2 Solid States and Description of Crystals

2.1 Please estimate the number of biological cells and the number of atoms within an average human being in Switzerland (75 kg, 1.71 m). Compare this number with other large numbers such as total number of humans, stars in the Milky Way, etc. Give an estimate of the size of a computer tomogram, which represents the entire human on the cellular level. Which possibilities do you see for reducing this size?

We assume the cell is cubic and eukariotic $a = 10\ \mu m$ and $V = a \times a \times a = 10^{-15}\ m^3$ and $75\ kg \cong 0.075\ m^3$, so the number of cells$=\frac{Vhuman}{V} = \frac{0.075\ m^3}{10^{-15}\ m^3} = 7.5 \times 10^{13}$.
We assume the human body mainly consists of water, so the considered human is 75 liters, the weight of the considered body in grams $\rightarrow 75 \times 1000 = 75000\ g$, the number of moles in the considered body$\rightarrow\ 75000 \div 18 = 4166.66\ mol$. So the number of water molecules of water (1 mol = 18 g) in the considerd body $\rightarrow 4166.66 \times 6.022 \times 10^{23} = 2.5 \times 10^{27}$. Since every water molecule has 3 atoms, the number of atoms within human body is $\rightarrow 2.5 \times 10^{27} \times 3 = 7.5 \times 10^{27}$.

The total number of humans is $\rightarrow 6.97 \times 10^9$. The number of stars in the milky way is $\rightarrow 3 \times 10^{11}$ stars.

We already know the number of cells in the human body, the number of voxels is the number of cells times the number of "gray values", assuming we take one voxel per cell. Then we can estimate the size of a computer tomogram. If we assume 1 byte per voxel (256 gray values), then 1 entire tomogram is 7.5×10^13 bytes, or 75 TB.
Reduction of this size can be made using symmetries (such as right-left) and identical units such as the kind of cells (around 100).

2.2 The ideal close-packed hcp structure has the important c/a ratio. Please verify that this value corresponds to 1.633.

When considering only one plane of the *hcp* lattice, connecting the center ponts of the spheres of radius r yields an equilateral triangle with side length $2r$. Adding a third sphere on top and connecting its center to the others yields a tetrahedron (cp. Figure 1). The c/a-ratio corresponds to twice the height of this tetrahedron. First consider the in-plane triangle (Figure 1a).

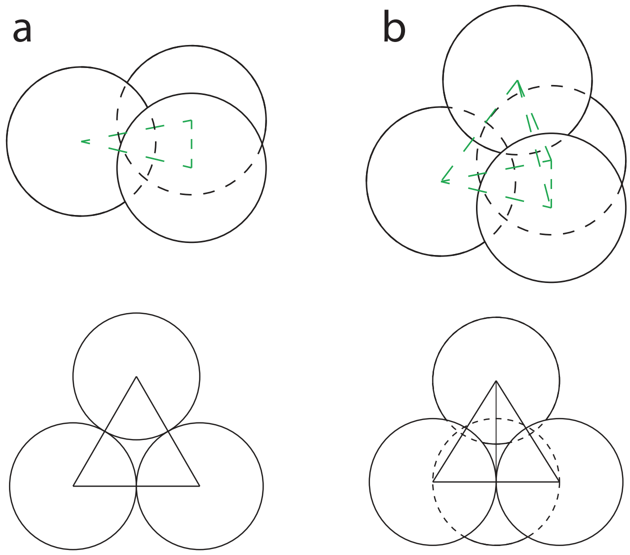


Figure 1: a) top view of one plane of close packed spheres. b) side view of close packed spheres.

Let a be its side lenght. Its height h is

$$h = a \cdot cos(30°) = \frac{\sqrt{3}}{2}a \tag{1}$$

The height of the tetaedron impinges in the center of the base triangle. The length of the segment s (cp. Figure 2) can be obtained by solving

$$s \cdot cos(30°) = \frac{a}{2}$$

for s. Thus

$$s \cdot cos(30°) = s \cdot \frac{\sqrt{3}}{2} = \frac{a}{2}$$

$$s = \frac{\sqrt{3}}{3}a \tag{2}$$

and therefore for h

$$h = \sqrt{a^2 - s^2} =$$

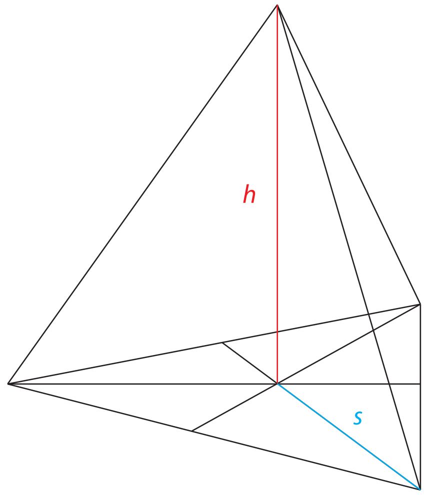


Figure 2: Tetrahedron connecting the centers of close packed spheres.

$$\sqrt{a^2 - \frac{3}{9}a^2} =$$

$$\frac{\sqrt{6}}{3}a = 0.8165 \cdot a \tag{3}$$

Setting $a = 1$ yields $h \cdot 2 = 1.633$.

2.3 Explain the construction of the Wigner-Seitz-cell within the two-dimensional plane in the quantitative manner.

The Wigner-Seitz cell around a lattice point is defined as the locus of points in space, which are closer to that lattice point than to any of the other lattice points. It can be shown mathematically that a Wigner-Seitz-Cell is a primitive unit cell spanning the entire Bravais lattice without leaving any gaps or holes. To create a Wigner-Seitz cell simply complete the four steps:

(a) Choose any lattice site as the origin.

(b) Starting at the origin draw vectors to all neighbouring lattice points.

(c) Construct a plane perpendicular to and passing through the midpoint of each vector.

(d) Construct a plane perpendicular to and passing through the midpoint of each vector.

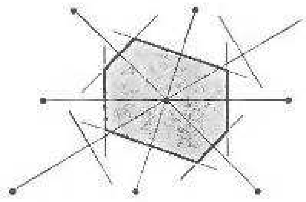
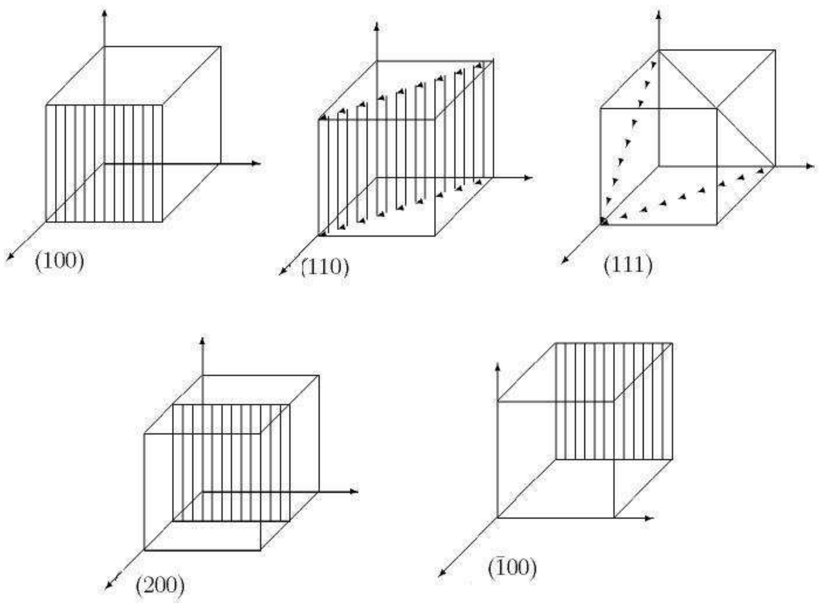


Figure 3: Plane view of a Wigner-Seitz-Cell

2.4 **Draw the following lattice planes in the cubic crystal:** $(100), (110), (111), (200), (\bar{1}00)$



2.5 **Please explain, why 5- and 7-fold rotational symmetries do not exist.**

Consider two neighbouring lattice points, A and B, of a lattice with a rotational symmetry, connected by the lattice vector of length r. Given the rotational symmetry, a lattice point A' exists that can be obtained by rotating A aroud B by the angle α. Equivalently, a lattice point B' can be obtained by rotating B around A by $-\alpha$. As A' and B' are lattice points, they are connected by a lattice vector of length r' which must be an integer multiple of r

$$r' = n \cdot r, \quad n = 0, 1, -1, 2, -2, \ldots \tag{4}$$

From figure 4 it is clear that

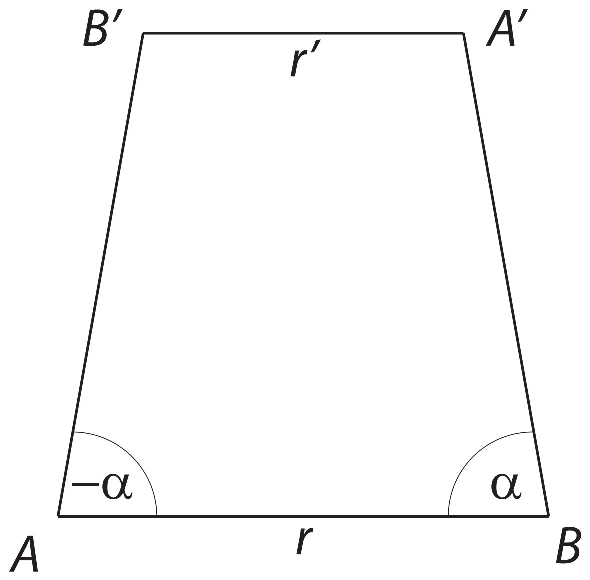


Figure 4: Lattice points A' and B' can be obtained by rotating A around B and vice versa.

$$r' = r - 2r \cdot cos(\alpha) \tag{5}$$

Combining equations 4 and 5 one obtains for $cos(\alpha)$

$$1 - 2cos(\alpha) = n$$

$$cos(\alpha) = \frac{(1-n)}{2} \tag{6}$$

As $|cos(\alpha)| \leq 1$ this cas be satisfied only by $n = -1, 0, 1, 2, 3$. Solving for α gives the possible rotation angles $0°, 60°, 90°, 120°, 180°$. Thus no 5- or 7-fold

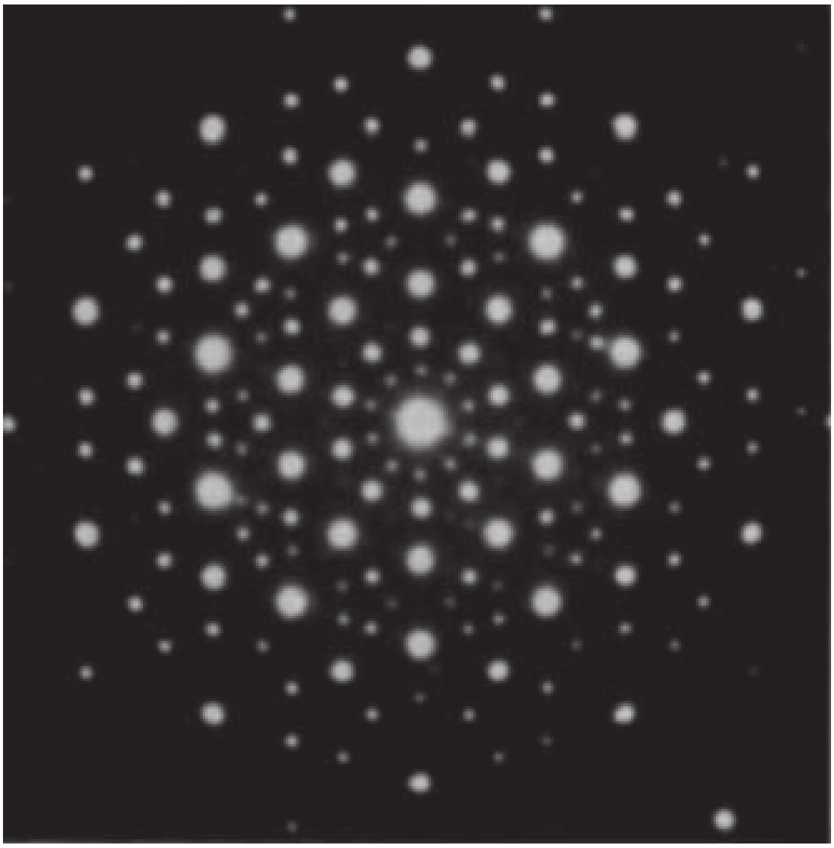


Figure 5: The electron diffraction pattern generated by Dan Shechtman's Al_6Mn quasicrystal along an axis of five-fold symmetry.

rotational symmetries are possible in crystals although objects themselves may appear to have 5-fold, 7-fold, 8-fold, or higher-fold rotational symmetries.

However, the Nobel prize winner Dan Shechtman realized that solids need not to be translationally periodic. These so-called quasicrystals may appear to have the forbidden rotational symmetry values. His investigation on aluminum manganese alloys, containing six Al atoms for every Mn atom and building an icosahedron, produced the crystallographically forbidden, tenfold symmetric diffraction pattern shown in figure 5. Icosahedra are actually fivefold symmetric about axes that intersect their vertices, but a diffraction

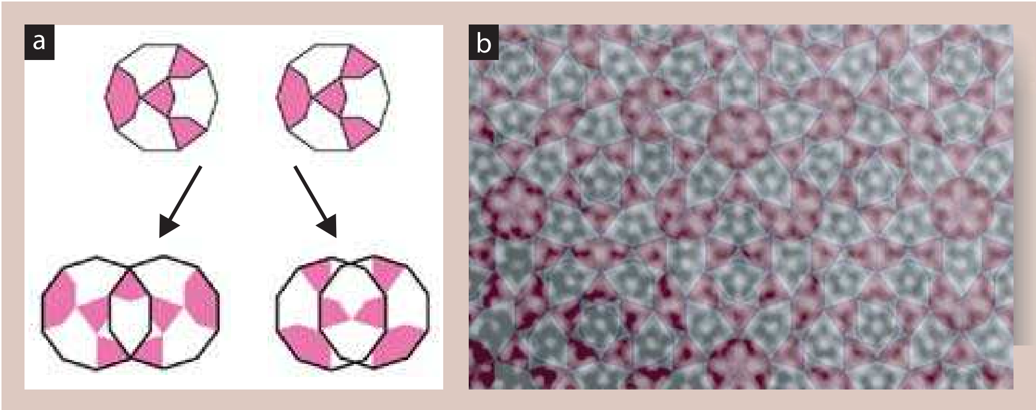


Figure 6: (a) A new order.

pattern taken along any one of those axes would show tenfold symmetry. However, icosahedra cannot be packed to fill space.

The model developed by Shechtman and Blech (figure 6) explained the experimantal results. In a variation of Penrose tiling, neighboring decagonal tiles are allowed to overlap in one of two ways. Maximization of the tiling density then yields a perfect quasiperiodic tiling. (b) Superimposed on a scanning electron microscope image of an $Al_{72}Ni_{20}Co_{8}$ quasicrystal, the tiling maps to the underlying atomic lattice. Atoms appear as white circles.