[1] Face centered cubic interstices

Consider a face centered cubic lattice of conventional lattice constant \( a \) with a hard sphere centered on each lattice point with a radius \( R \) such that each sphere touches its nearest neighbors.

![Figure 1: Face Centered Cubic conventional unit cell.](image)

(a) Express the sphere radius \( R \) in terms of \( a \).

The distance between the centers of two spheres touching is

\[ 2R = \frac{a}{\sqrt{2}} \]

so

\[ R = \frac{a}{2\sqrt{2}} = \frac{a\sqrt{2}}{4} \]

(b) Identify the two types of interstices where impurity atoms could be lodged between the normal crystal atoms.

(c) Modeling the interstitial atom as a hard sphere of radius \( r \), establish the maximal value of \( r \) in terms of the lattice constant \( a \) for both types of interstitial space.

First type of interstitial spaces

Think of one of the corner spheres & the three face centering spheres touching it in the conventional cell. These three spheres also touch each other, so the four spheres together form a tetrahedron at the center of which an interstitial impurity could lodge.

To find the maximal radius of a sphere that could fit in this space, consider the 3 spheres of radius \( R \) centered in \((t,0,0)\), \((0,t,0)\) & \((0,0,t)\). For them to just touch, we need \( \sqrt{2}t = 2R \) so \( t = \sqrt{2}R \).

Consider now the 4th sphere centered in \((t',t',t')\). For it to touch the three others, we need

\[ (2R)^2 = 2t' + (t-t')^2 \]

\[ = \frac{1}{2}t^2 + \left(\sqrt{2}R - t'\right)^2 = 3t'^2 + zR^2 - 2\sqrt{2}Rt' \]

So \( 3t'^2 - 2\sqrt{2}Rt' - zR^2 = 0 \) (yes there are two ways for the 4th sphere to touch the three others), and one solution is \( t' = \sqrt{2}R \) so this sphere has its center at a distance \( \sqrt{6}R \) from the origin of the coordinate system.
The center of the tetrahedron will be \((\lambda, \lambda, \lambda)\) with \(\lambda = \frac{R}{\sqrt{2}}\), which is at a distance \(\sqrt{\frac{3}{2}} R\) from the origin of the coordinate system. So the maximal radius \(R_{\text{max}}\) of the impurity lodging in the tetrahedral interstice is the distance between the center of the tetrahedron & the center of the system in \((\lambda, \lambda, \lambda)\) from which \(R\) must be subtracted, that is

\[
R_{\text{TETRA}} = (\sqrt{6} - \sqrt{\frac{3}{2}} - 1) R = \frac{\sqrt{3} - \sqrt{2}}{4} a = 0.07946 a
\]

**Note:** That was a lot of writing because a drawing was difficult.

- **Second type of interstitial spaces**

  → Consider now the four spheres at the centers of the faces of the conventional unit cell. They form an octahedron at the center of which an impurity can lodge.

  → The maximal radius can be obtained straightforwardly from the figure & is

\[
R_{\text{MAX}}^{\text{OCT}} = (\sqrt{2} - 1) R = \left(\frac{1}{2} - \frac{\sqrt{2}}{4}\right) a = 0.1464 a
\]

(d) What is the number of interstitial space of each type per conventional unit cell?

→ There is one tetrahedron for each corner of the conventional unit cell. That makes 8 tetrahedral interstices per conventional unit cell.

→ There is one octahedron at the center of the conventional unit cell plus one quarter of a tetrahedron on each corner edge of the conventional unit cell, so we have \(1 + \frac{12}{4} = 4\) octahedral interstices per conventional unit cell.
Crystal structure and density

Iron can be found under both body centered cubic (BCC) and face centered cubic (FCC) depending on temperature. We will assume each atom can be modeled as a hard sphere the radius \( R \) of which is the same in both phases and is such that each sphere just touches its direct neighbors.

(a) What is the ratio of densities between the two phases?

- **FCC**: In the previous exercise, we established \( a = \frac{4 \sqrt{2} R}{3} \) and there are \( \frac{8}{8} + \frac{6}{2} = 4 \) atoms per conventional unit cell.
- **BCC**: The body diagonal of the conventional unit cell is \( \sqrt{3} a = 4R \), so \( a = \frac{4}{\sqrt{3}} R \) and there are \( \frac{8}{8} + 1 = 2 \) atoms per conventional unit cell.

The density ratio then is

\[
\frac{\rho_{\text{FCC}}}{\rho_{\text{BCC}}} = \frac{4}{2} \left( \frac{4 \sqrt{3}/3}{2 \sqrt{2}} \right)^3 = \frac{4 \sqrt{2}}{3} \approx 1.0886
\]

(b) In its BCC phase, iron has a mass density of 7900 kg m\(^{-3}\). What is the conventional lattice constant?

The atomic mass of iron is \( 56 \times 10^{-3} \text{ kg mol}^{-1} \) and in the BCC phase, the density is:

\[
\rho_{\text{BCC}} = \frac{2 M_{\text{Fe}}}{a^3} \quad \text{so} \quad a = \left( \frac{2 M_{\text{Fe}}}{\rho} \right)^{1/3}
\]

Numerically:

\[
a = \left( \frac{2 \times 56 \times 10^{-3} / 6.02 \times 10^{23}}{7900} \right)^{1/3} = 2.866 \times 10^{-10} \text{ m} = 2.866 \text{ Å}
\]

Cubic crystals neighboring relations

We consider cubic lattices of conventional lattice constant \( a \). It may be helpful to consider the primitive vectors \( a \hat{x}; a \hat{y}; a \hat{z} \) along which the cubic lattice is aligned and one lattice point \( O \) in \((0;0;0)\) as the origin of the coordinate system.

(a) For the simple cubic lattice, establish the number and relative positions of the nearest and second nearest neighbors

- **First neighbors**: \( a(1,0,0); a(-1,0,0); a(0,1,0); a(0,-1,0); a(0,0,1) \) & \( a(0,0,-1) \)
- **Second neighbors**: \( a(1,1,0); a(1,-1,0); a(-1,1,0); a(-1,-1,0); a(-1,0,1); a(-1,0,-1); a(1,0,1); a(1,0,-1); a(-1,0,1) \) & \( a(-1,0,-1) \).
(b) For the body centered cubic lattice, establish the number and relative positions of the nearest and second nearest neighbors

There are 8 first neighbors in:

\[ \frac{a}{2} \left( 1, 1, 1 \right); \frac{a}{2} \left( 1, 1, -1 \right); \frac{a}{2} \left( 1, -1, -1 \right); \frac{a}{2} \left( 1, -1, 1 \right); \]
\[ \frac{a}{2} \left( -1, 1, 1 \right); \frac{a}{2} \left( -1, 1, -1 \right); \frac{a}{2} \left( -1, -1, -1 \right) \& \frac{a}{2} \left( -1, -1, 1 \right); \]

There are 12 second neighbors in:

\[ \frac{a}{2} \left( 1, 0, 0 \right); \frac{a}{2} \left( -1, 0, 0 \right); \frac{a}{2} \left( 0, 1, 0 \right); \frac{a}{2} \left( 0, -1, 0 \right); \]
\[ \frac{a}{2} \left( 0, 0, 1 \right) \& \frac{a}{2} \left( 0, 0, -1 \right); \]

(c) For the face centered cubic lattice, establish the number and relative positions of the nearest and second nearest neighbors

There are 12 first neighbors in:

\[ \frac{a}{2} \left( 1, 1, 0 \right); \frac{a}{2} \left( 1, -1, 0 \right); \frac{a}{2} \left( -1, -1, 0 \right); \frac{a}{2} \left( -1, 1, 0 \right); \frac{a}{2} \left( 1, 0, 1 \right); \frac{a}{2} \left( 1, 0, -1 \right); \]
\[ \frac{a}{2} \left( -1, 0, -1 \right); \frac{a}{2} \left( -1, 0, 1 \right); \frac{a}{2} \left( 0, 1, 1 \right); \frac{a}{2} \left( 0, 1, -1 \right); \frac{a}{2} \left( 0, -1, -1 \right) \& \frac{a}{2} \left( 0, -1, 1 \right); \]

There are 6 second neighbors in:

\[ a \left( 1, 0, 0 \right); a \left( -1, 0, 0 \right); a \left( 0, 1, 0 \right); a \left( 0, -1, 0 \right); a \left( 0, 0, 1 \right) \& a \left( 0, 0, -1 \right); \]