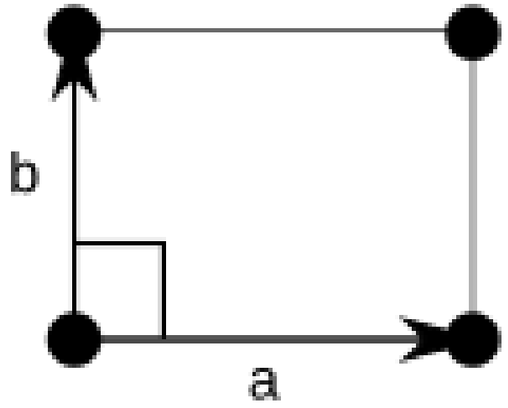
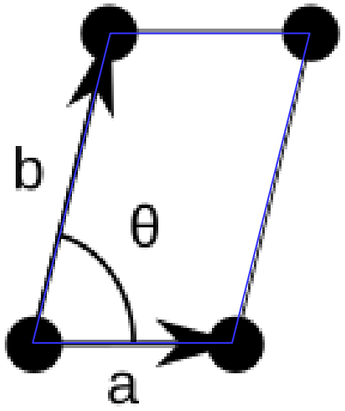
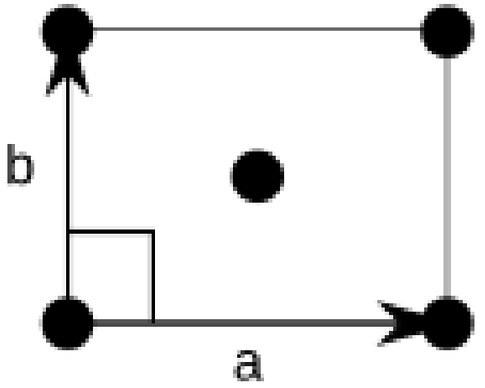
Homework 3.2

- Please identify and label the mirror planes in unit cell for the following 2D lattices ($a \neq b$):



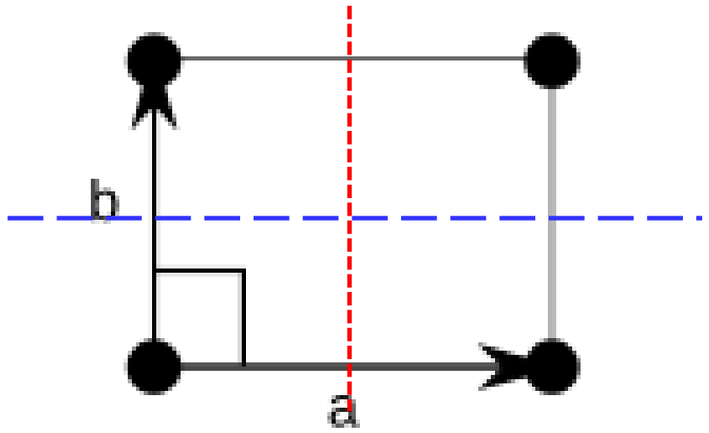




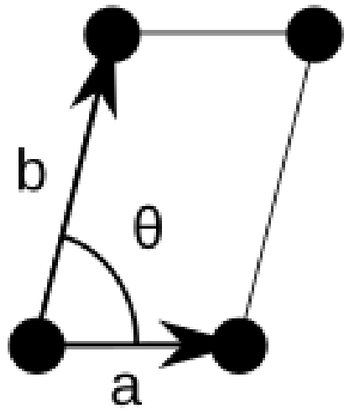
- For the above 2D unit cell, what rotational symmetry does the unit cells have? (e.g., a 6-fold rotational symmetry means a pattern rotates 60^o and would repeats itself)
- What is the coordination number (CN) for each of the above 2D lattices (**only counting the <u>nearest</u> neighbors**)? Please draw the pattern following the hard-circle (not sphere since 2D) model and give the math relationship, if applicable, between circle radius *R* and lattice constants (*a* or *b*)

Homework 3.2 (2)

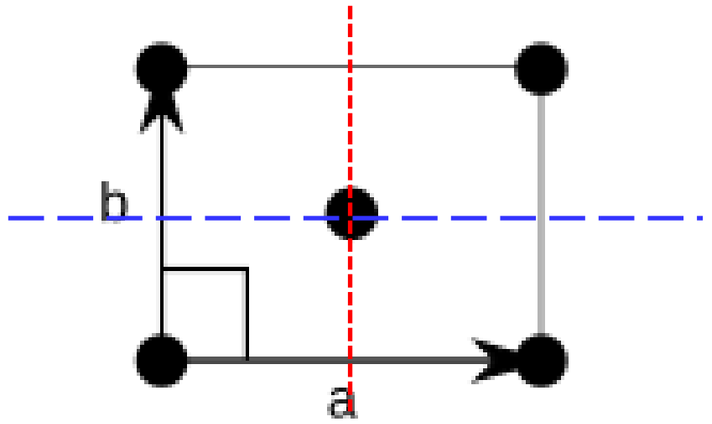
- Mirror planes in 2D unit cell ($a \neq b$):



2 mirror planes



NO mirror plane



2 mirror planes

- Rotation symmetry

2-fold rotation (apart from identity)

2-fold rotation (apart from identity)

2-fold rotation (apart from identity)

- Coordination number (CN), in 2D

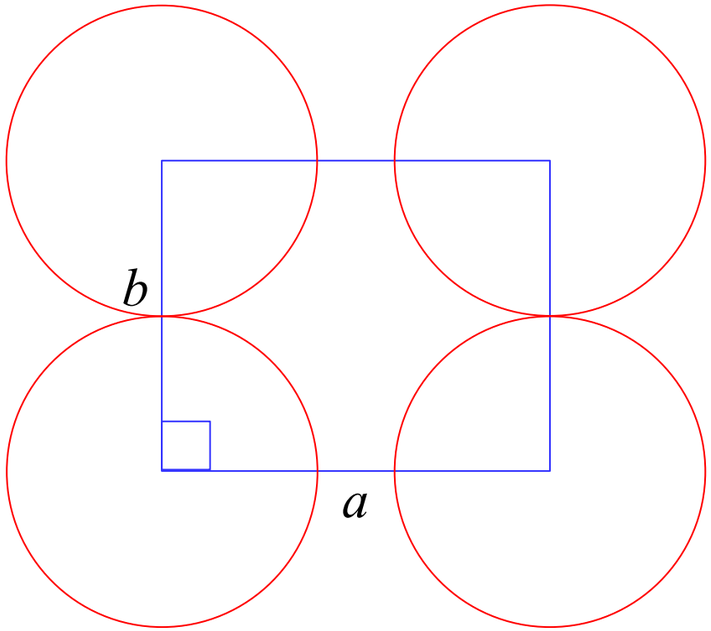
CN = 2
(Note: some sources claim CN = 4, when 2nd nearest neighbor is counted as well, since $a > b$)

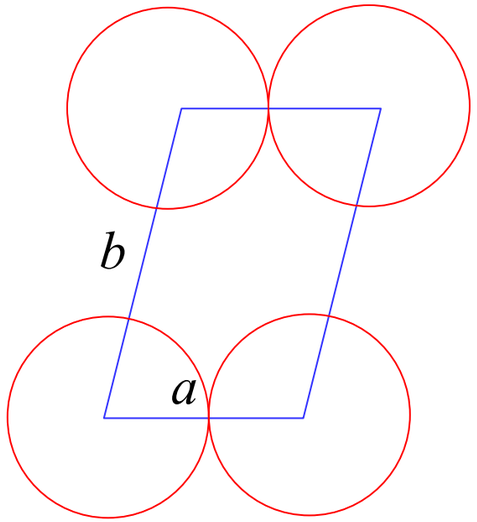
CN = 2

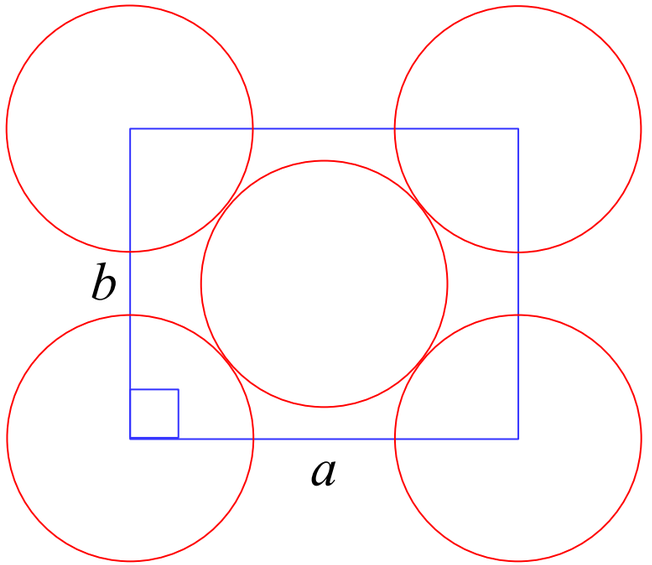
CN = 4

Homework 3.2 (3)

- Hard circle (i.e., 2D) model schematics







- Math relationship between circle radius R and 2D lattice constants (a or b)

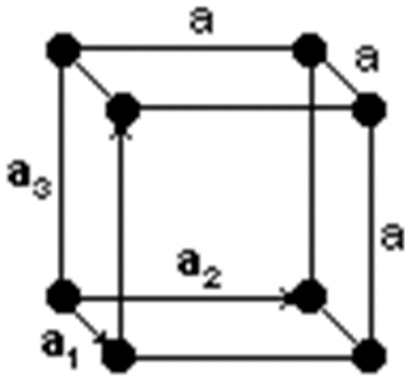
$b = 2R$

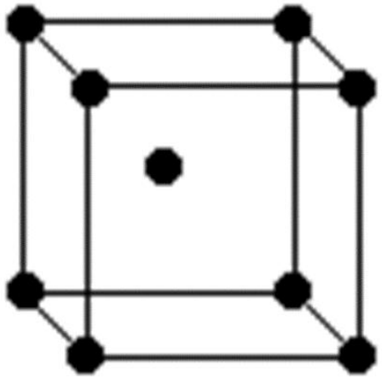
$a = 2R$

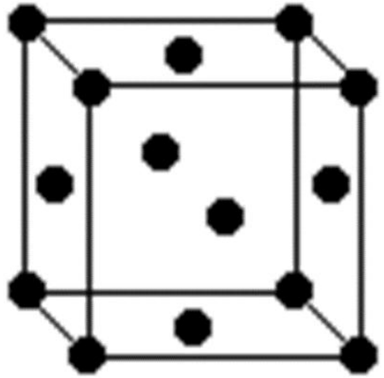
$\sqrt{a^2 + b^2} = 4R$

Homework 3.3

Please derive the mathematical relationship between lattice parameter *a* and atom radius *R* (e.g., *a* = ?? *R*) for the three cubic lattices: simple cubic, body centered cubic, and face-centered cubic. Make sure to draw 3D/2D figures to help show the validity of your derivation

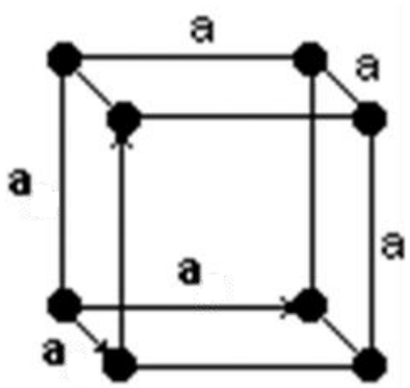


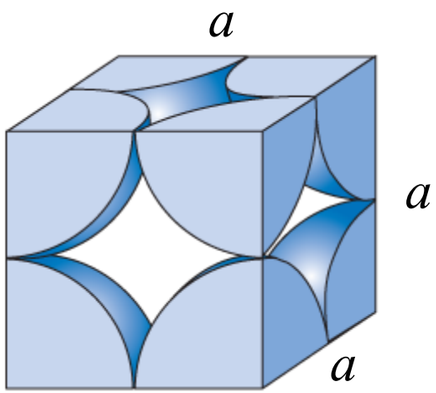


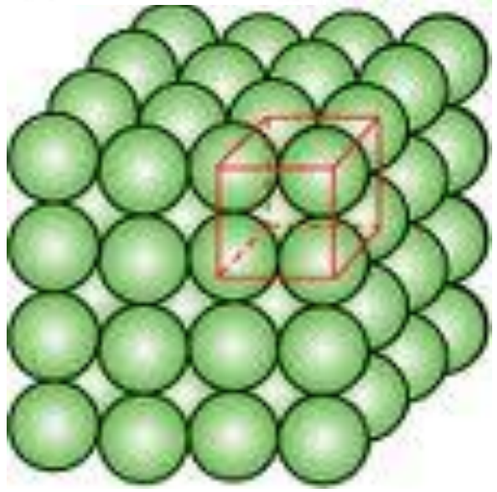


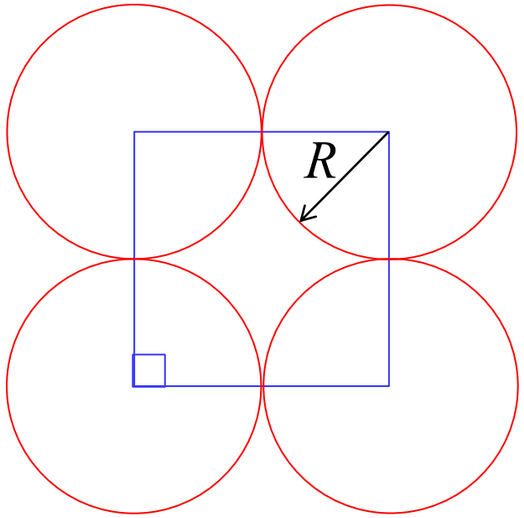
Homework 3.3 (2)

Simple cubic (SC)





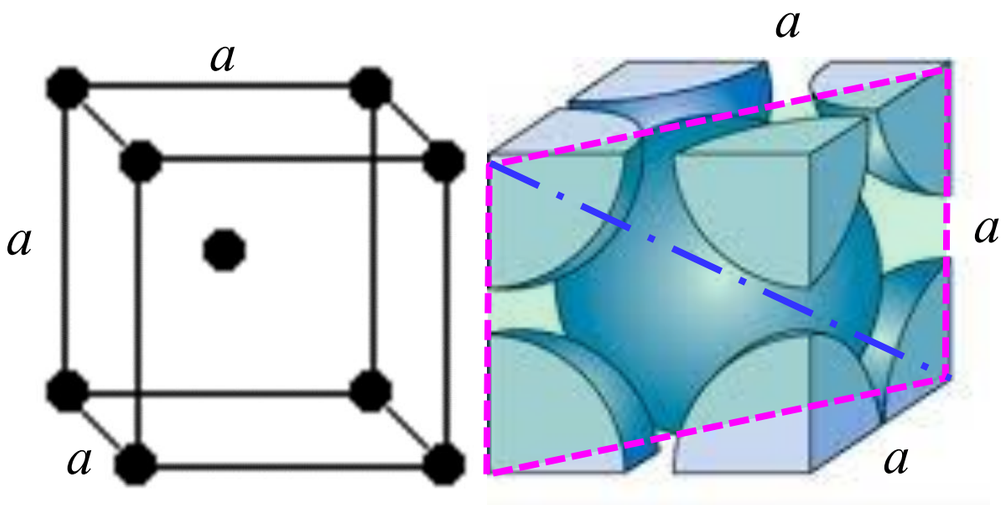


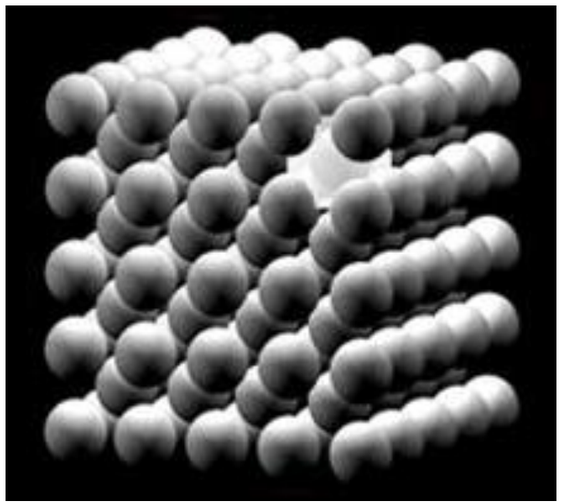


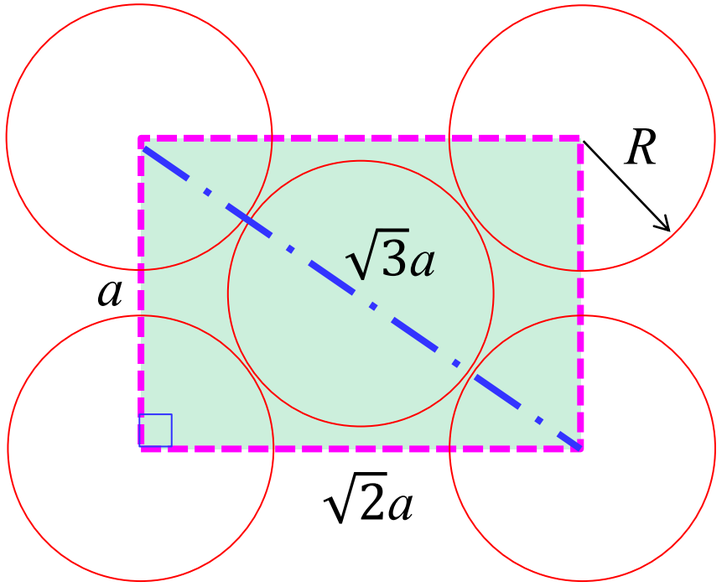
$$a = 2R$$

Homework 3.3 (3)

Body centered cubic (BCC)





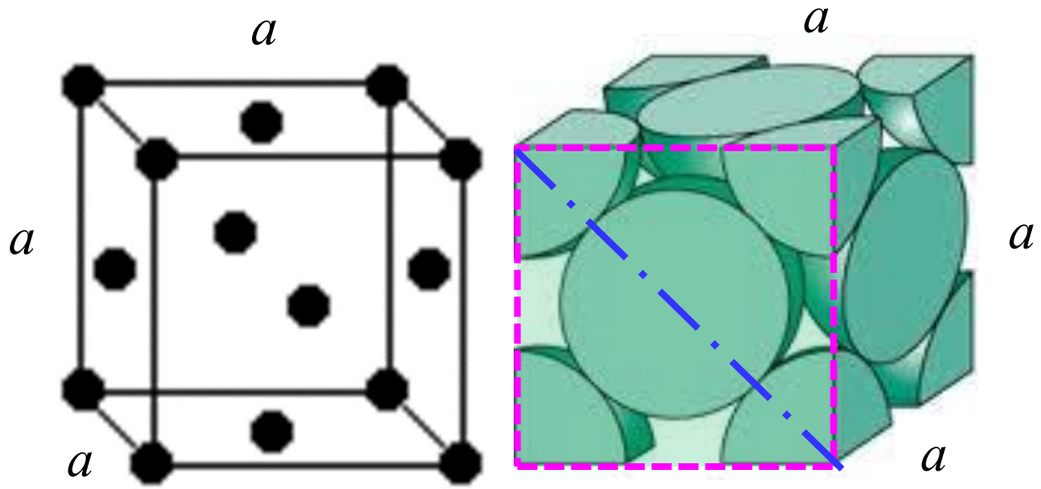


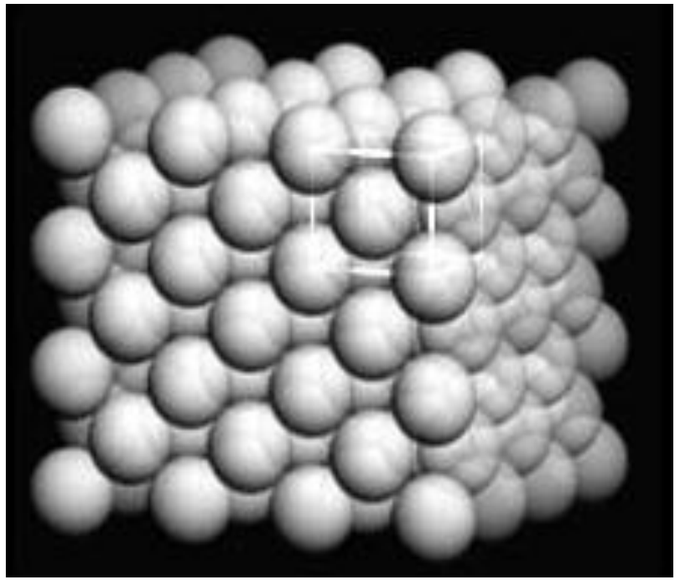
$$\sqrt{3}a = 4R$$

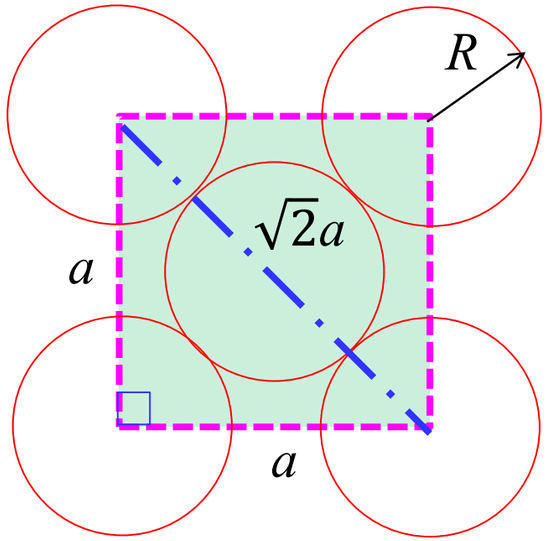
$$a = \frac{4}{\sqrt{3}}R$$

Homework 3.3 (4)

Face centered cubic (FCC)







$$\sqrt{2}a = 4R$$

$$a = 2\sqrt{2}R$$

Homework 3.4

Please estimate the density for solid aluminum metal, knowing that aluminum has face-centered cubic (FCC) crystal structure with a lattice constant of 0.405 nm. Refer to periodic table for information about aluminum atomic mass.

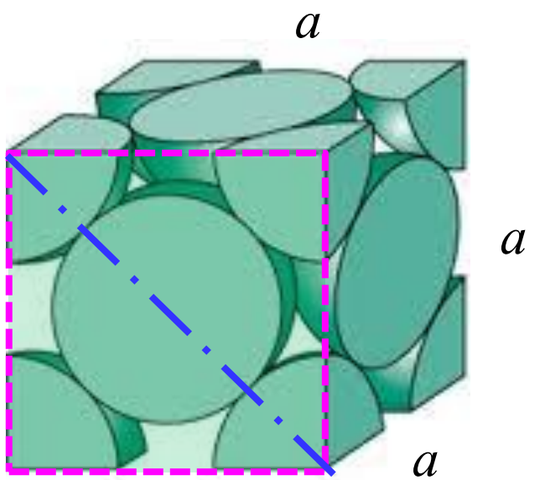
Volume of the metal aluminum unit cell $V_{Al} = ?? = ???$

Effective number of Al atoms WITHIN a unit cell: $N_{Al} = ? + \frac{1}{??} \times ?? + \frac{1}{???} \times ???? = ?????$

Mass of a single Al atom $m_{Al\ atom} = \frac{?}{??} = ??? \text{ unit?}$

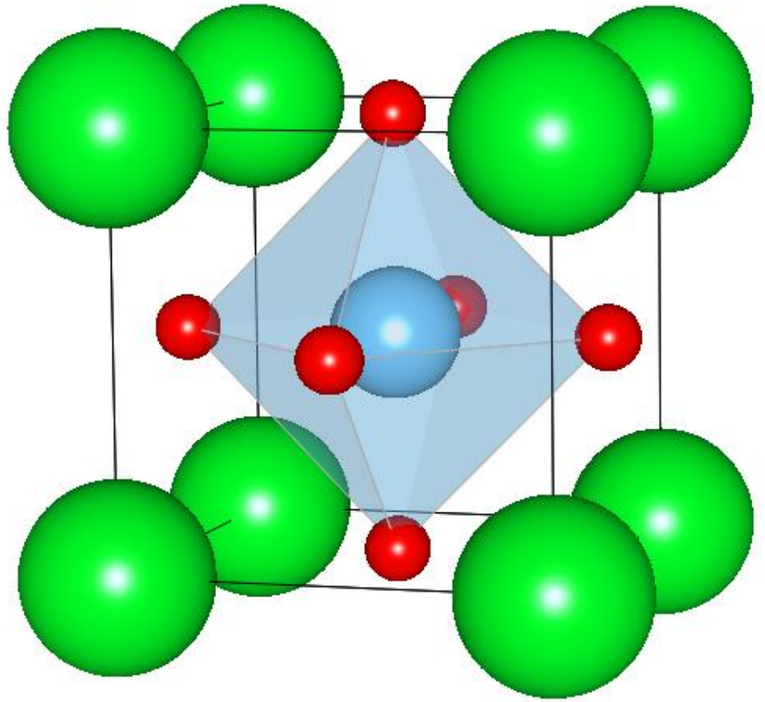
Aluminum theoretical density

$$\rho_{Al\_theory} = \frac{Total\ mass\ of\ Al\ within\ a\ unit\ cell}{Volume\ of\ a\ unit\ cell} = \frac{?}{??} = 2.699\ g/cm^3$$



Homework 3.5

The unit cell structure for a compound of Sr (in green large sphere), Ti (light blue medium sphere), and O (red smallest sphere) is shown below. Knowing that it is a **cubic** structure, with Sr at the corner, Ti at the cube center, while O are at the face center,



- Please give the chemical formula for the compound; be sure to explain it using the geometric information
- Please estimate the density for this material, if the lattice parameter is 0.3905 nm (refer to periodic table for atomic mass information)
- What are the length for the Sr-O bond? What about the Ti-O bond?
- What is the coordination number for Sr and Ti and why? Draw to help illustrate

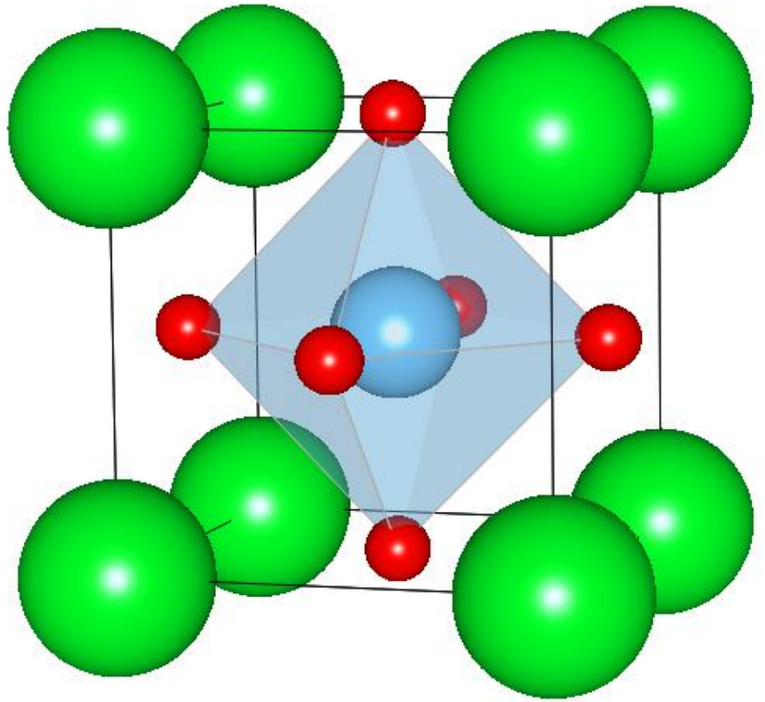
Homework 3.5 (2)

Chemical formula

Within a unit cell, there are

- ? Sr: ? corners, each counts as ??
- ?? Ti: ? at cube center
- ??? Oxygen: ? face center, each counts as ??

Therefore, atom ratio Sr : Ti : O = 1 : 1 : 3, i.e., chemical formula: **$SrTiO_3$**



Density

Unit cell volume: $V_{SrTiO3} = ? = ??$

Mass of a $SrTiO_3$ unit cell

$$m_{\text{SrTiO3 unit cell}} = \frac{(? + ?? + ??? \times ????)\ g/mol}{\#?\ /mol}$$

$SrTiO_3$ theoretical density

$$\rho_{\text{SrTiO3\_theory}} = \frac{\text{Total mass of Al within a unit cell}}{\text{Volume of a unit cell}} = \frac{?}{??} = \mathbf{5.119\ g/cm^3}$$

Homework 3.5 (3)

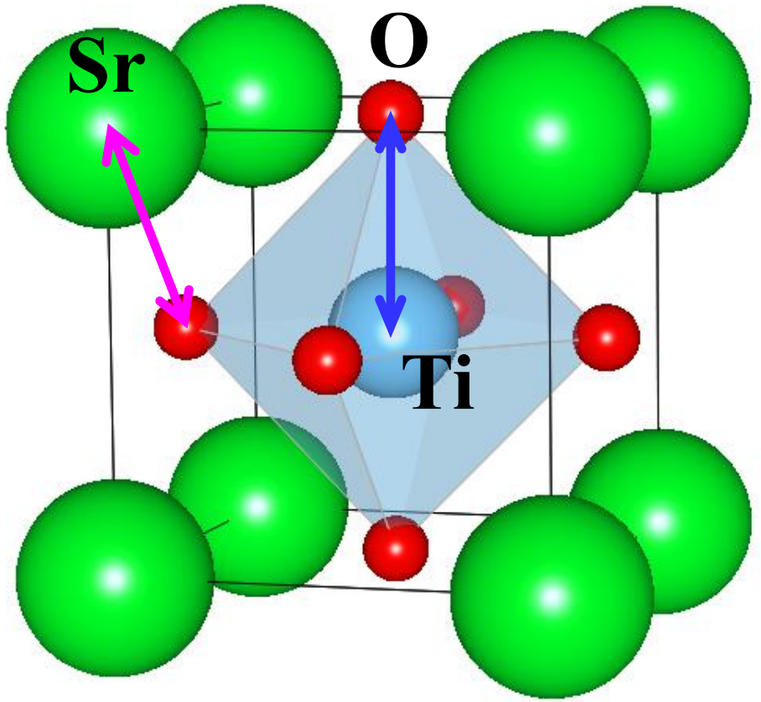
Bond length

Ti-O bond length is half of cubic unit cell edge length (or lattice constant)

$$L_{\mathrm{Ti-O}} = ?\ a = \cdots = \mathbf{0.1953\ nm}$$

Sr-O bond length is half of unit cell surface diagonal

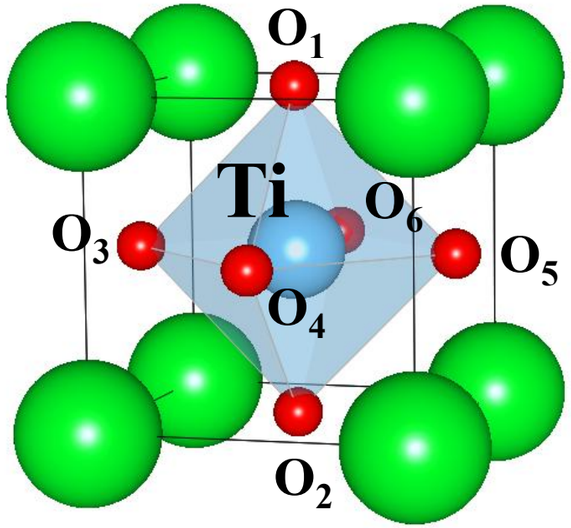
$$L_{\mathrm{Sr-O}} = ? \cdot ? \, ?\, a = \cdots = \mathbf{0.2761\ nm}$$



Coordination number

Ti is touching ? O (up/down, left/right, front/back):

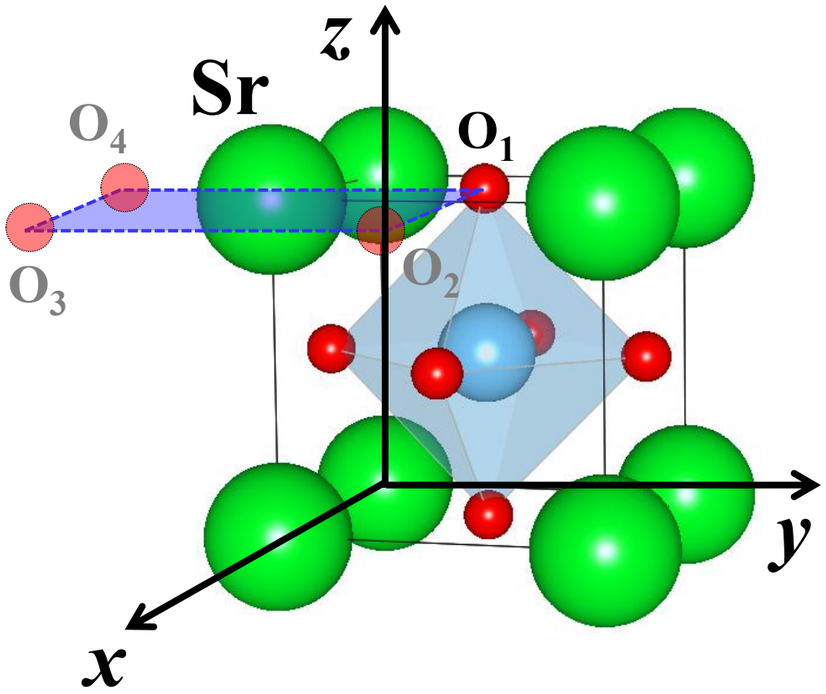
Therefore, **CN (Ti) = 6** (see below schematic)



Homework 3.5 (2)

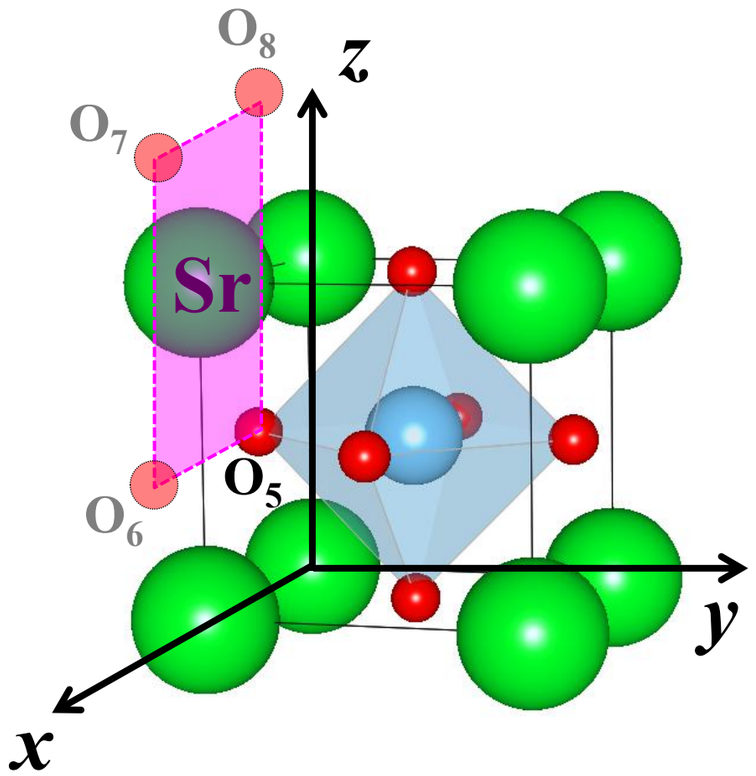
Coordination number

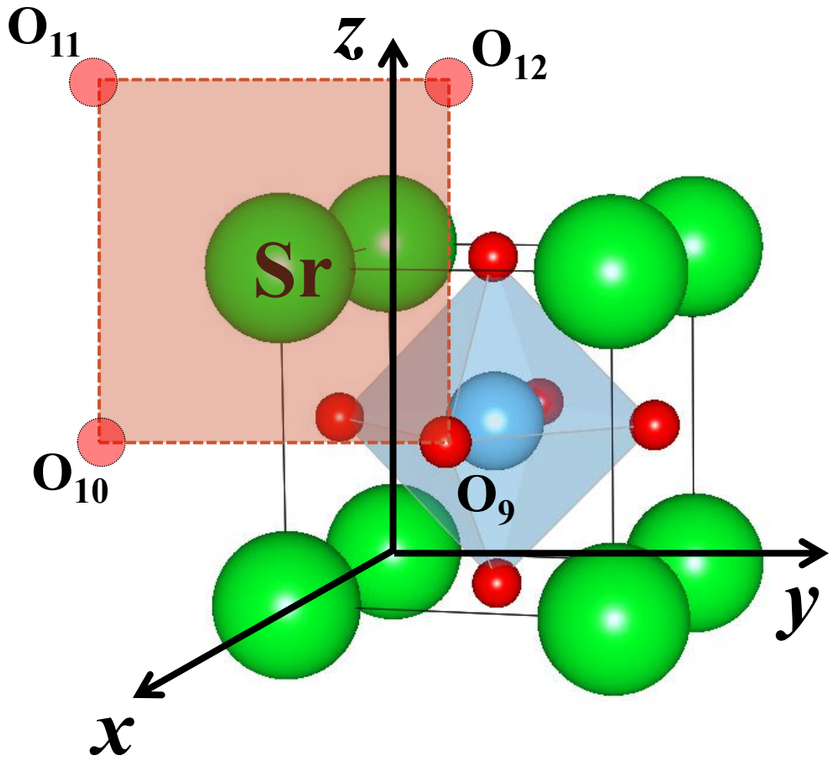
Sr is touching twelve (12) O: **CN (Sr) = 12** (4 in each plane: *x*-*y* plane, *x*-*z* plane, and *y*–*z* plane, as shown below)



O_2, O_3, O_4 are outside of the cubic unit cell

O_6, O_7, O_8 are outside of the cubic unit cell





O_{10}, O_{11}, O_{12} are outside of the cubic unit cell

Homework 3.6

Assuming the hard-sphere model for a pure element with body-centered cubic (BCC) structure, if **atomic packing factor (APF)** is defined as the ratio between volume occupied by all atoms within a unit cell to the total volume of that unit cell, i.e.,

$$APF = \frac{\text{Volume for all atoms } \mathbf{within} \text{ a unit cell}}{\text{Total volume of that unit cell}}$$

Please calculate the APF the body centered cubic structure and show your steps

The total volume for the cubic unit cell $V_{cell} = ?$

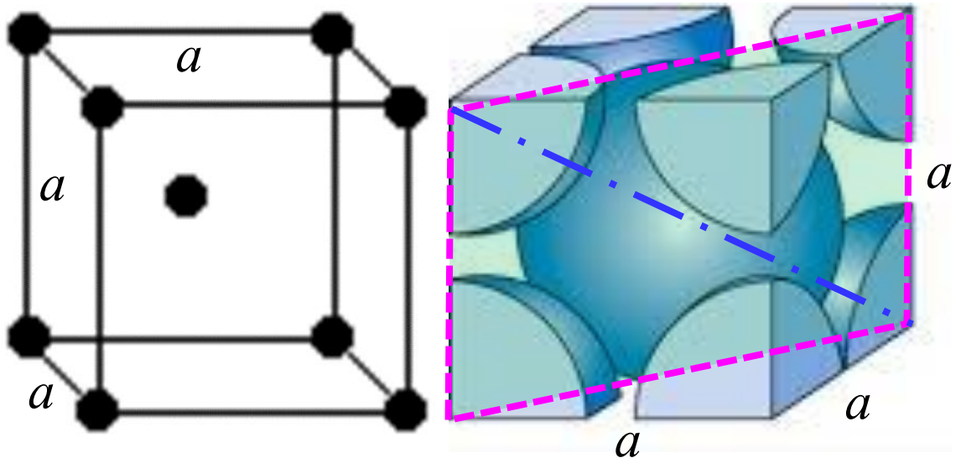
Effective number of atoms (or hard spheres) WITHIN a BCC unit cell:

$$N_{\text{atom in BCC}} = \ldots = 2$$

The total volume for ALL atoms (or spheres) WITHIN BCC unit cell

$$V_{\text{total atom}} = \cdots = ? \times ??$$

Body centered cubic (BCC)



Recall for BCC, $a = ??? \; R$ Therefore, $APF_{\text{BCC}} = \frac{?}{??} = \frac{???}{????} = \cdots = \frac{\sqrt{3}\pi}{8} \approx 68\%$