\mathbf{k}$ is the scattered wavevector, the angle between them is $\pi/2 - \theta$. So we have

$$\mathbf{k} \cdot \mathbf{G} = kG \cos\left(\frac{\pi}{2} - \theta\right) = kG \sin\theta.$$

Then (3.12) becomes

$$k \sin\theta = \frac{G}{2}.$$

Substituting the definition of λ and the result of 3(b), $d = 2\pi/G$, we have

$$\frac{2\pi}{\lambda} \sin\theta = \frac{\pi}{d}$$

as desired. □

References

[1] E. W. Weisstein, "Vector Quadruple Product." From MathWorld—A Wolfram Web Resource. `https://mathworld.wolfram.com/VectorQuadrupleProduct.html`.

[2] N. W. Ashcroft and N. D. Mermin, "Solid State Physics". Harcourt College Publishers, 1976.

[3] E. W. Weisstein, "Point-Plane Distance." From MathWorld—A Wolfram Web Resource. `https://mathworld.wolfram.com/Point-PlaneDistance.html`.