2.2. Basic Concepts

The idea of attributes is important in understanding materials. It is clear that the behaviour, i.e. the reaction of a material to external effects, is of utmost importance. Equally important is the reaction of the environment to the presence of some form of matter, but it is often more convenient to modify and control the agent rather than the ambient, in order to impose the desired reactions. The reactions related to certain material are conveniently defined by its attributes. The pertinent chemophysical and other attributes (such as the relative abundance or level of health hazard) are factors that distinguish one form of matter from another.

One of the principal attributes of matter is the amount (quantity) of a substance that exhibits certain consistent behaviour as an entity that can be distinguished from the ambient. Such entities of matter are modelled on an immense range of scales. Electrons, atoms and molecules can be placed at one end of such a range, while the planets, stars and galaxies belong to the other extreme.

Our knowledge of matter is conceptualised through defining the correlation between the geometric and kinetic features of its internal structure, the means needed to destroy or constitute them, and the scenarios of their formation or collapsing.

One classification convenient for understanding and use of materials defines so called states of matter such as solid, liquid, gas and plasma. Developing of these concepts is influenced by Mankind's initial perceptions of ambient and by historical evolution of the detecting and measuring techniques. Many strata of well verified knowledge and corresponding techniques make use of the above listed four concepts (i.e. solid, liquid, gas and plasma), however, the contemporary advances already promote yet further states of matter.

Pending on circumstances (purposes, limitations, intentions and beliefs), we can contemplate materials by departing from differing assumptions. For example, let assume that our solid product is intended for a use in which there is no exposure to any significant chemical deterioration or electromagnetic radiation (such as corrosion or gamma rays). In short, the only significant interaction with ambient can be represented by static mechanical forces that cause stresses well within the limits of elasticity. Finally, let us assume that the dimensions of our product are at the order higher than 10^{-4} m, and that its structure is homogeneous and continuous. Such solid can be described as a 3-dimensional set of points that obey a finite set of mathematical deterministic relations. Such a solid exhibits a resistance to change in its geometry when its motion collides with motion of other solids, i.e. when it comes into a contact with other solid that tends to follow a differing motion. Behaviour of this type of solids is quite successfully defined by so called theory of continuum mechanics, and in particular – solid mechanics. Deformation in such a solid must be less than 0.1 %, otherwise theory of elastoplasticity must be taken in account. Theory of solid mechanics allows for successful design of bridges, furniture, utensils, and variety of items and objects that can be classified as rigid bodies.

Numerous other applications, however, do not allow for the above simplifications. Indeed, some products are exposed to impacts or to fluctuating forces, and in such cases even the minute inhomogeneity and discontinuity becomes a significant factor. Stresses can reach levels far beyond the limits of elasticity and, in addition, various chemophysical phenomena such as oxidation, thermal and magnetic exposure can cause significant reactions in a solid material. Therefore we ought to understand the detailed structure of our product and the processes that take place in the ambient, in order to predict its behaviour.

The structure of matter in a solid material can be classified under four headings:

- **sub-atomic level**
- **atomic level**
- **super-atomic structures** and
- **more global configurations**.

Another way of looking at these levels is to allot the forms of matter to an appropriate scale

- **microscopic level (sub-atomic distances)**
- **human scale (macroscopic level)**
- **galactic and extragalactic scales.**

Since the **atom** is a fundamental concept, it is useful to note that some sources [287] define the atom as the 'smallest unit into which matter can be divided without the release of electrically charged particles'. The atom is also defined as the smallest fraction of matter that has the attributes of a chemical element. Sub-atomic structures are correlated to phenomena such as light or X-ray radiation, generally classified as electromagnetic radiation. The "upper level" of sub-atomic forms, namely quarks, electrons, protons and neutrons have only recently been detected and are by no means fully understood. Nevertheless, laser beams as well as magnetic fields are widely used in contemporary manufacturing processes, while gravitational fields have been exploited since the very beginning of human civilisation. The variety of applications continues to increase with our understanding of these phenomena, and vice versa.

When brought into certain mutual relations, electrons, protons, neutrons (probably further combined with additional sub-atomic particles) form together a family of differing chemical elements, methodically classified within chemistry and physics at the atomic level. The **periodic system of elements** provides a rational method for classifying elements into groups, where the common attributes can be understood, based on the model of the atom.

Simple geometric concepts of the atomic nuclei and corresponding electronic shells provide handy models for analysing and categorising different elements. It should be noted however, that even this atomic level of configuration is still a matter of intense study.

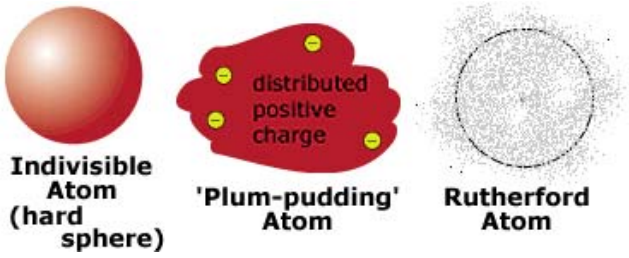

Fig 2.0 a: Historical models of the atom

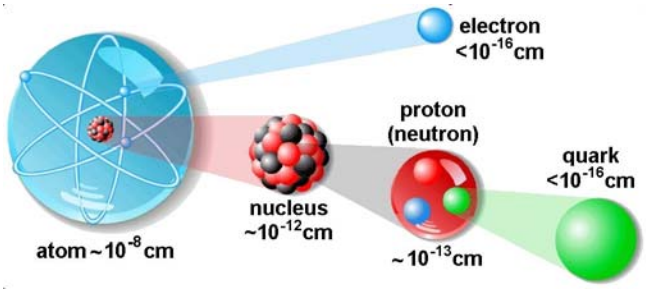

Fig 2.0 b: Structure of the atom
(contemporary models)

Contemporary materialography such as scanning tunnelling microscopy enables us to observe matter forms at the super-atomic level, Fig 2.1. Scientific models often translate these observations into geometric configurations of spheres "frozen" within crystal lattices, Fig 2.2.

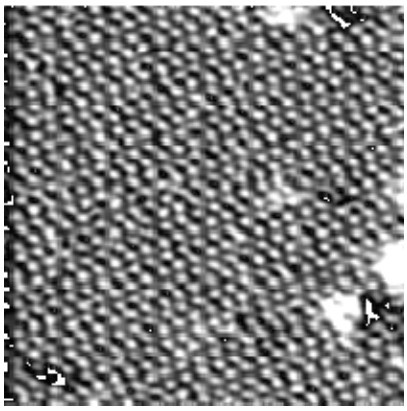

Fig 2.1: Scanning Tunneling Microscope picture of Germanium crystal plane (111) [121]

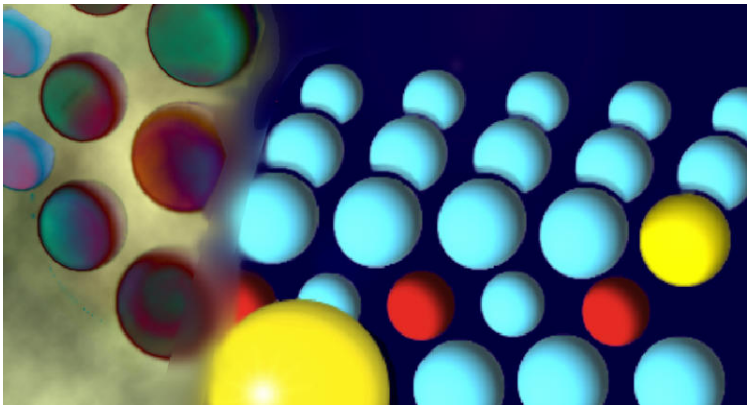

Fig 2.2: A model of "frozen" structure of a solid material

The modelling at sub-atomic and atomic levels is based on indirect observations of radiation phenomena, and on concepts of sub-atomic particles.

In 1910s Nagaoka and Rutherford proposed the model of an atom as a dense, positively charged nucleus, in which nearly all the mass is concentrated; the light, negatively charged electrons orbit the nucleus at some distance from it, Fig 2.3. This model, also called the planetary model, was based wholly on classical physics. It was superseded within a few years by the Bohr atomic model, Fig 2.4, incorporating some early quantum theory.

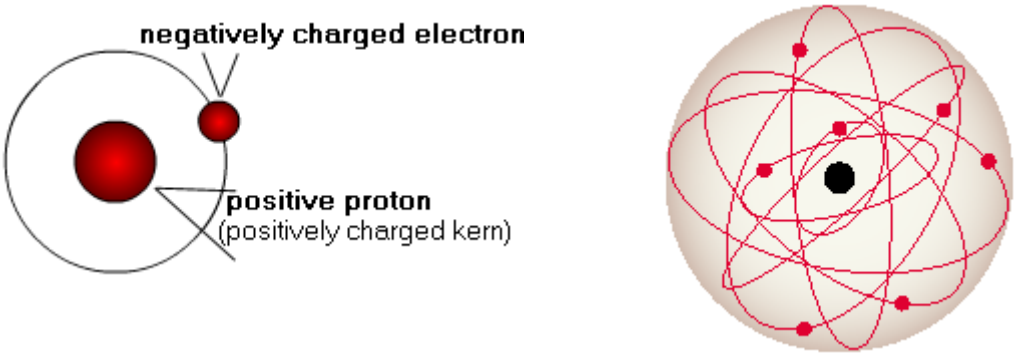

Fig 2.3: The Rutherford-Nagaoka atomic model

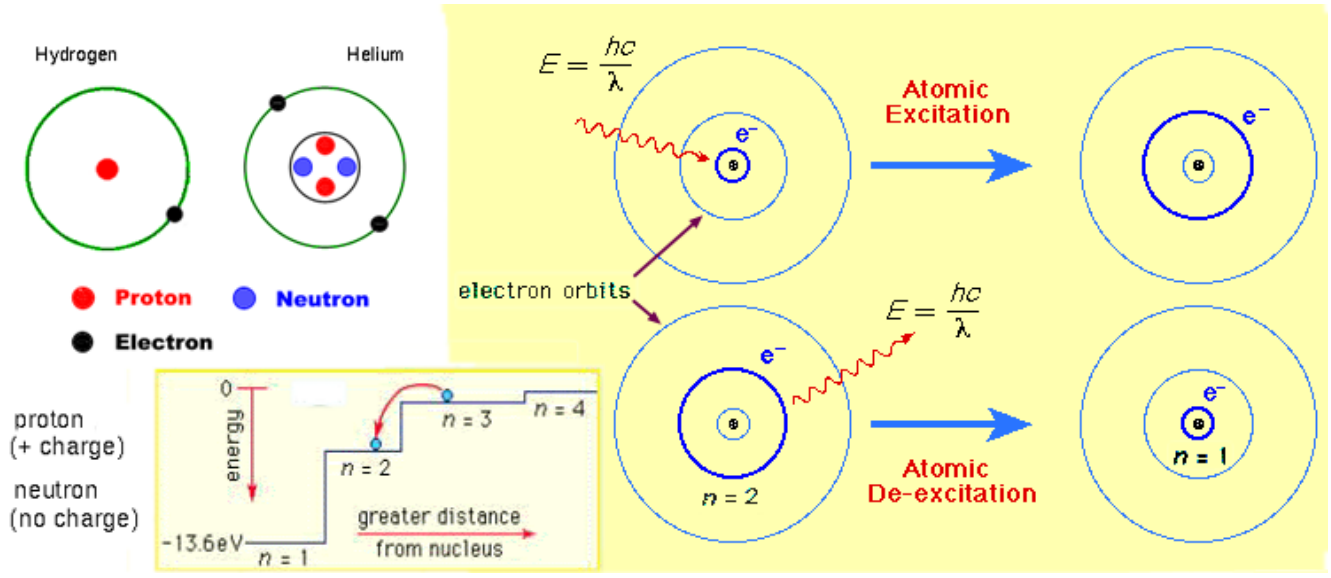

Fig 2.4: The Bohr atom. The electron travels in circular orbits around the nucleus. The orbits have quantized sizes and energies. "Energy" is emitted from the atom when the electron jumps from one orbit to another closer to the nucleus. Shown here is such a transition, in which an electron jumps from orbit n = 3 to orbit n = 2, producing a photon of red light with an energy of 1.89 eV and a wavelength of $656 \cdot 10^{-9}$ m. (Encyclopedia Britannica, Inc.) [11]

The Bohr model represents the atomic energy levels as discrete levels much like the orbits of planets around the sun. For many purposes of chemistry and materials science, this simple orbital model with its discrete energy levels is quite adequate.

A further concept is called the Shell Atomic Model. In this model, electrons in atoms are thought of as occupying diffuse shells in the space surrounding a dense, positively charged nucleus. The shells are filled in a systematic order, with each shell being extended outward from the nucleus. The shells are sometimes designated by capital letters beginning with **K** for the first shell, **L** for the second, **M** for the third, and so on. The maximum numbers of electrons that can occupy shells one through seven are, in sequence, 2, 8, 18, 32, 50, 72 and 98. Different atoms have different numbers of electrons, which are distributed in a characteristic electronic structure of filled and partially filled shells. The lightest element, hydrogen, has one electron in the first shell only. The heaviest elements in their normal states have only the first four shells fully occupied with electrons and the next three shells partially occupied.

Newer developments led to the so called Liquid Drop Model. Nuclear properties, such as the binding energy, are described in terms of volume energy, surface energy, compressibility, etc.— parameters that are usually associated with a liquid. This model has been successful in describing how a nucleus can deform and undergo fission. Yet another one — the Collective Model — includes motions of the whole nucleus such as rotations and vibrations. The Collective Model can be viewed as an extension of the Liquid Drop Model, and as an opposite extreme relative to the Shell Model; it explains why the energy levels show the characteristics of rotating or vibrating systems expected from the laws of quantum mechanics.

The more advanced contemporary models, known as Unified Models, propose theories such as Standard Model in an attempt to include both shell and collective behaviours.

The unified model describes the atomic nuclei by incorporating aspects of the shell model and so the called "liquid-drop" model to explain certain electromagnetic properties. In the shell model, nuclear behaviour is explained on the basis of unpaired nucleons (protons and neutrons) beyond the passive nuclear core composed of closed shells of paired protons and paired neutrons. In the liquid-drop model, nuclear behaviour is explained via statistical contributions of all the nucleons (much as the molecules of a spherical drop of water contribute to the overall energy and surface tension). In the collective model, high-energy states of the nucleus and certain magnetic and electric properties (moments) are explained by the motion of the nucleons outside the closed shells combined with the motion of the paired nucleons in the core. The nuclear core may be thought of as a liquid drop on whose surface circulates a stable tidal bulge directed toward the rotating unpaired nucleons outside the bulge. The tide of protons (positively charged particles) constitutes a current that in turn contributes to the magnetic properties (geometry) of the nucleus. These concepts are studied within the specialised streams of quantum chemistry and nuclear physics.

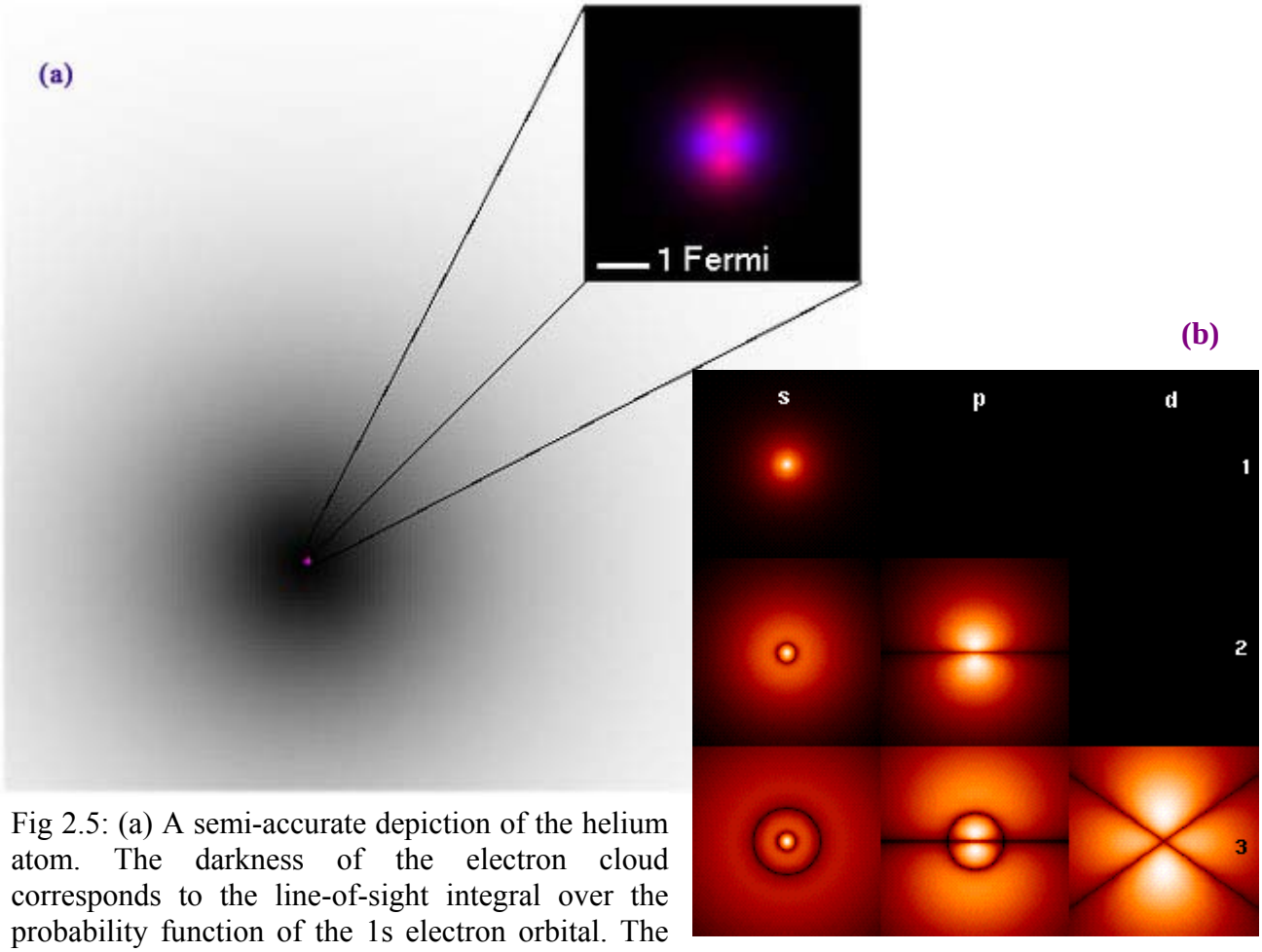

Fig 2.5: (a) A semi-accurate depiction of the helium atom. The darkness of the electron cloud corresponds to the line-of-sight integral over the probability function of the 1s electron orbital. The magnified nucleus is schematic, showing protons in pink and neutrons in purple.

(b) The atomic orbital wavefunctions of a hydrogen atom. The principal quantum number is at the right of each row and the azimuthal quantum number is denoted by letter at top of each column; The first few hydrogen atom orbitals (the cross-sections of the probability density that are color-coded:
black = zero density, white = highest density). The letters s, p, d and f are used to describe the shape of the atomic orbitals, and are called the orbital quantum numbers . [561]

The above theories provided explanations for variety of nuclear properties, especially energy levels in nuclei; they also provided more realistic picture of the electrons presenting them as probability clouds where the "orbit" is merely the most likely distance from the nucleus Fig 2.5.

The chemical properties of atoms are quite satisfactorily explained in terms of how the shells are occupied with electrons. For example, helium (atomic number 2) has a full first shell; neon (atomic number 10), with eight electrons in its outermost shell, has a full first and second shell. Other atoms that have eight electrons in their outermost shell, even though it is not full, chemically resemble helium and neon in their relative stability and inactivity. Thus, the arrangement of an atom's electrons determines its chemical properties.

Chemical elements can be characterised by the atomic number (number of protons or electrons) and atomic mass (sum of masses of protons and neutrons; for practical purposes the mass of electrons can be disregarded). The atomic mass (also "atomic weight") represents an average of the various isotopes (atoms of the same element which contain different numbers of neutrons) that may exist. The atomic mass of some amount of substance is measured in gram-moles.

The unit for the amount of matter is the mole. The mole is a dimensionless SI measure that denotes the amount of a substance containing the same number of chemical entities (atoms, molecules, ions, electrons, or other specified entities or groups of entities) as 12 grams of carbon-12. The number of entities in a mole is denoted by Avogadro's number (constant) N_A. Thus in a mole of carbon-12 there are $N_A = 6.0221367 \cdot 10^{23}$ atoms of carbon (this was determined experimentally using 12 grams of carbon-12). Carbon-12 was chosen arbitrarily to serve as the reference standard of the mole unit for the International System of Units. One mole of carbon-12 atoms has N_A atoms and mass of 12 grams. In comparison, one mole of Al consists of the same number of atoms as carbon-12, but it has a mass of 27 grams. The concept of the mole can be used to calculate the quantities involved in chemical reactions.

Example 2.2.1. Determine the mass of 0.72 mol of H_2ClO_4 (source of example: [325])

Solution: Since one mole has a mass of $2 \cdot 1 + 35.5 + 4 \cdot 16 = 101.5$ g, it follows that 0.72 mol corresponds to mass of $0.72 \cdot 101.5 = 73.1$ g

The interdependence of matter structure and its other properties continues at the super-atomic level. Based on their individual constellations, and the circumstances under which the different atoms are brought together, the resulting structures form entities such as molecules, crystals, clusters or glasses (amorphous substances). At a higher level (sometimes termed "macroscopic") the structural constituents such as 'dendrites', 'grains', 'grain boundaries', 'bands', 'networks', 'chains' and numerous combinations of these entities cause equally diverse permutations of attributes. Perhaps the "upper" boundary to such conceptual levelling, based on structures, are the foams and honeycomb macrostructures, which are still surpassed by complex structures called 'composites'.

The notions of "chemical" attributes linked to definition of chemical elements, and the "physical" attributes based on "laws governing matter and energy", have certainly brought in advances in understanding the matter forms. Further advances were brought about by combining chemical and physical theories, hence it is appropriate to denote this joint structure of relations ─ chemophysics.

Click here to return to Contents