IFES Report

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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

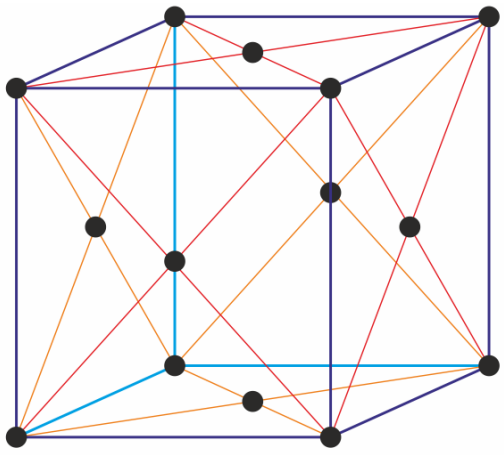

Figure 2: FCC-Lattice

Primitive Vectors

The three primitive vectors are

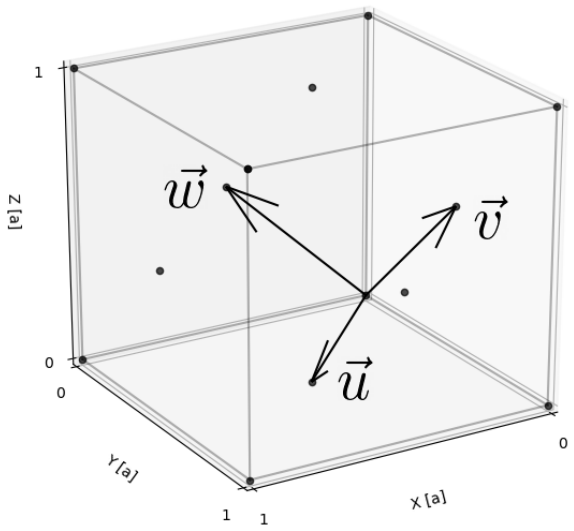

Figure 3: Primitive Vectors in a FCC-Lattice

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

The volume 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

The relationship between the parameter a and the radius of the Radius of the atomic sphere is given as:

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

$$APF = \frac{\pi}{3 \cdot \sqrt{2}} \approx 74\%$$

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:

$$P1: \quad z = \frac{2}{3}y$$
$$P2: \quad z = x - \frac{1}{2}y$$

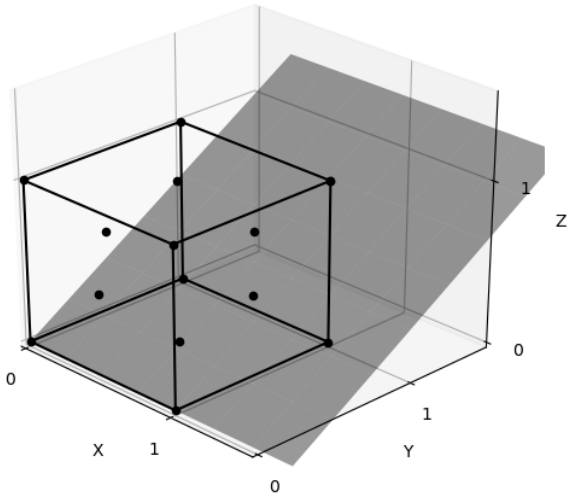

Figure 4: $(0\bar{3}2)$-Plane in a FCC-Lattice

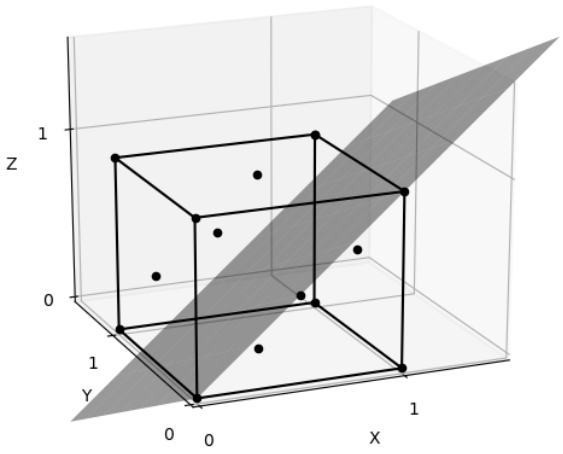

Figure 5: $(\bar{1}21)$-Plane in a FCC-Lattice

Linear Density [110]

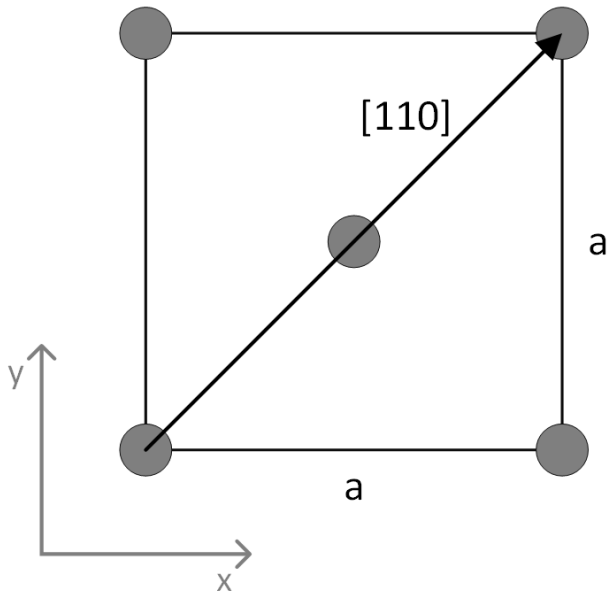

Figure 6: Linear Density of FCC in [110] Direction

$$\lambda = \frac{2 \cdot m_{Ca}}{\sqrt{2}a}$$

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

asdf

$$g(\omega) = \frac{L}{\pi}\frac{1}{v_s} \qquad \omega = k \cdot v_s \tag{2}$$

$$g(\omega) = \frac{V}{\pi}\frac{1}{v_s} \qquad \omega = k \cdot v_s \tag{3}$$

$x = 2$

$$x = 2$$

$$x = 2 \tag{4}$$

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