IFES Report

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Contents

ABSTRACT

1 Chapter 1

Structures and Cell Dimensions of Some Elements and Compounds

Element or compound	Structure	a, Å	c, Å
Al	fcc	4.04	
Be	hcp	2.27	3.59
Ca	fcc	5.56	

Figure 1

Unit Cell

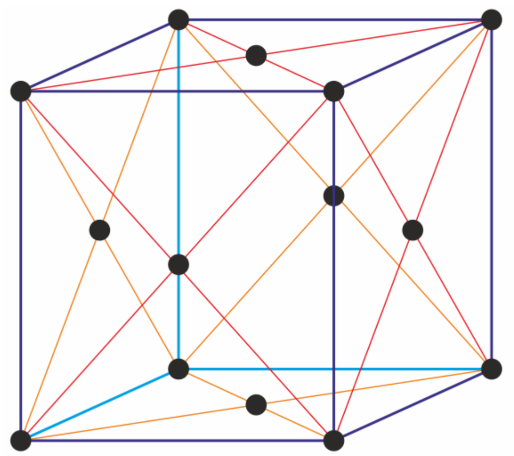

Figure 2: FCC-Lattice

Primitive Vectors

The three primitive vectors are

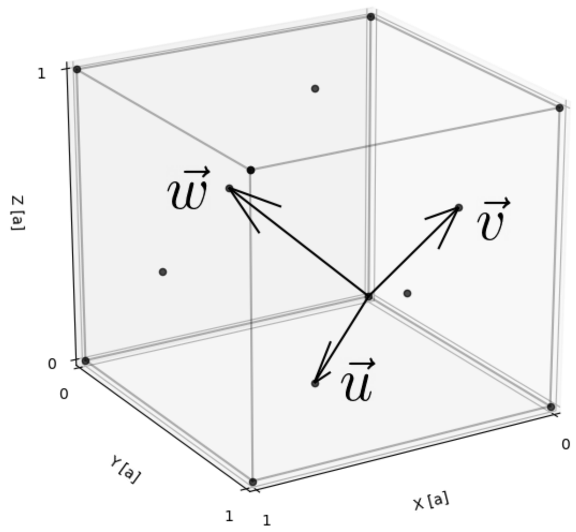

Figure 3: Primitive Vectors in a FCC-Lattice

$$\vec{u} = \frac{a}{2}\begin{pmatrix}1\\1\\0\end{pmatrix} \qquad \vec{v} = \frac{a}{2}\begin{pmatrix}0\\1\\1\end{pmatrix} \qquad \vec{w} = \frac{a}{2}\begin{pmatrix}1\\0\\1\end{pmatrix}$$

Whith these 3 base vectors a parallelepiped is given which is a primitive cell. The volume of the primitive cell can be calculated with the following formula

$$V_{PC} = |(\vec{u} \times \vec{v}) \cdot \vec{w}|$$

which equals (with $a = 5.56\,\mathring{A}$)

$$V_{PC} = \frac{a^3}{4} = 4.297 \cdot 10^{-30}\,m^3 = 4.297 \cdot 10^{-24}\,cm^3$$

Packaging Factor

The Packaging Factor can be calculated as the ratio between the volume of the atoms in the unit cell to the volume of the unit cell.

The volume of the unit cell can be calculated as:

$$V_{UC} = a^3$$

The unit cell containts 4 whole atoms. One eighth of a atomic sphere at each corner (8) and one half at each cube face (6).

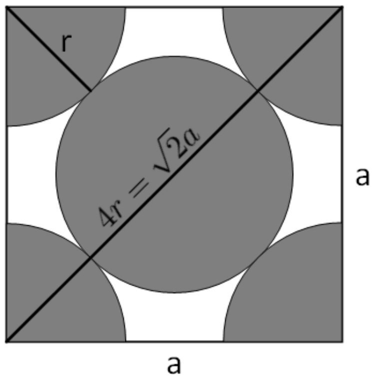

Figure 4: Relation between the atomic radius and the parameter a in a FFC

As Figure 4 shows the relationship between the parameter a and the radius of the atomic sphere is given as:

$$r = \frac{\sqrt{2}}{4}a$$

And further the volume of the sphere

$$V_{Atom} = \frac{4}{3}\pi r^3 = \frac{a^3\pi}{\sqrt{2^5}\cdot 3}$$

So the Atomic Packaging Factor APF can be calculated as ratio between the volume consumed by the atoms to the whole volume.

$$APF = \frac{4\cdot V_{Atom}}{V_{UC}} = \frac{\pi}{3\cdot\sqrt{2}} \approx 74\%$$

Density

The atomic mass of calcium us given as:

$$M_{Ca} = 40.078\frac{g}{mol}$$

$$\rho = \frac{4}{N_A}\cdot\frac{M_{Ca}}{V_{UC}} = 1.55\frac{g}{cm^3}$$

Planes

In the following the planes $P1 : (0\bar{3}2)$ and $P2 : (\bar{1}21)$ are drawn inside the unit cell. The Miller-Indices of the planes corresbond to the following plane equations:

$$P1: \quad -\frac{1}{3}y + \frac{1}{2}z = 1$$

$$P2: \quad -x + \frac{1}{2}y + z = 1$$

With respect of the fact that all parallel planes have the same Miller-Indices the planes which were drawn are:

$$P1: \quad z = \frac{2}{3}y$$

$$P2: \quad z = x - \frac{1}{2}y$$

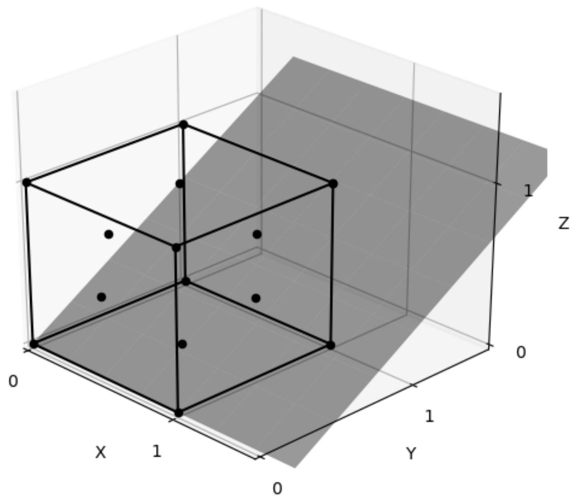

Figure 5: $(0\bar{3}2)$-Plane in a FCC-Lattice

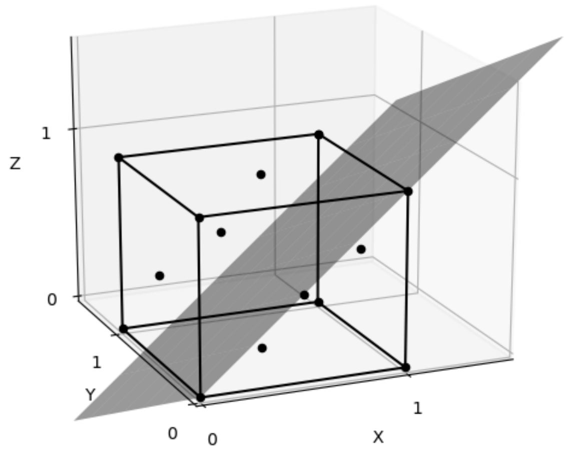

Figure 6: ($\bar{1}21$)-Plane in a FCC-Lattice

Linear Density [110]

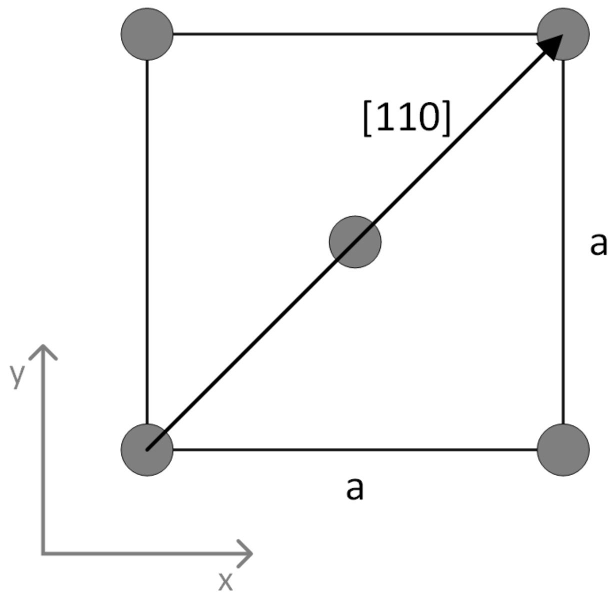

Figure 7: Linear Density of FCC in [110] Direction

Figure 7 shows the [110] direction in a FCC lattice. As you can see the [110] direction includes 2 atoms inside a length of $\sqrt{2}a$.

Therefore (with $a = 5.56\,\mathring{A}$)

$$\lambda = \frac{2\,Atoms}{\sqrt{2}a} = \frac{\sqrt{2}}{5.56}\frac{Atoms}{\mathring{A}}$$

Potential Energy

The potential energy between to adjacent ions can be represented by

$$E(r) = -\frac{A}{r} + \frac{B}{r^n} \tag{1}$$

To calculate the bonding energy $E_0 = E(r_0)$, which is a minimum of the function $E(r)$, the derivative has to equals zero. The negative derivative of the bonding energy equals the interatomic force.

$$F(r) = -\frac{\partial E(r)}{\partial r} = 0$$

$$-\frac{A}{r^2} + \frac{nB}{r^{n+1}} = 0$$

$$\Rightarrow r_0 = \left(\frac{A}{nB}\right)^{\frac{1}{n-1}}$$

By inserting the result for r_0 into Equation 1, the bonding energy E_0 in terms of A, B and n results as:

$$E_0 = E(r_0) = -\frac{A}{\left(\frac{A}{nB}\right)^{\frac{1}{n-1}}} + \frac{B}{\left(\frac{A}{nB}\right)^{\frac{n}{n-1}}}$$

2 Chapter 2

asdf

3 Chapter 3

Density of States (1D)

We start with the 1-D wave equation:

$$\frac{\partial^2 u}{\partial x^2} - \frac{\rho}{Y}\frac{\partial u}{\partial t} = 0$$

Which delivers a solution in the way of:
(The time depence is not needed for calculatiing the density of states)

$$u = Ae^{iqx} \tag{2}$$

By using the boundary conditions:

$$u(x = 0) = u(x = L)$$

We get:

$$e^{iqL} = 1$$

Due to Eulers-Equation we get for q

$$q = n\frac{2\pi}{L}$$

$$g(\omega) = \frac{L}{\pi}\frac{1}{\frac{d\omega}{dq}} \tag{3}$$

$$g(\omega) = \frac{L}{\pi}\frac{1}{v_s} \tag{4}$$

Density of States (3D)

Starting with the solution for the wave equation as same as in the 1-D case (Equation 2) we get:

$$u = Ae^{i(q_x x + q_y y + q_z z)} \tag{5}$$

By applying the same boundary conditions as in the 1-D case we get:

$$u = e^{i(q_x x + q_y y + q_z z)} = 1 \tag{6}$$

$$(q_x,\, q_y,\, q_z) = (n\frac{2\pi}{L},\, m\frac{2\pi}{L},\, l\frac{2\pi}{L})$$

$$g(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v_s^3} \tag{7}$$

As there are three different modes associated with the same value for q. (one longitudinal and 2 transversal modes). Equation 7 has to be multiplied by a factor of three to get the correct result.

$$g(\omega) = \frac{3V}{2\pi^2}\frac{\omega^2}{v_s^3} \tag{8}$$

Debye Frequency

Monoatomic 1D chain

We are going to consider elastic vibrations of the atomic network in classic terms. We assume that:

1. The average equilibrium position of each atom is placed at the Bravais network node.
2. Atomic deflections from equilibrium positions are small compared to the distances between atoms. This assumption leads to harmonic approximation allowing for simplification accounts
3. We will use the Born-Openhaimer adiabatic approximation: the velocities of electrons are on the order of $10^8 \frac{\mathrm{cm}}{\mathrm{s}}$, while the velocities of nuclei in atoms on the order of at most $10^5 \frac{\mathrm{cm}}{\mathrm{s}}$. When considering the motion of whole atoms or ions can therefore be assumed that electrons are always in their own ground state for a specific atom position.

If the waves propagate in a crystal with a regular structure the entire network planes move in phase, in direction or in parallel or perpendicular to the direction of the wave. After considering every of those statements the frequency of normal vibration modes $\omega(k)$ of modes with wave vector k (dispersion relationship) can be expressed by:

$$\omega^2 = 4K\sin^2\left(\frac{ka}{2}\right) \tag{9}$$

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