IFES Report

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Contents

ABSTRACT

The goal of this report is to show the basic concepts of Solid-State Physics in general and especially for Calcium. In Chapter 1 we will talk about Crystal Structure and how it is described, chapter two will provide further informations about how to determine these structures. To get further insides in the topic of Solid-State Physics Chapter 3, we will discuss some of the models which are used to describe Atoms which are not at rest at their lattice site.

1 Introduction

2 Results

2.1 Chapter 1

Calcium, as can be seen in the following table, has a FCC structure.

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

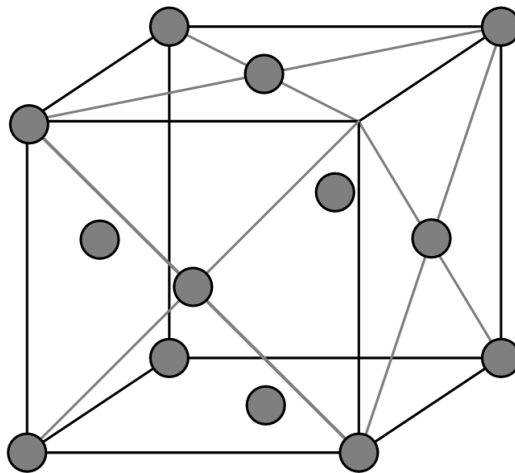The convential Unit Cell of a FCC lattice looks as follows:

Figure 2: FCC-Lattice

Primitive Vectors
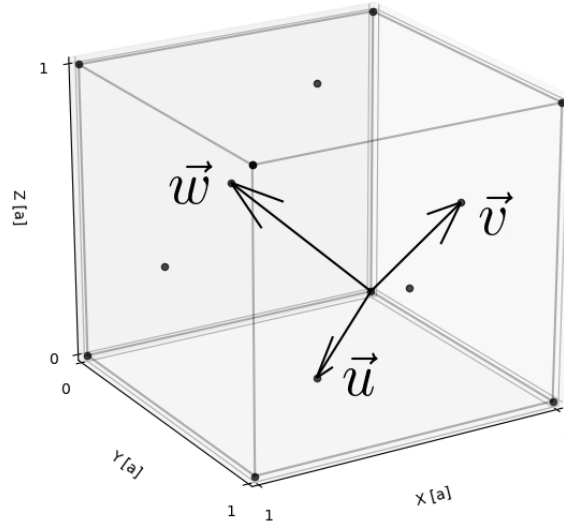
The three primitive vectors are

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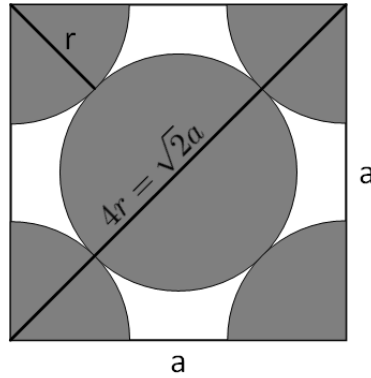
Figure 4: Relation between the atomic radius and the parameter a in a FFC

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:

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

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

(110) Plane

To show that the plane contains reticular rows of atoms in the specified directions, we need to calculate the normal vektor $\vec{n}$ of the plane, which we get by inverting the Miller Indices

$$\vec{n} = (\frac{1}{h}, \frac{1}{k}, \frac{1}{l}) = (1, 1, 0)$$

By knowing that the dot product between to orthogonal vectors is zero, we can show that the three directions lay orthogonal to $\vec{n}$ and further so parallel to the (110) plane.

- [001]
  $\vec{v_1} = (0,\ 0,\ 1)$
  $\vec{n} \cdot \vec{v_1} = 1 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 = 0$

- [1$\bar{1}$0]
  $\vec{v_1} = (1,\ -1,\ 0)$
  $\vec{n} \cdot \vec{v_1} = 1 \cdot 1 + 1 \cdot (-1) + 0 \cdot 0 = 0$

- [$\bar{1}$11]
  $\vec{v_1} = (-1,\ 1,\ 1)$
  $\vec{n} \cdot \vec{v_1} = 1 \cdot (-1) + 1 \cdot 1 + 0 \cdot 1 = 0$

By knowing that the three directions lay inside or parallel to the plane, we showed that the plane contains reticular rows of atoms in the [001], [1$\bar{1}$0] and [$\bar{1}$11] directions.

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:

$$P1 : \quad z = \frac{2}{3}y$$
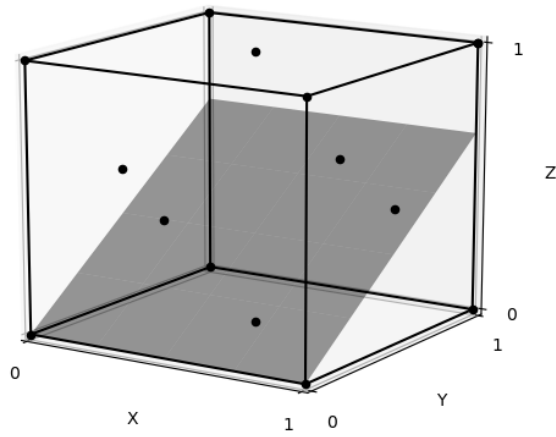
$$P2 : \quad z = x - \frac{1}{2}y$$
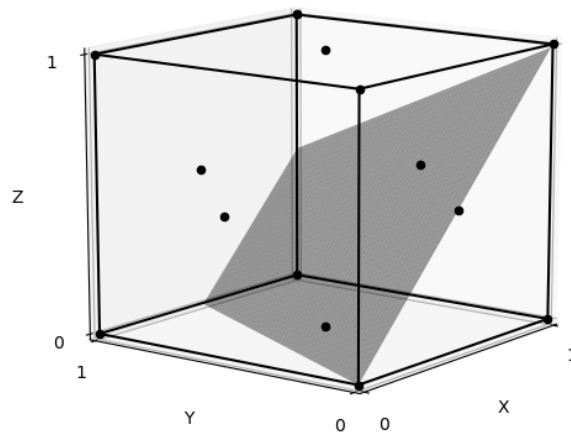
Figure 5: (0$\bar{3}$2)-Plane in a FCC-Lattice

Figure 6: ($\bar{1}$21)-Plane in a FCC-Lattice
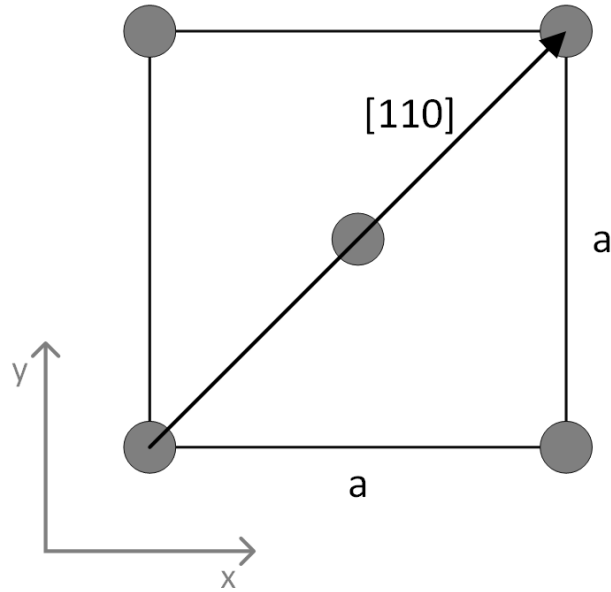
Linear Density [110]

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 $a = 5.56\,\text{Å}$)

$$\lambda = \frac{2\,Atoms}{\sqrt{2}a} = \frac{\sqrt{2}}{5.56}\frac{Atoms}{\text{Å}}$$

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:

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

2.2 Chapter 2

Geometric structure factor

The structure factor gives the amplitude of a scattered wave arising from the atoms with a single primitive cell.

$$\Phi_{\mathrm{k}} = \sum_j f_j(\mathrm{K})e^{i\mathrm{K}\cdot\mathrm{d}} \tag{2}$$

For crystals composed of only one type of atom, it's common to split the structure factor into two parts:

$$\Phi_{\mathrm{k}} = f_j(K)S_{\mathrm{K}} \tag{3}$$

,where f_j is atomic form factor and S_{K} is geometric structure factor. Now let's focus on the second one.

$$S_{\mathrm{K}} = \sum_{j=1}^{n} e^{i\mathrm{Kd}} \tag{4}$$

Calculations/needed

systematic/extinctions/needed

Diffraction

Bragg diffraction occurs when radiation, with a wavelength comparable to atomic spacings, is scattered in a specular fashion by the atoms of a crystalline system, and undergoes constructive interference. For a crystalline solid, the waves are scattered from lattice planes separated by the interplanar distance d. Bragg's law, describes the condition on for the constructive interference to be at its strongest by formula:

$$2d\sin\theta = n\lambda CALCULATIONS \tag{5}$$

Reciprocal lattice

Starting with a lattice whose basis vactors are **a**, **b**, and **c**, we can define a new set of basis vectors **a'**, **b'** and **c'**. according to the relations:

$$\mathbf{a'} = \frac{2\pi}{\Omega_c}(\mathbf{b} \times \mathbf{c}) \tag{6}$$

$$\mathbf{b'} = \frac{2\pi}{\Omega_c}(\mathbf{c} \times \mathbf{a}) \tag{7}$$

$$\mathbf{c'} = \frac{2\pi}{\Omega_c}(\mathbf{a} \times \mathbf{b}) \tag{8}$$

,where $\Omega_c = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$. So we can now calculate vectors of reciprocal lattice:

$$\mathbf{a'} = \frac{2\pi}{a}\begin{pmatrix}1\\1\\0\end{pmatrix} \qquad \mathbf{b'} = \frac{2\pi}{a}\begin{pmatrix}0\\1\\1\end{pmatrix} \qquad \mathbf{c'} = \frac{2\pi}{a}\begin{pmatrix}1\\0\\1\end{pmatrix}$$

2.3 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)

$$u = Ae^{ikx} \tag{9}$$

By using the boundary conditions:

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

We get:

$$e^{ikL} = 1$$

Due to Eulers-Equation we get for k

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

If you choose integer values for n and plot them along a k-axis, they form a one-dimensional mesh with a constants spacing $(2\pi/L)$ between the poins.
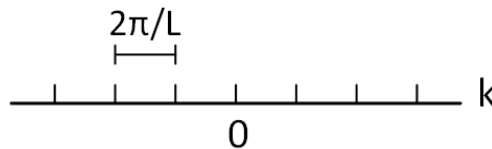

Figure 8: Allowed values of k

As we can see if L becomes large we get quasi-continous points for k. So the number of modes (points) in an interval dk in k-space equals:

$$\frac{L}{2\pi}dk$$

Using the dispersion relation we can find the number of modes in a frequency range $d\omega$, which lies within $(\omega, \omega + d\omega)$. This number is given as $(g\omega)d\omega$, with $g(w)$ defined as the density of states.

$$g(\omega)d\omega = \frac{L}{2\pi}dk$$

By solving for $g(\omega)$ and multipling with a factor of two. (Due to the fact that we have to include the modes lying the negative k-region)
We get:

$$g(\omega) = \frac{L}{\pi} \frac{1}{\frac{d\omega}{dk}} \tag{10}$$

By assuming that the dispersion in linear ($\omega = v_s k$) the density of states is

$$g(\omega) = \frac{L}{\pi} \frac{1}{v_s} \tag{11}$$

which is independet of ω

Density of States (3D)

Starting with the solution for the wave equation as same as in the 1-D case (Equation 9) we get:

$$u = A e^{i(k_x x + k_y y + k_z z)} \tag{12}$$

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

$$u = e^{i(k_x x + k_y y + k_z z)} = 1$$

$$(k_x,\ k_y,\ k_z) = (n\frac{2\pi}{L},\ m\frac{2\pi}{L},\ l\frac{2\pi}{L})$$

Each point in this k-space has a volume of $(2\pi/L)^3$. The number of modes that lie within a spherical shell with thikness dk with a radius k and a volume $4/3\pi k^3$, is given by:

$$\frac{d}{dk}(\frac{L}{2\pi})^3 \frac{4}{3}\pi k^3 = (\frac{L}{2\pi})^3 4\pi k^2 dk$$

And so with $L^3 = V$:

$$g(\omega)d\omega = \frac{V}{2\pi^2} k^2 dk \quad \Rightarrow \quad g(\omega) = \frac{V}{2\pi^2} k^2 \frac{dk}{d\omega}$$

By applying the linear dispersion relation, we get:

$$g(\omega) = \frac{V}{2\pi^2} \frac{\omega^2}{v_s^3} \tag{13}$$

As there are three different modes associated with the same value for q. (one longitudinal and 2 transversal modes). Equation 13 has to be multiplied by a factor of three to get the correct result.

$$g(\omega) = \frac{3V}{2\pi^2} \frac{\omega^2}{v_s^3} \tag{14}$$

Debye Frequency

In the Debye model the vibration frequency of the lattice covers a wide rang of values.

The total energy of the lattice is calculated by:

$$E = \int \overline{\epsilon}(\omega) g(\omega) \, d\omega \tag{15}$$

$g(\omega)$ ...   density of states
$\overline{\epsilon}(\omega)$ ...   energy of each mode

For various reasons a cutoff frequency is needed for example to not get infinit energys in Equation 15.

The upper cutoff frequency was defined, by requiring that the total number of modes included must be equal to the number of degrees of freedom for the entire solid.

$$\int_0^{\omega_D} g(\omega) \, d\omega = 3N_A \tag{16}$$

With inserting the Equation 13 into equation Equation 16 the integral can be solved and a expression for the Debye frequency w_D is obtained.

$$\int_0^{\omega_D} \frac{3V}{2\pi^2} \frac{\omega^2}{v_s^3} \, d\omega = \frac{3V}{2\pi^2} \frac{1}{v_s^3} [\omega]_0^{\omega_D} = \frac{V}{2\pi^2} \frac{\omega_D^3}{v_s^3}$$

$$\frac{V}{2\pi^2} \frac{\omega_D^3}{v_s^3} = 3N_A \qquad \Rightarrow w_D = (6\pi^2 n)^{\frac{1}{3}} v_s \text{ with } n = \frac{N_a}{V}$$

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 $10^8 \frac{cm}{s}$, while the velocities of nuclei in atoms on the order of at most $10^5 \frac{cm}{s}$. 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:

$$m\omega^2 = 4K \sin^2\left(\frac{ka}{2}\right) \tag{17}$$

$$v_G = \frac{\partial \omega}{\partial k} = \sqrt{\frac{K}{m}}\, a \cos\left(\frac{ka}{2}\right)$$

$$v_G(k = 0) = \sqrt{\frac{K}{m}}\, a$$

$$v_G\left(k = -\frac{\pi}{a}\right) = v_G\left(k = \frac{\pi}{a}\right) = 0$$

3 Conclusion

References

[1] M.A. Omar, Elementary Solid State Physics: *Principles and Applications*, Addison-Wesley, London, 1993.

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