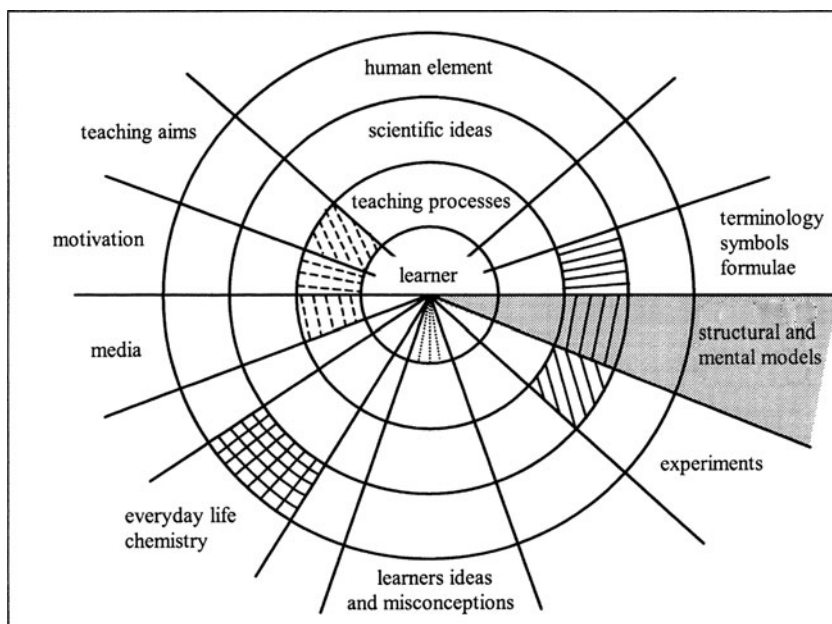


## Chapter 6

# Structural and Mental Models



*I once was invited to give a slide show about Germany in San Diego/California. One of the photos I found in an illustrated book called "Germany" represented the famous Neuschwanstein Castle near Füssen in Bavaria. I showed this picture first. As soon as it appeared on the screen a woman interrupted: "Beautiful – just like the castle in Disneyland." I tried to correct: "In Disneyland you find a copy of the castle – this photo shows the original in Bavaria" – but the woman did not listen. The difference between original and model was not important to her!*

In this example both the original and the model can be observed: the photo of the castle as well as the model in Disneyland can be compared to the Bavarian original in detail. In scientific models for chemical structures the spheres of the model cannot be compared to the submicroscopic original atoms, ions or molecules,

because it is impossible to see them – neither with a magnifying glass nor with the best microscope.

Because particles are not visible, one tried all times to develop suitable mental models. Demokritus and other Greek philosophers came up with the idea of the atom more than 2,000 years ago – simply by thinking about their observations concerning matter and trying to find out the composition and structure of matter. L  mery developed a particle model for the effects of acids [1]: “All acids are composed of particles like biting points, all experiences show that acids make pricks, which everyone can feel on the tongue.” L  mery had never seen acid particles, but he tried to transfer macroscopic characteristics of acids on the cited mental model.

Nevertheless structural and mental models are very important for the understanding of science, especially chemistry. One of the key questions of chemistry education deals with the scientific idea of models and how these can be transferred to young learners at school. To get the idea across, general characteristics of models have to be looked at first and later transferred to scientific models.

*General characteristics of models.* Following an empirical analysis of models in general Stachowiak [2] differentiates three basic characteristics:

- Feature of depiction: models are always a model of something, namely illustrations and therefore representations of certain natural or artificial originals.
- Feature of shortening: models do not cover all characteristics of the original, they represent only the ones that seem to be relevant in a particular context.
- Feature of subjectivity: models fulfil their functions of representation and substitution only for certain subjects, limited to certain mental or real operations, limited to certain time.

Take the picture of the Neuschwanstein Castle another time. It copies the building and the surrounding landscape with fields, trees, roads and mountains in the background downscaled: the feature of depiction is fulfilled. Some of the many shortenings of the original are the missing space dimension, the nonexistent patterns of light and shadow on walls and windows of the castle or the missing motion of trees and branches in the wind: feature of shortening. The specific view of the castle on the picture or the details of the landscape are subjectively chosen by the photographer for a special purpose: feature of subjectivity.

Taking two different maps of the London Underground show that feature 1 is fulfilled: they all show where the underground stations are located. Comparing them one shows the streets close to the stations, the other one not: the shortening is done differently. The differences are due to the users: some need the street maps around the stations, other ones not because they are traveling every day the same stations to work and back at home: feature of subjectivity.

## 6.1 Scientific Ideas: Thinking in Models

Chemistry found recognition and success, when it departed from trial and error approach of medieval alchemy. Starting with simple laboratory experiments for the description of substances it came to develop first mental models for the structure of matter in the eighteenth and nineteenth century. Some states of perception will be given exemplarily.

Dalton postulated in 1808 that there are as many kinds of atoms as there are known elements. He presented the first atomic mass table, which has been corrected and extended mainly by Berzelius in the next decade. The comparison of experimentally determined mass ratios of elements in compounds with their atomic masses made the empirical analysis possible and led to the knowledge of the composition of many substances as well as the first empirical formulae.

Kekulé deduced the theory of valence from his experience in 1865: He created a first concept of molecular structure with the four-bonding or the tetrahedral model of the carbon atom, the one-bonding model of the hydrogen atom, and the two-bonding model of the oxygen atom. With these mental models it became possible to predict structures of many molecules, verify them in experiments and plan targeted syntheses of new substances.

In 1912 Laue discovered three-dimensional crystal structures through the diffraction of X-ray radiation from salt crystals: he obtained X-ray diffraction patterns, calculated those three-dimensional interference patterns and deduced the structure of investigated salt crystals. Based on these results Bragg solved the crystal structure of sodium chloride in 1914. This destroyed the historical idea of NaCl molecules in table salt: sodium ions and chloride ions with the coordination number 6 form the salt crystals. All following structural analyses were based on Laue's and Bragg's fundamental discoveries, providing the chemical structure of many crystalline substances, in turn making the syntheses of new substances possible.

*Models and scientific perception.* The idea of models and the process of scientific perception will be explained with a diagram of Steinbuch [3] (see Fig. 6.1): "Any facts of reality, an original, can be transferred to an abstract mental model by taking only the essential and relevant parts of the given context. Certain information, for example generally accepted laws of logic or physics may be added. A mental model for future thinking processes is thereby available. For the purpose of illustration, this abstract mental model can be transferred back into reality by building a concrete display model or even by artistic representation. But these have unavoidable irrelevant components, which the mental model does not have."

This "thinking in models" can be transferred to Laue's way of perception (see Fig. 6.2): The interference pattern (original) that forms from a salt single-crystal in the Laue experiment is let through the filter as "essential." Interferences of light with two-dimensional diffraction gratings and their calculations are familiar (additional information). They are taken as a basis for the calculations of three-dimensional diffraction gratings. The result is a mental model for the three-dimensional symmetrical structure of salt crystals built of ions. The ions in the ionic

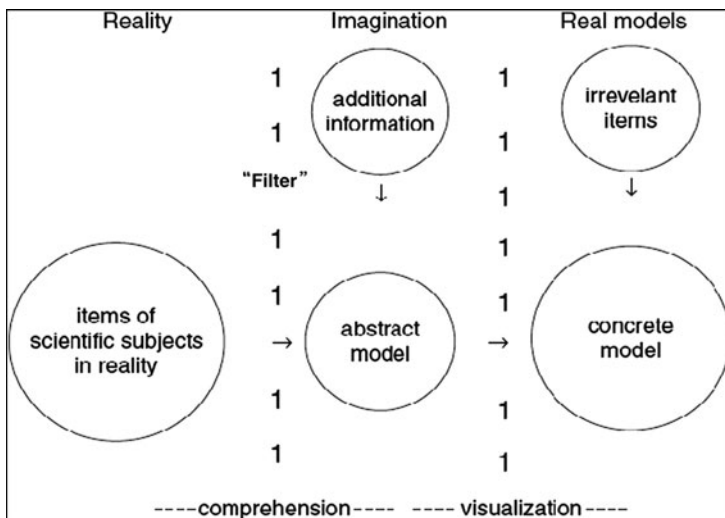


Fig. 6.1 Scheme of “thinking in models” according to Steinbuch [3]

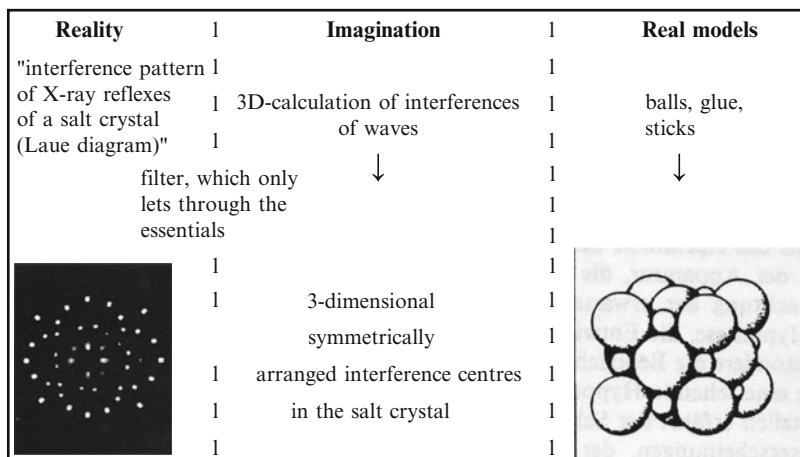


Fig. 6.2 Scheme of “thinking in models” applied to Laue’s way of X-ray analysis

structure function as diffraction centers for the X-ray radiation beam (abstract mental model).

For the illustration of this mental model, irrelevant components such as balls, sticks and glue can be used for the construction of display models: sphere packing or crystal structure models (see Fig. 6.3). In addition to sphere packing and crystal structure models, the resulting display model for the structure of crystals can also be a unit cell only (see Fig. 6.3).

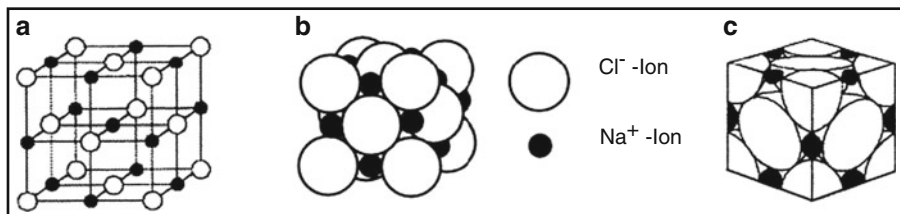


Fig. 6.3 NaCl-crystal structure: *ball-and-stick* model, cubic sphere packing and unit cell

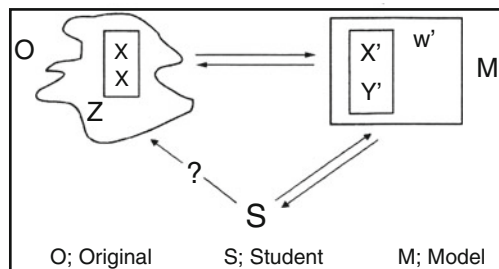


Fig. 6.4 Scheme of the way of perception by models, according to Kircher [4]

The process of perception through models is also described by Kircher [4]. His concept will be explained, using sodium chloride crystals and corresponding models (see Figs. 6.3 and 6.4):

- The original **O** is to be a natural rock salt crystal with a cubic shape, planar surfaces, straight edges and right angles
- The packing of spheres is to be chosen as the model **M** (see Fig. 6.3b). The chloride ions are represented by big balls and the sodium ions are represented by small balls
- The student **S** can now understand the original **O** with the help of the model **M**, the sphere-packing model works as a mediator between the student **S** and the original **O**

1. There are properties  $x$  and  $y$  of the crystal that have corresponding model characteristics  $x'$  and  $y'$ . For example,  $x$  is chosen for the spatial arrangement of sodium and chloride ions in the crystal,  $x'$  is then chosen for the corresponding arrangement of big and small balls with the coordination number 6 in the model. If  $y$  depicts the radius ratio of both types of ions in the sodium chloride crystal, then  $y'$  depicts the corresponding size ratio of the balls in the sphere-packing model. So  $x$  and  $y$  represent the parameters in the original,  $x'$  and  $y'$  those which are displayed in the model. According to Stachowiak  $x$  and  $y$  are the features of depiction, according to Steinbuch these are “the essentials, which are let through the filter.”
2. There exist characteristics  $z$  in the original that do not have an analogy in the model. The salty taste or the white color of the crystal, for example, are not

displayed in the model. The model is shortened by this characteristic: Stachowiak calls this “feature of shortening.” Similarly the density or melting points of crystals cannot be determined with models. The model builder, however, never had the intention to transfer these original characteristics to the model.

3. There may be characteristics  $w'$  in the model that do not have an analogy in the original. The choice of colors – for example white for the big balls and red for the small balls – represents a model characteristic, which is totally irrelevant and arbitrarily chosen by the model builder: Steinbuch calls these irrelevant components. Additional irrelevant components are model materials like wood, cellulose or styrofoam and an adhesive between the balls, such as glue or Velcro tape.

The crystal structure model (see Fig. 6.3a) only shows the cubic arrangement of ions in the crystals, not their size. The option of looking into the model, however, allows a better illustration of the coordination number 6. The connecting sticks between the junctions are only necessary for the stability of the model, they are totally irrelevant components towards the original and do not have a representation function.

The unit cell model (see Fig. 6.3c) shows three features of depiction: the cubic structure of the ionic compound, the size ratio of the ions and the correct 1:1 ratio of the number of ions. If all parts of the big and small balls of the model are summed up, it results in four big and four small balls. Transferred to the original, this shows a unit of four  $\text{Na}^+$  ions and four  $\text{Cl}^-$  ions corresponding to the symbol  $\{(\text{Na}^+)_4(\text{Cl}^-)_4\}$ .

The unit cell with this symbol can be regarded as the smallest unit of the NaCl-structure – just like the  $\text{C}_2\text{H}_5\text{OH}$  molecule is regarded as the smallest unit of the substance ethanol. Symbols like  $\{(\text{Na}^+)_1(\text{Cl}^-)_1\}$ ,  $(\text{Na}^+)(\text{Cl}^-)$  or  $\text{NaCl}$  can be derived from  $\{(\text{Na}^+)_4(\text{Cl}^-)_4\}$  – they are all shortened representations of the sodium chloride structure.

**Mental models in chemistry:** Due to improving knowledge, scientific models change continuously. Therefore it is not possible to speak of the current atomic model or the current model of chemical bonds.

*Quantum mechanical atomic model.* The structure of the electron shells of atoms or ions is described by the principal quantum number  $n$  (“K shell” or “L shell”), the angular momentum quantum number  $l$  (s, p, d and f sub-shell), the magnetic quantum number  $m$  and the spin quantum number  $s$ . A maximum of two electrons with different spins can form an electron cloud or an orbital (Pauli principle). Starting from the wave–particle duality, wave functions have been developed, which give information on energy levels and electronic orbitals (Schrödinger equation). The calculation of wave functions leads to the description of atoms by atomic orbitals and molecules by molecular orbitals. In this sense, covalent bonds in molecules can be described mathematically.

*Historical atomic models.* For educational reasons historical models are often used in chemistry education. For example:

- Mass model (Dalton, 1808)
- Mass–charge model (Thomson, 1897)
- Nucleus–shell model (Rutherford, 1911)
- Sub-shell model (Bohr, 1913)
- Electron-pair repulsion model (Gillespie, Kimball, 1966)

*Models of chemical bonding.* Mental models concerning this matter have to be viewed from two perspectives:

1. The effects of three-dimensional bonding forces are to be displayed with the model material:
  - (a) Directed bonding forces that work in designated directions of space are to be displayed by snap fasteners or sticks.
  - (b) Undirected bonding forces that work symmetrically around a particle are to be symbolized by spheres, which may be glued together.
2. Bonding forces are difficult to visualize and they are usually described by mathematical models with the distribution of electron densities. The following cases of chemical bonding are to be differentiated:
  - Ionic bonding
  - Covalent bonding
  - Metallic bonding
  - Hydrogen bonding
  - Van der Waals forces (intermolecular forces).

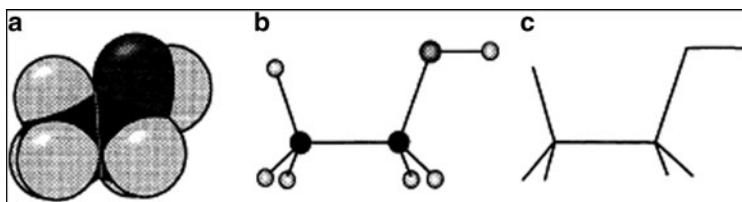
*Models of the chemical structure.* The mathematical calculation of atomic structure and chemical bonding is mostly a means to get information on the chemical structure. On this basis, it is the aim of many analytical procedures to determine and to describe the atomic or ionic arrangement in given substances, and derive the structural formulae from the determined structures. Different cases of chemical structures can be sketched in the following way:

- Molecular structure (atom types, bond length and bond angle)
- Atomic crystal structure (atom types and lattice constants, unit cell)
- Metal crystal structure (atom types and lattice constants, unit cell)
- Ionic crystal structure (types of ions and lattice constants, unit cell)
- Molecular crystal structure (types of molecules and lattice constants, unit cell)

*Models of the chemical reaction.* Arrangements of particles in chemical reactions can be described by mental models as well as shortened by reaction equations:

- Rearrangement of atoms in reactions of metals to alloys
- Rearrangement of ions in hydration and precipitation reactions
- Proton transfer in acid–base reactions
- Electron transfer in redox reactions
- Ligand transfer in complex reactions
- Addition, substitution and elimination reactions of organic molecules

**Display models in chemistry:** Chemists usually work with abstract mental models. For educational reasons appropriate display models are being developed (see Figs. 6.2, 6.3 and 6.5): concrete display models can be build, for example of molecules or crystal structures, in regard to many mental models of different chemical structures.



**Fig. 6.5** Space-filling, *ball-and-stick* and *stick* model of the structure of the  $C_2H_5OH$  molecule

*Models of molecule structures.* The spatial arrangement of atoms in a molecule is described with the help of space coordinates, bond lengths and bond angles, which are to be determined experimentally in the laboratory. It can be illustrated in different ways (see Fig. 6.5):

- Space-filling model (calotte model): the space filling of atoms is being displayed, atom calottes are connected to a molecular model, according to bond lengths and bond angles (a).
- Ball-and-stick model: all balls for the different kinds of atoms have the same size and are specially colored, they are being connected with connection sticks or snap fasteners (b).
- Stick model: instead of balls special sticks are used of appropriate lengths and connected with proper angles (c).

*Models of crystal structures.* The unit cell is sufficient for the expert to deduce the whole structure. To proceed graphically for the learner, certain parts of the lattice are being chosen to be displayed in models as a crystal structure or a packing of spheres (see Fig. 6.3):

- Crystal structure model: equal spheres, with different colors if applicable, are being connected by connection sticks until the desired part of the structure is being displayed, for example, the part corresponding to the NaCl unit cell (a).
- Packing-of-spheres model: the size ratio of the different atoms or ions is taken into account. The balls are to be glued or piled up according to familiar structure parameters until they display the desired part e.g. the NaCl unit cube (b).
- Unit cell model: it is derived from the corresponding unit cube model and guarantees a proper ratio of atoms or ions (c). Larger structures of any size can be derived by mental translation of unit cell models in all three directions in space.
- 3D-drawing model: red–green drawings of chemical structures are being fixed by both eyes until the three-dimensional picture appears; it can be interpreted spatially [5].

Besides the well-known molecular structure kits there exist a variety of model kits to build packings of spheres:



- “Metal structures” (see Fig. 6.6): this model kit allows to build the three common metal structures in the form of a packing of spheres with wooden balls of same size (diameter: 3 cm).
- “Model kit for crystal structures” (see Fig. 6.7): a base plate with slots in a triangular pattern for stacking colored plastic balls of the same size (diameter: 1 cm), only the close-packed structures can be built as shown in Fig. 6.6.
- “Solid-state model kit” (see Fig. 6.8): base plate with holes in different patterns to hold sticks with pierced glass spheres of different diameters. It is possible to build all metal structures with this kit as well as many salt structures with big and small glass spheres.

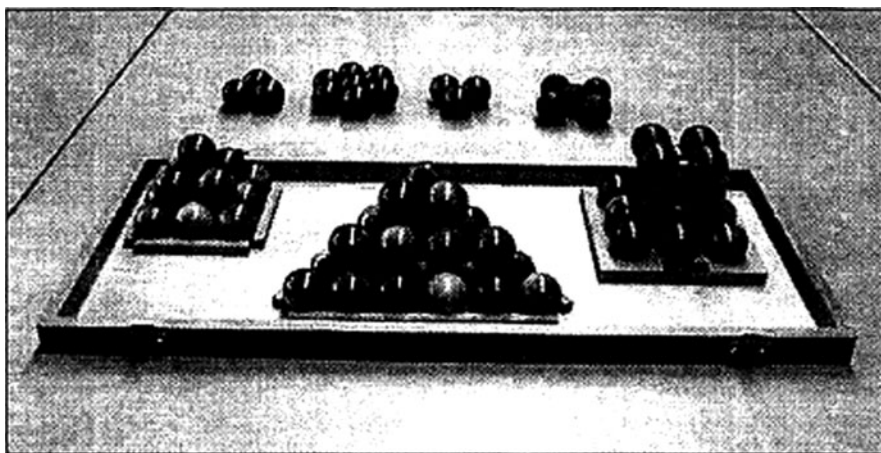


Fig. 6.6 Model kit “Metal Structures” by Geomix [6]

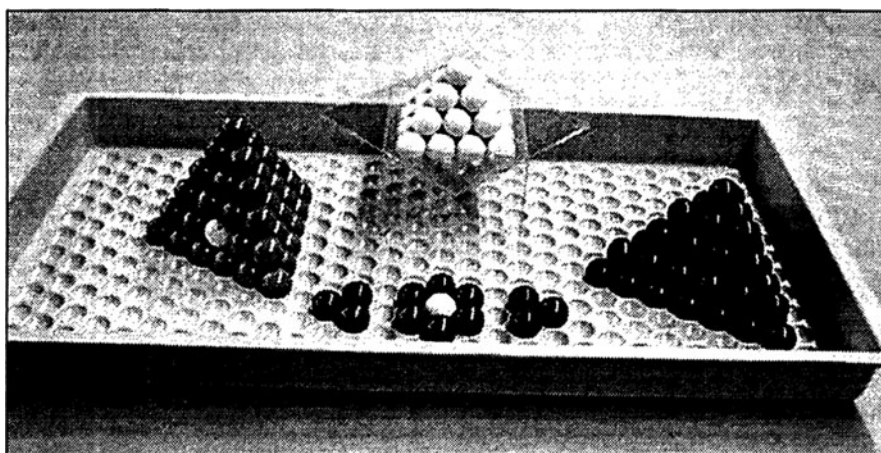


Fig. 6.7 “Crystal-Structure Model Kit” by Leybold [7]

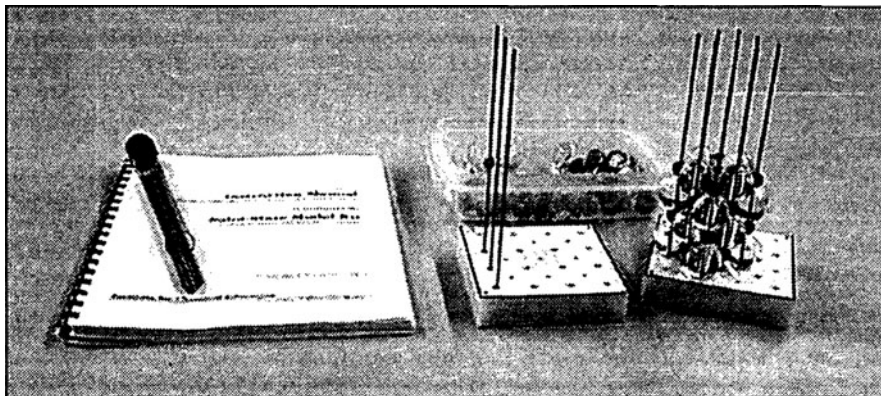


Fig. 6.8 “Solid-State Model Kit” of the Institute for Chemical Education, Univ. of Madison [8]

**Dynamic models:** Simulation games are dynamic models. They allow the demonstration and interpretation of physicochemical processes on the particle level, unlike the much discussed structural models, which only represent static and time-independent aspects of matter. The processes, which will be simulated on the model level below, can be divided into two categories:

- Processes in which particles (atoms, molecules, ions, photons, etc.) move in space without transforming into other particles. Examples: diffusion, chromatography, distribution equilibria, mixing and separation processes, light absorption.
- Processes in which particles transform into other particles during a chemical reaction. The time behavior of the system, i.e. the kinetics of these reactions are of particular interest. Examples: reactions of elements, consecutive reactions, competing reactions, balanced reactions, oscillating reactions.

The particles are being represented by simplest models in both categories. It is not so much the behavior of the single particle that is of primary interest, but the statistic behavior of a particle arrangement. From this point of view the simulation games can also be called statistic games. The rules for these games are simple, they can be described with the following basic points:

- One can either win tokens from a playboard (board model) or balls from a vessel (urn model).
- A randomly hit particle is considered to be activated – what happens to it next depends on the rules of the game: moving a sphere on the playboard, converting it into another kind of sphere by color change, etc. – the rules should be assigned to the simulated process in a comprehensible way.
- Every event that leads to an activation counts as one time unit, regardless of its specific consequences.
- The kinetics of the statistical process are being recorded by writing down the status of the game depending on the number of time units.

The following examples [9–11] illustrate the mathematical structures of these games as well as their contextualization in complex physicochemical theories (such as Maxwell velocity distribution, Boltzmann distribution, entropy, reaction kinetics). It is not necessary to teach the complex mathematical models as the basis of these games in chemistry lessons. The numerical interpretation of the games is usually enough to illustrate the core of the simulated issue. A mathematical understanding is helpful and even essential for anyone interested in creating computer simulations (see explanations in [9]). The visualization of radioactive decay might be a first qualitative interpretation.

Radioactive decay: Terms like “radioactivity,” “the unit Becquerel” or “half-life of isotopes” are part of the public discourse ever since the Chernobyl disaster on 26 April 1986. To enable students to participate in this discourse, it has to be ensured that they understand and use the technical terms in the correct way. This does not replace a further discussion about aims and risks of nuclear power as a basis for consensus building and social interaction.

The following simulation game, which is based on an idea by Eigen and Winkler [12], can be used to understand the process of a decomposition reaction, especially for teaching the term “half-life of isotopes”:

- 36 tokens are placed on a board with  $6 \times 6$  squares. These represent the atoms of a radioactive substance, which transforms to inactive atoms with a certain half-life (which is to be determined during the game).
- Coordinates on the board are being determined successively by rolling one dice twice. If there is a white token on the determined field (which will be the case in the beginning), it is to be replaced by a black token (inactive atom). If a field with a black token is being determined during the game, the token remains.
- Every double dice for both coordinates counts as one time unit, regardless of whether a black or a white token is hit.

A typical course of a game is displayed in Fig. 6.9: after about 100 time units almost all the white tokens are replaced by black tokens, i.e. almost all of the radioactive atoms have been transformed to inactive atoms.

The results of at least 10 players are being added up or averaged statistically for the quantitative analysis. An exponential curve progression with a half-life of  $t_{1/2} = 25$  time units results. It is important for students to realize that, despite the randomness of the single decay event, a lawful behavior of the overall process results: a curve progression with a constant half-life. If the students know the exponential function from their mathematics classes, the data can also be analyzed analytically (see Fig. 6.10).

Figure 6.10 also shows that the presentation of the data on a logarithmic scale results in a straight line: students can determine the rate constant  $k$  from the slope of the line; the value is  $k = 0.028$ . Since 0.028 is about equal to  $1/36$ , students are able to grasp the relevance of  $k$ :  $1/36$  is the probability with which a single token is taken after rolling the dice. This means that  $k$  is the probability with which a single radioactive atom decays per time unit.

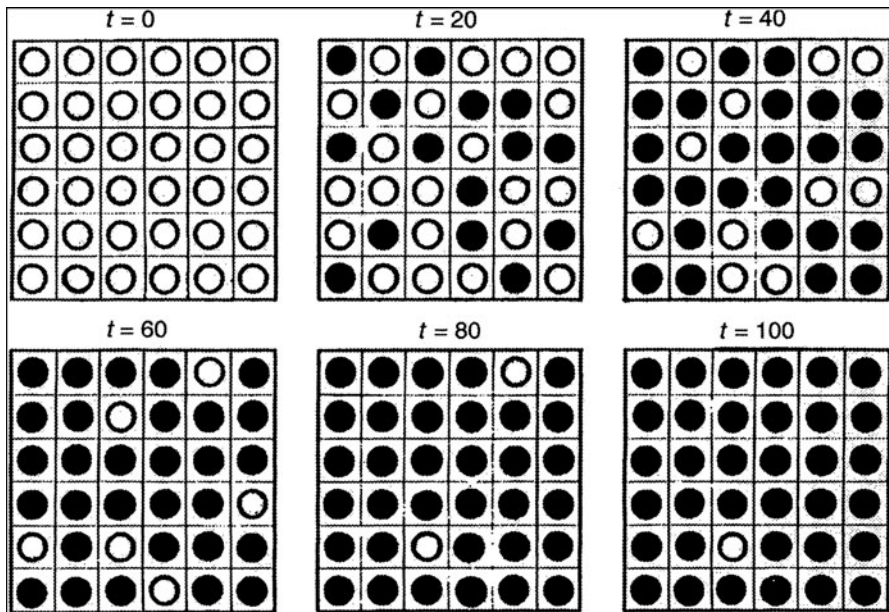


Fig. 6.9 Simulation game for radioactive decay

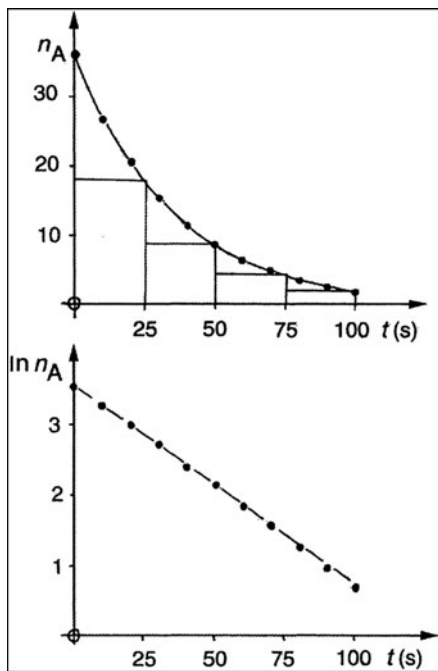


Fig. 6.10 Quantitative analysis of the data in normal and logarithmic presentation (mean values of at least ten games)

In connection with the Chernobyl disaster the caesium isotope Cs-137, which decays with a half-life  $t_{1/2} = 30$  years, was discussed in the newspapers. With the help of this game students will be able to grasp the consequences: it takes almost 100 years until the Cs-137 activity decays to 10% of the starting value. Luckily the clouds with radioactive particles spread widely over Western Europe so that experts predicted the dose of Cs-137 in food to be small despite its long half-life.

## 6.2 Teaching Processes: Models and Their Functions

Students already gained lots of experience in the field of natural phenomena: this field is concrete for them. Therefore they like the elementary lessons in biology, chemistry, geography and physics: they stay in the well-known field of direct illustration and tangible phenomena. As soon as formulae and reaction equations play a role in chemistry lessons, interest in chemistry dwindles: chemistry becomes dry and lifeless, becomes hard to understand. One reason is that formulae and equations belong to abstract mental models (see Chap. 6.1).

Therefore it is important for the education process to find out which display models, for example molecular models, packing of spheres or crystal structures, can be used, before mental models are being introduced. All bonding models or models of the structure of single atoms or ions are abstract mental constructs. They have to stand back until a first understanding of the structure of matter is build up with the help of illustrative structural models. First the chemical structure, then the chemical bond!

Some chemistry and physics educators see the use of particles and ball models for chemical structures with a critical eye. Buck [13], for example, calls the particle model a “nonmodel” and opposes the usual illustration with circles or balls and their arrangement for demonstrating models of the states of matter or aqueous solutions: “Actually we are not allowed to draw spheres, because we are dealing with centers of force. Teachers and authors who should know, accept without problems that atomic and molecular orbitals are asymptotic, can stretch across the whole universe, that limiting lines are drawn arbitrarily, mostly at 85%. To summarize it: the visualisation and illustration by particle pictures is a crucial mistake” [13].

He also recommends initiating “the jump” to the atoms by showing slides of increasing or decreasing complexity and a discussion of system characteristics: “egg → hen house → farm → village → country → earth → universe → earth → city → school → students → hair → ? What about the next slide? There is no next slide, because such a slide does not exist” [14].

This discussion might be very interesting, for sure. It can take place in class before the introduction of smallest particles. But the consequence of the “nonexistence of the next slide” cannot be to go over to the abstract “centers of force” or “endlessly widespread nucleus–shell systems” right away. For developmental psychological reasons concrete circles, balls, cubes or lego bricks have



to be chosen as models of smallest particles. Especially the discussion of form, color or material of the model as “irrelevant components” opens the chance to introduce the idea of the scientific model even on this level. In the beginning the particle model is used as a preliminary mental model. As lessons go along it advances via Dalton’s atomic model to the nucleus–shell model. At the end of this topic, “the randomly drawn limiting line” may be discussed with students and the demonstration of balls and circles should be critically evaluated.

*Understanding of chemistry through models:* Figure 6.1 shows the scheme “thinking in models” and thereby the process of perception in chemistry “from left to right”: with the help of additional information a chemist works out a mental model and transfers it to concrete models for visualization. Learners cannot go this way, but they can make their way through the diagram “from right to left,” by working first with concrete models: they observe and compare concrete models and develop advanced mental models for relevant issues. It is often the case that mental models interfere with irrelevant issues of display models, but an adequate abstraction happens more and more with time.

After the introduction of first mental models, for example the particle model of matter or the Dalton model of atoms or molecules, chemical facts are to be interpreted with those models, as long as it is possible on this level. Chemistry lessons should now proceed double-tracked, and they should be structure-oriented (see Chap. 10):

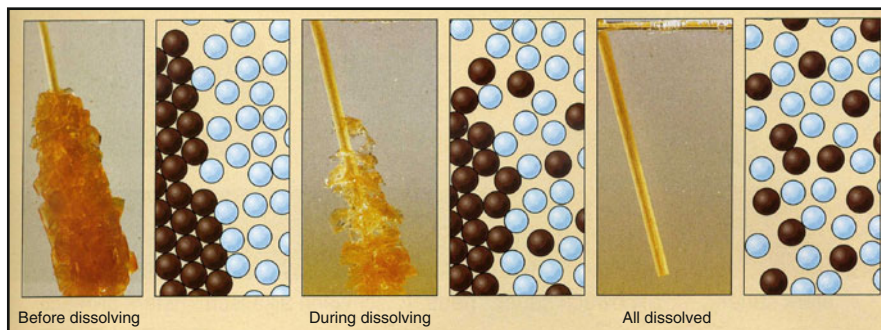
Track 1: phenomena and laboratory experience.

Track 2: structural models and mental models (see Table 6.1).

After the decision to introduce the *particle model of matter*, appropriate phenomena and experiments are to be chosen. It is possible to take snow flakes or crystals of sugar and to ask the reason why they have the same shape. The answer should be the symmetrical arrangement of particles: water particles are arranged in snow flakes in a special way, sugar particles in sugar crystals in a different way (see Table 6.1). It makes also sense to choose dissolution processes, for example the dissolution of sugar in water (see Fig. 6.11): the sugar particles are shown by dark spheres, the water particles by light spheres, the dissolving process should be interpreted by moving spheres: in the solution moving sugar and water particles

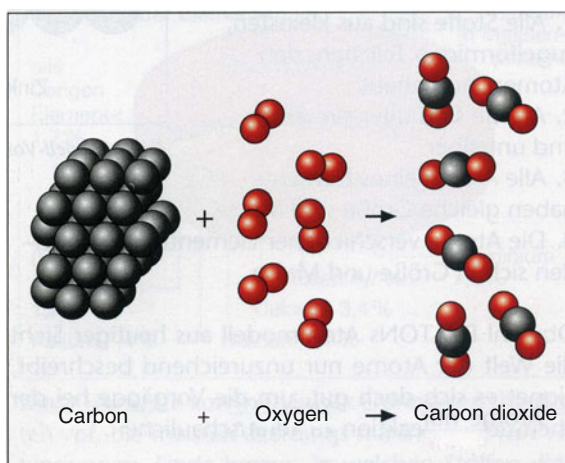
**Table 6.1** The two-tracked approach in chemistry lessons

Track 1:			
Phenomena and laboratory experience	Same shape of crystals, dissolving processes, diffusion, distillation	Chemical reactions of gases, gas laws, Avogadro’s law	Redox reactions of metals and salt solutions
Track 2:			
Mental and concrete models	Particle model: arrangement of particles before and after diffusion or dissolution	Dalton’s model: models for arrangements of atoms and molecules before and after chemical reactions	Atomic structure: electron transfer from metal atoms to ions in solution, from ions to atoms



**Fig. 6.11** Dissolving sugar crystals interpreted by the particle model of matter [15]

**Fig. 6.12** The carbon–oxygen reaction interpreted by Dalton’s atomic model [15]



are mixed. The motion can be visualized by shaking mixtures of two kinds of spheres in a glass bowl on the overhead projector.

If it is decided to introduce atoms and molecules with *Dalton’s atomic model*, reactions of carbon and oxygen may be conducted (see E1.9) and interpreted with C atoms and O atoms (see Fig. 6.12): C atoms in a carbon crystal are shown by big spheres in a closest sphere packing; two O atoms in one  $O_2$  molecule are presented by two linked smaller spheres. Carbon dioxide as the reaction product can be shown by  $CO_2$  molecules: molecular models consist of two small spheres with one big sphere in the middle. The reaction is interpreted by the rearrangement of C and O atoms.

*Packing of spheres.* Since metals are in the center of beginning chemistry lessons, it is possible to introduce the particle model (copper particles) or the Dalton model (Cu atoms) through the structure of metals. The advantage of this approach is that the three-dimensional arrangement of metal atoms in many metal crystals can be shown with close-packed spheres (see Fig. 6.13); learners accept

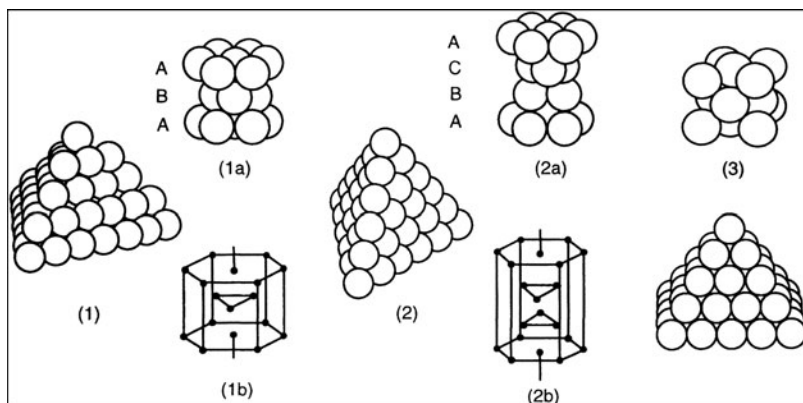


Fig. 6.13 Hexagonal and cubic close-packing as models of different metal structures [17]

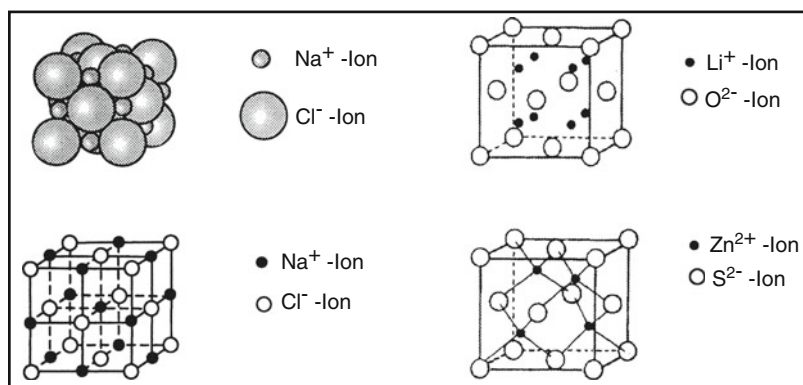


Fig. 6.14 Cubic-close-packing as models for salt crystal structures [18]

sphere packings easily when they have the opportunity to produce these models themselves by stacking spheres. With M6.1–M6.7 (see the “modeling course” at the end of this chapter) the building of sphere packings is suggested for the laboratory. Further information on metal structures can be found elsewhere (see also [5] or [17]).

If the holes in the cubic close-packing of spheres are introduced, one obtains the sodium chloride structure by filling out the octahedral holes with small balls (see Fig. 6.14). If the tetrahedral holes are being filled, the lithium oxide structure results. The zinc sulfide structure results in case that only half of the tetrahedral holes are filled. The construction of these salt structures is suggested for the lab with M6.8–M6.15 (see end of this chapter, also [5] or [18]).

*Molecular models.* As soon as gases are to be interpreted with the structure-oriented approach, the structures of appropriate molecules are to be demonstrated



with molecular models. Since the bonding of nonmetal atoms is usually represented by push buttons on balls in molecular kits, it is fairly easy for the learner to build molecular models independently. Thereby they become acquainted with atomic bonding over time (see Fig. 6.5 and [19]).

If the learner observes the directed sticks from ball to ball in the molecule model, these sticks can be interpreted as *directed bonding* between atoms. Subsequently it is possible to understand the bonding of metal atoms in metals or of ions in salts as *undirected bonding* and to separate this from the different bonding in molecules [16]. It is also possible to differentiate the *finite* arrangement of atoms in molecules from the *infinite* one of atoms or ions in crystals.

If at least two molecule kits are available and two different models are being built for the same molecule, the fixation of one single model with all irrelevant components can be prevented. In a discussion of these models the learner has to find out similarities in both models and recognize them as the feature of depiction. The same applies to sphere packings later on: if two models of different colors and materials are being built for the same metal or salt structure, a one-sided internalization of material or color can be avoided.

In conclusion it should be pointed out that the spatial ability of the learner can be enhanced with these three-dimensional structural models (see Chap. 10). Empirical research has shown [20–22] that spatial ability increases with the construction and discussion of structural models, with building up sphere packings to show metal structures, with the comparison of octahedral or tetrahedral holes and coordination numbers in ionic structures, with the intensive use of three-dimensional models of the structure of matter in chemical education.

*Adaptation and extension of models in chemistry lessons:* In most cases chemistry lessons start with the simple particle model of matter: one smallest particle is chosen for every pure substance, for the substance copper the copper particle, for water the water particle, for sugar the sugar particle. The assignment of carbon particles causes difficulties since there are two substances: diamond and graphite.

But there are no specific graphite particles and different diamond particles. Carbon particles exist in both substances: they build the diamond structure in a specific way and the graphite structure in another way (see Fig. 6.15). Carbon particles are therefore neither colorless nor black – colors are characteristics of substances and not characteristics of particles. The same applies to densities or melting temperatures: they are not particle characteristics, but substance characteristics!

*Applications and limits of models.* Table 6.2 shows that a specific model is not fixed for every time: there are spiral curricular changes depending on purpose and level of knowledge. Thereby one can indicate to the learner in chemistry lessons that models and mental models have to be extended according to latest understanding and knowledge – as it was the case historically.

In history the Greek philosophers were already discussing the atoms as “smallest particles of matter.” In 1808 Dalton got the big idea that there are as many kinds of atoms as elements, after discovering more and more elements. He brought us the first table of atomic masses and the sphere as the first mental model of one atom. In 1884 Arrhenius postulated ions as smallest particles of salts, acidic and basic

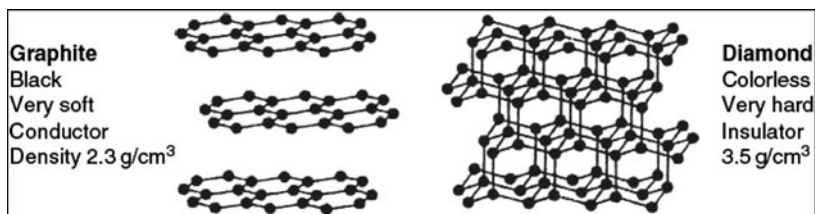


Fig. 6.15 Arrangement of C atoms in the graphite and diamond structure [19]

**Table 6.2** Concrete models and mental models, their application and limits

Particle model of matter	Interpretation: state of matter, change of state, kinetic theory of gases, diffusion and solution processes, chemical reaction without change of particles (e.g. formation of alloys), etc. Limits: ↓
Mass-charge model (Dalton)	Atom, atomic mass, element, compound, periodic table, chemical reactions: regrouping of atoms and ions, law of conservation of mass in chemical reactions, ions, ionic symbols, ion lattice, undirected bond, molecule, molecule symbol, molecule structure, directed bond, empirical and structural formula, reaction equation, etc. Limits: ↓
Nucleus and shell model (Rutherford)	Nucleus, protons, neutrons, isotopes, radioactivity, atomic shell, moving electrons, electron density, electron clouds, electrolysis, metal–nonmetal-reaction, redox reaction, electron transfer, etc. Limits: ↓
Nucleus and sub-shell model (Bohr)	Ionic charge number, periodic table and octet rule, chemical bond, ionic bond, covalent bond, hydrogen bond, etc. Limits: ↓
Valence shell electron pair repulsion model (VSEPR, Gillespie)	Electron clouds, repulsion of electron clouds, bond angle, bond length, spatial structure of molecules, etc. Limits: ↓
Atomic orbital model (Schroedinger)	Orbital, hybridization, delocalization, structure of the benzene molecule, calculation and prediction of lattice or molecule structures, molecular design with computers, etc.

solutions – from now atoms and ions should be called the basic particles of all substances, and the ions may be added to Dalton’s model. Following Rutherford’s discovery of the nucleus of atoms with his famous experiment in 1911, the nucleus–shell model was created. Subsequently Bohr and Schroedinger described and calculated the arrangement of electrons in sub-shells and orbitals.

Further functions of display and mental models: Models have not only the function to understand the structure of matter – there are other functions to understand chemistry better.

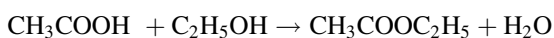
*Reduction of the learner’s anthropomorphic conceptions.* Preconceptions like “sunbeams clear the puddle” or “acids eat up metals” have been described in Chap. 1 “students’ alternative conceptions.” These or similar comments can be

discussed and challenged with the help of display models. Despite initial difficulties with scientific models, the learner is open to give up his alternative conception for a new mental model, when concrete models of the structure of matter are consequently used. Advanced mental models can be developed afterwards.

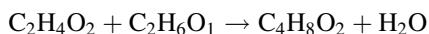
*Reduction of complex contexts.* The reduction of difficult contexts is a fundamental teacher's task: wherever possible complex contexts have to be reduced without losing the essentials. If the definition of element and compound is being reduced to the mental model of elements being built of atoms and compounds being built of molecules – as it happened in the 1950s – this reduction has to be avoided. If the chemical bonding of atoms in molecules is being reduced to the mental model of atomic valences and one introduces the bonding number 4 for the C atom or the bonding number 1 for the H atom, the reduction is reasonable and easily applicable to the methane molecule CH<sub>4</sub>, and other hydrocarbon molecules. This conception is acceptable – it can be extended in lessons on the nucleus–shell model later on to form the mental model of binding electron pairs between the atoms in molecules.

*Generalization of facts.* Beginning with the use of models, students are often able to generalize. If the CH<sub>4</sub>-tetrahedron is being introduced as a model of the methane molecule and the extension to the ethane molecule is demonstrated, then students are able to deduce all homologues of the alkane series by generalization. They develop a spatial ability for the structure of molecules and are more and more able to understand usual structural formulae or even half-structural symbols.

*Illustration of reactions.* If a chemical reaction is to be interpreted, structural models of the substances before and after the reaction can be demonstrated to the learner (see Chap. 7). Before the reaction to prepare and illustrate ester formation, for example, the structure of the involved acetic acid molecule and alcohol molecule has to be demonstrated with the molecular model kit. The elimination of a water molecule and the reaction equation using half-structural formulae can be written and illustrated with structural models:



No expert would describe the ester formation with empirical formulae only:



It is easy for reactions of organic chemistry: molecular structures before and after the reaction have to be taught and half-structural symbols have to be derived – otherwise empirical formulae of the above kind have to be memorized. In inorganic chemistry it is often thought that one can use symbols like Na, Zn or Al for metals and NaCl, ZnS or Al<sub>2</sub>O<sub>3</sub> for the corresponding salts. Without illustrating the structure of metals and salts by sphere packings and crystal structure models, however, learners will develop misconceptions of molecules: NaCl molecules or ZnS molecules. The empirical formulae lack any structural information and therefore these formulae are not helpful to understand substances and reactions: mental models of the structure of metals and salts have to be demonstrated (see [16–19, 23] and also Chaps. 7 and 10).

*Illustration of mathematical logical facts.* Descriptions of many chemical facts are based on abstract mathematical terms. Substantial mathematical reasoning is necessary for the deduction and use of equilibrium constants, for example, to recognize that the equilibrium of a weak acid is almost completely on the side of the molecules. The “glass-tube-cylinder model” (see E4.2) should be introduced, before equilibrium constants come into play. It is to demonstrate that equilibria do not only occur with a ratio of 50:50 (glass tubes of equal size in the model experiment), but also with ratios of 20:80 or 10:90 (glass tubes with different diameters). If the single steps of this experiment are plotted in a graph ( $x$ -axis) with the measured volumes in both cylinders ( $y$ -axis), two pairs of curves can be observed (see Fig. 6.16): equilibria and corresponding equilibrium constants can be understood with this model experiment. Another statistical game can show the same mathematical relationship.

The following rules regulate the game with A- and B-spheres:

- At the beginning 140 A-spheres are located in a glass bowl, no B-spheres are present
- Per time unit one sphere is taken out of the bowl: in case it is an A-sphere (that is certain at the start), it is changed to a B-sphere
- If it is a B-sphere, it is changed with the probability of 1:2 (throw a coin!) into an A-sphere. In case the coin decision is negative, the B-sphere is put back into the bowl

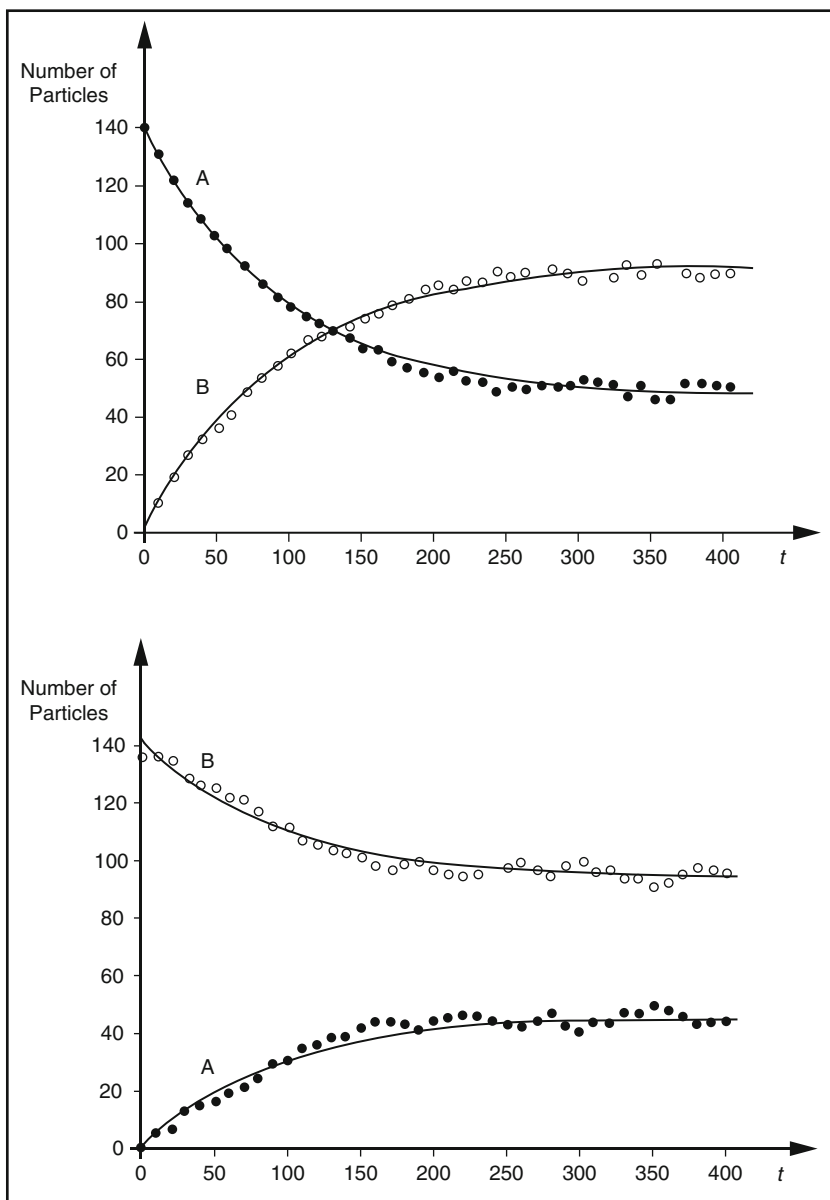
The result after 400 time units is shown in Fig. 6.16 (top): the model equilibrium is reached after about 300 time units, the number of B-spheres in the bowl is double that of the A-spheres.

If one starts with 140 B-spheres instead of A-spheres and plays with the same rules, the same model equilibrium as before is reached (see bottom of Fig. 6.16):  $n(\text{B}):n(\text{A}) = 2:1$ . If equilibrium is reached you can continue and play another 200 time units: the ratio of 1:2 will not change.

The transfer to reality shows the properties of a *dynamic* equilibrium: the forward reaction and the backward reaction are going on and on, but the concentrations of particles stay constant. The mathematical terms for these observations are the equilibrium constants: they are easier to understand with those models than without. Another nice model experiment shows the “Apple fight” of Dickerson and Geis [24] in Fig. 6.17.

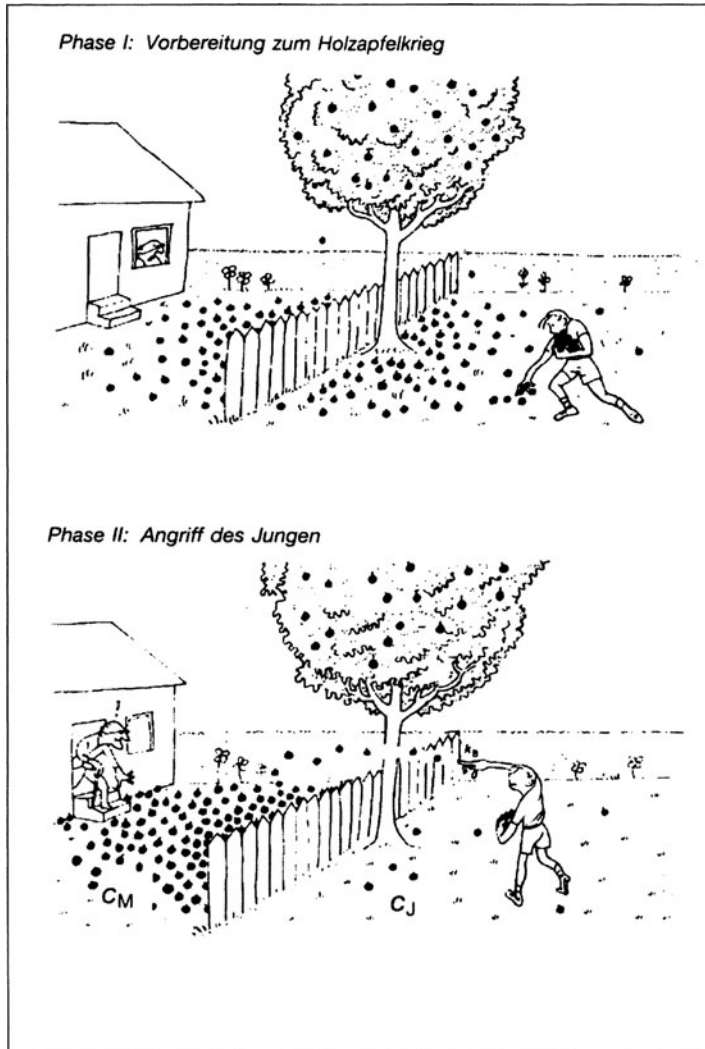
*Illustration of processes in chemical engineering.* If a production process for plastics is to be discussed in class, an experiment takes the part of a model. The experimental production of a nylon thread from the simple starting chemicals adipic acid and hexamethylene diamine, for example, can be demonstrated by pouring some mL acid on top of some mL hexamethylene diamine. A thin film forms at the interface, a thread can be drawn out of the beaker with the help of a glass rod. This model experiment serves as a basis for demonstrating the production of nylon or other polymers in chemical engineering.

*Construction of hypotheses.* Mental models of molecules allow the prediction of characteristics and specific reactions. If students are already familiar with the



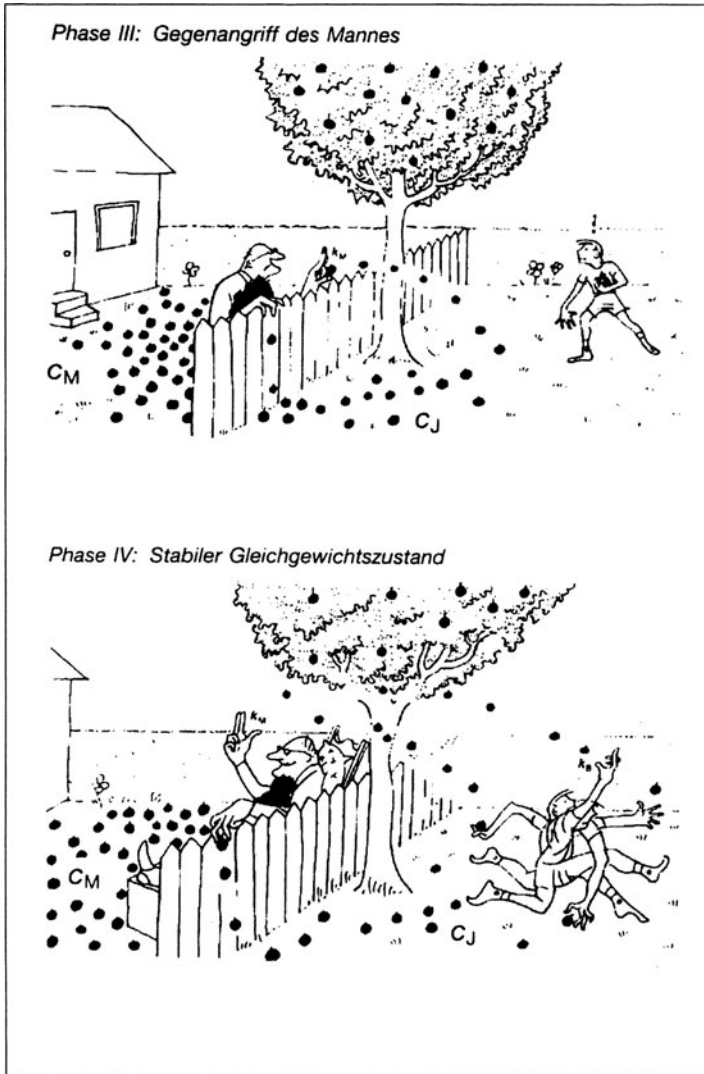
**Fig. 6.16** Simulation of an equilibrium [9]

structure of alkane or alkanol homologues, they are able to devise a hypothesis for the solubility of these homologues with the help of appropriate mental models concerning structures of molecules: alcohols with short carbon chains are not soluble in petrol, but in water; alcohols with long carbon chains are not soluble in water, but in petrol. Appropriate experiments can be planned for testing hypotheses.



**Fig. 6.17 (a)** An illustration of the equilibrium with the “Apple fight,” Part 1 [24]. Continued.

Science history also offers many examples. Watson [25], to only name one, cut out the shapes of base molecules from cardboard for the prognosis of base-combinations in the assumed DNA double helix: “The purine and pyrimidine models that I needed were not ready in time. So I used the whole afternoon to cut out exact models from thick cardboard. I started to move the base models back and forth and arranged them in pairs in every possible combination. Suddenly I realized that an adenine–thymine pair, which was held together by two hydrogen bonds, had the same shape as a guanine–cytosine pair” [25]. These sentences indicate the importance of very simple



**Fig. 6.17 (b)** An illustration of the equilibrium with the "Apple fight," Part 2 [24]

cardboard models for the understanding of the structure and function of nucleic acids. Thanks to this model conception, Watson and Crick were able to build a complete structural model of the DNA. They also formulated hypotheses that were in accord with all known facts and looked for new hypotheses, namely for the reduplication of DNA and the processes for the development of life.

### 6.3 Learner: Experience with Models

Students come to chemistry lessons with their experience of models in three areas: their own toy models, for example, soft toys, car or ship models. They also know concrete models of other school subjects like biology or geography, in mathematics they may even be used to mental models: most graphs can be shown by mathematical terms or formulae.

*Toys.* Children like to compare their dolls with themselves or others. They find out that many characteristics are the same in model and in the original: for example place and form of mouth, nose, eyes and ears. They also realize that there are functions, which the doll does not have: the doll does not eat or breath.

This experience is contrary to the understanding of scientific models. If young students take a structural model, they cannot compare it to the original: they are not able to look into the salt crystal, to recount the coordination number 6/6 of ions in common salt crystals. They find coordination numbers only in structural models. Due to the learners experience of concrete toy models the scientific model has to be developed and defined step by step.

*Fun with models.* The fun that children have playing with their dolls or car and ship models can be used for working with models of the structure of matter in chemistry. It has to be connected to an activity-oriented introduction to the scientific world of models, for example by building close-packed sphere models or crystal structure models.

If you show the packing of spheres for the sodium chloride structure to students (see Fig. 6.3b) and ask them to build this model with white and red spheres from cellulose (diameter: 30 mm and 12 mm, respectively), they have a lot of fun and proudly present this model at home. They might even discuss this model with their parents and siblings and might explain to them what it is a model for: now they are the experts, who explain chemical ideas to others! Instructions for model building exercises can be found at the end of this chapter.

If you show a model of the sodium chloride structure (see Fig. 6.3a) and ask them to rebuild this model with tooth picks and soft candy of two colors (for example red and black “strawberries” from sweet producers) they like to do this – and after the hard work and explanations of the coordination number 6 they may eat their model.

Older students, prospective teachers or even teachers at meetings for teacher training also like to work with structural models of all kinds, according to our experience. They convince themselves of the number and kinds of isomers in alkane molecules or special alcohol molecules, by building molecular models with the help of molecular model kits. If you offer even spheres of foam, of styrofoam, or of plexiglass to teachers, they like to build the different sphere packings (see the modeling course at the end of this chapter), and even like to build difficult models of unit cells (see Fig. 6.3c). At the end of the course they can take their self-built models to the school collection and use them in their chemistry lectures.

*Models from other subjects.* Students have lots of experience with models from other subjects. *Biology:* The school collection normally holds models of eyes, ears



or the human skeleton (only rarely an original). Model character, shortenings and irrelevant components of the models are very evident in these cases. These models are very illustrative and motivating due to the relevance for oneself: they can be used for a discussion of the idea of scientific models. But since visible body parts of the original can be compared with the corresponding model, this kind of biological model is not to be transferred to the models of chemical structures: no one is able to directly observe original structures of matter!

*Geography:* Maps, for example those of their home town or familiar hiking trails, are also models that are easy to understand for the students. Even the globe as a model can be compared to the original: pictures of Earth, seen from space, can be shown to the students today. Before the time of space travel the globe was nearly a mental model that could not be compared to the original directly. Models of Earth's interior cannot be obtained by optical comparison: they are derived from empirical analysis of experiments on Earth's surface.

*Mathematics:* Geometric drawings can be regarded as models. Certain triangles, for example rectangular triangles or equilateral triangles, are models for different patterns, and students can reproduce them for drawing special parquetry layers on the basis of these triangles. When students build three-dimensional models of cubes, cuboids, octahedra or tetrahedra with the help of given cardboard pattern and try to fill the whole space with them, the transfer of these models to chemical structures is possible and very useful. Structural models can be explained on this mathematical basis in chemistry lessons.

When students start to draw these cubes, tetrahedra and octahedra in three dimensions in their math class, these skills can be transferred to chemistry lectures to develop the ability to also draw three-dimensional models of the structure of matter. Moreover this trains and advances their spatial ability. The advancement of these skills is an important interdisciplinary task for mathematics, but also in chemistry: spatial ability is important for everyone's life!

## 6.4 Human Element: Interdisciplinary Mental Models

Working with models has an interdisciplinary character and makes a contribution to general education. Besides the understanding of the importance of scientific models, especially for chemistry, one can reflect on the relevance of models in many other fields. Models and mental models play an important role in

Industry: cycles of material

Economy: cycles of money and goods

Sociology: behavior patterns of specific groups of people

Politics: voting behavior of special groups of people

Ecology: cycles of substances in nature and ecological systems

## Appendix A. Problems and Exercises

- P6.1 You will find models in your chemistry collection at school: NaCl packing of spheres, NaCl crystal structure and NaCl unit cell (see Fig. 6.3). Give the features of depiction of the three models. Discuss and compare the irrelevant components of these models.
- P6.2 The NaCl-structure can be described by the cubic face-centered lattice of chloride ions where the octahedral holes are filled with sodium ions. Describe the  $\text{Li}_2\text{O}$ -structure and the ZnS-structure in a similar way and draw the corresponding models (see Fig. 6.13).
- P6.3 Planning of chemistry lessons applies two levels: level 1 deals with phenomena and lab experiences, level 2 with structural and mental models (see Fig. 6.11). Describe and draw your mental model of the diffusion of hydrogen sulfide ( $\text{H}_2\text{S}$ ) in air on the basis of (a) the particle model of matter, (b) Dalton's atomic model.
- P6.4 Usually mental models are introduced in chemistry lessons from the particle model, via Dalton's atomic model to the nucleus-shell model. Chose (a) a substance and (b) a chemical reaction and make model drawings on the basis of these three models. Discuss the differences in interpretation based on those models.
- P6.5 The chemical equilibrium can be illustrated with model experiments or with every-day experiences. Give one example for each and establish connections to an example of a real chemical equilibrium.

## Appendix B. Modeling Course: Structures of Metals and Salts

Material: 100 white cellulose balls  $d = 30$  mm [26], 50 red cellulose balls  $d = 12$  mm [26], triangular wooden frame ( $a = 17.5$  cm), square wooden frame ( $a = 15$  cm), modeling clay, glue, two equilateral ball-triangles (six balls with  $d = 30$  mm each).

Structure the plural: Close-packing of spheres (1 metal atom  $\equiv$  1 sphere) are structural models to describe the structure of many metal crystals (find drawing models at the end of this sheet).

- M 6.1: Fill up the triangular wooden frame with a closest layer of balls in the triangular pattern. Put as many layers of balls on top as possible. Draw the layers of balls.
- M 6.2: The coordination number stands for the number of balls that touch one ball in the middle of the packing. Find out the coordination number of one sphere in the close-packing of spheres. Draw three layers of balls to visualize this number.
- M 6.3: Two different close-packings of spheres with the coordination number 12 are possible:

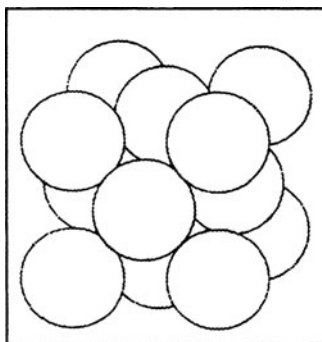
(a) With the layer sequence ABCABC..., (b) with the layer sequence ABAB...

Build both packings! Draw the layers of balls with triangular pattern so that (a) and (b) become apparent.

Definition: A layer sequence ABCA... exists, when the fourth layer of balls is congruent with the first layer – seen from above. The layer sequence ABA... exists, when the third layer of balls is already congruent with the first layer (the layers in triangular pattern are meant).

Information: An elementary cube (see picture) can be found in the ABCA-packing of spheres. Therefore this packing is also called *cubic close-packing* of spheres.

M 6.4: Draw the crystal structure model next to the shown packing. Draw a perspective cube: instead of the balls only give the central points of the balls and connect these points.



M 6.5: Put together the shown model with the help of the two equilateral 6-spheres triangles and two additional spheres.

Try to build this cube into the closest ABC-packing (M 6.3).

Draw two possible ways for building the elementary cube:

(a) Connect layers in a triangle pattern (1 + 6 + 6 + 1), (b) in a square pattern (5 + 4 + 5).

M 6.6: Take the square wooden frame. Build the cubic close-packing of spheres beginning with the square pattern. Try to get the elementary cube into the packing. Determine the coordination number. Draw the sphere layers so that the coordination number can be determined.

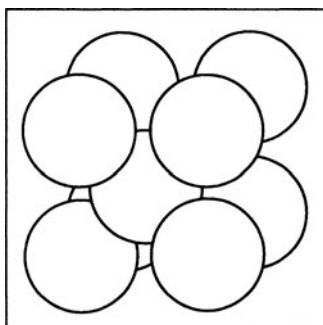
Information: The following models show the structure of metal crystals:

1. The hexagonal close-packing of spheres with the layer sequence ABA: it shows how crystals of magnesium and zinc are built up of atoms. One can say that there are crystals with hexagonal symmetry or crystals of the *Mg-type*.
2. The cubic close-packing of spheres with the layer sequence ABCA in triangular pattern: it shows in which way crystals of copper, silver or gold are built up of atoms. One can say that there are crystals with cubic

symmetry or crystals of the *Cu-type*. The elementary cube has one sphere in every face center – therefore this structure is also called *face-centered cubic*.

3. The name “face-centered cubic” is possible to point out the difference to the *body-centered* cubic packing of spheres. It is not a close-packing anymore, the coordination number is 8 (see picture). Metal crystals of tungsten and alkaline metals have this structure, the *W-type*.

M 6.7: The nine-spheres packing shows the elementary cube of body-centered cubic metal structures. Draw the crystal structure next to the picture: draw a perspective cube, instead of the balls only give the central points of the balls and connect these points. Compare it with M6.4.



**Structures of salt crystals:** The structure of many metal crystals can be illustrated by packings of spheres of *one* kind – the structure of salt crystals needs *two* kinds of spheres. Models for the sodium chloride structure and three other salt crystals will be built in the following (drawing models of the crystal structures are shown at the end of this section).

- M 6.8:  $\text{Na}^+$  ions in sodium chloride are to be represented with red balls ( $d = 12 \text{ mm}$ ),  $\text{Cl}^-$  ions with white balls ( $d = 30 \text{ mm}$ ). With the help of the triangle frame build a close-packing of spheres with both kinds of balls. Draw the layers of balls.
- M 6.9: Determine the coordination number for both kinds of balls. Draw the layers of balls to visualize the coordination number of both kinds of balls.
- M 6.10: In the close-packing of spheres there are two different-sized kinds of holes or gaps. Determine the number of balls that form those two different gaps. Draw the gap-producing balls for both kinds of holes in the form of the layers of balls: (a) for big gaps, (b) for small gaps.
- Information: Two different types of holes can be found in the close-packing of spheres. Convince yourself with the help of the model M 6.8:
1. Big holes are formed by six balls with octahedral geometry: octahedral gaps (OG)
  2. Small holes are formed by four balls with tetrahedral geometry: tetrahedral gaps (TG)

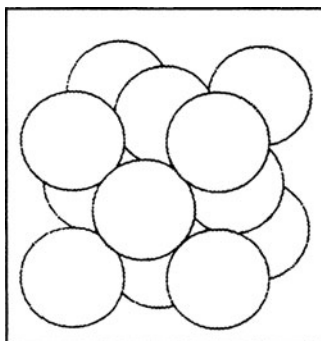
3. Spheres, OG and TG exist in a ratio of 1:1:2 in the close-packing of spheres.

The structure of the sodium chloride crystal can therefore be explained like this:  $\text{Cl}^-$  ions form a cubic close-packing of spheres, all octahedral gaps are occupied by smaller  $\text{Na}^+$  ions. The coordination numbers are 6 and 6, the ion ratio is 1:1, the ratio symbol should be  $(\text{Na}^+)_1(\text{Cl}^-)_1$

Explain the cubic shape of the sodium chloride crystal.

M 6.11: Take the elementary cube from M6.5, look for octahedral gaps and fill them with small red balls.

(a) Complete the model drawing by filling the gaps with small spheres (see picture).



(b) Draw the crystal structure next to the picture. Draw a perspective cube: instead of the balls only give the central points of the balls and connect these points (see M6.4).

M 6.12: Build the cubic close-packing of spheres with the help of the square frame and with both kinds of spheres. Draw the sequence of the 2-spheres layers.

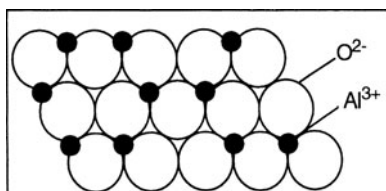
M 6.13: Convince yourself that the elementary cube can be build into the packing of spheres beginning with the triangle pattern (M 6.8) as well as the one beginning with the square pattern (M 6.12). Which position does it take in both models?

Draw the elementary cube with the help of (a) layers of spheres in the triangular pattern, (b) layers of spheres in the square pattern.

M 6.14: A model for the aluminium oxide structure (corundum structure) may be built:

(a) Stick together three layers with 15 white balls each (see picture).

(b) Add ten small balls in the shown pattern (see picture).

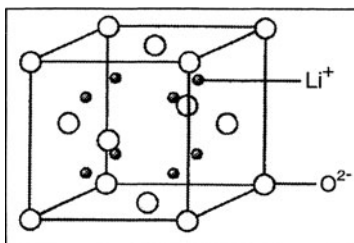
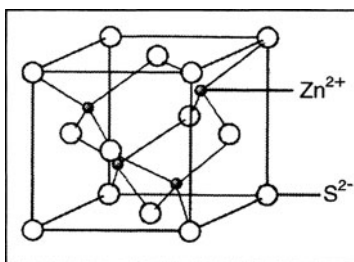


- (c) Stack up three layers so that the sequence is ABA. The coordination number of the small balls has to be six, of the big balls has to be four. What is the ratio of the balls?

Information: The  $O^{2-}$  ions form a hexagonal close-packing in aluminium oxide crystals, only  $2/3$  of octahedral gaps are occupied by  $Al^{3+}$  ions. The coordination is  $6/4$ , the ratio of ions is  $2:3$ . Therefore the models have to be abbreviated to formulae like  $\{(Al^{3+})_2(O^{2-})_3\}$  or  $Al_2O_3$ .

M 6.15: Form a few small balls with modeling clay that fit into the tetrahedral gaps of big spheres. With the small and the big spheres build an elementary cube

- (a) For the zinc sulfide structure (see picture).  
 (b) For the lithium oxide structure (see picture).

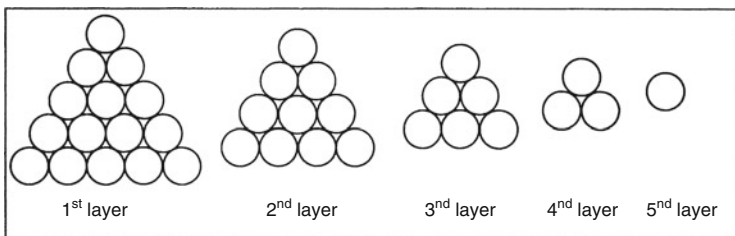


Information: zinc sulfide can be described as a cubic close-packing of  $S^{2-}$  ions, half of the tetrahedral gaps are occupied by  $Zn^{2+}$  ions. The coordination is  $4/4$ , the formula for the unit cell is  $\{(Zn^{2+})_4(S^{2-})_4\}$ , the empirical formula  $ZnS$ .

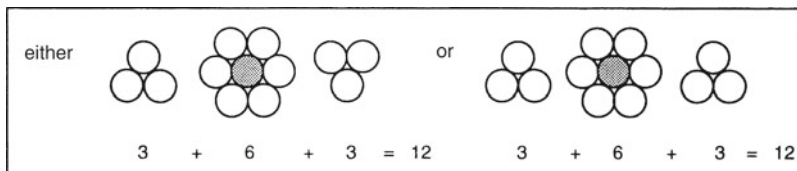
Lithium oxide can be shown as a cubic close-packing of  $O^{2-}$  ions, all of the tetrahedral gaps are occupied by  $Li^+$  ions. The coordination is  $4/8$ , the formula for the unit cell is  $\{(Li^+)_8(O^{2-})_4\}$ , the empirical formula  $Li_2O$ .

On the following two pages you will find the expected model drawings for the models M6.13 to M6.15. Compare your own drawings with these.

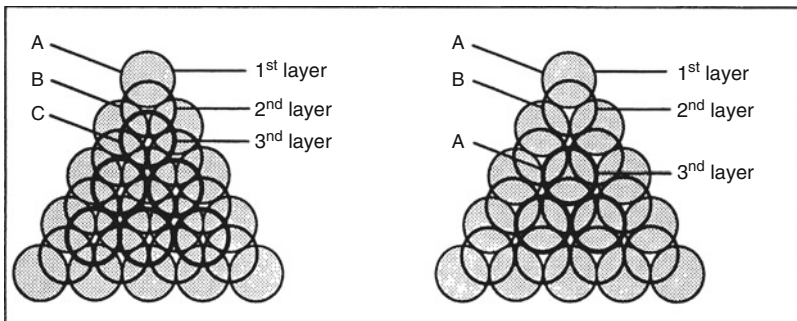
M 6.1:



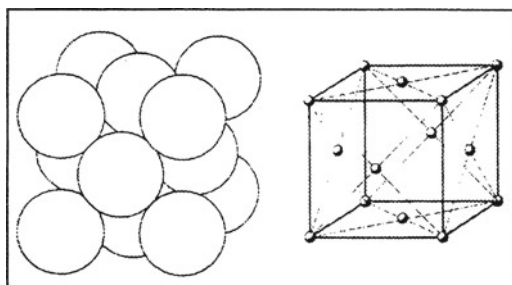
M 6.2:



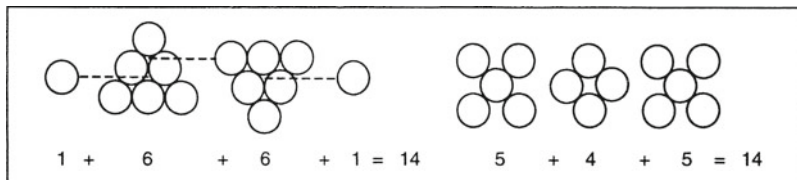
M 6.3:

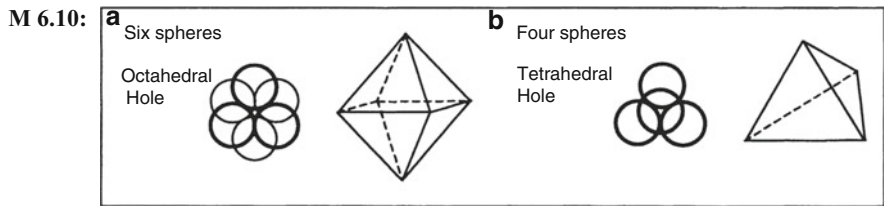
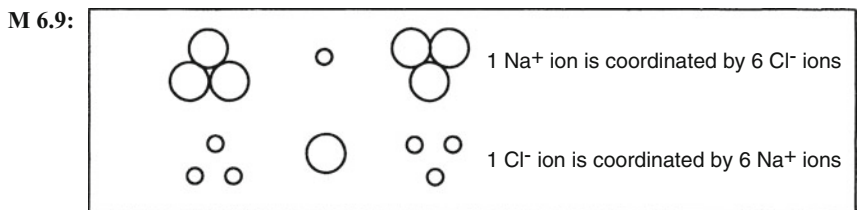
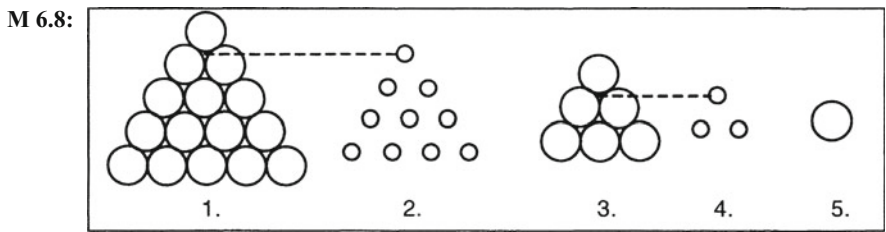
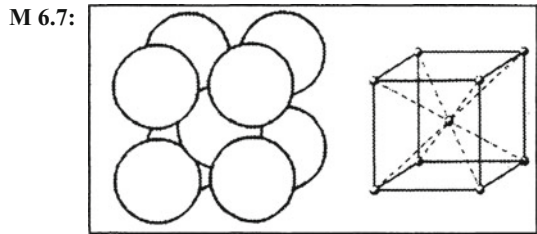
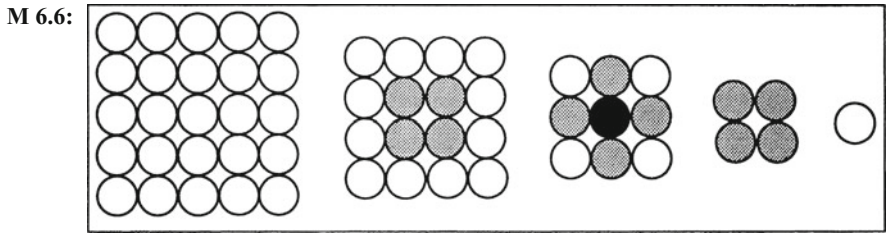


M 6.4:



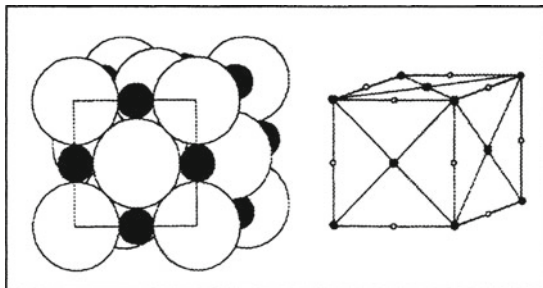
M 6.5:



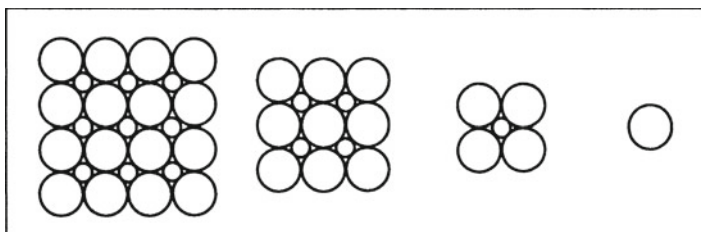




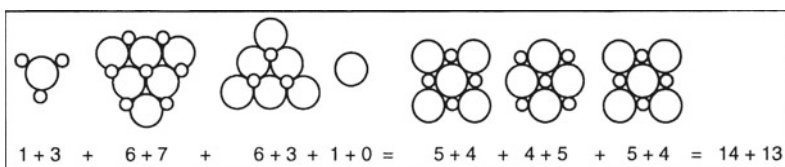
M 6.11:



M 6.12:



M 6.13:



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## ***Further Reading***

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