IFES Report

Patrick Jenny
Filip Banasiak

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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

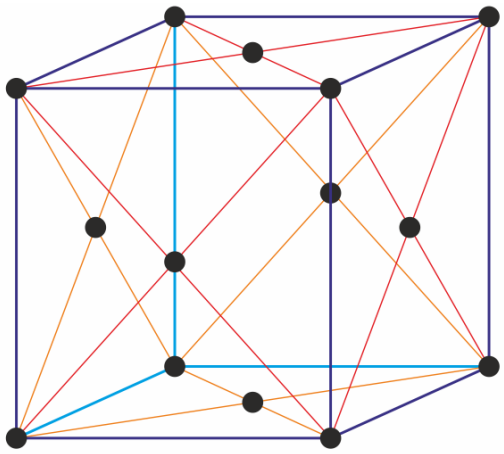

Figure 2

Primitive Vectors

The three primitive vectors are

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

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:

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

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

Linear Density [110]

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

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