

ELEMENTS OF THE PHYSICAL MECHANISMS OF DEFORMATION AND FRACTURE

*Lorsqu'un théoricien trouve un résultat nouveau personne n'y croit,
sauf lui! lorsqu'un expérimentateur trouve un résultat nouveau tout
le monde y croit, sauf lui!*

The aim of this first chapter is to give nonspecialists in physics and metallurgy a general idea of the structure and mechanisms of deformations and fracture of the principal materials used in ordinary structures. Therefore, it consists of a brief summary of the classical knowledge as found in specialized works. The main references among these are given in the bibliography. Knowledge of these basic physical mechanisms is necessary for the formulation of hypotheses upon which the macroscopic phenomenological theories of deformation and fracture can be based. These theories, presented in Chapters 4–8, must indeed integrate the phenomena associated with discrete entities such as atoms, crystals, molecules, cells, etc., to the level of homogeneous continuum models. In metals, the introduction of the concept of dislocations by Taylor and several others in 1934 marked the first decisive step in explaining the phenomenon of plastic deformation. In a more general way, the invention of transmission and scanning electron microscopes has permitted, during the 1960s, an understanding of the main mechanisms of deformation and fracture.

It must, however, be remembered that in the field of fracture where these phenomena occur at the much larger scale of crystal or molecular arrangements, there are several unresolved questions, and for this reason the schematic treatment given in this chapter remains very rudimentary.

Paradoxically, despite the large differences in the nature and structure of materials such as metals and alloys, polymers and composites, concrete, wood, there is a great unity displayed in their macroscopic behaviour. With different orders of magnitude, terms like elasticity, viscosity, plastic or permanent deformation, consolidation or hardening, brittle fracture and ductile fracture can be applied to all these materials. This is what justifies 'a priori' the global approach to the mechanics of materials which, with the aid

of concepts from continuum mechanics and thermodynamics in Chapter 2, and from rheology in Chapter 3, allows the construction of models independent of the nature of materials in their basic properties (but not in their analytical formulations).

1.1 Metals and alloys

1.1.1 Structure

Elements of crystallography

Atoms

Metals and alloys are made up of arrangements of atoms held together by electromagnetic forces between the electrons of neighbouring atoms. The order of magnitude of the 'radius' of an atom varies from 10^{-7} to 10^{-6} mm ($1-10 \text{ \AA}$). Stable arrangements are determined by a minimum energy condition of the atomic packing, which is a function of thermal activation. In metals, the bonds result from a sharing of electrons in the outer shells of the atoms. Metals and alloys are normally found to consist of closely packed crystals. The amorphous state can only result from complex processes requiring extremely fast cooling.

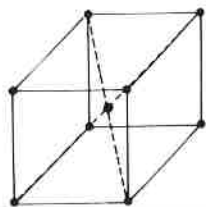
Monocrystals

The crystalline state is characterized by the regularity of the atomic arrangement; an elementary parallelepipedic pattern or lattice repeats itself periodically in all three directions.

Most of the metallic lattices belong to one of the three following systems:

- Cubic centred (CC) crystals (Fig. 1.1) e.g., Fe α , Cr, Mo
- Face centred cubic (FCC) crystals (Fig. 1.2) e.g., Cu, Ag, Al, Ni
- Close packed hexagonal (CPH) crystals (Fig. 1.3) e.g., Mg, Zn, Ti α , Co α .

Fig. 1.1. CC crystals.



These lattices possess axes and planes of symmetry, the latter being in general the planes in which the atoms are most densely packed and which possess a lower resistance to shear. Their conventional representation is by means of Miller indices: the plane to be characterized is identified by the coordinates of its intersection with the axes of an orthogonal reference system, with the reciprocals of these numbers reduced to the three smallest integers which have the same ratios (Fig. 1.4).

Fig. 1.2. FCC crystals.

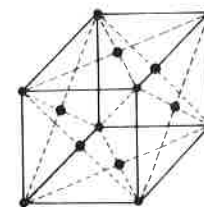


Fig. 1.3. CPH crystals.

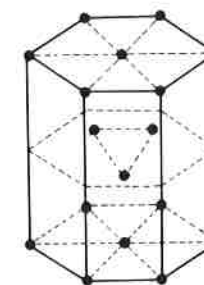
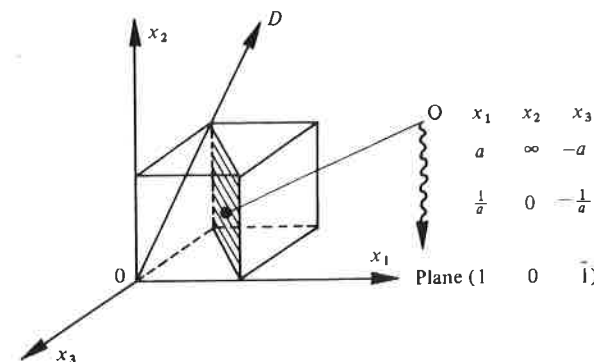


Fig. 1.4. Miller indices.



A crystallographic direction is characterized by a straight line emanating from the origin of the reference system and passing through the position of an atom. It is designated by the coordinates of that atom expressed in terms of interatomic distances. For example, the direction OD in Fig. 1.4 is expressed as $\langle 01\bar{1} \rangle$.

The structure of an alloy can be either that belonging to one of the constitutive elements or an entirely different crystalline structure. In solid solutions, it is possible to have the substitution of an atom from the lattice (for example aluminium in iron) or the insertion of small atoms in the network of the solvent (for example carbon in iron for austenite (Fig. 1.5)). Metals can take different forms or phases depending on the temperature. The most common phases for steels are the γ and α phases (respectively FCC for austenite and CC for the ferrite of the carbon-iron system). It is also possible to have stable or unstable secondary phases, phases β , δ , ϵ , σ , and in a particular phase it is possible to distinguish the cases in which the substitute atoms occur in a disordered state (for example phase γ) or in an ordered state (for example phase γ').

Polycrystals

Metals and alloys are generally produced in a liquid state, and their structure is formed as they solidify when cooled. As the temperature of the liquid decreases, the interatomic distances become smaller; the critical distance, at which bonding occurs, is reached at several, randomly distributed sites, and these constitute the first germs or nuclei of crystal growth. The lattices are formed in the same crystalline system but in random directions. Each nucleus develops into a crystal whose growth is limited by neighbouring crystals. A polycrystal is made up of several monocrystals oriented randomly. The size of such monocrystals varies from a few microns (10^{-3} mm) to a few millimetres depending on the nature of the constituent elements of the metal, as well as on the thermal and mechanical treatments to which the polycrystal has been subjected (Fig. 1.6). It is therefore

Fig. 1.5. Solid solution of substitution (S) or insertion (I).

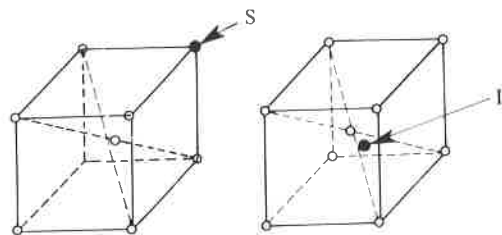
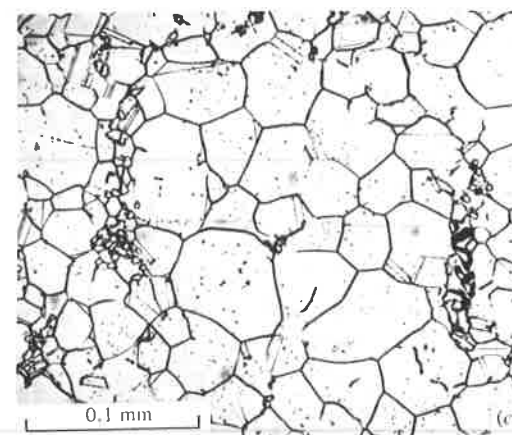
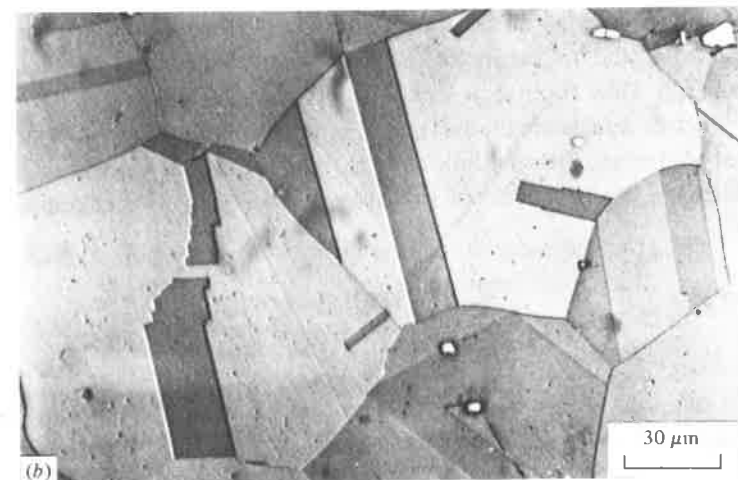
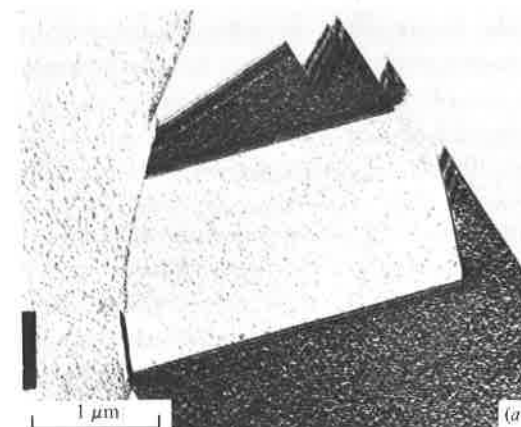


Fig. 1.6. Examples of crystals (after A. Pineau): (a) nickel based Inconel 718 alloy, transmission electron microscopy; (b) nickel Waspaloy alloy, optical microscopy; (c) nickel based Inconel 718 alloy, optical microscopy.



understandable that although a polycrystal consists of essentially anisotropic monocrystals, it can often be regarded as macroscopically isotropic, i.e., without any preferred direction for the properties under consideration.

Crystal defects

The structure of the perfect crystal as described above can only account for elastic deformations and for so-called brittle fracture in which the loss of cohesion occurs without noticeable macroscopic deformation. Plastic deformations and tensile fracture can only be explained by the presence of defects that disturb the crystal lattice.

Point and surface defects

Atomic point defects consist of atoms inserted or substituted in solid solutions and of vacancies (i.e. points in the lattice where atoms are missing). They result in a local distortion of the lattice.

Surface defects are the surfaces of separation between crystals or parts of a crystal where the orientations or natures of the phases are different. Their thickness is of the order of 4–5 atomic 'diameters'. For example,

grain boundaries (or crystal boundaries) in polycrystals,
dislocation loops and cells,
twin crystal boundaries,
interfaces between two phases.

Cohesion defects, consisting of the surfaces of separation in a material which lead to fracture, are micro-cracks and cavities.

Dislocations (line defects)

These are the defects which are mainly responsible for plasticity of metals. A line of dislocation is a defect in the arrangement of atoms which is repeated periodically and which represents the equilibrium state of atoms with slightly different magnetic fields. It is possible to give a schematic representation of such defects in the case of simple cubic crystals:

An edge dislocation or defect which would be created by the translation of the upper part of the crystal (Fig. 1.7).

A screw dislocation or defect which would be created by a local rotation of the upper part of the crystal (Fig. 1.8).

A dislocation loop or line which, for example, joins a pure edge dislocation to a pure screw dislocation (Fig. 1.9).

Dislocations are created during the growth of the crystals; their density, which is very high in most metals and alloys, varies from 10^6 km cm^{-3} for well-annealed crystals to 10^7 km cm^{-3} for heavily cold-worked samples. Fig. 1.10, which was obtained by scanning electron microscopy, shows a dislocation configuration. Prolonged heat treatments favour the arrangement of dislocations in the form of almost regular three-dimensional cells consisting of crystal planes and nodes, called *Frank networks*.

Fig. 1.7. Edge dislocation of line DC.

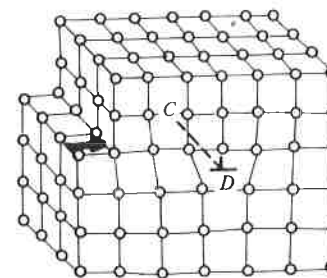


Fig. 1.8. Screw dislocation of line DV.

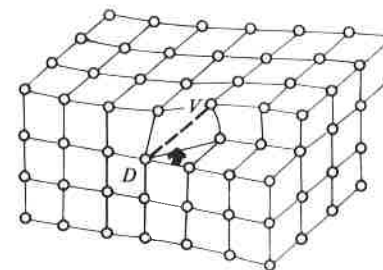
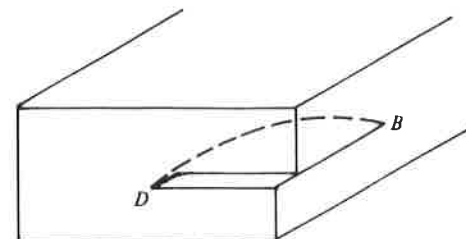


Fig. 1.9. Dislocation loop of line BD.



Burgers vector

A dislocation can be characterized by the 'lack of closure' vector of a contour encircling the dislocation line. Let us consider two simple cubic crystals one perfect and the other with an edge dislocation L (Fig. 1.11). In the latter, let us consider a closed loop $ABCD$ around the point L with the sense of traverse defined with respect to an orthogonal reference system. Now let us, reproduce this contour in the perfect crystal by counting the same number of interatomic distances: $A'B'C'D'E'$. To close the contour, the vector $\vec{E'A'}$ should be added. This vector by definition is the Burgers vector \vec{b} .

Burgers vectors have the following properties:

- they are independent of the contour;
- their magnitude defines the translation which would be necessary to create a dislocation;

Fig. 1.10. Dislocations in a stainless steel. Fe20 Cr-Ni-Al hardened by precipitation in the ordered phase Ni-Al (after Pineau).

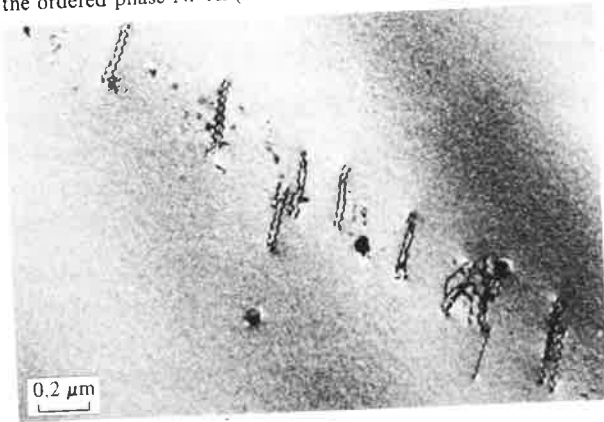
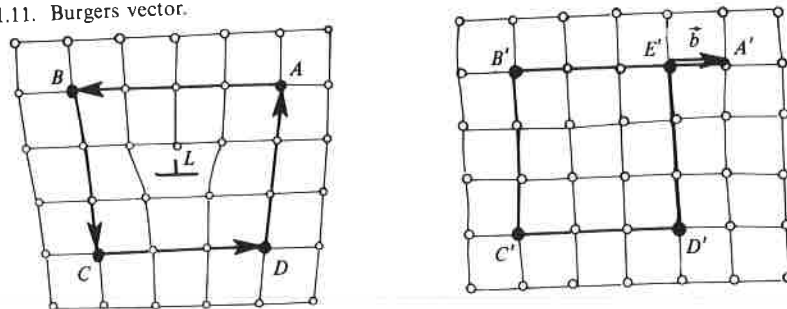


Fig. 1.11. Burgers vector.



they are constant along the whole dislocation line;

if $\vec{\tau}$ is a unit vector on the dislocation line then:

if $\vec{\tau}$ and \vec{b} are perpendicular to each other, the dislocation is an edge dislocation;

if $\vec{\tau}$ and \vec{b} are parallel, the dislocation is a screw dislocation;

if $\vec{\tau}$ and \vec{b} are at some angle to each other, the dislocation is a mixed one;

the closing vector of a contour surrounding several dislocations is the sum of the Burgers vector of these dislocations.

Energy associated with dislocations

Since dislocations produce purely elastic distortions of the lattice, and since the neighbourhood of a dislocation can be considered to be a linear elastic continuum, we can calculate the elastic energy w_e stored in the material in the form of internal stresses and strains. For an edge dislocation or a screw dislocation (Fig. 1.12) of unit length and a Burgers vector of magnitude b in a medium with shear modulus μ , we find that the stored energy is of the order of

$$w_e = \mu b^2 \text{ Jm}^{-1}.$$

In the same way, it is possible to calculate the force \vec{F}_D which would be exerted on a dislocation of unit vector $\vec{\tau}$ and Burgers vector \vec{b} in a uniform stress field σ . This is the Peach-Koehler relation

$$\vec{F}_D = (\sigma \cdot \vec{b}) \wedge \vec{\tau}.$$

1.1.2 Physical mechanisms of deformation**Elastic deformation**

Elastic deformations occur at the atomic level. The observed macroscopic effect is the result of the variations in the interatomic spacing necessary to balance the external loads, and also of the reversible movements of dislocations. These geometrical adjustments are essentially reversible. In a

Fig. 1.12. Energy associated with dislocations.



purely elastic deformation, the initial configuration of atoms is restored upon the removal of the load.

Permanent deformations

Plastic or viscoplastic permanent deformations occur at the crystal level, and are in addition to elastic deformations; they correspond to a relative displacement of atoms which remains when the load is removed. Depending on the case, the deformations are either purely intragranular (inside the grains) or involve intergranular displacements. The ratio of joint deformation to grain deformation remains small, but it generally increases with increasing temperature and also with decreasing strain rate.

Deformation by slip and twinning

Symmetry planes of the crystal lattice, which are also the reticular planes of the most densely packed atoms, form the parallel planes with the greatest distance between them. It is therefore in these planes that slip due to shear can occur in the direction of maximum shear stress, e.g., planes (1, 1, 1) in FCC crystals; and planes (1, 1, 0) and (1, 1, 2) in the BCC crystals. They occur in the form of parallel slip bands which result in steps on the exterior surface of the samples (Fig. 1.13(a)) or in the form of twins which consist of slips symmetric with respect to a plane (Fig. 1.13(b)).

Twinning is more characteristic of deformations which occur at average or room temperature. It occurs in CC and CHP crystals in conjunction with slips, but also in FCC crystals where the energy of stacking defects is low. These defects, slips or twinings, are, in fact, heterogeneous deformations at the crystal level, but may be considered homogeneous at the macroscopic level.

Deformation by dislocation movements

The presence of dislocations considerably reduces the stability of the crystal lattice. Their mobility is the essential cause of permanent deformations, homogeneous at the macroscopic scale.

Slip displacement: when, under an external load, an edge or screw dislocation moves across a crystal, irreversible displacement occurs which is equal to the Burgers vector. Fig. 1.14 shows an edge dislocation in a cubic crystal subjected to a shear stress σ_{12} . The plane defined by the unit vector \vec{l} and the Burgers vector \vec{b} is called the slip plane.

This displacement mechanism requires the breaking of bonds only in the vicinity of the dislocation line, and successively from one atom to the next.

Fig. 1.13. (a) Slip bands in nickel based Waspaloy (after Pineau). (b) Twinning deformation in zinc (after Pineau).

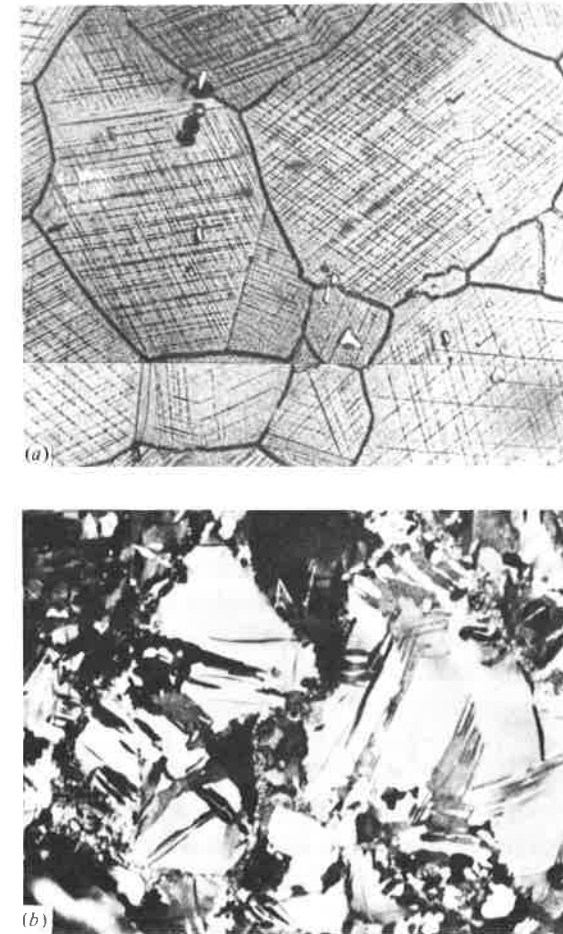
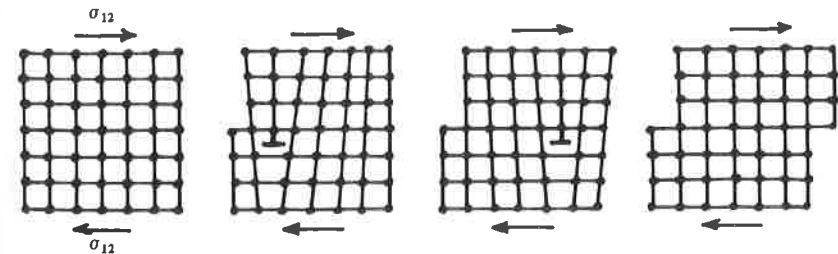


Fig. 1.14. Slip displacement of a dislocation.



In the more complex case of a dislocation loop, the plane of the loop can digress into another plane (a perpendicular one for example) arising from its 'pure screw' point to avoid an obstacle such as an impurity; this is called a deviated slip.

Climb displacement: an edge dislocation can move perpendicularly to its slip plane with the transport of material. If a void is close to a dislocation line, then a distortion of the lattice resulting from the application of an external load can cause an atom of the lattice to jump by half a plane on the empty side of the crystal and result in the rearrangement of the whole row of atoms. Thus, in this mechanism, the dislocation climbs up by one interatomic space (Fig. 1.15). This displacement mechanism, linked to the diffusion of vacancies or foreign atoms, is favoured by thermal activation; it, therefore, occurs mostly at high temperatures ($T > \frac{1}{3} T_M$, where T_M is the melting temperature).

The rate of dislocation displacement (slip or climb) can be very low or very high depending upon the applied stress, but it cannot be higher than the speed of sound in the material under consideration.

Fig. 1.15. Climb displacement of a dislocation.

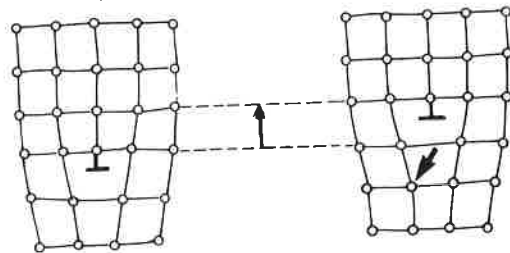
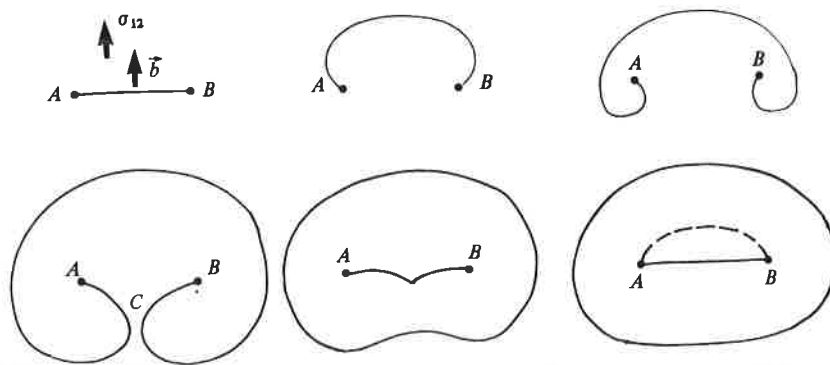


Fig. 1.16. Generation of dislocations by the Frank-Read mechanism.



Sources of dislocations

Dislocation movements cause permanent deformations; conversely, large plastic deformations increase the density of dislocations which, in turn, increases the number of blockings and contributes to further hardening. The most important source of dislocations is that described by the Frank-Read mechanism. Let us consider a dislocation segment anchored at A and B , the points of intersection with other dislocations or impurities (Fig. 1.16), of Burgers vector \vec{b} normal to AB and subjected to a shear stress σ_{12} in the same direction as \vec{b} . Under the applied stress, the dislocation is forced to move around the points A and B . When the two branches rejoin at C , they have the same Burgers vector but opposite unit vectors. They combine to create a large loop and a new segment AB which in turn generates another loop and so on...

Elasticity limit

It is easy to calculate the elastic limit of a perfect stack of atoms assuming that the shear stress causing one set of atoms to glide over another in a plane, is a sinusoidal function of a period equal to the interatomic distance (the Frenkel hypothesis). Assuming that in the vicinity of the equilibrium position, this shear stress is linearly related to the corresponding deformation through the shear modulus μ , the maximum τ_Y of this stress corresponding to the limit of reversibility of the movement is found to be

$$\tau_Y = \mu/2\pi.$$

This value is of the order of 100 times higher than the elastic limit in shear of common metals, but it is very close to the values observed for 'whiskers' or thin fibres which consist of perfect stacks of atoms. For example,

Theoretical elastic limit	{ pure iron whiskers of iron }	$\tau_Y = 84700/2\pi = 13550 \text{ MPa}$
Measured elastic limit	{ pure iron whiskers of iron }	$\tau_Y = 28 \text{ MPa}$ $\tau_Y = 11000 \text{ MPa}$

The elastic limit of a real single crystal is very difficult to evaluate because of the different mechanisms which can occur:

the dislocation loops generated by the Frank-Read mechanism and which emerge at the free surface of the crystal create an irreversible deformation. The shear stress required to initiate this mechanism is of the order of

$$\tau_y = 2\mu(b/L) \quad (L \text{ is the length of the source})$$

a value much lower than the observed elastic limit;

in fact, due to the interatomic bonds broken at the core of dislocations, the so-called Peierls–Nabarro forces prevent the slip and give rise to a higher elastic limit;

the decomposition of dislocations leads to the creation of barriers which also restrict the slip;

the Frank networks offer a resistance to shear with an order of magnitude

$$\tau_y = \frac{\mu b}{2\pi L} \quad (L \text{ is the length of the Frank cells});$$

in alloys, solid solutions or precipitates contribute to an increase in the resistance to dislocation movements.

Several of these mechanisms can occur simultaneously to give the values of elastic limit as measured macroscopically. In the case of polycrystals, the disorientation between the crystals and the grain boundaries, prevents the progress of irreversible deformation. Therefore, in this case we must add to the mechanisms described above a mechanism for crossing the grain boundary. By considering the equilibrium of forces due to the blocking of dislocations at the grain boundaries and those applied externally, and taking into account the fact that τ_y , the shear elastic limit, is the stacking stress in a crystal which can activate a dislocation source at a distance r in an adjacent crystal of mean length d , we obtain the following relation known as the Petch equation

$$\tau_y = \tau_0 + \tau^*(r/d)^{1/2}.$$

It is evident from this equation that the elastic limit varies in direct proportion to the square root of the distance r , and in inverse proportion to the square root of the average crystal length d ; τ_0 and τ^* are coefficients which are characteristics of the metal or the alloy.

Deformation of polycrystals

In order to define the basic assumptions of a model well, it is necessary to examine in a schematic way the sequence of mechanisms which occur in the deformation of a polycrystal during a uniaxial external loading, which first increases and then decreases (see Fig. 1.17).

Elastic deformation (OY in Fig. 1.17)

Elastic deformations result from reversible relative movements of atoms. They are almost independent of the permanent deformations except as regards the microscopic residual stresses which result from the irreversible crystalline slips causing the macroscopic elastic deformations to be slightly different from the sum of the microscopic elastic deformations.

Elastic limit (Point Y in Fig. 1.17)

The elastic limit is characterized by the state of stress or strain which causes the first irreversible movements of dislocations. As they are difficult to detect, we define the elastic limit or the yield stress, σ_y , by convention to be the stress for a fixed amount of permanent strain; $\epsilon^p = 0.02\%$ or 0.05% or 0.2% depending upon the precision required (see Chapter 5).

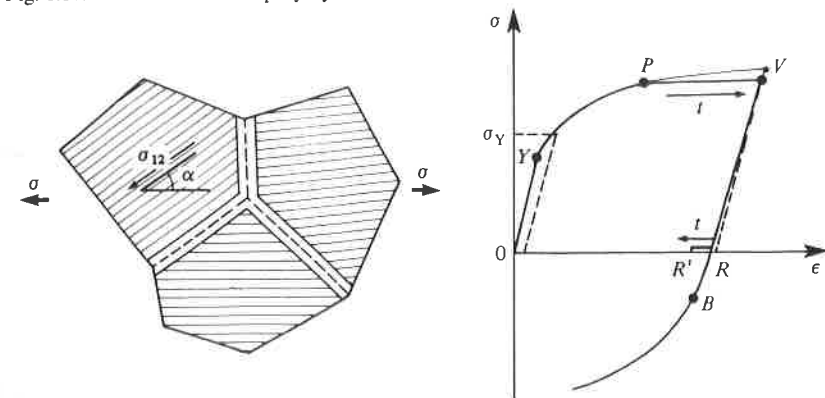
Plastic deformation (YP in Fig. 1.17)

The first slips occur in crystals with crystallographic slip planes oriented at $\alpha = \pi/4$ to the direction of applied stress σ , where the shear stress σ_{12} is maximum. The reorientation of crystals, necessary to ensure compatibility of deformations, activates other slip systems and the deformation appears macroscopically homogeneous. It is a stable deformation and each state is that of an elastoplastic equilibrium.

Hardening or consolidation (YP in Fig. 1.17)

If the stress continues to rise, the dislocation density is increased but the number of barriers is increased even more, so that the deformation

Fig. 1.17. Deformation of a polycrystal.



cannot progress unless the load is increased. This increased resistance to slip deformation is the phenomenon of hardening which can also result from the presence of intercrystalline microstresses induced by the incompatibility of grain to grain deformations.

Viscoplastic deformation (PV in Fig. 1.17)

If the stress continues to rise, the slips can cross and follow the grain boundaries. This phenomenon of intergranular slip is favoured by thermal activation and is especially significant at temperatures higher than one third of the absolute melting temperature. A large part of the deformation, however, remains intragranular and is comprised of slip and climb of dislocations. When the deformation can progress under constant stress with no possibility of equilibrium, we have creep flow the rate of which depends on the applied stress; this is the domain of viscoplasticity.

Restoration or recovery (RR' in Fig. 1.17)

The modifications produced in an aggregate of polycrystals by deformation represent a deviation with regard to the thermodynamic equilibrium which tends to decrease under zero or reversed loading; the concentration of the vacancies or of the interstitial atoms decreases, dislocations of opposite signs neutralize each other, and recrystallization can occur. The recovery is a function of time and is favoured by thermal activation. On a macroscopic level, it manifests itself in a partial recovery of the deformation or in a decrease in the hardening. This description also applies to microstructurally stable materials. However, the phenomenon of ageing can occur which involves instabilities of structures or chemical compositions over a short or a very long time (e.g. ageing of some alloys after heat treatment).

Plastic or viscoplastic incompressibility

Since slip deformations do not alter the crystal structure, the total volume of an aggregate remains unchanged. Only elastic deformations produce a noticeable volume change; the change due to the increase of the density of dislocations, always remains very small. In the same way, a normal stress on the slip plane or a state of hydrostatic stress ($\sigma_1 = \sigma_2 = \sigma_3$) has no effect on permanent deformations. This has been experimentally verified up to pressures of 30 000 atmos (3000 MPa).

Anisotropy induced by permanent deformations

As permanent deformations differ from one crystal to the next, the

compatibility of deformations at grain boundaries is assured only by elastic microdeformations; these remain partially locked when the load is removed resulting in self-equilibrated microscopic residual stresses. These microscopic stresses in effect load the crystal at a neutral state and can increase or decrease the external load necessary to produce new slips in a way which varies according to the direction considered: this is the anisotropy which results from permanent deformations. The Bauschinger effect, which is the lowering of the absolute value of the elastic limit in compression following a previous tensile loading, is its simplest manifestation (point B in Fig. 1.17).

Microstructural instabilities

These correspond to an instability of the metallurgic state of the microstructure and manifest themselves in the course of time by variations in strength. They are frequently induced by temperature variations (phase changes, precipitation).

Phase and structural changes generally take place during a variation of temperature. The structure of steel reveals, for example, phase δ (BCC) at very high temperatures, phase γ (FCC) at high temperatures, and phase α (BCC) at low temperatures. Precipitation (precipitate γ' for example, in a phase γ) occurs during a lowering of the temperature, after a partial dissolution of the phase γ' at the higher temperature. The new structure is extremely fine and produces significant hardening (higher resistance to deformation) but it is unstable.

Growth of precipitates occurs under constant temperature when the microstructure is initially in an unstable state. This phenomenon is thermally activated. It manifests itself by an increase in resistance to deformation in the region where dislocations can cross precipitates only by shear and then, for more important precipitate sizes, by a decrease in resistance to deformation when dislocations can go around the particles.

Ageing corresponds to an instability of microstructure which occurs at constant temperature with or without load and usually results in an increase in resistance (precipitation of carbides, for example, the precipitation of $M_{23}C_6$ at the grain boundaries of non-oxydizing austenitic steels). It is possible to demonstrate this phenomenon (as well as that of the precipitate growth) by heating a sample for some time before a creep or hardening test.

1.1.3 Physical mechanisms of fracture

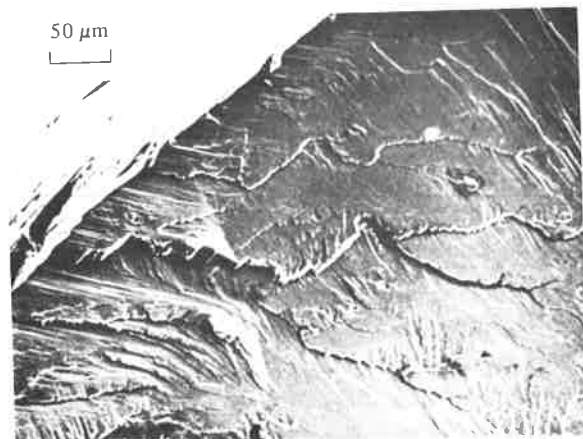
Elastic and permanent deformations, which take place at atomic and crystalline levels respectively maintain the cohesion of the matter. Fracture, by definition, destroys this cohesion by creating surface or volume discontinuities within the material. Therefore, fracture occurs at the larger scale of crystals: we will be concerned with microcracks or cavities of a size expressed in microns or hundredths of a millimetre, with macrocracks of the order of a millimetre, and with cracks which occur at the scale of mechanical structures, measurable in centimetres or decimetres.

The two main basic mechanisms of local fracture are brittle fracture by cleavage and ductile fracture resulting from large localized plastic deformations.

Brittle fracture

In so-called brittle fracture, only the fracture of interatomic bonds, without noticeable overall plastic deformations, is involved. These fractures occur when the local strain energy due to the external loads becomes equal to the energy necessary to pull the atom layers apart. Lattice defects or accidental geometrical imperfections result in stress concentration, and hence they play an essential part in the initiation of the fracture process. Brittle fracture by cleavage consists in a direct separation of particular crystallographic planes (for example, the plane (100) for iron). In a crystal, several parallel

Fig. 1.18. Brittle fracture by cleavage in a weak alloyed steel, scanning micrograph (after Pineau).



surfaces of cleavage can develop which join each other perpendicularly in the form of 'steps' arranged in 'rivers'. At grain boundaries the cleavage surfaces change direction in order to follow the crystallographic cleavage planes of the next crystal (Fig. 1.18).

FCC crystals are less vulnerable to cleavage; this occurs mostly in CC crystals such as steel with a low carbon content and in CPH crystals such as zinc and magnesium which fracture by cleavage.

Intergranular fracture is a cleavage that follows the grain boundaries. It occurs in two forms:

Brittle fracture itself which occurs at low temperature when impurities segregated at the grain boundaries lower the energy of cohesion at these boundaries.

Intergranular fracture due to creep, observed mostly at average and high temperatures (more than one third of the absolute melting temperature). It can be present with or without significant overall viscoplastic deformation, which justifies the term 'brittle' (Fig. 1.19). The defects leading to this mode of fracture are initially in the form of cavities at the boundaries where dislocations have piled up, subsequently increasing in volume and reproducing themselves, or in the form of decohesions called triple points, which result from the intersection of three crystals, following intercrystalline slips. This intergranular decohesion occurs over a period of time and can be caused, for example, by high temperature creep. When decohesion occurs at several adjacent grain boundaries, we may say that a crystalline crack has been initiated.

Ductile fracture

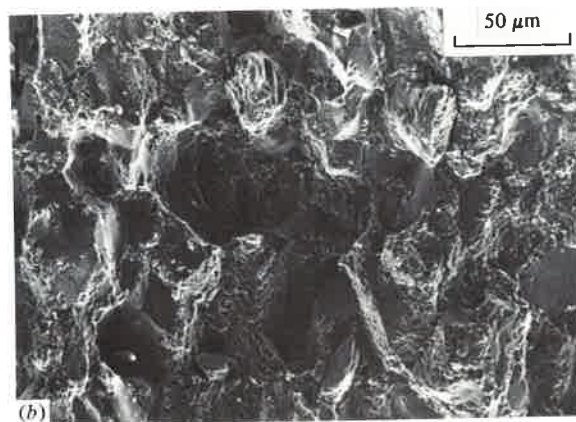
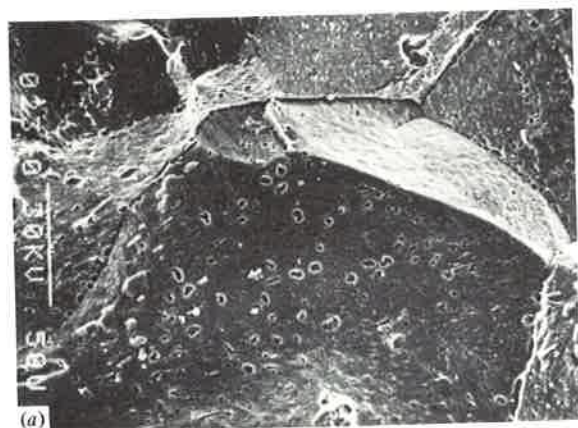
Ductile fracture arises from the instability which results when very large local deformations occur in the vicinity of crystalline defects. Depending upon the density of these defects, the overall macroscopic deformations may or may not be significant so that a material which shows signs of ductile fracture can have either a ductile or brittle global behaviour. The defects responsible for initiating ductile fracture are:

- particles of added elements in alloys;
- inclusions;
- solution precipitates resulting from a heat treatment;
- piling up of dislocations;
- grain boundaries and triple points.

In the vicinity of the defects, the external loads create stress concentrations which lead to large plastic deformations. The particle or foreign defect, being generally less ductile than the matrix, produces an instability which results in decohesion at the interface or in fracture due to cleavage and thus initiating a microcrack or a cavity.

The growth of these cavities takes place through plastic slips with local strains that can well exceed 100% to the point where the peduncles of metal separating the holes reach a condition of instability by necking. Their brittle fracture causes coalescence of the cavities which leads to the final fracture. The fracture surface very often looks like a juxtaposition of cups having a precipitate or an inclusion at their bottoms (Fig. 1.20).

Fig. 1.19. (a) Intergranular brittle fracture by creep in a Cr-Mo steel (after Pineau). The small cavities on the boundaries are creep cavities. (b) Intergranular ductile fracture in a Nickel based Inconel 718 alloy (after Pineau).



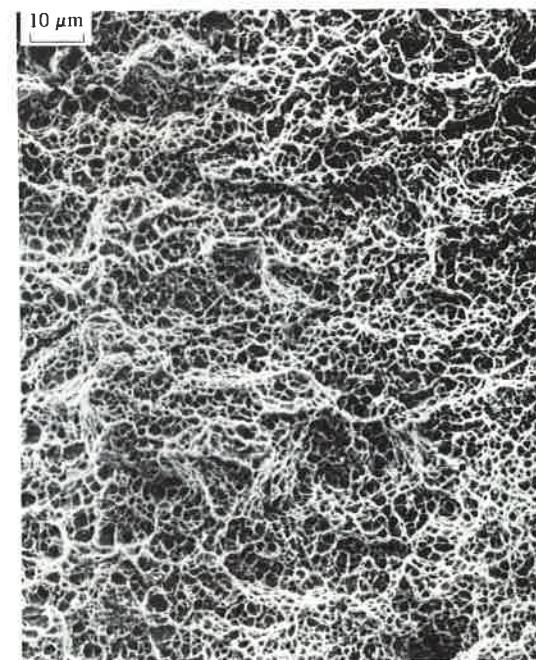
Fatigue fracture of a polycrystal

The fracture of an element under service conditions usually involves different interacting mechanisms. Fatigue failure under cyclic loads is an example worth describing because it clearly distinguishes for modelling purposes the different stages of fracture. Let us consider therefore a polycrystal subjected to a periodic load.

Accommodation stage (or nucleation)

Even if the maximum load is lower than the usual elastic limit, locally, in the vicinity of the defects the stress concentrations create cyclic plastic microdeformations, which, in turn, block further slip by virtue of multiplication of dislocation nodes. This dissipative mechanism produces a local rise in temperature which can then induce the relaxation of microstresses. Depending upon the relative importance of these two processes of hardening and relaxation, a hardening or softening of the material takes place. During this phase slip bands can form, resulting in steps on the surface of the sample.

Fig. 1.20. Transgranular ductile fracture in a 0.30 C-1 Cr-0.25 Mo steel (after Pineau).



Initiation phase of microcracks (stage 1)

It is difficult to demonstrate and to study the initiation of microcracks due to fatigue. Depending upon the material and the level of the load, several mechanisms can influence the initiation:

dislocation climbs accompanied by the formation of voids;
the formation of permanent slip bands and decohesion, very often at the surface of the sample;
intrusion-extrusion mechanisms.

During this initiation phase, the defects usually follow planes with $\pm 45^\circ$ inclination to the direction of the largest principal stress. Their presence is likely to be accelerated by a hostile environment (oxidation or corrosion).

Growth phase of microcracks (stage 2)

The initiation stage corresponds to progression from stage 1 to stage 2. Schematically, the microcracks have a tendency to orient themselves perpendicular to the direction of the maximum principal stress. This stage usually corresponds to the crossing of the first grain. Thereafter, the microcracks move through the successive grains or, less often, along the grain boundaries. When the crack size becomes significant and has acquired a well-defined direction, it grows in a preferential way, partially unloading other microcracks and generating a high stress concentration at its front. In this stage a macroscopic initiation is taking place: the material can no longer be considered as a homogeneous macroscopic medium.

Growth phase of a macrocrack

The cyclic opening and closing of cracks results in alternating plastic slips at the crack-tip, which in different crystallographic planes form a ridge of cleavage at each growth of the crack. The fractured surface reveals a succession of striations which often (but not always) permits a measurement of the crack-tip progress in each cycle (two good examples are given in Fig. 1.21).

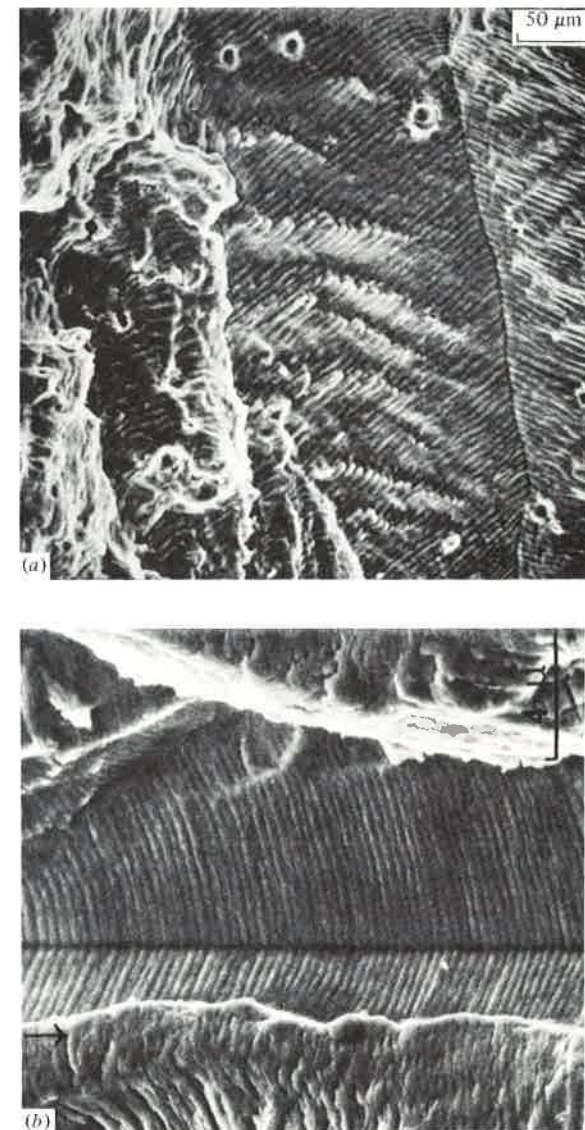
The crack grows in this way until it reaches a critical size at which the cracked part becomes unstable. The crack then propagates rapidly, breaking the work-piece into two or more pieces.

Effects of the environment

The fracture mechanisms described above are influenced by chemical reactions generated by a hostile environment. Corrosion, more particularly

stress-corrosion, affects grain boundaries and accelerates intergranular fracture. The presence of hydrogen in steel, even in small amounts, is conducive to formation of cracks by diffusion and concentration in highly stressed zones.

Fig. 1.21. Fatigue ridges (after Pineau): (a) stainless austenitic steel; (b) Inconel 718 alloy.



The most affected damage phenomenon is that of fatigue in view of the preferential localization of defects which occurs at the surfaces of areas easily accessible to corrosive agents. Generally it is observed that fatigue life in a vacuum (or in an inert gas) is longer than that in the air, the latter being higher than that in a corrosive medium (salt water, media with high sulphur content). The mechanisms involved are of an electrochemical nature resulting in the formation of passive protective layers which can break under the action of mechanical loads (stress-corrosion).

For fatigue cracks, the effect of the environment can result in either slowing down or accelerating the crack growth rate depending on whether the crack-tip has been blunted or whether there has been an increase in stress concentration by virtue of the edge effect of a partial penetration. These phenomena are not yet well known and are difficult to model.

1.2 Other materials

1.2.1 Polymers

Structures

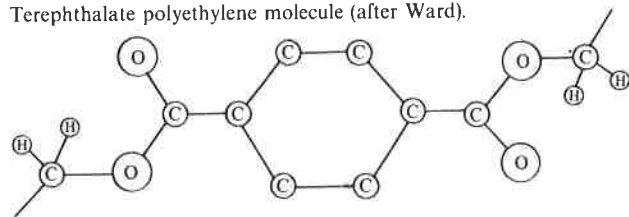
Molecules

High polymer solids consist of chain-like molecules. The chain backbone is mostly made up of carbon atoms linked by carbon-carbon covalent bonds with a fracture energy which is of the order of 300 kJ mole^{-1} . Other atoms of hydrogen, oxygen, nitrogen are linked to the atoms of the chain and eventually to the neighbouring atoms by covalent links or by van der Waal type bonds; the latter have a fracture energy which is only in the order of 10 kJ mole^{-1} (Fig. 1.22).

Amorphous and semicrystalline arrangements

The flexibility of polymer molecules allows different types of arrangement. However, as a result, molecules possess a much less regular character than metal crystals.

Fig. 1.22. Terephthalate polyethylene molecule (after Ward).



In an amorphous polymer the chains are packed randomly at the molecular scale but have a certain order at a smaller scale (Fig. 1.23). On the macroscopic scale, the amorphous materials are isotropic and often transparent. Examples of such polymers include plexiglass and polystyrene.

During polymerization and under thermomechanical effects the long-chain molecules of certain polymers tend to arrange themselves in packs to form crystallites separated by amorphous areas.

The crystalline wafers form a superstructure with a mean lattice size of $1 \mu\text{m}$. They are more resistant than the amorphous zones and have arrangement defects. Partially crystallized polymers are

Fig. 1.23. Diagrams of (a) amorphous and (b) crystalline arrangements.

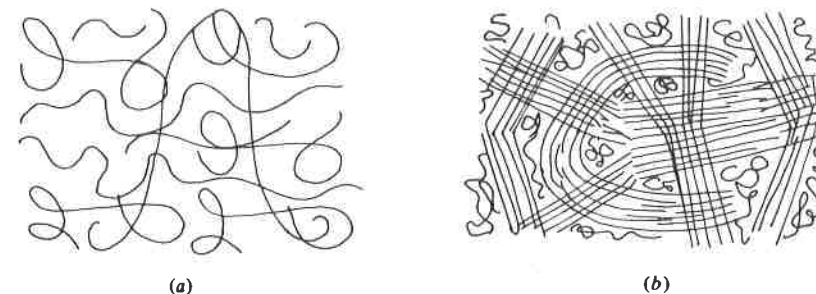
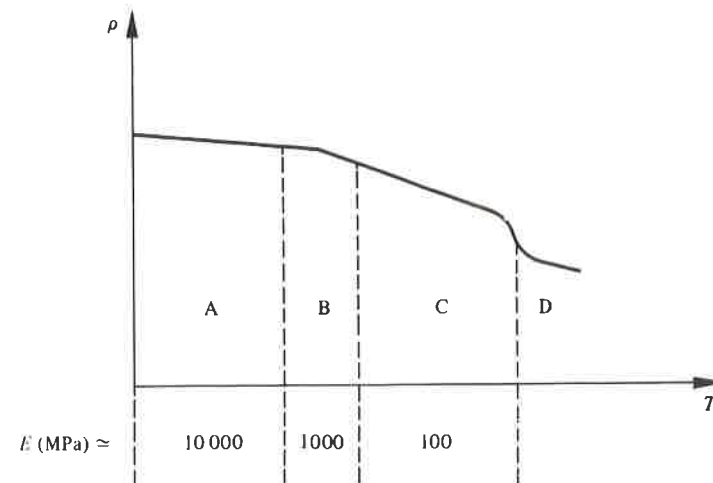


Fig. 1.24. States of polymers.



translucent or opaque. Examples of such polymers include nylon, polythene.

Different polymers

Depending upon the temperature, a polymer can occur in four different states corresponding to an increase in the free intermolecular volume with the temperature, and a decrease in the strength of the bonding forces. We may represent these states by following the graph of density ρ or of the elastic modulus E , for example, as a function of the temperature (Fig. 1.24). Room temperature could lie in any one of the four zones depending upon the polymer considered.

Glass state (A): organic glasses allow only very small deformations.

Transition state (B): in this state, we encounter linear thermoplastic polymers (cellulose, polyamides, polyesters, polyvinyls) and cross-linked polymers in which chemical decomposition occurs before melting (phenolic plastics or aminoaldehydic resins).

Rubbery state (C): elastomers consist of very long molecular chains linked together at relatively few junction points.

Fluid state (D).

Fibre-resin composites

The combination of fibres embedded in a resin results in composite materials with a specific resistance which may be higher than that of certain metals. The most commonly used fibres are of glass, Kevlar, boron, and carbon. Their diameters range from a few hundredths of a millimetre to tens of millimetres. The most frequently used resin is epoxy resin. The fibre-matrix interfaces are the weakest zones as regards resistance to deformation and to fracture. The volume of the fibres in the composite varies from 50 to 70% depending on the manner of their arrangement which can be:

unidirectional: the composite consists of parallel fibres in the form of bars or plates (Fig. 1.25(a));

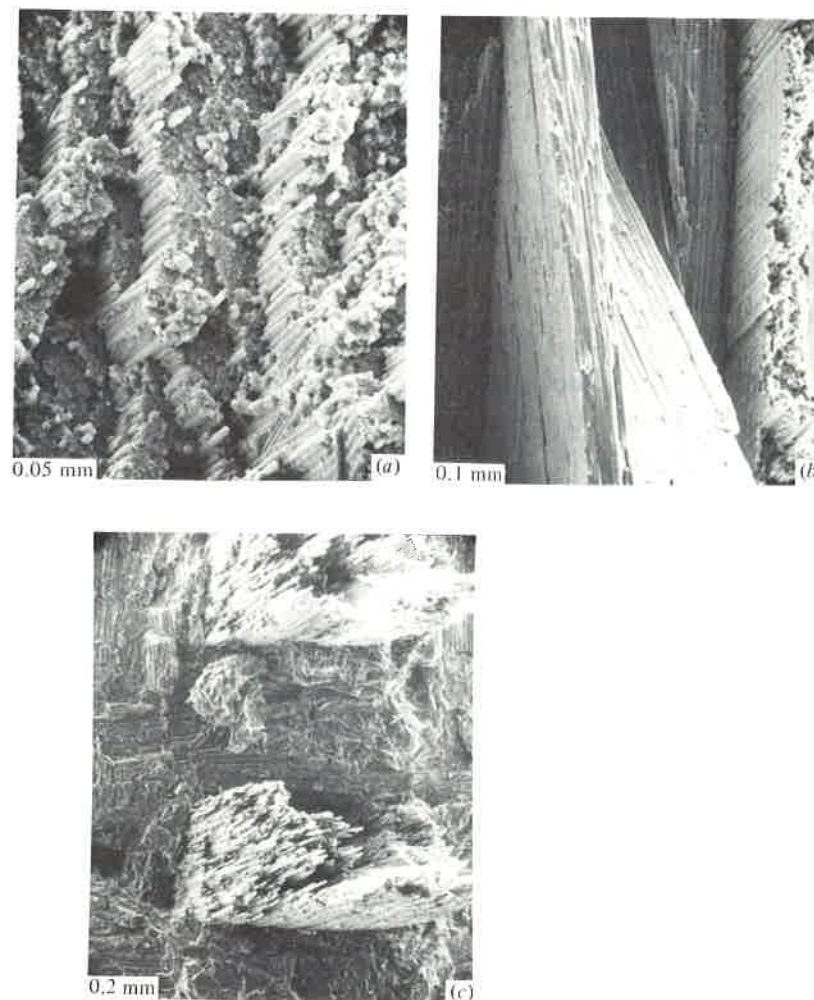
bidirectional: by superposition of crossing unidirectional sheets or by means of tissue impregnation, plates or shells are fabricated whose stiffness and resistance vary with the direction of the load (Fig. 1.25(b));

tridirectional: it is also possible to manufacture composites with

fibres in three directions, for example a composite with a carbon matrix and carbon fibres in three perpendicular directions (Fig. 1.25(c)).

By virtue of their construction, all these composites are strongly anisotropic as the stiffness and the strength of the fibres are 50–100 times higher than those of resins.

Fig. 1.25. Structures of composites: (a) unidirectional; (b) bidirectional; (c) tridirectional (after Vançon).



*Physical mechanisms of deformation**Viscoelastic deformations*

For most polymers, as long as the load remains below a certain value, deformations are elastic but involve dissipation which is globally expressed by viscosity. These deformations result from the relative movement of chain segments in which the bonds are not really destroyed but the rearrangement is thermally activated. The number of atoms free to jump per second is a function of the stress and the temperature; this gives a relation between the strain rate and the stress. This is the phenomenon of viscosity. The deformation, though reversible, stabilizes itself or disappears only after the lapse of a certain time. The limit of reversibility is of the order of a few per cent, but with a low density of bonds (as in elastomers) it can reach 50–100%.

Elastic limit

Above a characteristic load, irreversible reorientation of chain segments and crystallite wafers occurs resulting in strains which occur in addition to the elastic ones and which persist long after the removal of the load.

Permanent deformations

Permanent deformations originate both in the crystallites where dislocations are present and in amorphous regions by rotations of the bonds. Application of a high load initiates the destruction of the substructure by breaking the weakest link while new bonds can develop simply by the coming together of active elements.

Reorientations promote the creation of new crystallites which act as reinforcement. Under constant stress, consolidation or hardening occurs with asymptotic plastic equilibrium as a function of time.

As the density of the crystallites becomes stable, creep flow under constant stress can occur.

Finally, as for metals, plastic deformation is accompanied by anisotropy by virtue of directional consolidation.

All these mechanisms take place in the domain of very large strains (several tens to several thousands per cent).

Physical mechanisms of fracture

In a very schematic way, we may say that fracture initiation in polymers is marked by the disappearance of molecular bonds under the combined effect of external load and thermal activation. As in the case of deformations, this phenomenon is sensitive to strain rate.

The initiation zones are mainly those zones with defects, impurities or crystalline flaws in crystallites. Fracture development can take the form of a brittle fracture for polymers in the transition or rubbery state.

1.2.2 *Granular material: concrete**Constitution of hydraulic concrete*

Concrete used in construction is composed of aggregates, cement and water. For the occasional handyman, good concrete is made with (by volume) one part cement, two parts dry sand, four parts gravel, and a 'large' amount of water.

Aggregate

Natural aggregates are obtained from rolled alluvial materials or from crushed rocks of very different natures (silicon limestone, granite, ...). An aggregate is characterized by its granular curve which gives, as a function of the mean grain size, the percentage of grains with sizes smaller than a given value.

To make mortar, only sand with a grain diameter less than 5 mm is used. For concrete, fine gravel is also used with a grain diameter up to 25 mm. In very special cases, for example in construction of dams, rocks (up to 100 mm) and rubble (160 mm and more) can be used.

The maximum size d of the aggregate to be used depends on the characteristic size of the work-piece. If h is the smaller dimension of the concrete structure under consideration and e is the distance between the reinforcing bars to be provided, then

$$d \leq \frac{1}{4}h \quad \text{or} \quad d \leq \frac{3}{4}e.$$

Cement

Portland cement essentially consists of tricalcium silicate ($\approx 60\%$), bicalcium silicate ($\approx 20\%$), gypsum ($\approx 3\%$), tricalcium aluminate ($\approx 10\%$) and tetracalcium aluminoferrite ($\approx 7\%$) ground into a powder with a grain

size of the order of 10–50 μm . The process of hydration renders these constituents into a truly artificial stone.

Hydration of the cement powder

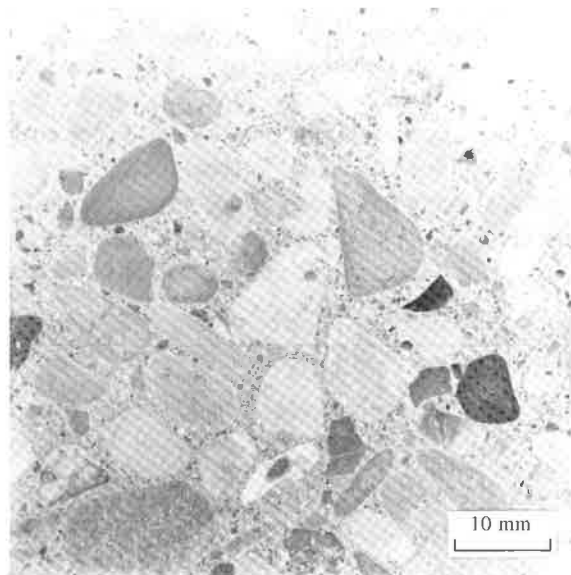
A mixture (by weight) of 66% cement and 33% water yields a paste that hardens with time. At the start of the setting, dry compounds are dissolved to the point of saturation and these then react in solution to give hydrates that precipitate coatings around the dry grains. The crystals which are formed in this process are hydrates of calcium silicate, hydroxide of lime, and various aluminates. The paste remains fluid for a few hours and then hardens with the growth of tobermorite crystals and postlandite originating from silicates. Hydration gives rise to the following phenomena:

an increase in the specific surface of the grains by a factor which might be as high as 100;

shrinkage or contraction of the order of 0.3 mm per metre;

hardening with time: the crushing strength in compression normalized to 1 on the seventh day, is 0.35 on the second day, 1.5 on the 28th day, 1.8 at the end of a year, and 2.2 at the end of a decade.

Fig. 1.26. An example of the structure of concrete (after Mazars, Lab. Audio-visuel ENS de Cachan).



Finally the structure of hardened concrete consists of the following (Fig. 1.26):

aggregates of different sizes,

cement paste binding the aggregates,

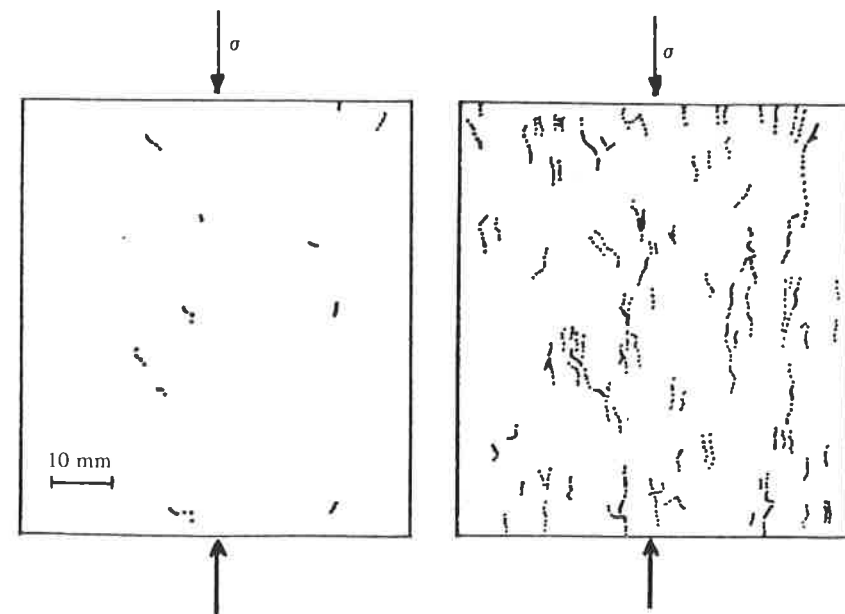
flaws consisting of microcracks in the paste–grain bond caused by shrinkage and voids caused by air bubbles entrapped during casting.

Physical mechanisms of deformation and fracture

It is difficult to separate the phenomena of deformation and fracture, because the microcracks and the initial voids, present before any load is applied, grow through the mechanism of brittle fracture and generate permanent deformations (Fig. 1.27).

The phenomenon of permanent deformation, however, is not significant when the load is below a certain value. Deformation in this first stage is the result of almost reversible movements of atoms and can be considered elastic with a low viscosity.

Fig. 1.27. X-ray observations of the evolution of microcracks in concrete under compression (after Robinson).



Brittle fracture which arises from a decohesion of the paste-grain is the essential phenomenon of permanent deformation and fracture and is strongly influenced by the nature of the load. The elastic limit or the fracture strength is of the order of 12 times higher in compression than in tension, which explains why concrete is used essentially in compression.

Beyond the load which corresponds to the elastic limit, microcracks in the bonds between the paste and the bigger grains begin to spread toward the periphery of the grains thus generating, at the macroscopic level, permanent deformations in conjunction with the elastic ones. For even higher loads loss of cohesion means that the microcracks reach the paste and in the case of compression loadings, assume a direction parallel to the stress. Slips appear in the crystals of the grains and thus contribute to the permanent deformation which occurs at constant volume. The microcrack damage becomes strongly anisotropic. The final stage is the fracture stage: macroscopic cracks appear, the stress necessary to produce further deformation decreases, the specific volume increases, and the final fracture occurs when microcracks join to form a surface discontinuity through the whole object.

We will see in Chapter 7 that the theory of damage coupled with that of

Fig. 1.28. Cross-section of the trunk of an Oak tree (after Lab. Audio-visuel ENS de Cachan).



elasticity is sufficient to model the nonlinear deformation behaviour of concrete.

1.2.3 Wood

Anatomical structure of wood

Within a broad classification, there are two kinds of wood; resinous and foliaceous, which have different structures, but nevertheless possess common characteristics due to the mode of growth of trees.

Heterogeneity and anisotropy

The growth in diameter of trees results from the proliferation of cells in the cambium which is located under the bark of the tree, with growth activity depending on the season. In spring, the cellular tubes have a large diameter and consist of soft tissue (spring wood); at the end of summer, when the growth activity stops, the tissue becomes lighter and more fibrous (summer wood). These alternate formations result in the concentric annular rings characteristic of the macroscopic appearance of the cross-sections of trees (Fig. 1.28).

To this pseudo-periodic radial inhomogeneity is added another kind which results from the ageing of the central part (or the heartwood) with tissue in this area becoming thicker than in the periphery (the sapwood). The anisotropy of formation is therefore essentially axisymmetric, although with many imperfections which result from knots at the root of the branches, differences of exposure, internal longitudinal compressive stresses and forces and local biological accidents.

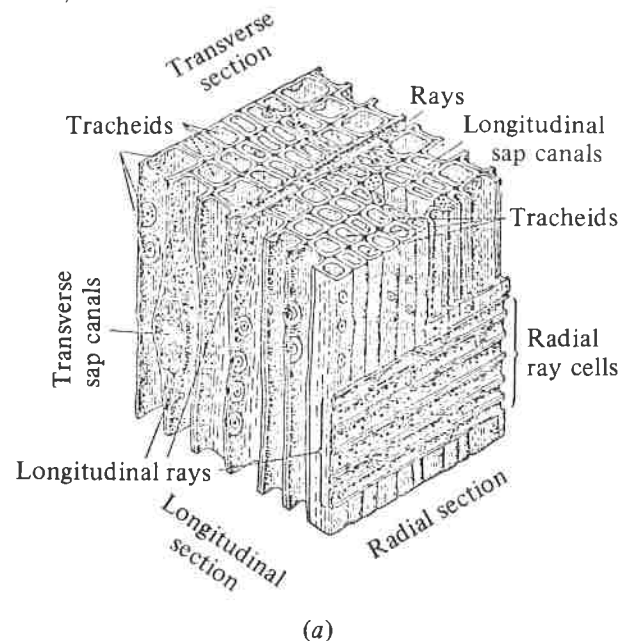
Fibres and cells

The macroscopic fibres consist of cells a few hundredths of a millimetre wide and a few millimetres long arranged parallel to the axis of the trunk. The strength of the wood increases as the cross-section of the cells decreases.

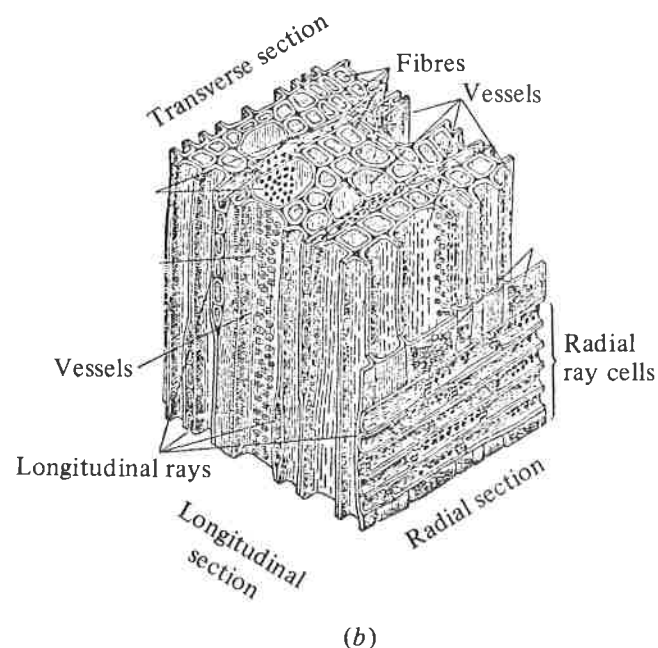
In resinous wood, the branches and the conduction tissue through which the sap circulates consist of only one type of cells. In addition, there are resinogen canals which produce the resin and the 'rays' of the wood, which consist of more dense cells arranged in the form of radial laminae (Fig. 1.29(a)).

Folliaceous woods have a more complex structure with three or

Fig. 1.29. Structure of wood: (a) resinous: epicea; (b) foliaceous: poplar (after M. T. Gautherin).



(a)



(b)

four types of cells with different functions: mechanical support, conduction, and storage (Fig. 1.29(b)).

Humidity

Wood cells consist mainly of cellulose (40–50% by weight) and lignin (25–30%). To these two polymers it is necessary to add water which can reach a moisture percentage of 100% of the dry weight. Water exists in chemical combination with lignin, or impregnated in cell membranes, or even in the free form in the cavities of the tissues. Moisture plays a large part in determining the mechanical properties, and therefore, drying of wood is very important. At moisture contents which are below the saturation of the fibres, the elastic characteristics and the resistance to fracture increase as the moisture content decreases.

Physical mechanisms of deformation and fracture

Elastic deformations are caused by reversible deformations of the cells, which are highly dependent upon the moisture content. They can reach 0.1–0.5%, without noticeable permanent deformation, depending upon the type of wood and the direction of the load with regard to the axis of the tree. The viscosity effect is weak.

As with concrete, it is difficult to separate the mechanisms of permanent deformation and fracture, both because macroscopic permanent deformations result from microfractures and because macroscopic fracture occurs, before noticeable deformations are produced. In any case, the principal mechanism of plastic deformation in wood consists of the slip of cells over one another, while fracture is caused by the breaking of cellulose chains, the breaking of a bond by a very high stress in the direction of fibres, and cleavage fracture at much lower stresses perpendicular to the fibres.

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2

*ELEMENTS OF CONTINUUM MECHANICS
AND THERMODYNAMICS*

A chaque phénomène sa variable

A chaque variable sa loi d'évolution

To model the physical phenomena of deformation and fracture, described briefly in Chapter 1, a method based upon general principles which govern the variables representative of the state of the material medium is needed. The objective of this chapter is to present in a condensed form all the basic concepts that will be used in the following chapters. Two types of modelling are necessary: one, the so-called kinematical or mechanical modelling is concerned with the motions and forces in the continuum, and the second, the so-called phenomenological or physical modelling introduces the variables characterizing the phenomena under study.

The presentation given here is the result of the work of Germain as presented in a post graduate course and subsequently incorporated by one of the authors (Lemaitre) in his course, and also contained in *Cours de mécanique des milieux continus* cited in the bibliography of this chapter. This reference contains the details necessary for a deeper understanding of the concepts. Here, only the essential results are given, and the mathematical derivations have been largely omitted. The notation used is almost identical to that in the work referred to above which should help the reader who is anxious to go deeper into the subject.

The framework of mechanics presented here is based on the principle of virtual power. Although the basic idea was presented by D'Alembert as long ago as 1750, it is only, with the development of the variational methods of functional analysis in around 1970 (Duvaut, Lions, Nayroles), that systematic use of this principle has been made. The choice of a particular virtual movement for a given medium leads naturally to consistent definitions of stresses and strains, and to equations of equilibrium with corresponding boundary conditions.