Chapter 1
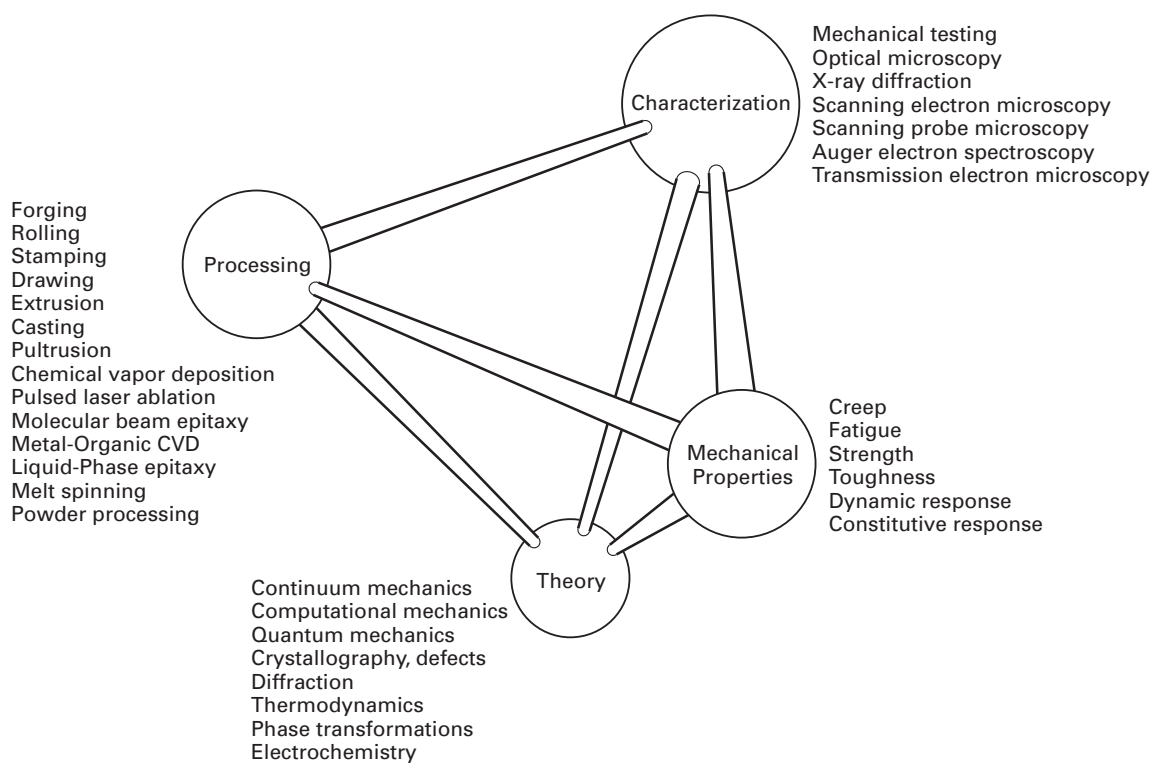
Materials: Structure, Properties, and Performance

1.1 | Introduction

Everything that surrounds us is matter. The origin of the word matter is *mater* (Latin) or *matri* (Sanskrit), for *mother*. In this sense, human beings anthropomorphized that which made them possible – that which gave them nourishment. Every scientific discipline concerns itself with matter. Of all matter surrounding us, a portion comprises materials. What are materials? They have been variously defined. One acceptable definition is "matter that human beings use and/or process." Another definition is "all matter used to produce manufactured or consumer goods." In this sense, a rock is not a material, intrinsically; however, if it is used in aggregate (concrete) by humans, it becomes a material. The same applies to all matter found on earth: a tree becomes a material when it is processed and used by people, and a skin becomes a material once it is removed from its host and shaped into an artifact.

The successful utilization of materials requires that they satisfy a set of properties. These properties can be classified into thermal, optical, mechanical, physical, chemical, and nuclear, and they are intimately connected to the structure of materials. The structure, in its turn, is the result of synthesis and processing. A schematic framework that explains the complex relationships in the field of the mechanical behavior of materials, shown in Figure 1.1, is Thomas's iterative tetrahedron, which contains four principal elements: mechanical properties, characterization, theory, and processing. These elements are related, and changes in one are inseparably linked to changes in the others. For example, changes may be introduced by the synthesis and processing of, for instance, steel. The most common metal, steel has a wide range of strengths and ductilities (*mechanical properties*), which makes it the material of choice for numerous applications. While low-carbon steel is used as reinforcing bars in concrete and in the body of automobiles, quenched and tempered high-carbon steel is used in more critical applications such as axles and gears. Cast iron, much more brittle, is used in a variety of applications, including automobile

Characterization

Mechanical testing
Optical microscopy
X-ray diffraction
Scanning electron microscopy
Scanning probe microscopy
Auger electron spectroscopy
Transmission electron microscopy

Forging
Rolling
Stamping
Drawing
Extrusion
Casting
Pultrusion
Chemical vapor deposition
Pulsed laser ablation
Molecular beam epitaxy
Metal-Organic CVD
Liquid-Phase epitaxy
Melt spinning
Powder processing

Processing

Mechanical
Properties

Creep
Fatigue
Strength
Toughness
Dynamic response
Constitutive response

Theory

Continuum mechanics
Computational mechanics
Quantum mechanics
Crystallography, defects
Diffraction
Thermodynamics
Phase transformations
Electrochemistry

Fig. 1.1 Iterative materials tetrahedron applied to mechanical behavior of materials. (After G. Thomas.)

engine blocks. These different applications require, obviously, different mechanical properties of the material. The different properties of the three materials, resulting in differences in performance, are attributed to differences in the internal structure of the materials. The understanding of the structure comes from *theory*. The determination of the many aspects of the micro-, meso-, and macrostructure of materials is obtained by *characterization*. Low-carbon steel has a primarily ferritic structure (body-centered cubic; see Section 1.3.1), with some interspersed pearlite (a ferrite–cementite mixture). The high hardness of the quenched and tempered high-carbon steel is due to its martensitic structure (body-centered tetragonal). The relatively brittle cast iron has a structure resulting directly from solidification, without subsequent mechanical working such as hot rolling. How does one obtain low-carbon steel, quenched and tempered high-carbon steel, and cast iron? By different *synthesis* and *processing* routes. The low-carbon steel is processed from the melt by a sequence of mechanical working operations. The high-carbon steel is synthesized with a greater concentration of carbon (>0.5%) than the low-carbon steel (0.1%). Additionally, after mechanical processing, the high-carbon steel is rapidly cooled from a temperature of approximately 1,000 °C by throwing it into water or oil; it is then reheated to an intermediate temperature (tempering). The cast iron is synthesized with even higher carbon contents (∼2%). It is poured directly into the molds and allowed to solidify in them. Thus, no mechanical working, except for some minor machining, is needed. These interrelationships among

structure, properties, and performance, and their modification by synthesis and processing, constitute the central theme of materials science and engineering. The tetrahedron of Figure 1.1 lists the principal processing methods, the most important theoretical approaches, and the most-used characterization techniques in materials science today.

The selection, processing, and utilization of materials have been part of human culture since its beginnings. Anthropologists refer to humans as "the toolmakers," and this is indeed a very realistic description of a key aspect of human beings responsible for their ascent and domination over other animals. It is the ability of humans to manufacture and use tools, and the ability to produce manufactured goods, that has allowed technological, cultural, and artistic progress and that has led to civilization and its development. Materials were as important to a Neolithic tribe in the year 10,000 BC as they are to us today. The only difference is that today more complex synthetic materials are available in our society, while Neolithic tribes had only natural materials at their disposal: wood, minerals, bones, hides, and fibers from plants and animals. Although these naturally occurring materials are still used today, they are vastly inferior in properties to synthetic materials.
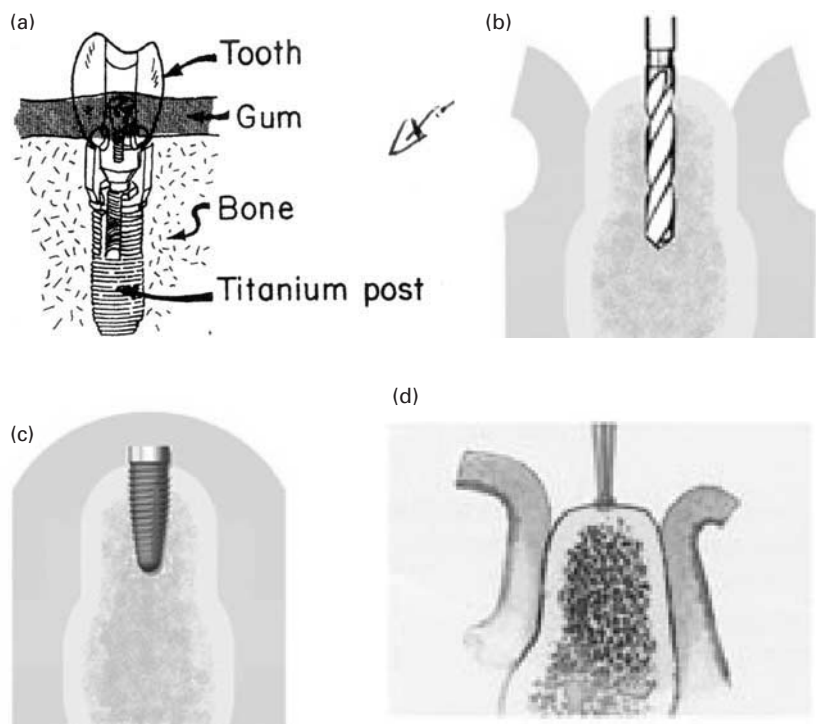
1.2 | Monolithic, Composite, and Hierarchical Materials

The early materials used by humans were natural, and their structure varied widely. Rocks are crystalline, pottery is a mixture of glassy and crystalline components, wood is a fibrous organic material with a cellular structure, and leather is a complex organic material. Human beings started to synthesize their own materials in the Neolithic period: ceramics first, then metals, and later, polymers. In the twentieth century, simple monolithic structures were used first. The term *monolithic* comes from the Greek *mono* (one) and *lithos* (stone). It means that the material has essentially uniform properties throughout. Microstructurally, monolithic materials can have two or more phases. Nevertheless, they have properties (electrical, mechanical, optical, and chemical) that are constant throughout. Table 1.1 presents some of the important properties of metals, ceramics, and polymers. Their detailed structures will be described in Section 1.3. The differences in their structure are responsible for differences in properties. Metals have densities ranging from 3 to 19 g/cm^{-3}; iron, nickel, chromium, and niobium have densities ranging from to 7 to 9 g/cm^{-3}; aluminum has a density of 2.7 g/cm^{-3}; and titanium has a density of 4.5 g/cm^{-3}. Ceramics tend to have lower densities, ranging from 5 g/cm^{-3} (titanium carbide; TiC = 4.9) to 3 g/cm^{-3} (alumina; Al$_2$O$_3$ = 3.95; silicon carbide; SiC = 3.2). Polymers have the lowest densities, fluctuating around 1 g cm^{-3}. Another marked difference among these

Table 1.1 Summary of Properties of Main Classes of Materials

Property	Metals	Ceramics	Polymers
Density (g/cm^3)	from 2 to 20	from 1 to 14	from 1 to 2.5
Electrical conductivity	high	low	low
Thermal conductivity	high	low	low
Ductility or strain-to-fracture (%)	4–40	<1	2–4
Tensile strength (MPa)	100–1,500	100–400	–
Compressive strength (MPa)	100–1,500	1,000–5,000	–
Fracture toughness (MNm$^{-3/2}$)	10–30	1–10	2–8
Maximum service temperature (°C)	1,000	1,800	250
Corrosion resistance	low to medium	superior	medium
Bonding	metallic (free-electron cloud)	ionic or covalent	covalent
Structure	mostly crystalline (Face-centered cubic; FCC Body-centered cubic; BCC Hexagonal closed packed; HCP)	complex crystalline structure	amorphous or semicrystalline polymer

three classes of materials is their ductility (ability to undergo plastic deformation). At room temperature, metals can undergo significant plastic deformation. Thus, metals tend to be ductile, although there are a number of exceptions. Ceramics, on the other hand, are very brittle, and the most ductile ceramics will be more brittle than most metals. Polymers have a behavior ranging from brittle (at temperatures below their glass transition temperature) to very deformable (in a nonlinear elastic material, such as rubber). The fracture toughness is a good measure of the resistance of a material to failure and is generally quite high for metals and low for ceramics and polymers. Ceramics far outperform metals and polymers in high-temperature applications, since many ceramics do not oxidize even at very high temperatures (the oxide ceramics are already oxidized) and retain their strength to such temperatures. One can compare the mechanical, thermal, optical, electrical, and electronic properties of the different classes of materials and see that there is a very wide range of properties. Thus, monolithic structures built from primarily one class of material cannot provide all desired properties.

In the field of biomaterials (materials used in implants and life-support systems), developments also have had far-reaching effects. The mechanical performance of implants is critical in many applications, including hipbone implants, which are subjected to high stresses, and endosseous implants in the jaw designed to serve as the base for

Fig. 1.2 (a) Complete enclosures implant, (b) A hole is drilled and (c) a titanium post is screwed into jawbone. (d) Marking of site with small drill. (Courtesy of J. Mahooti.)

teeth. Figure 1.2 (a) shows the most successful design for endosseous implants in the jawbone. With this design, the tooth is fixed to the post and is effective. A titanium post is first screwed into the jaw-bone and allowed to heal. The tooth is then fixed to the post, and is effectively rooted into the jaw. The insertion of endosseous implants into the mandibles or maxillae, which was initiated in the 1980s, has been a revolution in dentistry. There is a little story associated with this discovery. Researchers were investigating the bone marrow of rab-bits. They routinely used stainless steel hollow cylinders screwed into the bone. Through the hole, they could observe the bone marrow. It so happened that one of these cylinders was made of titanium. Since these cylinders were expensive, the researchers removed them periodically, in order to reuse them. When they tried to remove the titanium cylinder, it was tightly fused to the bone. This triggered the creative intuition of one of the researchers, who said "What if . . .?"

Figure 1.2(c) shows the procedure used to insert the titanium implant. The site is first marked with a small drill that penetrates the cortical bone. Then successive drills are used to create the orifice of desired diameter (Figure 1.2(d)). The implant is screwed into the bone and the tissue is closed (Figure 1.2(c)). This implant is allowed to heal and fuse with the bone for approximately six months. Chances are that most readers will have these devices installed sometime in their lives.

Hip- and knee-replacement surgery is becoming commonplace. In the USA alone between 250,000 and 300,000 of each procedure are carried out annually. The materials of the prostheses have an

Fig. 1.3 (a) Total hip replacement prosthesis; (b) total knee replacement prosthesis.
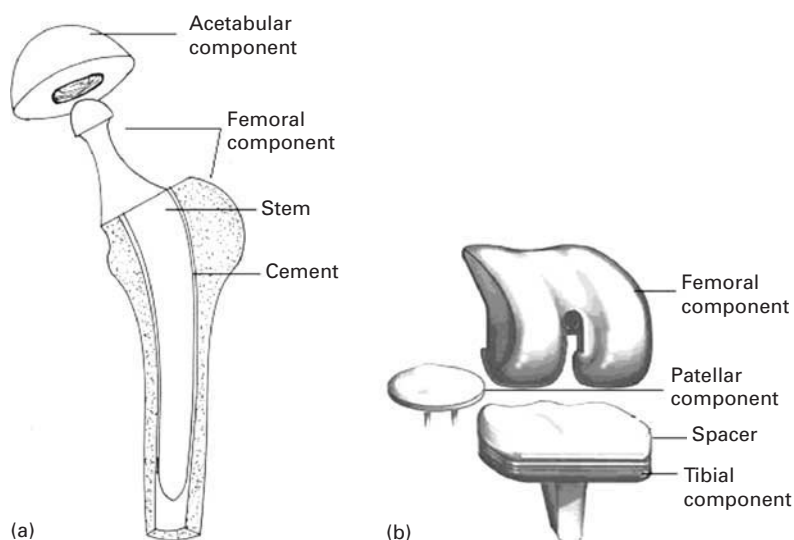
important bearing on survival probability. Typical hip and knee prostheses are shown in Figure 1.3.

The hip prosthesis is made up of two parts: the acetabular component, or socket portion, which replaces the acetabulum; the femoral component, or stem portion, which replaces the femoral head.

The femoral component is made of a metal stem with a metal ball on the extremity. In some prostheses a ceramic ball is attached to the metal stem. The acetabular component is a metal shell with a plastic inner socket liner made of metal, ceramic, or a plastic called ultra-high-molecular-weight polyethylene (UHMWP) that acts like a bearing. A *cemented* prosthesis is held in place by a type of epoxy cement that attaches the metal to the bone. An *uncemented* prosthesis has a fine mesh of holes on the surface area that touches the bone. The mesh allows the bone to grow into the mesh and become part of the bone. Biomaterial advances have allowed experimentation with new bearing surfaces, and there are now several different options when hip-replacement surgery is considered.

The metal has to be inert in the body environment. The preferred materials for the prostheses are Co–Cr alloys (Vitalium) and titanium alloys. However, there are problems that have not yet been resolved: the metallic components have elastic moduli that far surpass those of bone. Therefore, they "carry" a disproportionate fraction of the load, and the bone is therefore unloaded. Since the health and growth of bone is closely connected to the loads applied to it, this unloading tends to lead to bone loss.
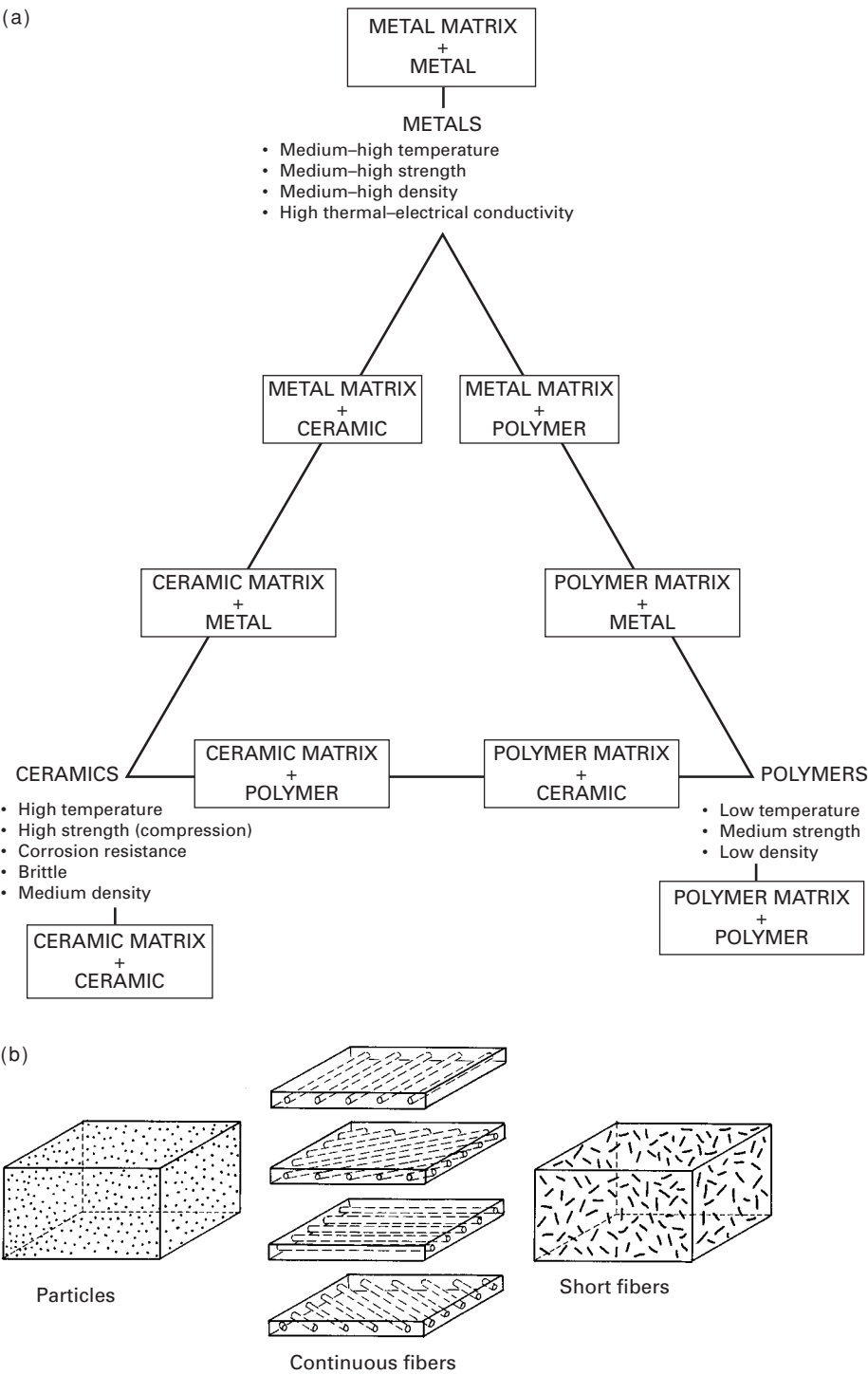
The most common cause of joint replacement failure is wear of the implant surfaces. This is especially critical for the polymeric components of the prosthesis. This wear produces debris which leads to tissue irritation. Another important cause of failure is loosening of the implant due to weakening of the surrounding bone. A third source of failure is fatigue.

Biocompatibility is a major concern for all implants, and ceramics are especially attractive because of their (relative) chemical inertness. Metallic alloys such as Vitalium® (a cobalt-based alloy) and titanium alloys also have proved to be successful, as have polymers such as polyethylene. A titanium alloy with a solid core surrounded by a porous periphery (produced by sintering of powders) has shown considerable potential. The porous periphery allows bone to grow and affords very effective fixation. Two new classes of materials that appear to present the best biocompatibility with bones are the Bioglass® and calcium phosphate ceramics. Bones contain calcium and phosphorus, and Bioglass® is a glass in which the silicon has been replaced by those two elements. Thus, the bone "perceives" these materials as being another bone and actually bonds with it. Biomechanical properties are of great importance in bone implants, as are the elastic properties of materials. If the stiffness of a material is too high, then when implanted the material will carry more of the load placed on it than the adjacent bone. This could in turn lead to a weakening of the bone, since bone growth and strength depends on the stresses that the bone is subjected to. Thus, the elastic properties of bone and implant should be similar. Polymers reinforced with strong carbon fibers are also candidates for such applications. Metals, on the other hand, are stiffer than bones and tend to carry most of the load. With metals, the bones would be shielded from stress, which could lead to bone resorption and loosening of the implant.

Although new materials are being developed continuously, monolithic materials, with their uniform properties, cannot deliver the range of performance needed in many critical applications. *Composites* are a mixture of two classes of materials (metal–ceramic, metal–polymer, or polymer–ceramic). They have unique mechanical properties that are dependent on the amount and manner in which their constituents are arranged. Figure 1.4(a) shows schematically how different composites can be formed. Composites consist of a matrix and a reinforcing material. In making them, the modern materials engineer has at his or her disposal a very wide range of possibilities. However, the technological problems involved in producing some of them are immense, although there is a great deal of research addressing those problems. Figure 1.4(b) shows three principal kinds of reinforcement in composites: particles, continuous fibers, and discontinuous (short) fibers. The reinforcement usually has a higher strength than the matrix, which provides the ductility of the material. In ceramic-based composites, however, the matrix is brittle, and the fibers provide barriers to the propagating cracks, increasing the toughness of the material.

The alignment of the fibers is critical in determining the strength of a composite. The strength is highest along a direction parallel to the fibers and lowest along directions perpendicular to it. For the three kinds of composite shown in Figure 1.4(b), the polymer matrix plus (aramid, carbon, or glass) fiber is the most common combination if no high-temperature capability is needed.

(a)

METAL MATRIX
+
METAL

METALS
• Medium–high temperature
• Medium–high strength
• Medium–high density
• High thermal–electrical conductivity

METAL MATRIX
+
CERAMIC

METAL MATRIX
+
POLYMER

CERAMIC MATRIX
+
METAL

POLYMER MATRIX
+
METAL

CERAMICS
• High temperature
• High strength (compression)
• Corrosion resistance
• Brittle
• Medium density

CERAMIC MATRIX
+
POLYMER

POLYMER MATRIX
+
CERAMIC

POLYMERS
• Low temperature
• Medium strength
• Low density

POLYMER MATRIX
+
POLYMER

CERAMIC MATRIX
+
CERAMIC

(b)

Particles

Continuous fibers

Short fibers

Fig. 1.4 (a) Schematic representations of different classes of composites. (b) Different kinds of reinforcement in composite materials. Composite with continuous fibers with four different orientations (shown separately for clarity).

Table 1.2	Specific Modulus and Strength of Materials Used in Aircraft	
	Elastic Modulus	Tensile Strength
Material	Density ($GPa/g \cdot cm^{-3}$)	Density ($MPa/g \cdot cm^{-3}$)
Steel (AISI 4340)	25	230
Al (7075-T6)	25	180
Titanium (Ti-6Al-4V)	25	250
E Glass/Epoxy composite	21	490
S Glass/Epoxy composite	47	790
*Axamid/Epoxy composite	55	890
HS (High Tensile Strength) Carbon/Epoxy composite	92	780
HM (high modulus) Carbon/Epoxy composite	134	460

Composites are becoming a major material in the aircraft indus-
try. Carbon/epoxy and aramid/epoxy composites are being introduced
in a large number of aircraft parts. These composite parts reduce
the weight of the aircraft, increasing its economy and payload. The
major mechanical property advantages of advanced composites over
metals are better stiffness-to-density and strength-to-density ratios
and greater resistance to fatigue. The values given in Table 1.2 apply to
a unidirectional composite along the fiber reinforcement orientation.
The values along other directions are much lower, and therefore the
design of a composite has to incorporate the anisotropy of the mater-
ials. It is clear from the table that composites have advantages over
monolithic materials. In most applications, the fibers are arranged
along different orientations in different layers. For the central com-
posite of Figure 1.4(b), these orientations are 0°, 45°, 90°, and 135° to
the tensile axis.

Can we look beyond composites in order to obtain even higher
mechanical performance? Indeed, we can: Nature is infinitely
imaginative.

Our body is a complex arrangement of parts, designed, as a whole,
to perform all the tasks needed to keep us alive. Scientists are looking
into the make-up of soft tissue (skin, tendon, intestine, etc.), which
is a very complex structure with different units active at different
levels complementing each other. The structure of soft tissue has
been called a *hierarchical* structure, because there seems to be a rela-
tionship between the ways in which it operates at different levels.
Figure 1.5 shows the structure of a tendon. This structure begins
with the tropocollagen molecule, a triple helix of polymeric protein
chains. The tropocollagen molecule has a diameter of approximately

Fig. 1.5 A model of a hierarchical structure occurring in the human body. (Adapted from E. Baer, *Sci. Am.* 254, No. 10 (1986) 179.)
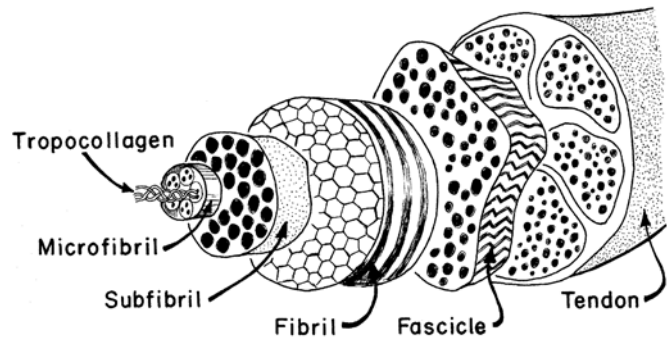
Fig. 1.6 Schematic illustration of a proposed hierarchical model for a composite (not drawn to scale). (Courtesy of E. Baer.)
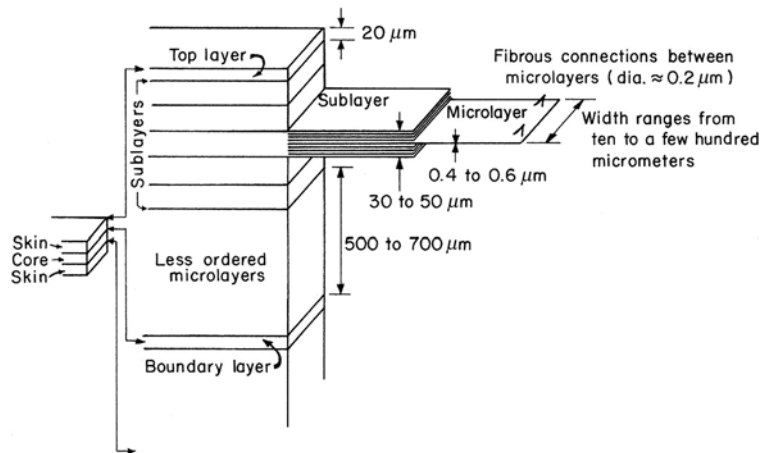
1.5 mm. The tropocollagen organizes itself into microfibrils, sub-fibrils, and fibrils. The fibrils, a critical component of the structure, are crimped when there is no stress on them. When stressed, they stretch out and then transfer their load to the fascicles, which compose the tendon. The fascicles have a diameter of approximately 150–300 μm and constitute the basic unit of the tendon. The hierarchical organization of the tendon is responsible for its toughness. Separate structural units can fail independently and thus absorb energy locally, without causing the failure of the entire tendon. Both experimental and analytical studies have been done, modeling the tendon as a composite of elastic, wavy fibers in a viscoelastic matrix. Local failures, absorbing energy, will prevent catastrophic failure of the entire tendon until enormous damage is produced.

Materials engineers are beginning to look beyond simple two-component composites, imitating nature in organizing different levels of materials in a hierarchical manner. Baer[1] suggests that the study of biological materials could lead to new hierarchical designs for composites. One such example is shown in Figure 1.6, a layered structure of liquid-crystalline polymers consisting of alternating core and skin layers. Each layer is composed of sublayers which, in their

[1] E. Baer, *Sci. Am.* 254, No. 10 (1986) 179.