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],

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

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.

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.