

Minerals and the crystalline state



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Introduction

Rocks are made of minerals and, as minerals are natural crystals, the geological world is mostly a crystalline world. Many large-scale geological processes, such as the movement of continents and the metamorphism of large volumes of rock during mountain building, represent the culmination of microscopic processes occurring inside minerals.

Minerals and rocks are also natural resources that provide the inorganic raw materials for almost everything humans use. A good scientific understanding of their origins, occurrence and properties helps to maximise their potential benefits to humanity.

In this free course, you will study mineral and rock (and fossil) specimens as interactive images in a resource called the Digital Geology Kit, which is described briefly in the box below and then in more detail in a subsequent activity.

Accessing the Digital Geology Kit

The Digital Geology Kit is one of a number of interactive, practical science resources that you can access from [The OpenScience Laboratory](#) website: a collaborative initiative of The Open University and The Wolfson Foundation. Here you will find investigations, tools and activities covering a broad range of scientific fields, including Earth science, astronomy and health.

Links to the Digital Geology Kit appear at relevant points within this course. When you first access the tool you will be prompted to either sign in (if you are already an Open University student), or to register with your email address to create an account free of charge. This only takes a few minutes to do.

Note that the interactive activities on the OpenScience Laboratory website require a modern web browser, such as Mozilla Firefox, Google Chrome, Apple Safari or Microsoft Internet Explorer 9 or later.

This OpenLearn course is an adapted extract from the Open University course S209 [Earth science](#).

Learning Outcomes

After studying this course, you should be able to:

- give, with an appropriate example, the meaning of the terms phase, phase boundary and phase transformation, and interpret stability fields in terms of pressures and/or temperatures using a phase diagram
- describe and recognise, giving examples, various physical properties of minerals, including lustre, cleavage, hardness and density
- describe, giving mineral examples, the main differences between metallic, ionic and covalent structures and their type of bonding
- explain the significance of various types of defects in crystals
- explain the meaning of the terms lattice, unit cell, reflections and rotational symmetry, and how these relate to crystal systems.

1 Introducing crystals

Three distinct types of crystal, each of which is a different mineral, can be seen in the granite shown in Figure 1: shiny black *biotite mica*; cloudy white *feldspar* and translucent grey *quartz*.



Figure 1 A close-up of a piece of granite, 7 cm across, showing interlocking, intergrown crystals of several different minerals, including grey quartz.

The junction between any two adjacent crystals in the rock is called a **grain boundary**. Grain boundaries occur where crystals develop in contact with each other - here, during the cooling and crystallisation of magma to form granite. Grain boundaries also develop when minerals grow in the solid state during metamorphism.

Where the crystals form an interlocking mass, as in granite or marble, they rarely have the opportunity to develop good crystal faces. By contrast, the best-formed crystals are often ones that have grown into cracks or cavities (such as a gas bubble in a lava flow). Figure 2 shows several such quartz crystals that have grown into a cavity.



Figure 2 Well-formed quartz crystals. The largest crystal is 6 cm long.

Crystals may be objects of great beauty, in part because of their almost perfectly flat crystal faces and geometric shapes. This regular external appearance is caused by a highly ordered internal arrangement of atoms known as the crystal structure, which leads to distinct, and to some extent predictable, physical and chemical properties.

Minerals, by definition, are solid substances. Before looking at the crystalline world in more detail, the next section considers briefly the various physical states that matter can have, and the transition from one state to another. These are concepts that are relevant at various stages throughout the course.

2 States of matter

Substances generally exist in one of three different states: as a gas, liquid or solid. Figure 3 illustrates these states in terms of their atomic arrangements, with small black arrows representing relative velocities of atoms or molecules in the liquid and gas. Atoms or molecules in a gas move at high velocities, and the distances between them are large, so gases have low densities. In a liquid, the atomic motions are slower, and the atoms are closer together (producing a higher density).

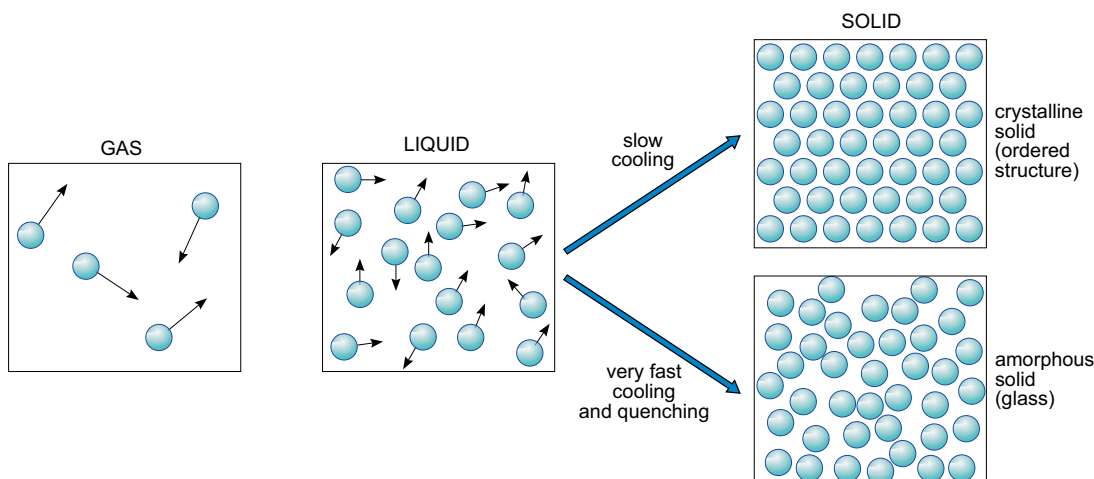


Figure 3 Schematic diagrams of atomic arrangements in the gas, liquid and solid states. The small black arrows represent relative velocities of atoms or molecules in the liquid and gas.

If you could take a snapshot of the atoms in a liquid or a gas, you would see a random or disordered arrangement. Another snapshot, taken a fraction of a second later, would look different. So, the internal structures of liquids and gases are disordered both in space and time.

A kind of real-life snapshot of a liquid structure can be taken by very rapidly cooling the liquid to quench it, so that it solidifies before the atoms have had time to rearrange themselves. At low temperatures, there is not enough thermal energy for the atoms to move relative to each other. The quenched material is a disordered solid, known as an **amorphous** solid or **glass** (Figure 3).

By contrast, slow cooling of a liquid allows atoms to arrange themselves into an ordered pattern, which may extend over a huge number of atoms. This kind of solid is called **crystalline**. So if a melt of a given composition (e.g. SiO_2) is cooled very rapidly it will produce a silica glass, whereas if it is cooled slowly it will produce a crystalline solid composed of quartz crystals.

It is important to note that compared with crystalline solids, glass is not a particularly stable form of matter. Over many years, glass may slowly convert into a crystalline form in a process called **devitrification**. This can sometimes be observed in centuries-old window panes, where circular frosted patches of tiny crystals have formed within the glass.

The states in which a single substance can exist - gas, liquid or solid - are referred to as **phases** of matter. The range of pressures and temperatures over which a particular phase is stable (i.e. its **stability field**) can be shown on a **phase diagram**. The stability

fields of different phases may be represented as areas separated by boundary lines on a pressure-temperature diagram, as illustrated in Figure 4, a phase diagram for H₂O. A change of temperature (or pressure) may result in a **phase transformation**; for example, liquid H₂O (water) can be heated to form a gas (steam), or cooled to form a solid (ice).

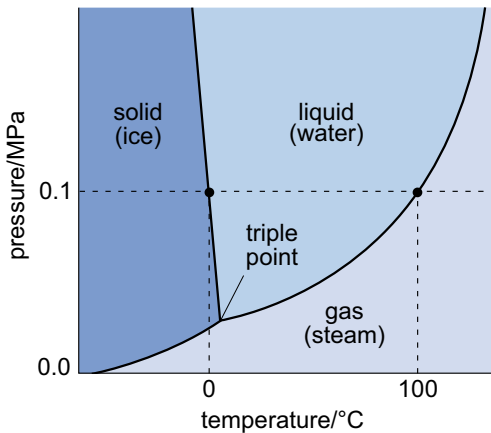


Figure 4 A phase diagram for the three phases of H₂O, showing their stability fields over a range of pressures, measured in MPa, and temperatures, measured in °C. (The SI unit of pressure is the pascal, abbreviated to Pa; 1 Pa = 1 N m⁻²; atmospheric pressure is approximately 10⁵ Pa, or 0.1 MPa.) Axes are not drawn to scale.

At the surface of the Earth, with a typical pressure of one atmosphere (approximately 10⁵ Pa), a crystalline solid, ice, is the stable phase of H₂O at temperatures below 0 °C. Above this temperature (the melting point of ice), solid ice transforms to liquid water. The boundary between the solid and liquid stability fields is a **phase boundary**, and is indicated by a solid line in Figure 4. If the temperature continues to increase at constant pressure (along the horizontal dashed line in Figure 4), the phase boundary between the liquid (water) stability field and the gas (steam) stability field is reached. This boundary represents the boiling temperature of water.

Although only the effect of *changing temperature* has been considered so far, it is important to note that both the melting temperature and the boiling temperature vary with pressure. The point where all three phase boundaries for H₂O meet is called the **triple point**, a unique pressure and temperature where solid (ice), gas (steam) and liquid (water) can coexist.

- How would the boiling temperature of water, measured at the top of a high mountain, where the atmospheric pressure is low, compare with its boiling temperature at sea level (where atmospheric pressure is relatively much higher)?
- The H₂O phase diagram (Figure 4) shows that the boiling temperature of water (indicated by the liquid/gas phase boundary) decreases with decreasing pressure. Thus, on top of a mountain, where atmospheric pressure is lower, water boils at a lower temperature.

3 Physical properties of minerals in hand specimen

Physical properties, such as colour and density, are those that can be observed without causing any change in the chemical composition of a specimen, whereas chemical properties determine how a substance behaves in a chemical reaction. Many of the physical properties of minerals can be predicted from a detailed knowledge of their crystal structures, which can be obtained by various analytical techniques. Alternatively, physical properties can be used to infer particular aspects of a mineral's internal structure.

Several physical properties of minerals can be readily observed in hand specimen and can be used for recognising and distinguishing different minerals. In this course you will do this using the [Digital Geology Kit](#), which is introduced in the next activity.

Activity 1 Introduction to the Digital Geology Kit

Allow about 40 minutes.

Task 1

Begin by watching Video 1 to familiarise yourself with the functionality of the Digital Geology Kit. (You will need to view it in 'Full Screen' mode in order to see in detail the various tools and features.) Then answer the associated questions.

Video content is not available in this format.

[Video 1 Introduction to the Digital Geology Kit.](#)

Question 1

Select the specimen 'Variety amethyst' from the 'Quartz' list of minerals in the [Digital Geology Kit](#). How long is the amethyst crystal on the far left? Measure it using the graticule.

Answer

It is about 16 mm. Note that there are large divisions on the graticule every 10 mm.

Question 2

Now go to 'Red crystals in gneiss' in the 'Garnet' list. Go to coordinates X = 1860, Y = 930. (Note that, hereafter, the X and Y labels will be omitted on all coordinates, e.g. this point would be '(1860, 930)'). Is any red garnet visible at the point denoted by the cross hairs?

Answer

No, garnet is not visible at this point; only a white mineral is visible at the stated coordinates.

3.1 Crystal shape

Well-developed crystals show a number of flat faces and a distinct shape. The shape of the crystal and the precise arrangement of its crystal faces relate to its internal structure, and are expressions of the regular way the atoms are arranged.

Many terms are used to describe the shapes of different crystals. These can be broadly grouped into three categories:

- **prismatic** (the crystal is stretched out in one direction; Figure 5a)
- **tabular** (the crystal is squashed along one direction, so appears slab-like or 'platy'; Figures 5b and c)
- **equidimensional** (the crystal has a rather similar appearance in different directions, e.g. cubes, octahedra, and 'rounded' crystals with many faces of similar size; Figures 5d and e).

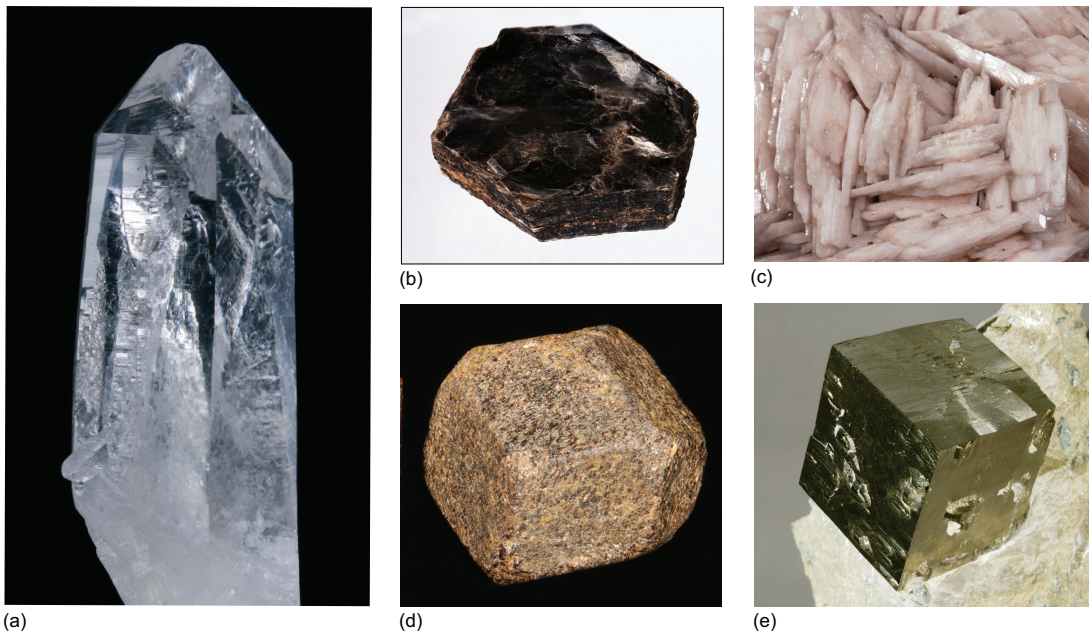


Figure 5 Some examples of crystal shapes: (a) prismatic (quartz, 6 cm long); (b) tabular (mica, 9 cm across); (c) tabular (barite, field of view 10 cm across); (d) equidimensional (garnet, 4 cm); (e) equidimensional (pyrite, 2 cm).

Crystals of the same mineral tend to show the same general crystal shape. Quartz, for example, is almost always prismatic, rather than tabular or equidimensional. However, the *exact* shape of crystals of the same mineral can vary depending on the conditions at the time of growth. Two crystals of the same mineral may differ in the relative sizes of specified crystal faces, or some faces may not be present.

Although the relative *sizes* of specific crystal faces often vary, the *angles* between such faces are always fixed as they are defined by the crystal structure. This consistency of angles may be verified by measuring the angle between crystal faces with, for example, a protractor (Figure 6) or a more accurate device called a **goniometer**.

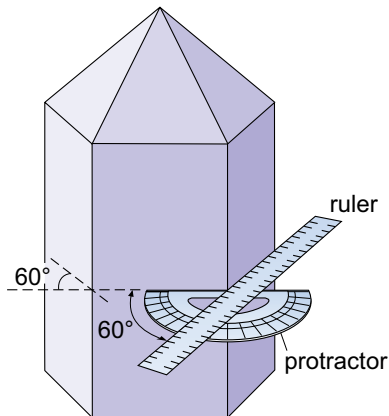


Figure 6 Idealised quartz crystal showing that the prism faces are 60° apart. The prism faces may vary in size, but the angles between them are all exactly 60° .

- Some minerals have a crystal shape that is best described as **acicular** (i.e. needle-like). In which of the three general categories of crystal shape mentioned above do acicular crystals lie?
- Acicular crystals belong to the prismatic category as they are stretched out in one direction.

Note that there is often a distinction between the shape of *individual* crystals and the form they may take when many crystals are assembled into an *aggregate*. For example, some minerals have acicular crystals that radiate in all directions away from a central point, forming a **globular** (i.e. spherical) aggregate. Aggregates may also be, for example, fibrous, columnar or **dendritic** (clusters of crystals in fern-like branches). When crystals grow together in a solid mass, in which individual crystals cannot clearly be seen, aggregates are described as **massive**.

3.2 Colour

The colour of a mineral can be its most obvious feature, but colour can also be one of the least reliable properties for identifying minerals. Many minerals show a wide range of coloration, often caused by tiny amounts of impurities.

For example, pure quartz (SiO_2) is colourless, but minute quantities of Fe^{3+} iron induce a purple coloration, characteristic of the variety of quartz known as amethyst (Figure 7a). Small amounts of aluminium cause the dark coloration of smoky quartz when the crystal has been exposed to natural radioactivity (Figure 7b). The reason for the pink colour in rose quartz (Figure 7c) is not fully understood; titanium or manganese may be involved, as may minute fibrous crystals of a complex mineral within the quartz.

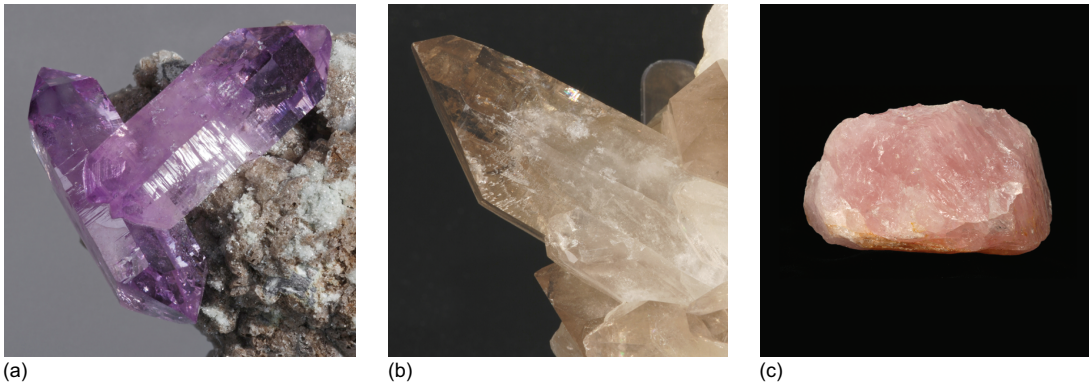


Figure 7 Some coloured varieties of quartz: (a) purple amethyst (crystals 1.5 cm long); (b) grey smoky quartz (5 cm long); (c) pink rose quartz (8.5 cm long).

The yellow colour of citrine (another quartz variety) is probably due to minute amounts of iron hydrates dispersed within the crystal. (Many examples of citrine for sale are actually artificially heated or irradiated amethyst.) Milky quartz is white and cloudy as a result of tiny bubbles of fluid (liquid and/or gas).

In a few minerals, such as tourmaline, an individual crystal may be multicoloured (Figure 8), reflecting subtle changes in chemical composition as it grew. Although most commonly black, other colours of tourmaline include brown, green, pink, blue or yellow. Here, a single crystal varies markedly in colour along its length (5 cm). In this case, the green part has the most iron, and the pink colour is due to trace amounts of manganese.

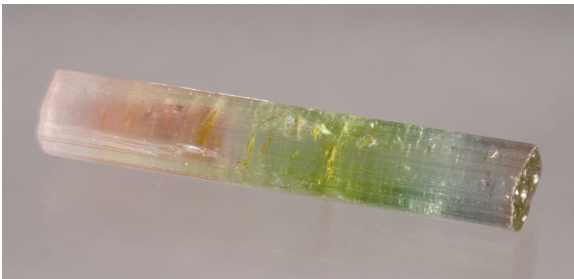


Figure 8 Tourmaline, a complex silicate mineral that shows a variety of colours. (Sample is 5 cm long.)

Some minerals do, however, have reliable and distinctive colours. Silicate minerals that contain large amounts of iron are typically dark green or black. These minerals, which often also contain magnesium, are called **ferromagnesian minerals**; they include olivine, pyroxene, amphibole and biotite mica.

3.3 Lustre

The term **lustre** refers to the surface appearance of a mineral, which depends on the way it reflects light. Quartz (Figure 5a) has a vitreous lustre, as do many other silicate minerals, such as feldspar. When transparent, like window glass or clear coloured glass, the term 'glassy' lustre may be used instead of vitreous: quartz, for example, often has a glassy lustre. Some opaque minerals scatter light very strongly, giving rise to shiny, reflective surfaces and a metallic lustre, such as seen in pyrite (Figure 5e) and magnetite (Figure 9a).

Other examples are pearly lustre (looking like pearls; Figure 9b), silky lustre (like shiny threads or fibres; Figure 9c), and a dull or earthy lustre (Figure 9d). Note that, as in the case of gypsum (Figures 9b and c), different varieties of the same mineral may show different types of lustre.

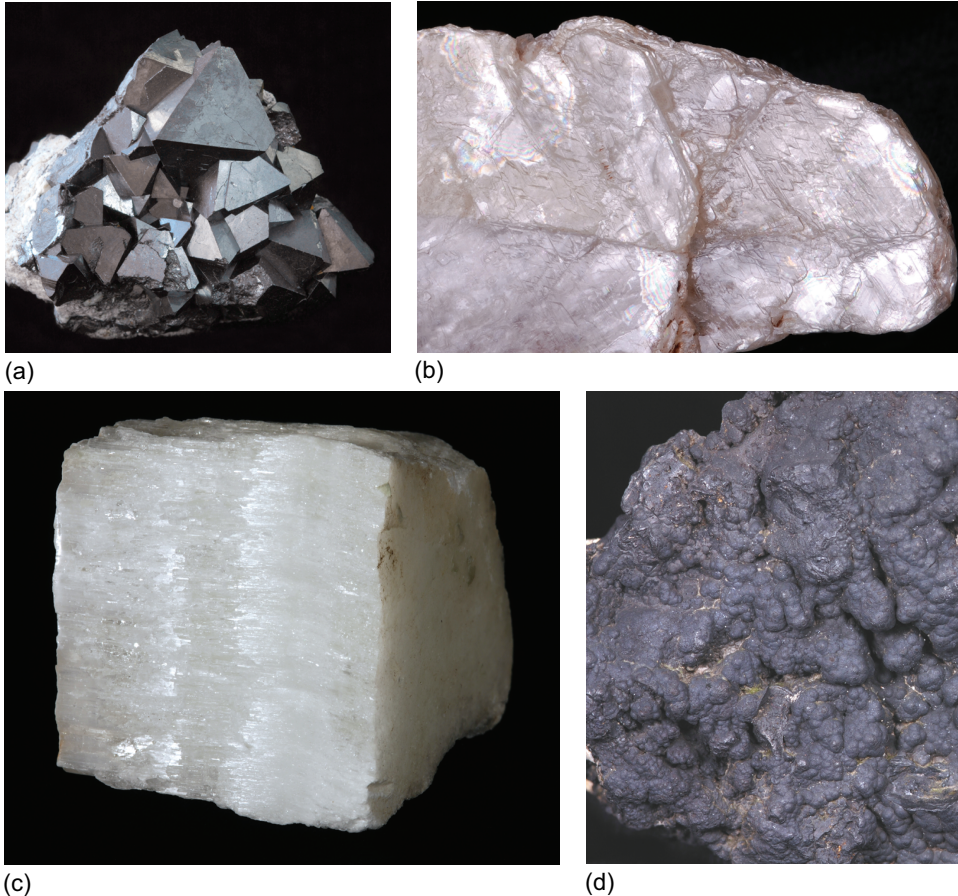


Figure 9 Some examples of lustre: (a) metallic (magnetite) (specimen 4 cm across); (b) pearly (gypsum, variety selenite) (field of view 7 cm across); (c) silky (gypsum, variety satin spar) (5.5 cm); (d) dull or earthy (psilomelane, a form of manganese oxide) (field of view 4.5 cm across).

3.4 Cleavage

If a crystal is struck with a hammer, it will probably shatter into many pieces. Some minerals, such as calcite, break into well-defined blocky shapes with flat surfaces. These are called **cleavage fragments** (Figure 10b) and the flat surfaces are called **cleavage planes** (Figure 10a). Note that cleavage planes, which occur *within* a crystal, are not the same as crystal faces. **Cleavage** arises when the crystal structure contains repeated parallel planes of weakness (due to weak chemical bonds), along which the crystal will preferentially break.

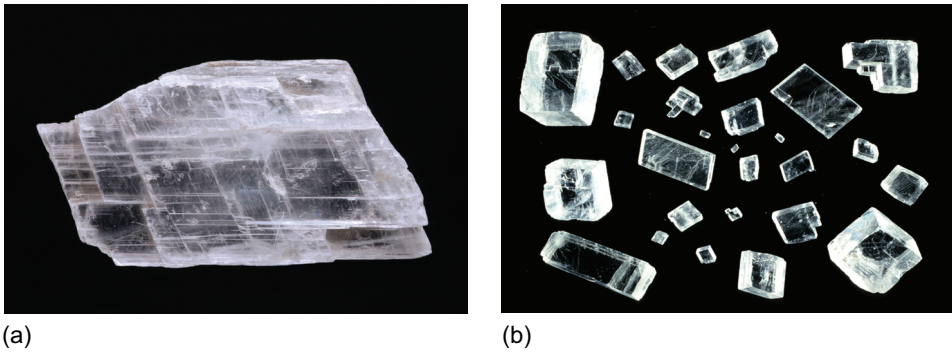


Figure 10 (a) Cleavage planes within a gypsum crystal (11 cm). (b) Cleavage fragments (rhombs) of calcite. Each piece is bounded by three sets of cleavage planes (no two of which intersect at right angles). The largest fragment is 2 cm long.

The mineral mica (which includes biotite and muscovite) has such perfect cleavage in one direction that it can be readily split, or cleaved, into wafer-thin sheets, as shown in Video 2.

Video content is not available in this format.

Video 2 Cleavage in mica. (There is no voice-over in this video.)

Some minerals break into irregular fragments that lack flat surfaces (except for any remnants of original crystal faces). In the case of quartz (Figure 11), which has no cleavage, the broken pieces have a curved pattern and this is called a **conchoidal fracture** ('conchoidal' is pronounced 'con-koi-dal').



Figure 11 A broken quartz fragment showing an absence of any cleavage planes, and conchoidal fracture (5 cm).

Some minerals have only one set of cleavage planes, others have two sets, and a few (such as calcite) have three. In minerals with only one or two sets of cleavage planes, some broken surfaces will show just fracture.

- Look at the video of the galena below. How many cleavage orientations does galena exhibit?

Video content is not available in this format.

Video 3 Rotating view of galena. (There is no sound in this video.)

- Galena has three sets of cleavage planes at right angles to each other.

3.5 Density

Density is a measure of how heavy an object is for a given volume. You can get a general idea of the relative densities of different minerals just by picking them up: a piece of galena (PbS) feels heavier than a piece of quartz (SiO₂) *of the same size*.

The density of a mineral depends on its chemical composition, the type of bonding and its crystal structure. The standard unit of density is kg m⁻³. Examples of the relative densities of various minerals compared with water at room temperature (about 1000 kg m⁻³) are shown in Table 1. The relationship between density and crystal structure is explored further in Section 4.

Table 1 Relative densities of various minerals.

Mineral	Symbol/ formula	Relative density at room conditions (compared with water = 1.0)
Graphite	C	2.2
Quartz	SiO ₂	2.65
Diamond	C	3.5
Barite	BaSO ₄	4.5
Galena	PbS	7.6
Silver	Ag	10.5
Gold	Au	19.3

- According to the information provided in the [Digital Geology Kit](#), which of the following minerals has the highest density and which has the lowest density: garnet, gypsum and quartz?
- Garnet has the highest density (3.6-4.3); gypsum has the lowest density (2.3). Quartz is in between (2.65). (Density values quoted are relative to water.)

3.6 Hardness

Hardness is loosely defined as the resistance of a material to scratching or indentation. The absolute hardness of a material can be determined precisely, using a mechanical instrument to measure the indentation of a special probe into a crystal surface. However, you can get a general idea of a mineral's *relative* hardness by undertaking a few simple scratch tests.

The nineteenth-century German mineralogist, Friedrich Mohs, devised a useful scale of mineral hardnesses, consisting of well-known minerals ranked in order of increasing hardness, from talc, with a hardness of 1, to diamond, with a hardness of 10 (Table 2).

Table 2 Mohs' hardness scale.

Mohs' hardness	Reference mineral	Non-mineral example (hardness in brackets)
1	talc	
2	gypsum	
		fingernail (2.5)
3	calcite	
		copper coin ¹ (3.5)
4	fluorite	
5	apatite	
		window glass/ ordinary knife blade (5.5)
6	orthoclase feldspar ²	
		hardened steel (6.5)
7	quartz	
8	topaz	
9	corundum	
10	diamond	

¹ Many of today's 'copper coins' are copper-plated steel and are harder below the copper coating. ² Other types of feldspar may have a slightly greater hardness, between 6 and 6.5.

Compared with an absolute hardness scale, **Mohs' scale** is highly non-linear (diamond is about four times harder than corundum; Figures 12c and b) but, because the scale uses familiar minerals, it provides a quick and easy reference for geologists in the field.

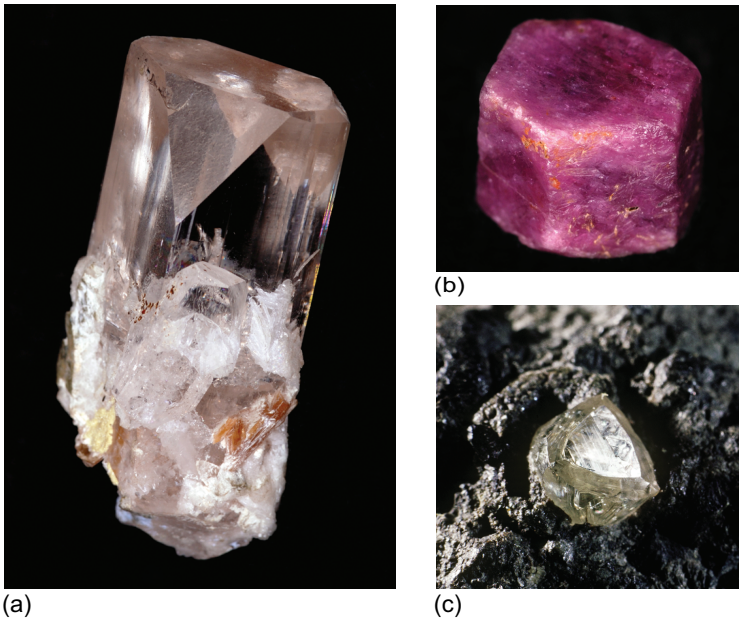


Figure 12 Three very hard minerals: (a) topaz (5 cm long); (b) corundum (variety ruby) (1 cm); (c) diamond (6 mm).

Minerals with a hardness of less than 2.5 may be scratched by a fingernail (Video 4), whereas those with a hardness of less than 3.5 may be scratched by a copper coin (Video 5), and so on.

Video content is not available in this format.

Video 4 Scratch test on gypsum. (There is no voice-over in this video.)

Video content is not available in this format.

Video 5 Scratch test on calcite. (There is no voice-over in this video.)

- Will quartz scratch topaz (Figure 12a)?
- The hardness of quartz is 7 whereas topaz has a hardness of 8, so topaz will scratch quartz, but not the other way round.
- Using evidence from the [Digital Geology Kit](#), which of the following minerals is the hardest, and which is the softest: galena, hematite, pyrite?
- Pyrite is the hardest (6-6.5), galena the softest (2.5). Hematite has hardness 5-6.

Hardness should not be confused with **toughness**, which is the resistance of a material to breaking. Many minerals are hard, but they may not be tough. Diamond, for example, is the hardest known material, but it is not tough: it will shatter if dropped onto a hard surface.

4 The atomic structure of crystals

The atomic structure of a mineral influences many of its physical and optical properties. This section briefly considers some of the main ways in which atoms are arranged, and how they are bonded, starting with metals, which have some of the simplest atomic arrangements possible. Variations on these arrangements provide the structural foundations of many common minerals.

4.1 Metallic structures and bonding

Metal crystals are built from layers of densely packed metal **cations** (atoms that have lost one or more electrons, leaving them positively charged). The ions are organised in regular, *close-packed* arrangements.

In close-packing, a layer of identically sized atoms (or ions) occupies the minimum possible space - like a raft of hard spheres (e.g. marbles) in contact with each other. Each atom has six neighbours in a plane. The three-dimensional structure of a metal involves the successive stacking of close-packed layers on top of each other.

In **metallic bonding**, atoms donate one or more outer electrons to a free electron 'sea' (Figure 13), which flows between and around the cations and acts as a kind of glue, holding them together. This kind of bonding is uniform in all directions, so that metallic structures are dense and close-packed. The electron mobility renders metals both malleable and ductile, which are vital properties for producing thin sheets and for stretching out to form thin cables or filaments (e.g. copper wire).

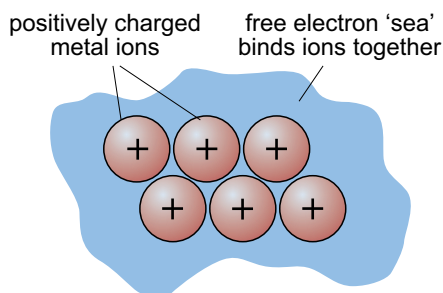


Figure 13 Metallic bonding.

4.2 Ionic structures and bonding

About 90 per cent of all minerals are essentially ionic compounds. **Ionic bonding** is generated by the *transfer* of one or more electrons from one atom to another. This creates two ions of opposite charge, which are attracted to each other (Figure 14). For example, in **halite** (sodium chloride, NaCl) there is a positively charged sodium cation, Na^+ , and a negatively charged chlorine **anion**, Cl^- .

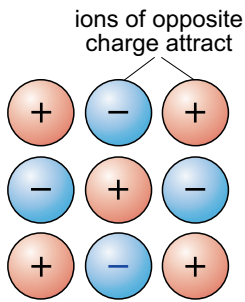


Figure 14 Ionic bonding.

As with metallic bonding, ionic bonds are non-directional, so ionic crystals tend to have fairly dense, close-packed structures. However, ionic bonds tend to be stronger than metallic bonds, so crystals containing ionic bonds tend to be unmalleable and much more brittle than metal crystals.

Even though a close-packed structure looks densely packed, there are actually lots of spaces between the atoms. These spaces are called **interstices** and are important in metallic structures because they provide sites for smaller atoms to reside. Interstices also provide a basis for many ionic structures: they provide locations for smaller ions, in the presence of large ions. There are two kinds of interstices:

- a tetrahedral interstice, surrounded by four atoms, one at each of the corners of an imaginary tetrahedron (Figure 15a)
- an octahedral interstice, surrounded by six atoms, arranged at the corners of an imaginary octahedron (Figure 15b).

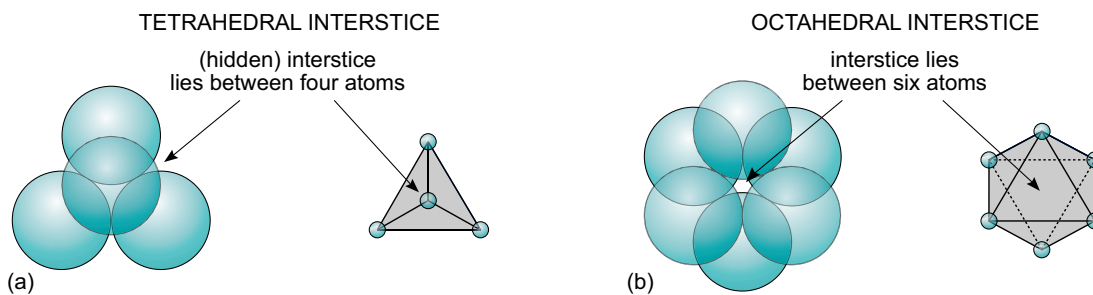


Figure 15 Interstices (vacant sites) between two close-packed planes of spheres: (a) tetrahedral interstice; (b) octahedral interstice.

The mineral halite (Figure 16) is an example of a structure with octahedral interstices (as in Figure 15b). The chlorine ions are arranged a bit like the atoms in a metal - although they do not quite touch each other. The sodium ions, which are much smaller, fit snugly between the large chlorine ions, as illustrated in a space-filling model (Figure 16a).

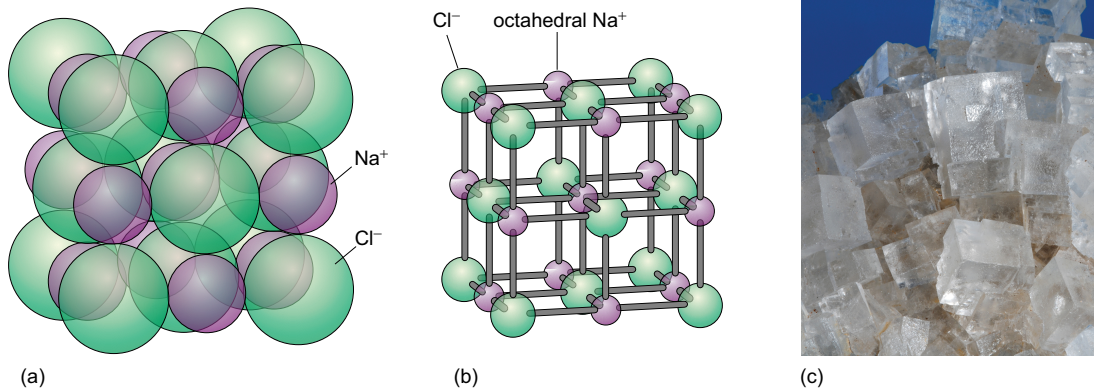


Figure 16 The structure of halite (sodium chloride, NaCl): (a) space-filling model (sodium and chlorine ions shown at their correct relative sizes); (b) ball-and-stick model; (c) cubic crystals of halite (field of view 10 cm across).

The structure of **sphalerite** (zinc sulfide, ZnS) (Figure 17) has a close-packed arrangement of sulfur ions, a structure in which zinc ions fill half of the tetrahedral interstices (as in Figure 15a).

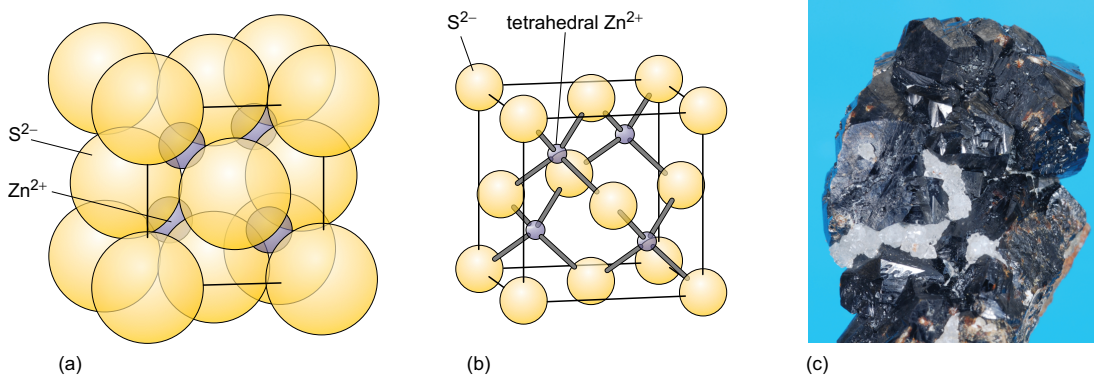


Figure 17 The structure of sphalerite (zinc sulfide, ZnS): (a) space-filling model; (b) ball-and-stick model - the unit cell (Section 6.2) is shown by black lines in both (a) and (b); (c) sphalerite (with white quartz) (2 cm across).

4.3 Covalent structures and bonding

Covalent bonding is formed when two atoms *share* two electrons (one from each atom) through overlap and merging of two electron orbitals (Figure 18). Crystals containing covalent bonds tend to have more complex structures than those of ionic or metallic structures.

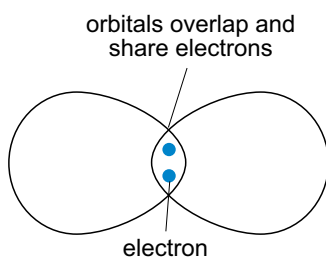


Figure 18 Schematic representation of covalent bonding.

Covalent bonding requires the *precise overlap* of electron orbitals, so if an atom forms several covalent bonds, these are usually constrained to specific directions. As covalent bonds are directional, unlike metallic or ionic bonds, this places additional constraints on the arrangements of atoms within such a crystal. One result is that covalent structures tend to be more open, and hence have lower densities than do metallic or ionic structures.

Diamond is an example of a covalently bonded solid. In this form of carbon, each atom is covalently bonded to four other carbon atoms, arranged at the corners of a tetrahedron (Figure 19a). The resulting structure, which has a repeating cubic shape, is illustrated in Figure 19b. The structure contains much more unoccupied space than do close-packed metal structures.

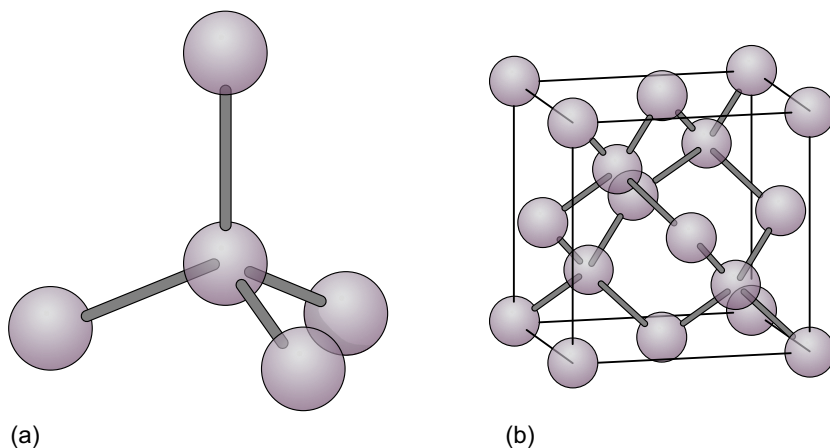


Figure 19 The diamond structure: (a) tetrahedral arrangement of covalent bonds around a carbon atom; (b) arrangement of carbon atoms and bonds in the unit cell (Section 6.2) - the unit cell is shown by black lines.

Another form of solid carbon with covalent bonding is **graphite** (Figure 20). Unlike those in diamond, the carbon atoms in graphite are covalently bonded to *three* neighbours in the same plane (Figure 20a), producing a strong sheet of carbon atoms. However, each carbon atom has one extra electron available for bonding that forms very weak bonds, which serve to keep the carbon sheets together (Figure 20b).

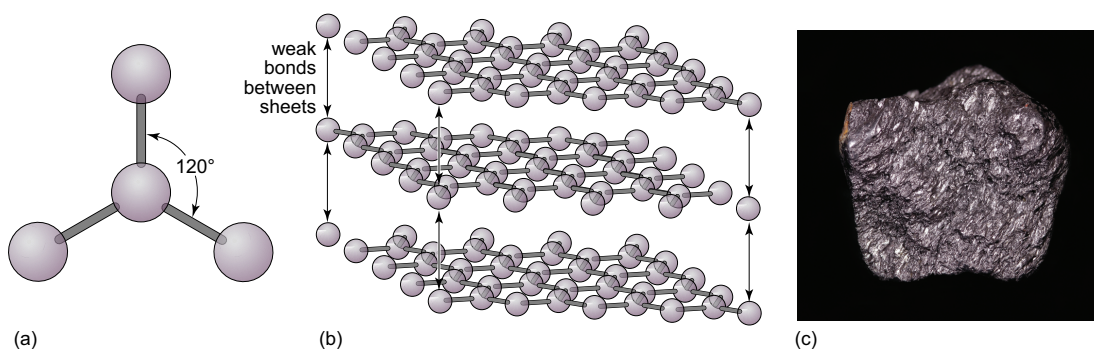


Figure 20 The graphite structure: (a) triangular arrangement of covalent bonds around a carbon atom in the same plane; (b) part of the 3D structure of graphite, showing strongly bonded hexagonal sheets of carbon atoms, connected by weak bonds; (c) specimen of graphite (3.5 cm across).

- How do the crystal structures of diamond and graphite account for the differences in hardness between the two minerals?
- Diamond has a three-dimensional bonding pattern, with identical bonding in all directions, and no 'weak' directions. Graphite has a mainly two-dimensional pattern, with sheets of C-C bonds. Bonds between the sheets are very weak, so sheets can easily slide past each other, explaining graphite's use as a lubricant and why it is soft enough to mark paper.

Diamond and graphite have the same chemical composition (pure carbon) but different crystal structures. They are known as **polymorphs** of carbon. Diamond is formed under higher pressures than graphite (Figure 21), and is less stable than graphite at the surface of the Earth. Indeed, temperature and pressure conditions within the Earth are such that diamond tends to form only at depths greater than 150 km. However, because of the strong bonding, it is very difficult to break down the diamond structure, so diamonds (fortunately) will not spontaneously transform into graphite! Note that not only is diamond harder than graphite, but it is also denser, as predicted by its structure (Table 3).

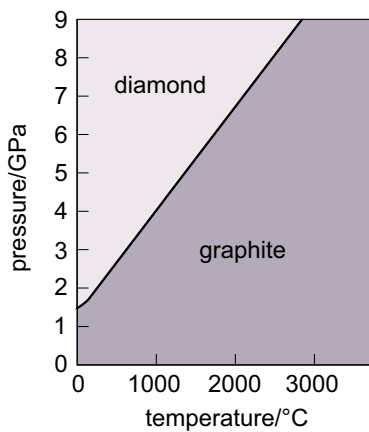


Figure 21 Phase diagram illustrating the stability fields for graphite and diamond.

Table 3 Relative densities of various minerals and ice, and notes on their structure and bonding.

Substance	Relative density at room conditions (compared with water = 1.0)	Structure and bonding
Ice, H ₂ O	0.9	open structure; covalent bonds plus weak bonds between H ₂ O molecules
Graphite, C	2.2	open structure; covalent bonds plus weak bonds between layers
Feldspar, KAISi ₃ O ₈	2.5	open structure; predominantly covalent bonds
Quartz, SiO ₂	2.7	open structure; predominantly covalent bonds
Olivine, Mg ₂ SiO ₄ –Fe ₂ SiO ₄	3.2-4.4	structure based on close-packing, but with ionic and covalent bonds; density increases as Fe content increases
Diamond, C	3.5	structure based on close-packing, but with covalent bonds
Barite, BaSO ₄	4.5	ionic bonds between barium and sulfate groups
Hematite (iron oxide), Fe ₂ O ₃	5.3	structure based on close-packing; ionic and metallic bonds
Galena (lead sulfide), PbS	7.6	structure based on close-packing; ionic and metallic bonds
Silver, Ag	10.5	close-packed structure; metallic bonds
Gold, Au	19.3	close-packed structure; metallic bonds

Minerals are never chemically pure; they always contain some foreign atoms. These impurity atoms may simply squeeze into the interstices. Another possibility is that certain elements may be able to directly replace (substitute for) the normal atoms in the ideal structure - although, for a comfortable fit, the substituting element must have a similar size and charge to the original atom. This phenomenon is called **ionic substitution**. An example is the substitution of Fe²⁺ for Mg²⁺, or Mg²⁺ for Fe²⁺, which occurs in the mineral olivine.

5 Crystal defects and twinning

Virtually all crystals contain minute imperfections or defects. The effect of defects on the physical and chemical properties of a crystal can be out of all proportion to their size.

Defects come in several types. *Point defects* may involve missing or displaced atoms in the crystal structure, giving empty sites, or vacancies. Such defects make it much easier for atoms to diffuse through the crystal structure by moving between vacant sites. This is important because the rate of diffusion of atoms through a crystal structure can determine the speed at which processes such as weathering, or other chemical reactions (e.g. during metamorphism) proceed.

Minerals in deformed rocks, such as those from mountain belts, contain large numbers of *line defects* caused by rows of atoms that are out of place in the crystal structure.

Figure 22 shows an artificial example based on an alloy used in semiconductors, where each dark line represents a strained part of the crystal. Such defects affect the mechanical strength of a crystal, which determines the strength of rocks and how they deform under intense pressure. During deformation, progressive movement along flaws in crystals takes place in tiny steps, as bonds are broken and re-formed.



Figure 22 Transmission electron microscope image showing many line defects in a crystal of indium aluminium arsenide (an alloy used in semiconductors). The width of this image is about 1 μm .

A third type of defect is called a *planar defect*. Crystals grow by the progressive addition of atoms onto a surface. 'Mistakes' in the stacking of new planes with respect to previously formed planes are common during crystal growth. These planar defects can have a profound effect on the way atoms are stacked, and can produce distinct regions called *domains* within a single crystal. One such planar defect is a boundary that separates two domains of a crystal that are mirror images (Figure 23). The result is called a twinned crystal.

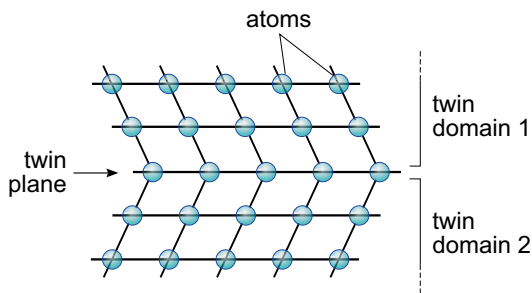


Figure 23 Example of crystal twinning, in which a twin plane separates two regions of a single crystal that are mirror images. The two regions are referred to as twin domains.

Various types of crystal **twinning** exist, and in each case a single crystal consists of two or more regions with different orientations. The different regions of the twinned crystal may be related in various ways, such as by rotation about a symmetry axis (Section 6.2). Twinning is especially common in feldspar. Orthoclase feldspar often displays *simple twinning*, in which the crystal is divided into two domains with a different structural orientation (Figure 24).

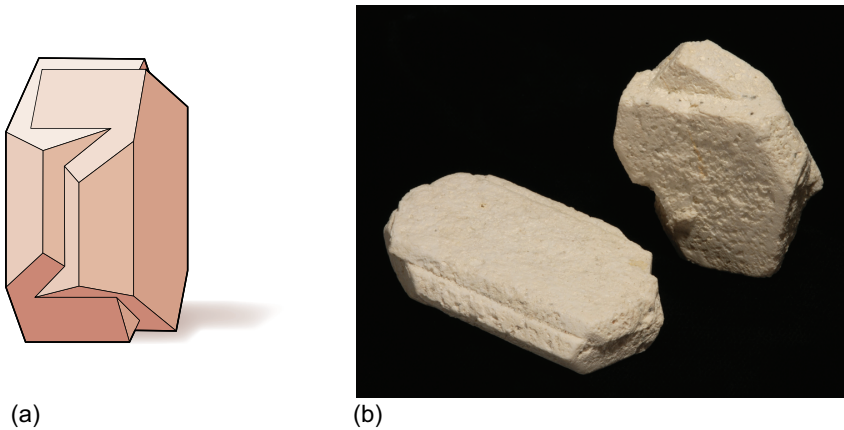


Figure 24 (a) Example of simple twinning. (b) Two crystals of orthoclase feldspar showing simple twinning. The left-hand one is 5 cm long.

Other types of feldspar (e.g. plagioclase feldspar) may have a more complex type of twinning, called *multiple twinning*, in which a single crystal has many different domains (Figure 25).

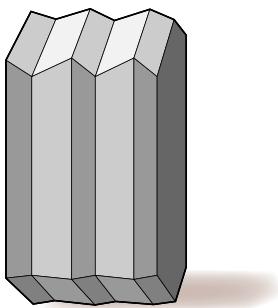


Figure 25 Example of multiple twinning.

Grain boundaries are different from twin boundaries because there is no orientation relationship between crystals on either side of the grain boundary. There are two distinct grains, with the same, or a different, mineral composition (Figure 26).

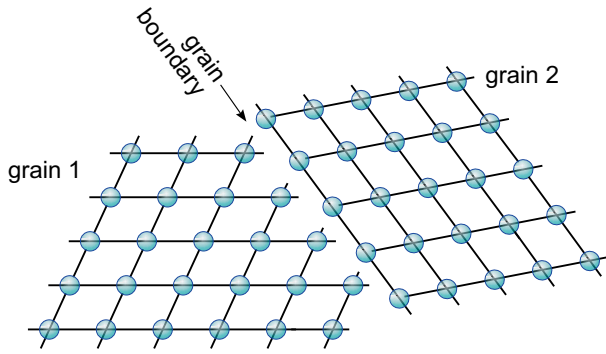


Figure 26 Grain boundary between two distinct crystals.

6 Crystal symmetry and shape

In this section you investigate the relationship between the shape and symmetry of crystals, consider why minerals have only a limited number of crystal shapes, and discover how the shape of a mineral relates to its internal structure.

6.1 Crystal symmetry

When you first look at a collection of minerals in a museum, there may seem to be an infinite variety of crystal shapes. However, on closer inspection there is an underlying order, and this is best seen by the consistency in the angles between crystal faces for particular groups of minerals. Crystals possess a variety of symmetries, and it has been demonstrated by X-ray methods that symmetry visible in hand specimen relates to the internal arrangement of atoms.

Most people have an idea of what is meant by symmetry, as many everyday objects and living things possess it. There are two main types of symmetry:

- **reflection symmetry**, where one side of an object is the mirror image of the other side (e.g. insects, birds and spoons)
- **rotational symmetry**, where an object looks the same after a certain amount of rotation (e.g. many flowers, starfish and bicycle wheels).

Many complicated patterns such as carpet or wallpaper designs have symmetry, but these can sometimes be a little difficult to discern. Consider, therefore, an object with obvious symmetry, such as a snowflake (Figure 27).

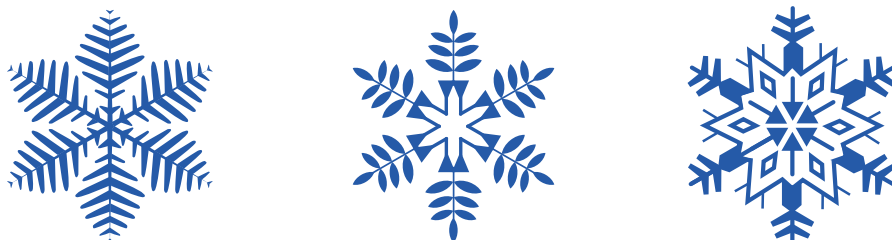


Figure 27 Examples of snowflakes, displaying perfect six-fold rotational symmetry.

Each snowflake can be rotated by 60° about an axis perpendicular to the page and it will look exactly the same as it did before. The operation can be repeated six times in a full 360° rotation, and at each 60° interval the snowflake will look the same. Thus the snowflake has a six-fold rotational symmetry. A snowflake also possesses reflection symmetry: if you 'split' the snowflakes along certain planes, called **mirror planes**, the two halves are mirror images of each other.

Some examples of rotational and reflection symmetry found in crystals are illustrated in Figure 28. The first three shapes are bisected with examples of mirror planes to illustrate reflection symmetry. Placed at the centre of each shape is the appropriate symbol for their rotation axis.

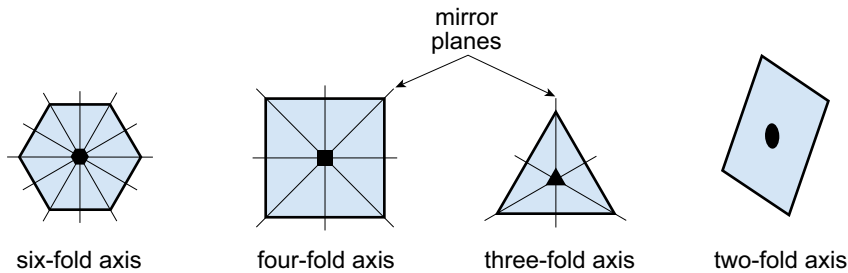


Figure 28 Examples of rotational and reflection symmetries shown by crystals.

6.2 Crystal lattices and unit cells

A typical crystal contains billions of atoms in a highly ordered structural arrangement. Perhaps, surprisingly, the essence of such a complex structure can be described relatively simply. How is this possible?

If you tried to tile a two-dimensional area such as a bathroom floor without any gaps, you would do this by adding tiles that fitted together. In fact, only tiles with two-, three-, four- and six-fold symmetry allow for successful tiling (Figure 29). Similarly, if you tried to produce a three-dimensional structure (like a crystal) without any gaps it would require the repetition of building blocks (i.e. 3D repeating units) with particular shapes. As with two-dimensional tiling, the only kinds of rotational symmetry axis possible in three-dimensional crystals are two-, three-, four- and six-fold axes.

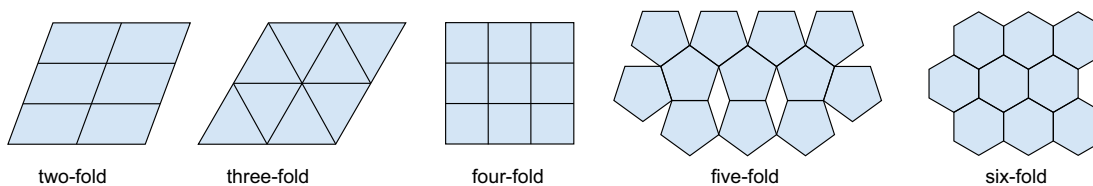


Figure 29 Two-dimensional tiling. Some shapes cannot be tiled without gaps appearing. Only two-, three-, four- and six-fold symmetry are consistent with periodic repetition without gaps.

A **lattice** is an array of objects or points that form a periodically repeating pattern in two or three dimensions. In a crystal lattice, the repeating pattern is simply an arrangement of atoms (or ions) that is located at regular points, called lattice points.

Figure 30a shows a three-dimensional lattice, the building of which can be envisaged by simply stacking a series of identical two-dimensional lattices on top of each other. A crystal is, in effect, a structure formed by countless numbers of identical tiny building blocks, called **unit cells** (Figure 30b), and these make up the crystal lattice. Each mineral has a specific unit cell, which is defined according to the lengths of its sides and their angular relationships. Each unit cell contains one or more different kinds of atoms joined to each other by chemical bonds. Shapes of unit cells vary from one mineral to another; all have six sides (three sets of parallel faces, though not necessarily perpendicular to each other).

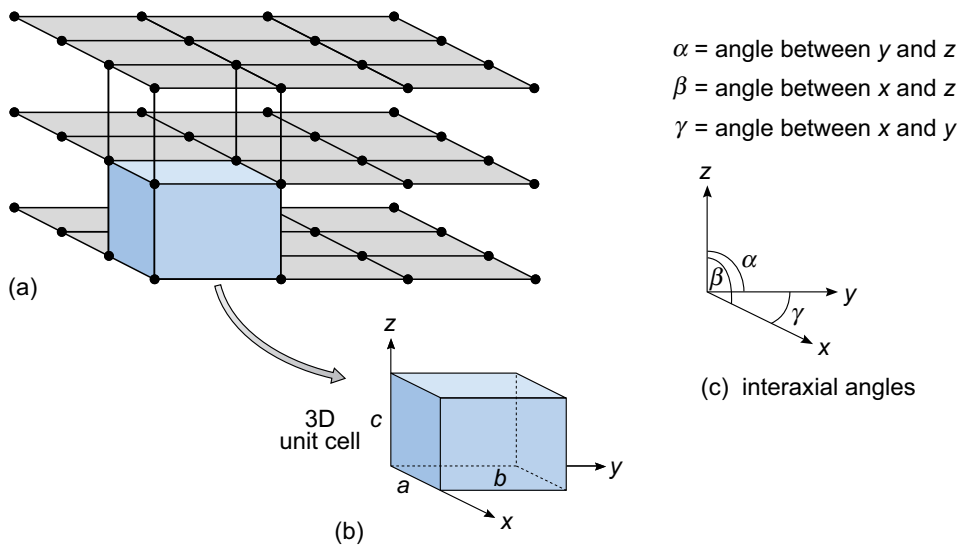


Figure 30 Anatomy of a three-dimensional lattice. (a) Stacking 2D lattices results in a 3D lattice made of tiny building blocks. (b) The 3D unit cell is the basic building block of the crystal lattice. (c) Angles between the three crystallographic axes.

To define the resulting 3D lattice, it is convenient to specify reference directions, x , y and z , which are chosen to be parallel to three edges of the unit cell (Figure 30b). These are known as **crystallographic axes**, and it is important to remember that they are not always at 90° to each other. The angles between the axes are denoted by the Greek letters α , β and γ (alpha, beta and gamma), as shown in Figure 30c. The size of the unit cell is given by the lengths of the three edges, a , b and c , as shown in Figure 30b.

The unit cell is extremely small - typically less than 1 nm (10^{-9} m) in any direction. It is therefore a huge jump in scale from a single unit cell to a single crystal visible to the naked eye. With an edge length of 1 nm, a crystal only 1 mm³ requires 10^{18} unit cells to build it: a vast number.

So a three-dimensional lattice (which may have billions of lattice points) can be represented by just six numbers: the lattice parameters a , b , c , α , β and γ . In the next section you will see how the shape of the unit cell relates to a crystal's symmetry, and what this means for the external shapes of crystals.

6.3 Crystal systems

Most three-dimensional lattices display some symmetry, although the symmetry elements (e.g. rotation axes and mirror planes) can be in any direction. Some arrangements of symmetry elements place special constraints on the shape of the unit cell. For example, a four-fold rotation axis requires the unit cell to have a square section at right angles to the symmetry axis (Figure 31a). Three four-fold axes at right angles to each other imply that the unit cell must be a cube, and so on.

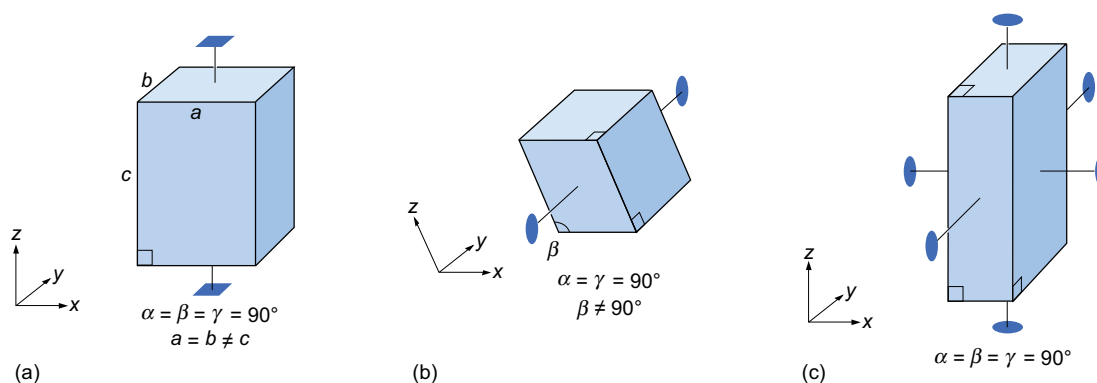


Figure 31 Symmetry and shape of some unit cells corresponding with certain rotation axes (reflection planes are not shown): (a) four-fold rotation axis - crystallographic axes at 90° to each other, and the unit cell has a square cross-section; (b) single two-fold rotation axis - constrains two of the crystallographic axes to be at 90° to each other; (c) three two-fold rotation axes at 90° to one another - implies that three crystallographic axes are also at 90° to each other.

Crystals are classified on the basis of this three-dimensional symmetry (and hence the shapes of their unit cells) into one of seven different **crystal systems** (Figure 32).

Crystal system	Unit cell	Essential symmetry	Example of everyday object with essential symmetry	Mineral example
triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ 	none	a packet of envelopes pushed askew in two directions 	plagioclase feldspar, kyanite
monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$ 	one two-fold axis	a partially squashed matchbox cover, flattened to one side 	gypsum, biotite mica, muscovite mica, orthoclase feldspar, hornblende (amphibole), augite (pyroxene), talc
orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ 	three two-fold axes (at 90° to each other)	a matchbox 	barite, topaz, olivine, andalusite
tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ 	one four-fold axis	two sugar cubes stuck together 	chalcocopyrite, zircon
cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$ 	four three-fold axes (through corners)	a sugar cube 	galena, halite, pyrite, fluorite, garnet, diamond, sphalerite, magnetite, silver, gold
trigonal	$a = b = c$ $120^\circ > \alpha = \beta = \gamma \neq 90^\circ$ 	one three-fold axis	a triangular prism 	calcite, tourmaline, hematite, corundum (e.g. ruby, sapphire)
hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$ 	one six-fold axis	unsharpened pencil 	graphite, apatite, beryl (e.g. emerald, aquamarine)

Figure 32 Illustration of the seven crystal systems in relation to some everyday objects,

and mineral examples. Note that only the diagnostic axes of symmetry have been shown - there are many others, as well as numerous mirror planes. The trigonal system is closely related to the hexagonal system, and is sometimes considered a subsystem of it. All the minerals mentioned in this course (except quartz) are given, along with a few others.

- Study the three unit cell shapes shown in Figure 31. To which of the seven crystal systems would each belong?
- Figure 31a: tetragonal; Figure 31b: monoclinic (note that while two axes are at 90° to each other, one axis is inclined - hence the term 'monoclinic'); Figure 31c: orthorhombic. See Figure 32.

- What would be the shape of the cross-section, at right angles to the longest side, of a crystal with a unit cell like that in Figure 31a?
- The cross-section would be square.

The beauty of crystallography is that you do not need to see the lattice, the unit cell, or the atoms in order to deduce this symmetry. The extent of symmetry varies from the cubic system, which has the most symmetry, to triclinic, which has the least.

Generally, the more symmetry a crystal has, the more constraints this places on its external shape. Crystals belonging to the cubic system tend to have equidimensional shapes, such as cubes, octahedra (with eight faces), or rather rounded-looking crystals with many faces (e.g. dodecahedra, with 12 faces). Pyrite and galena, for example, can have very simple cube-shaped crystals, which clearly indicate their underlying cubic symmetry. These same minerals may also have more complex shapes, with many more faces, but each shape still has the symmetry that places the mineral within the cubic system.

The same possibility for variation within certain limits applies to other minerals in different crystal systems. Despite their complexity, by focusing on the symmetry relationships between faces, you may still be able to determine the crystal system.

Sometimes a crystal has less symmetry than first appearance suggests. For example, quartz crystals are usually prismatic, and often have a hexagonal appearance in cross-section. At first, quartz thus appears to have a six-fold rotation axis. However, in some well-developed quartz crystals there are a number of small faces that present the same appearance only three times in a full 360° rotation, revealing that the true symmetry is less.

- Given this information, to which crystal system does quartz belong?
- The trigonal system (Figure 32), as this is the only system in which only one three-fold axis is present.

It is important to realise that conditions during the growth of a crystal often prevent some faces from developing as perfectly as they might, which results in individual crystal faces having different sizes. Some crystal faces may not be developed at all. Therefore, when looking at crystal symmetry, the *angles* between faces should be considered (Figure 33), not the absolute sizes of individual faces.

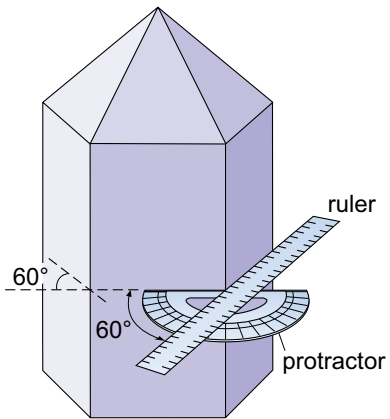


Figure 33 Idealised quartz crystal showing that the prism faces are 60° apart. The prism faces may vary in size, but the angles between them are all exactly 60° .

Conclusion

This free course provides the necessary background to enable you to progress with further study of the main mineral groups and the identification of minerals and rocks in this section using the Digital Kit. It has addressed the following points.

- Matter exists in the form of gases, liquids and solids, and the arrangement of atoms becomes progressively more ordered from gases to solids. The stability fields for the three states of a chemical element or compound are shown in a pressure-temperature plot known as a phase diagram.
- Physical characteristics of minerals evident in hand specimen include crystal shape, colour, lustre, cleavage, density and hardness. Colour may be misleading, as minute amounts of impurities can affect the colour of some minerals. Cleavage, density and hardness are strongly related to the underlying atomic structure.
- Atoms are bonded together by three different mechanisms: metallic bonding, in which a 'sea' of electrons holds the metal cations strongly together, giving dense, closely packed structures; ionic bonding, where electrons are transferred between atoms, producing positive and negative ions that are strongly attracted to each other; and covalent bonding, where electrons are shared, resulting in open, low-density crystal structures, which are strongly bonded. About 90 per cent of all minerals are essentially ionic compounds.
- Crystals may have several different types of defect that can strongly influence the mineral's physical and chemical properties.
- Many geological processes - rock formation, rock deformation, weathering and metamorphism - are controlled by processes operating at very small scales, such as the movement of atoms in crystals (diffusion), the breaking of atomic bonds within crystal structures, the initiation and growth of new crystals, and phase transformations.
- Various types of crystal twinning exist. In each case, the twin is a single crystal that consists of two or more regions in which the crystal lattice is differently orientated.
- The external shape of a crystal (i.e. the arrangement of crystal faces) is controlled by its internal structure. Crystals are composed of atoms arranged in repeating patterns that can have two-, three-, four- or six-fold symmetry. Each repeating pattern is located at a lattice point. A three-dimensional crystal lattice is a structure formed by countless numbers of identical, tiny building blocks, called unit cells. Unit cells have a box shape, which can be defined by the length of the three sides of the unit cell (a , b and c) and the angle between the axes of the unit cell (α , β and γ). Variation in the shape of the unit cell results in different symmetry elements (rotation axes and reflection planes), but *all* crystals may be ascribed to one of seven crystal systems.
- When looking at crystal symmetry, the *angles* between faces are more important to consider than the absolute sizes of individual faces, as conditions during the growth of a crystal often prevent some faces from developing as perfectly as they might, or from developing at all.

Glossary

acicular

Needle-shaped.

anion

An atom (or group of atoms) that carries a negative charge.

amorphous

A description of a substance that is without shape; a material that is structurally disordered, e.g. glass.

cations

An atom (or group of atoms) that has lost one or more electrons, to give it a positive charge.

cleavage

Planes of weakness in the crystal structure of a mineral allowing it to fracture along smooth parallel surfaces (cleavage planes). Also planes of weakness in metamorphic rocks, notably slates, caused by the alignment of fine-grained, platy materials. See also slaty cleavage.

cleavage fragments

Broken piece of a crystal with a well-defined, blocky shape and a flat surface.

cleavage planes

A term used in minerals for flat surfaces formed along planes of structural weakness when a crystal is broken. A term used in rocks for a plane along which platy minerals are aligned and splitting tends to occur; most well-developed in slates.

conchoidal fracture

A curved (shell-like) pattern developed on the fractured surface of fine-grained and glassy rocks and some minerals (such as quartz) that lack cleavage. (Pronounced '*con-koi-dal*'.)

covalent bonding

A type of bonding in a mineral structure in which most, or all, of the chemical bonds between atoms involve sharing of electrons.

crystal systems

The classification scheme for crystals, based on symmetry elements.

crystalline

A term used to describe solid material composed of crystals, formed when atoms are arranged in a structurally ordered pattern, as occurs when a liquid cools more slowly. Also used to describe the rock texture when crystals have grown together to form an interlocking mass, as occurs in crystallisation from liquid (igneous crystallisation) and solid (metamorphic crystallisation) states.

crystallographic axes

A set of three directions in a crystal (labelled *x*, *y* and *z*) that are parallel to the edges of a unit cell.

dendritic

Descriptive term for a mineral with clusters of crystals in fern-like branches.

density

A measure of how heavy an object is for a given volume.

devitrification

The slow transformation of glass to a crystalline form.

equidimensional

Term used to describe a crystal that has a rather similar appearance in different directions.

ferromagnesian minerals

Silicate minerals rich in iron and magnesium, including olivine, pyroxene, amphibole and biotite mica. See also mafic minerals.

glass

A structurally disordered solid formed by quenching of a liquid.

globular

Descriptive term for a mineral with acicular (needle-like) crystals radiating in all directions from a central point to form a spherical aggregate.

goniometer

Device for measuring the angle between crystal faces.

grain boundary

The line of contact between adjacent crystals in a rock.

graphite

A polymorph of carbon that consists of sheets of atoms tightly bonded in a hexagonal structure with only weak bonds between sheets. It is stable at low temperatures and pressures.

halite

A mineral form of sodium chloride (NaCl), also known as rock salt. It is an example of purely ionic bonding between Na^+ cations and Cl^- anions.

hardness

The resistance of a material to scratching or indentation.

interstices

The spaces in a close-packed crystal structure that can accommodate small atoms or ions.

ionic bonding

A type of bonding in a mineral structure, generated by the transfer of one or more electrons from one atom to another, creating two ions of opposite charge which are attracted to each other.

ionic substitution

The replacement of ions of one element by those of another in a crystal structure. Ions most likely to substitute for one another have similar sizes and electrical charges.

lattice

An array of objects or points in space that form a repeating pattern in two or three dimensions.

lustre

The surface appearance of a mineral that depends on the way it reflects light. Typical terms used to describe a mineral's lustre include: glassy, resinous, metallic.

massive

Descriptive term for crystals that have grown together in a solid mass, in which individual crystals cannot clearly be seen.

metallic bonding

A type of bonding in a mineral structure involving atoms donating one or more electrons to a 'sea' of free electrons that flows between and around the cations. Such structures are dense and close-packed, yet malleable and ductile.

mirror planes

A plane of symmetry, dividing two halves of an object that are mirror images of each other.

Mohs' scale

A scale of mineral hardness devised by Friedrich Mohs and consisting of ten well-known minerals, ranked in order of hardness from the softest, talc (hardness 1) to the hardest, diamond (hardness 10).

phase boundary

The dividing line between two stability fields on a phase diagram.

phase diagram

A diagram showing the stability fields over which different phases of matter can exist (at equilibrium) and the phase boundaries between them. Usually, such a diagram is plotted for a fixed chemical composition over a range of pressure and temperature, in which case the axes of the graph represent pressure and temperature.

phase transformation

An event involving the conversion of one phase into another phase having the same chemical composition (but with a different crystal structure, if any).

phases

The state in which a particular substance can exist - as gas, liquid or solid. Also used to refer to a mineral with a definite chemical composition.

polymorphs

Substances that have the same chemical composition, but different crystal structures. For example, diamond and graphite are both polymorphs of carbon.

prismatic

Term used to describe a crystal stretched out in one direction.

reflection symmetry

The property where one side of an object is a mirror image of the other (e.g. insects, birds).

rotational symmetry

The property of an object that produces an identical arrangement of crystal faces at regular intervals of rotation.

sphalerite

A mineral form of zinc sulfide, ZnS.

stability field

The range of temperatures and pressures over which a particular phase or phase assemblage is stable.

tabular

Term used to describe a slab-like or platy crystal.

toughness

Term used to describe the resistance of a material to breaking or shattering.

triple point

The point of intersection of three phase boundaries on a phase diagram representing the pressure and temperature conditions at which solid, liquid and gas phases can coexist.

twinning

The term used to describe a type of crystalline defect, in which a crystal contains different regions in which crystal lattices are related in a predictable way (e.g. by reflection in a mirror plane, or rotation about a symmetry axis).

unit cells

The basic building block of a 3-dimensional crystal lattice with three sets of parallel sides and a lattice point at every corner.

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