

Problem 1 (Problem 1 from Chapter 5 of Ashcroft and Mermin, page 93)

(a) Prove that the reciprocal lattice primitive vectors defined in (5.3) satisfy

$$\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}. \quad (5.15)$$

(*Hint:* Write \mathbf{b}_1 (but not \mathbf{b}_2 or \mathbf{b}_3) in terms of the \mathbf{a}_i , and use the orthogonality relations (5.4).)

(b) Suppose primitive vectors are constructed from the \mathbf{b}_i in the same manner (Eq. (5.3)) as the \mathbf{b}_i are constructed from the \mathbf{a}_i . Prove that these vectors are just the \mathbf{a}_i themselves; i.e., show that

$$2\pi \frac{\mathbf{b}_2 \times \mathbf{b}_3}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} = \mathbf{a}_1, \text{ etc.} \quad (5.16)$$

(*Hint:* Write \mathbf{b}_3 in the numerator (but not \mathbf{b}_2) in terms of the \mathbf{a}_i , use the vector identity $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$, and appeal to the orthogonality relations (5.4) and the result (5.15) above.)

(c) Prove that the volume of a Bravais lattice primitive cell is

$$v = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|, \quad (5.17)$$

where the a_i are three primitive vectors. (In conjunction with (5.15) this establishes that the volume of the reciprocal lattice primitive cell is $(2\pi)^3/v$.)

Problem 2(Problem 2 from Chapter 5 of Ashcroft and Mermin, page 93)

(a) Using the primitive vectors given in Eq. (4.9) and the construction (5.3) (or by any other method) show that the reciprocal of the simple hexagonal Bravais lattice is also simple hexagonal, with lattice constants $2\pi/c$ and $4\pi/\sqrt{3}a$, rotated through 30 degrees about the c -axis with respect to the direct lattice.

(b) For what value of c/a does the ratio have the same value in both direct and reciprocal lattices? If c/a is ideal in the direct lattice, what is its value in the reciprocal lattice?

(c) The Bravais lattice generated by three primitive vectors of equal length \mathbf{a} , making equal angles θ with one another, is known as the trigonal Bravais lattice (see Chapter 7). Show that the reciprocal of a trigonal Bravais lattice is also trigonal, with an angle θ^* given by $-\cos \theta^* = \cos \theta / [1 + \cos \theta]$, and a primitive vector length a^* , given by $a^* = (2\pi/a)(1 + 2 \cos \theta \cos \theta^*)^{-1/2}$.

Problem 3

X-ray diffraction. The X-ray wavelengths used to obtain the data in Fig. 1 are 0.153 93 nm (denoted K_α) and 0.139 02 nm (K_β). Decide which of the peaks correspond to the K_α

radiation. Given that the first K_α peak with $\theta \neq 0$ occurs at $\theta = 15.80$ degrees, determine a value of d for the sodium chloride crystal used in this experiment. Assuming that there is no error in the measurement of θ and that the width of the peak at half maximum intensity is 0.1 degrees, estimate the uncertainty in the value of d .

Problem 4* (Extra credit problem)

The crystal structure of the superconducting K_3C_{60} is shown in Fig. 2 . Find the underlying Bravais lattice.