4261 HW 5

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1a

This is a face-centered cubic lattice.

1b

Taking the origin to be the lower-left atom, we take the basis vectors $[\frac{1}{2}, \frac{1}{2}, 0]a$, $[\frac{1}{2}, 0, \frac{1}{2}]a$, $[0, \frac{1}{2}, \frac{1}{2}]a$, where a is the lattice constant. The atoms in the conventional cell that aren't at one of these basis vectors may be readily constructed from them.

1c

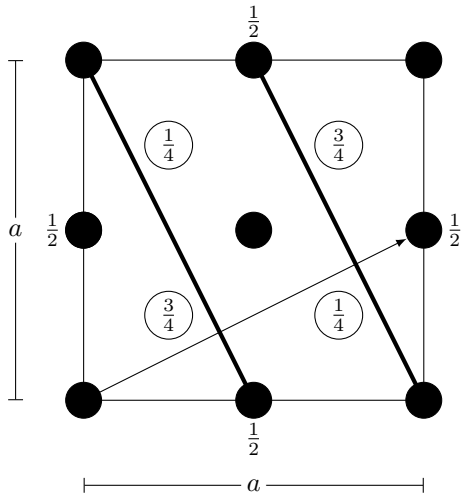
Looking at the fcc conventional cell, it is evident that adjacent Zn atoms are spaced by the distance from the center of the face to the corner; in terms of the lattice constant, this is

$$\ell = a/\sqrt{2} = (0.54\,\mathrm{nm})/\sqrt{2} = 0.38\,\mathrm{nm}$$

The S atoms will be spaced by the same amount, since their primitive unit cell is that of the Zn atoms translated by $[1/4, 1/4, -1/4]a$. The Zn-S spacing is the magnitude of this translation,

$$\sqrt{3a^2/16} = a\sqrt{3}/4 = (0.54\,\mathrm{nm})\sqrt{3}/4 = 0.23\,\mathrm{nm}$$

1d



Note that the arrow lies parallel to the xy-plane and the lattice planes are pointing out of the page from the lines representing them.

1e

Notice from the image that the arrow representing the given direction has length $\sqrt{a^2 + a^2/4} = a\sqrt{5}/2$, and along its length there are two and a half instances of the lattice plane spacing. The spacing between planes is then $a\sqrt{5}/25$.

2

A crystal plane is a plane overlaying a crystalline lattice that intersects at least three non-collinear points of the lattice. Miller indices describe lattice planes by first constructing a reciprocal-space basis corresponding to a direct-space basis of choice, and denoting points of the reciprocal lattice by (hkl) where the numbers are the coefficients of the linear combination of the reciprocal basis vectors that equals the point.