

PHY801: Survey of Atomic and Condensed Matter Physics
Michigan State University

Homework 5 – Solution

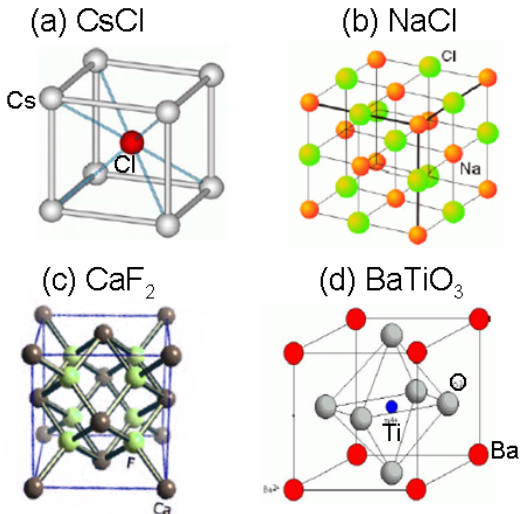
5.1. In each of the following cases indicate whether the structure is a primitive Bravais lattice. If so, provide the three primitive vectors. If not, then describe it as a Bravais lattice with as small a basis as possible.

- (i) Base centered cubic lattice (simple cubic with two additional lattice points at the center of the horizontal faces)
- (ii) Side centered cubic lattice (simple cubic lattice with additional lattice points at the center of four vertical faces)
- (iii) Edge centered cubic lattice (simple cubic lattice with additional lattice points at the centers of the 12 edges of the cube)

Solution:

- (i) Bravais; $\vec{a}_1 = a(1, 0, 0)$, $\vec{a}_2 = a\left(\frac{1}{2}, \frac{1}{2}, 0\right)$, $\vec{a}_3 = a(0, 0, 1)$.
- (ii) Non-primitive lattice with a 3-atom basis. The primitive lattice vectors are $\vec{a}_1 = a(1, 0, 0)$, $\vec{a}_2 = a(0, 1, 0)$, $\vec{a}_3 = a(0, 0, 1)$. The basis vectors are $\vec{r}_1 = a(0, 0, 0)$, $\vec{r}_2 = a\left(\frac{1}{2}, 0, \frac{1}{2}\right)$, $\vec{r}_3 = a\left(0, \frac{1}{2}, \frac{1}{2}\right)$.
- (iii) Non-primitive lattice with a 4-atom basis. The primitive lattice vectors are $\vec{a}_1 = a(1, 0, 0)$, $\vec{a}_2 = a(0, 1, 0)$, $\vec{a}_3 = a(0, 0, 1)$. The basis vectors are $\vec{r}_1 = a(0, 0, 0)$, $\vec{r}_2 = a\left(\frac{1}{2}, 0, 0\right)$, $\vec{r}_3 = a\left(0, \frac{1}{2}, 0\right)$, $\vec{r}_4 = a\left(0, 0, \frac{1}{2}\right)$.

5.2. For the four crystal structures below, identify (i) the type of the underlying Bravais lattice (simple cubic, fcc, bcc, etc.), (ii) the three primitive lattice vectors, (iii) position of the atoms in the basis, (iv) concentration of atoms using a , the side of the unit cube, as the length unit.



Solution:

(a) CsCl: Simple Cubic (SC),

$$\vec{r}_{Cs} = a(0, 0, 0), \vec{r}_{Cl} = a\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right).$$

$$n = (\text{number of atoms/unit cell volume}) = \frac{2}{a^3}.$$

(b) NaCl: Face-Centered Cubic (FCC),

$$\vec{r}_{Na} = a(0, 0, 0), \vec{r}_{Cl} = a\left(\frac{1}{2}, 0, 0\right).$$

$$n = (\text{number of atoms/unit cell volume}) = \frac{2}{a^3/4} = \frac{8}{a^3}.$$

(c) CaF₂: Face-Centered Cubic (FCC),

$$\vec{r}_{Ca} = a(0, 0, 0), \vec{r}_{F_1} = a\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right), \vec{r}_{F_2} = a\left(\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right).$$

$$n = (\text{number of atoms/unit cell volume}) = \frac{3}{a^3/4} = \frac{12}{a^3}.$$

(d) BaTiO₃: Simple Cubic,

$$\vec{r}_{Ba} = a(0, 0, 0), \vec{r}_{Ti} = a\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), \vec{r}_{O_1} = a\left(\frac{1}{2}, \frac{1}{2}, 0\right), \vec{r}_{O_2} = a\left(0, \frac{1}{2}, \frac{1}{2}\right), \vec{r}_{O_3} = a\left(\frac{1}{2}, 0, \frac{1}{2}\right).$$

$$n = (\text{number of atoms/unit cell volume}) = \frac{5}{a^3}.$$

5.3. Consider a two-dimensional triangular lattice described by the two primitive vectors (in an orthogonal coordinate system)

$$\vec{a}_1 = a(1, 0); \quad \vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right).$$

Find the two primitive lattice vectors \vec{b}_1, \vec{b}_2 describing the reciprocal lattice. Find the area of the 1st Brillouin zone and find its relation with the area of the direct lattice unit cell.

Solution:

$$\vec{b}_2 \cdot \vec{a}_1 = 0 \Rightarrow \vec{b}_2 = \beta \hat{y}$$

$$\vec{b}_2 \cdot \vec{a}_2 = 2\pi \Rightarrow \beta \hat{y} \cdot \left(\frac{a}{2} \hat{x} + a \frac{\sqrt{3}}{2} \hat{y}\right) = \beta a \frac{\sqrt{3}}{2} = 2\pi.$$

Thus,

$$\beta = \frac{4\pi}{a\sqrt{3}},$$

$$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}(0, 1).$$

Next,

$$\vec{b}_1 \cdot \vec{a}_2 = 0 \Rightarrow \vec{b}_1 = \gamma \left(\frac{\sqrt{3}}{2} \hat{x} - \frac{1}{2} \hat{y}\right)$$

$$\vec{b}_1 \cdot \vec{a}_1 = 2\pi \Rightarrow \gamma a \frac{\sqrt{3}}{2} = 2\pi.$$

Thus,

$$\gamma = \frac{4\pi}{a\sqrt{3}} = \beta,$$

$$\vec{b}_1 = \frac{4\pi}{a\sqrt{3}} \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right).$$

The 2D reciprocal lattice (net) is spanned by the two primitive vectors \vec{b}_1 and \vec{b}_2 of length $\beta = \frac{4\pi}{a\sqrt{3}}$.

The area of the 1st BZ is the area of the primitive cell in the reciprocal lattice space. This is given by $A_{BZ} = \beta^2 \frac{\sqrt{3}}{2} = \frac{8\pi^2}{a^2\sqrt{3}}$. The area of the primitive cell in the direct lattice space is $A = a^2 \frac{\sqrt{3}}{2}$. Thus we find $A_{BZ} = \frac{(2\pi)^2}{A}$.
