The geometry of perfect crystals

Problem 1:
Find primitive cell to the unit cell of the Bravais face centered cubic lattice, find its volume, the number of contained atoms and shows that the number of atoms to the volume unit is the same in both of cells.
Prove (by algebraic calculation) that founded primitive cell is rhombohedron and find the angles between generating vectors.

Solution:
Let denote the elementary translation vectors as **a**, **b** a **c**, their length are the same, i.e. $a = b = c$. To find the elementary translation vectors of the primitive cell, we have to investigate three of the linear independent vectors **u**, **v**, **w** that connect the closest neighbor atoms. Such three pairs apparently forms closest site-centered atoms with the atom situated in the vortices of the cube. In the base $A = \{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ they are the vectors

$$\mathbf{u}_A = \left(\tfrac{1}{2},\ \tfrac{1}{2},\ 0\right),\ \mathbf{v}_A = \left(\tfrac{1}{2},\ 0,\ \tfrac{1}{2}\right),\ \mathbf{w}_A = \left(0,\ \tfrac{1}{2},\ \tfrac{1}{2}\right).$$

Triple of vectors **u**, **v**, **w** unambiguously defines parallelepiped with the volume

$$V_{\mathbf{uvw}} = \left|\mathbf{u}\cdot\left(\mathbf{v}\times\mathbf{w}\right)\right|.$$

Remember that term inside the absolute value is the triple scalar product that is invariant to the cyclic permutation and antisymmetric to the pair commutation. Geometrical meaning is the oriented volume of the generated parallelepiped. In Cartesian base it could be expressed as determinant with the rows from vector components. Our base is orthogonal but not orthonormal, the unit of the base vectors is a, so to take the proper value of the volume we have to multiply the result with the factor of a^3. Thus

$$V_{\mathbf{uvw}} = \mathrm{abs}\begin{vmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{vmatrix} a^3 = \mathrm{abs}\begin{vmatrix} \tfrac{1}{2} & \tfrac{1}{2} & 0 \\ \tfrac{1}{2} & 0 & \tfrac{1}{2} \\ 0 & \tfrac{1}{2} & \tfrac{1}{2} \end{vmatrix} a^3 = \left|-\frac{1}{4}\right| a^3 = \frac{1}{4}a^3.$$

There are 4 atoms per volume $V_{\mathbf{abc}}$, from them 8 atoms are at the vortices, but every of them is counted as 1/8 because it is always shared with the 8 neighbor cells and 6 atoms in the center of sides but counted as 1/2 because each is shared with the opposite cell touching the side.

There is 1 atom per volume $V_{\mathbf{uvw}}$, because it the case of primitive cell there are present only atoms in vortices.

Because the primitive cell's volume $V_{\mathbf{uvw}}$ is four time smaller than the cubic one $V_{\mathbf{abc}}$, the concentrations of atoms are the same calculated from both primitive and cubic cell respectively, as was expected.

Lengths of **u**, **v** and **w** are the same and equal of $a/\sqrt{2}$, because their end-points are situated in the half of the side-diagonals, what could be also proved from calculation from their components.

Angles between vectors **u** and **v** could be expressed with the scalar product

$$\cos\gamma = \frac{\mathbf{u}\cdot\mathbf{v}}{uv} = \frac{\tfrac{1}{2}\tfrac{1}{2}a^2}{\frac{a^2}{2}} = \frac{1}{2}.$$

Similarly the remaining angles α a β a we have $\alpha = \beta = \gamma = \pi/3$, that means **the rhombohedral cell** (remember that defined with the same length of the generating vectors and with the same angels between them but various from the right angle $\pi/2$.

Problem 2:

Cooper has a density of about 8 885 kg/m^3. Its atomic weight is 63.57.

a) About how many moles of Cu are contained in 1 m^3 of the solid?
b) About how many atoms are contained in 1 m^3?
c) Calculate the size of the unit cube for this fcc metal.
d) Calculate the atomic radius of Cu.
e) What is the weight of a single atom of Cu?

Problem 3:

Iron is bcc below 910 °C and is fcc above 910 °C. The atomic radius is the same in both structures. Calculate the ratio of the densities of bulk iron in the two structures at 910 °C.

Problem 4:

The diamond lattice may be considered to be a combination of two interpenetrating sublattices. One sublattice has its origin at the point (0, 0, 0) and the other at a point one-quarter of the way along the body diagonal.

a) Write the positions of all the atoms in the unit cell.
b) How many atoms are contained in this unit cell?

Problem 5:

Prove that the direction [$h\ k\ l$] is the normal to the plane ($h\ k\ l$) for the cubic lattice.

Problem 6:

An orthorhombic structure is one in which the unit-cell edges are mutually orthogonal but are unequal in length. Draw a (321) plane and a [321] direction. Find the angle between the [3 2 1] and the normal to the (3 21) plane for the ratio of unit-cell edge lengths of 1:1:2.

Problem 7:

Show that the distance d between adjacent planes of types ($h\ k\ l$) in a cubic lattice of cubic edge a is given as

$$d = \frac{a}{\left(h^2 + k^2 + l^2\right)^{\frac{1}{2}}}.$$

Problem 8:

How many planes of type {$h\ k\ l$} are found in the cubic systems? Of type {$h\ k$ 0}?