

Materials on an Atomic Level

1 Bonding Types

Atoms are bonded together to form materials. They can be bonded in multiple ways. The three strongest bonding types, the primary bonding types, are:

- Ionic Bonding - When metallic elements give up their electrons to nonmetallic elements, the metallic elements become positively charged, while the nonmetallic elements get a negative charge. These different kinds of charges attract each other.
- Covalent Bonding - In covalent bonding, stable electron configurations are assumed by the sharing of electrons between adjacent atoms.
- Metallic Bonding - Metallic bonding is, more or less, caused by a negative electron cloud (consisting of valence electrons), holding together the positive ion cores, consisting of nonvalence electrons and atomic nuclei.

Next to the primary bonding types, there are also secondary bonding types. These van der Waals-bonds are weak in comparison to the primary bonds, and are caused by atomic or molecular dipoles, existing whenever there is a separation of positive and negative portions of an atom or molecule.

2 Crystallinity

Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. If the atoms are situated in a repeating or periodic array over large atomic distances, it is called a crystalline material. Otherwise it is a noncrystalline or amorphous material. All metals, many ceramics, and also certain polymers form crystalline structures under normal solidification conditions.

The crystal structure of a material is the manner in which atoms, ions or molecules are spatially arranged. Some of the properties of a material depend on this crystal structure.

3 Unit Cells

The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. It is often handy to look for a small unit cell that, when put together multiple times, forms the regular pattern in which the atoms are arranged. Unit cells have multiple properties:

- The crystal system the unit cell belongs to. This depends on the shape of the unit cell.
- The size of the unit cell. (Also the shape can be important, if this has not been set by the crystal system the unit cell is a member of.)
- The atoms per unit cell.
- The atomic packing factor (APF). This is the part of the unit cell filled by atoms, and can be calculated by dividing the volume of atoms in a unit cell by the total unit cell volume.
- The coordination number. This is the amount of neighboring atoms every atom has.

There are three kinds of metallic crystal structures: the face centered cubic (FCC), the body centered cubic (BCC) and the hexagonal close packed (HCP). Their properties can be found in table 1.

Also the crystal structure density ρ can be determined, using the following formula:

$$\rho = \frac{nA}{V_c N_A} \quad (1)$$

Structure	Shape	Size ($R = \text{Atom radius}$)	Atoms/cell	APF	Coordination #
FCC	Cubic	Cube length = $2\sqrt{2}R$	4	$\frac{\pi}{3\sqrt{2}} \approx 0.74$	12
BCC	Cubic	Cube length = $\frac{4R}{\sqrt{3}}$	2	$\frac{\sqrt{3}\pi}{8} \approx 0.68$	8
HCP	Hexagonal	Hexagon Length = $2R$ Height = $4\sqrt{\frac{2}{3}}R \approx 3.266R$	6	$\frac{\pi}{3\sqrt{2}} \approx 0.74$	12

Table 1: Properties of the FCC, BCC and HCP crystal structures.

Where n is the amount of atoms per unit cell, A is the atomic weight, V_c is the volume of a unit cell and N_A is Avogadro's number ($6.022 \cdot 10^{23}$ atoms/mol).

4 Amount of Crystals

Some materials may have more than one crystal structure. This phenomenon is known as polymorphism, and is sometimes also termed allotropy. The prevailing structure depends on both temperature as external pressure.

Most materials only have one crystal structure, but are composed of a collection of many small crystals or grains. This means that there are multiple grains inside the specimen, each having the same crystal structure, but are orientated in a different way. Every crystal or grain itself is therefore anisotropic. But since there often is an extreme high amount of different grains in a specimen, all having random orientations, the specimen itself is isotropic.

When a specimen is made in such an ordered way that all grains have equal orientation, and therefore become one grain or crystal, the specimen becomes a single crystal. Single crystals exist in nature, and can also be produced artificially, but they are rather difficult to grow. In single crystals the crystal structure extends itself throughout the entirety of the specimen without interruption. Materials not consisting of a single crystal are termed polycrystalline materials.

The place where two grains meet is called a grain boundary. More about this will be explained in paragraph 8.

5 Irregularities

Only under perfect situations is the atom pattern in a material perfectly regular. Many irregularities or imperfections may occur. It might occur that there is an empty spot in the atom roster, where normally an atom should have been. This is called a vacancy. It is also possible that there is an atom in a place where normally there would not be an atom. This event, which occurs in only very small concentrations, is called a self-interstitial. Naturally, materials consisting of only one element are impossible to make as well. Impurities always occur in a metal. Sometimes this is done intentionally, for example in the creation of an alloy. The addition of impurity atoms to a metal will often result in the formation of a solid solution (also a new phase might form, but that is an entirely different topic). In a solution, the solvent is the compound present in the greatest amount, while the solute is the compound present in minor concentrations.

The solute can dissolve in the solvent in multiple ways. The solute can consist of substitutional impurity atoms. These atoms take up the place of one or more solvent atoms. The solute can also consist of interstitial impurity atoms, which take up a position between the solvent atoms. The way in which the solute dissolves in the solvent depends on multiple parameters, of which the most important one is the atomic size factor.

6 Specification of Composition

In the case of an alloy, it is often necessary to express the composition of an alloy. The most common way is to use the weight percentage (wt%) or the atom percentage (at%), which are, respectively:

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100\% \quad C'_1 = \frac{n_1}{n_1 + n_2} \times 100\% \quad (1)$$

Where C_1 , m_1 , C'_1 and n_1 are the weight percentage, the mass, the atom percentage and the number of atoms/moles, respectively, of a certain element 1. m_2 and n_2 naturally are the mass and the number of atoms/moles, respectively, of a certain element 2. The percentages of element 2 can be calculated in a similar way.

7 Dislocations

A dislocation is a linear or one-dimensional defect around which some of the atoms are misaligned. One type of dislocation is when the edge of an extra plane of atoms terminates within the crystal. This is termed an edge dislocation. The line at which the edge terminates is termed the dislocation line.

Another type of dislocation, called a screw dislocation, exists, which may be thought of as being formed by a shear stress that is applied to produce a distortion. However, most dislocations found in crystalline materials exhibit components of both types. These dislocations are termed mixed dislocations.

As was previously mentioned, the dislocations cause an irregularity in the crystal structure. This irregularity causes internal strains in the crystal structure, called lattice strains. The term lattice is sometimes used that it means a three-dimensional array of points coinciding with atom positions (or sphere centers).

To indicate the amount of dislocations, the dislocation density is defined as the length of the dislocations per unit volume or, equivalently, the number of dislocations that intersect a unit area of a random section. The dislocation density therefore has as unit m^{-2} (per square meter).

8 Interfacial Defects

Interfacial defects are boundaries that have two dimensions, and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations. One of the most obvious boundaries is the external surface, along which the crystal structure terminates.

Inside a specimen are also boundaries between multiple grains, called grain boundaries. (Single crystals are an exception.) These boundaries separate two small grains or crystals having different crystallographic orientations. Grain boundaries aren't necessarily flat planes. Various degrees of misalignment between adjacent grains are possible. When the orientation mismatch is small (in the order of a few degrees), then the term low-angle grain boundary is used. Otherwise the term high-angle grain boundary is used.

Other types of grain boundaries are tilt boundaries and twin boundaries. Also other miscellaneous interfacial defects may occur in a material.

9 Diffusion

Diffusion is material transport by atomic motion. There is no external force in diffusion. For example, when two types of metal are held together and heated, diffusion usually occurs (depending on things as material type, of course). The atoms of one metal start mixing up in the other. This process of migration of impurity atoms is called interdiffusion or impurity diffusion. A migration of the host atoms itself is called self-diffusion. This kind of diffusion does not cause concentration changes. Diffusion is caused by the fact that the atoms of a material are always moving (the higher the temperature, the faster the atoms move).

Two diffusion mechanisms are possible. One mechanism of diffusion is vacancy diffusion, where an atom adjacent to a vacancy, moves to the vacancy, leaving a new vacancy on its former position. Another mechanism of diffusion is interstitial diffusion, where interstitial atoms change position between the other atoms.

If M is the mass diffusing through and perpendicular to a unit cross-sectional area A of solid per unit time, and t is the elapsed diffusion time, then the diffusion flux J is defined as:

$$J = \frac{M}{At} \quad (1)$$

If the diffusion flux does not change with time, a steady-state diffusion exists. Otherwise a nonsteady-state diffusion exists. This diffusion flux also has a relation with the rate at which diffusion occurs. This rate is indicative of the rate of atomic motion, being strongly dependent on the temperature.

10 Dislocation Movement

Dislocations can move around in a crystal structure. This is often caused by external forces, but sometimes also by internal strain energy. When some of the internal strain energy is relieved by virtue of dislocation motion, there is some reduction in the number of dislocations, and dislocation configurations are produced having low strain energy. This process is called recovery.

Even after recovery, the grains are still in a relatively high strain energy state. When there is enough energy (which is the case when the temperature is high enough), recrystallization occurs. Recrystallization is the formation of a new set of strain-free grains that have low dislocation densities. The average size of the new grains is a function of the temperature. The recrystallization behavior of a particular metal alloy is sometimes specified in terms of a recrystallization temperature, which is the temperature at which recrystallization just reaches completion in one hour.

Dislocations often have a certain plane in which they 'prefer' to move, the so-called slip plane, and also a certain direction in which they prefer to move, which is called the slip direction. This combination of the slip plane and the slip direction is termed the slip system. The slip system is such that the atomic distortion that accompanies the motion of a dislocation is a minimum.

11 Strain Hardening

Strain hardening, also called cold working, is the phenomenon whereby a ductile metal becomes harder and stronger as it is plastically deformed. Percent cold work is defined as:

$$\%CW = \left(\frac{A_0 - A_d}{A_0} \right) \times 100\% \quad (1)$$

Where A_0 is the original area of the cross-section that experiences deformation, and A_d is the area after deformation. Strain hardening increases yield strength and tensile strength, but decreases the ductility. The dislocation density increases because of cold working, causing dislocation multiplication and the formation of new dislocations. Since the dislocations are packed closer together, their ability to move decreases, which hardens the material, but also makes it brittle.

The effects of strain hardening can be removed by an annealing heat treatment, i.e., an exposure to an elevated temperature followed by cooling at a slow rate. This often causes recrystallization, decreasing the amount of dislocations in the material. The new-formed grains during recrystallization are characteristic of the pre-cold-worked condition.