By Lect. Adwaa M. Al Nasrawee

Lecture No.1

Introduction to Materials Science and Engineering

1.1 Introduction:

Materials science underlies most technological advances. Transportation, housing, clothing, communication, recreation, and food production– virtually every segment of our everyday lives is influenced to one degree or another by materials. Understanding the basics of materials and their applications will help us during the design process. In order to be a good designer, you must learn what materials will be appropriate to use in different applications.

1.2 Materials Science and Engineering:

Materials science involves investigating the relationships that exist between the structures and properties, processing, and performance of materials. In materials engineering, the focus is on how to translate or transform materials into a useful device or structure. Virtually all-important properties of solid materials may be grouped into six different categories: mechanical, electrical, thermal, magnetic, optical, and deteriorative. Mechanical properties relate deformation to an applied load or force; examples include elastic modulus (stiffness), strength, and toughness. For electrical properties, such as electrical conductivity and dielectric constant, the stimulus is an electric field. The thermal behavior of solids can be represented in terms of heat capacity and thermal conductivity. Magnetic properties demonstrate the response of a material to the application of a magnetic field. For optical properties, the stimulus is electromagnetic or light radiation; index of refraction and reflectivity are representative optical properties. Finally, deteriorative characteristics relate to the chemical reactivity of materials.

1.3 Atomic Structure and the Elements

The basic structural unit of matter is the atom. Each atom is composed of a positively charged nucleus, surrounded by a sufficient number of negatively charged electrons so that the charges are balanced. The number of electrons identifies the atomic number.

Many of the similarities and differences among the elements can be explained by their respective atomic structures. The simplest model of atomic structure, called the planetary model, shows the electrons of the atom orbiting around the nucleus at certain fixed distances, called shells, as shown in Figure 1.1.

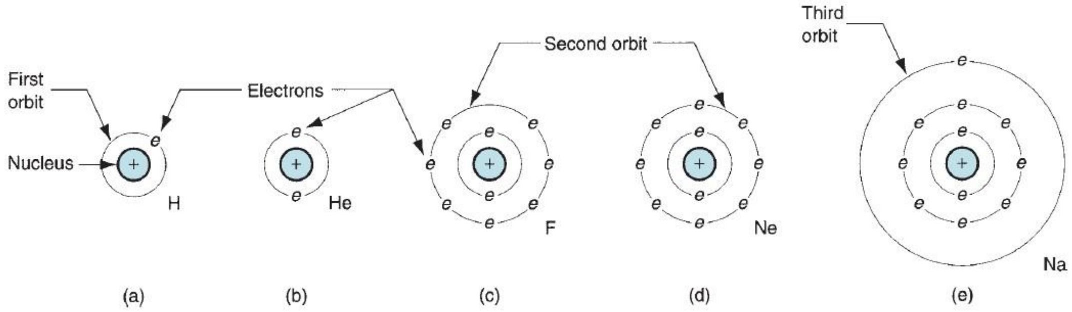


Fig. 1.1 Simple model of atomic structure for several elements: (a) hydrogen, (b) helium, (c) fluorine, (d) neon, and (e) sodium.

The hydrogen atom (atomic number 1) has one electron in the orbit closest to the nucleus. Helium (atomic number 2) has two. Also shown in the figure are the atomic structures for fluorine (atomic number 9), neon (atomic number 10), and sodium (atomic number 11). One might infer from these models that there is a maximum number of electrons that can be contained in a given orbit. This turns out to be correct, and the maximum is defined by:

$$\text{Maximum number of electrons in an orbit} = 2n^2$$

where n identifies the orbit, with n = 1 closest to the nucleus. The number of electrons in the outer most shell, relative to the maximum number allowed, determines to a large extent the atom's chemical affinity for other atoms. These outer-shell electrons are called valence electrons. For example, because a hydrogen atom has only one electron in its single orbit, it readily combines with another hydrogen atom to form a hydrogen molecule H_2. For the same reason, hydrogen also reacts readily with various other elements (e.g., to form H_2O). In the helium atom, the two electrons in its only orbit are the maximum allowed ($2n^2=2(1)^2=2$), and so helium is very stable. Neon is stable for the same reason: Its outermost orbit (n=2) have eight electrons (the maximum allowed), so neon is an inert gas.

Fluorine has one fewer electron in its outer shell (n = 2) than the maximum allowed and is readily attracted to other elements that might share an electron to make a more stable set. The sodium atom seems divinely made for the situation, with one electron in its outermost orbit. It reacts strongly with fluorine to form the compound sodium fluoride, as pictured in Figure 1.2.

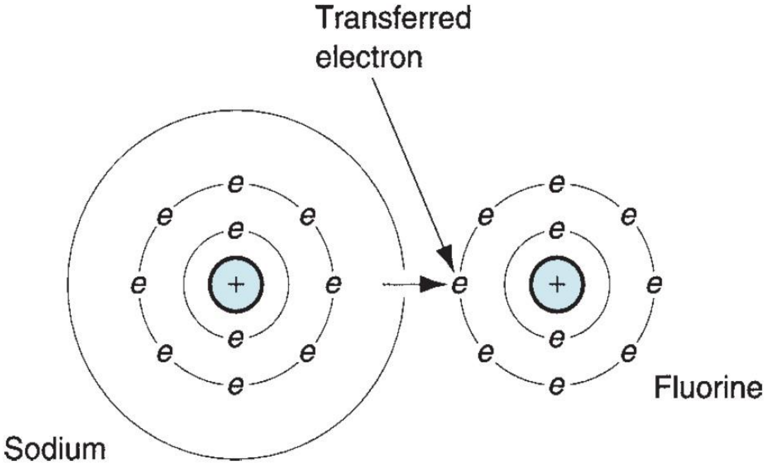


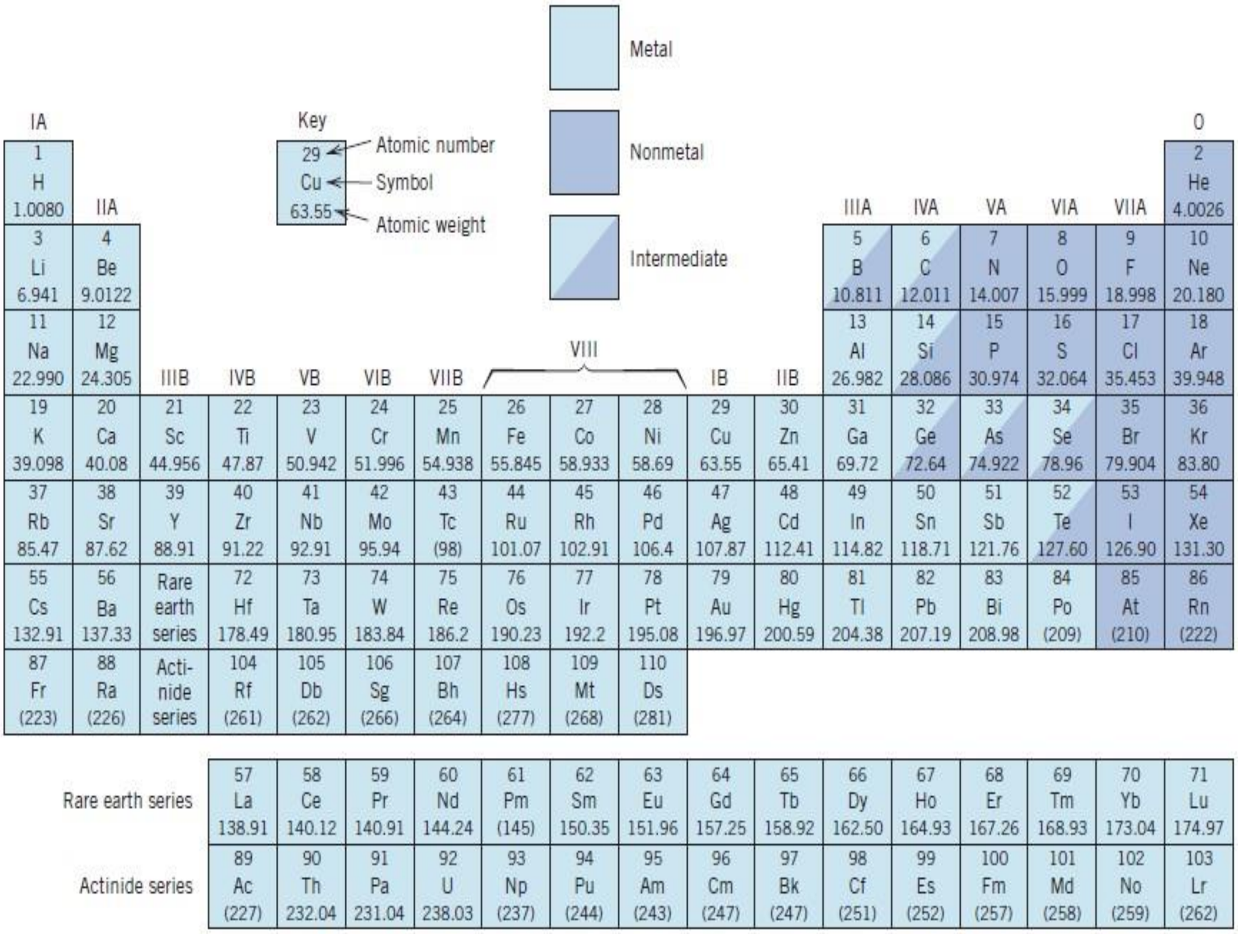
Figure 1.2: The sodium fluoride molecule, formed by the transfer of the ‘‘extra’’ electron of the sodium atom to complete the outer orbit of the fluorine atom.

1.4The Periodic Table

All the elements have been classified according to electron configuration in the **periodic table** (Figure 1.3). The periodic table contains a wealth of useful information (e.g., atomic mass, atomic number of different elements, etc.). The elements are situated, with increasing atomic number, in seven horizontal rows called periods. The arrangement is such that all elements arrayed in a given column or group have similar valence electron structures, as well as chemical and physical properties. These properties change gradually, moving horizontally across each period and vertically down each column.

Metallic elements occupy the left and center portions of the chart, and nonmetals are located to the right. At room temperature and atmospheric pressure, they each have a natural phase; e.g., iron (Fe) is a solid, mercury (Hg) is a liquid, and nitrogen (N) is a gas.

In the table, the elements are arranged into vertical columns and horizontal rows in such a way that similarities exist among elements in the same columns. For example, in the extreme right column are the noble gases (helium, neon, argon, krypton, xenon, and radon), all of which exhibit great chemical stability and low reaction rates. The halogens (fluorine, chlorine, bromine, iodine, and astatine) in column VIIA share similar properties (hydrogen is not included among the halogens). The noble metals (copper, silver, and gold) in column IB have similar properties. Generally, there are correlations in properties among elements within a given column, whereas differences exist among elements in different columns.



IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080																	2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.87	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.33	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.2	76 Os 190.23	77 Ir 192.2	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.19	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti- nide series	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)								

Rare earth series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
Actinide series	89 Ac (227)	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

Figure 1.3: The periodic table of the elements.

1.5 Iron ores:

Iron was discovered sometime during the Bronze Age. It was probably uncovered from ashes of fires built near iron ore deposits. In the nineteenth century, industries such as railroads, shipbuilding, construction, machinery, and the military created a dramatic growth in the demand for iron and steel in Europe and America. Although large quantities of pig iron could be produced by blast furnaces, the subsequent processes for producing wrought iron and steel were slow.

Iron ores are rocks and minerals from which metallic iron can be economically extracted , also, it is the raw materials used to make pig iron, which is one of the main raw materials to make steel. About 98% of the mined iron ore is used to make steel

Iron ore is a combination of iron with oxygen and various other unwanted substances, generally known as "gangue. The compounds of iron best suited to smelting in a blast furnace are the oxides, although carbonates and silicates are sometimes used. There are various types of iron ore, classified chiefly according to iron (Fe) content (see Table 1 below). It is evident, then, that from the point of richness, oxides are far superior to carbonates and silicates. Table 1: Iron Ore Classification

Name	Classification	Theoretical Max. Iron Content(%)
Hematite	Fe_2O_3	70
Magnetite	Fe_3O_4	72.4
Goethite	FeO.OH	62.8
Siderite	$FeCO_3$	48.3

The impurities in iron ore fines include SiO_2, Al_2O_3, S, P, MgO and CaO, As well as varying amounts of components responsible for loss ignition

1.6 Engineering materials:

Most engineering materials can be classified into one of three basic categories :(1) metals, (2) ceramics, and (3) polymers. Their chemistries are different, their mechanical and physical properties are different, and these differences affect the manufacturing processes that can be used to produce products from them. In addition to the three basic categories, there are (4) composites-nonhomogeneous mixtures of the other three basic types rather than a unique category. The classification of the four groups is pictured in Figure 1.4.

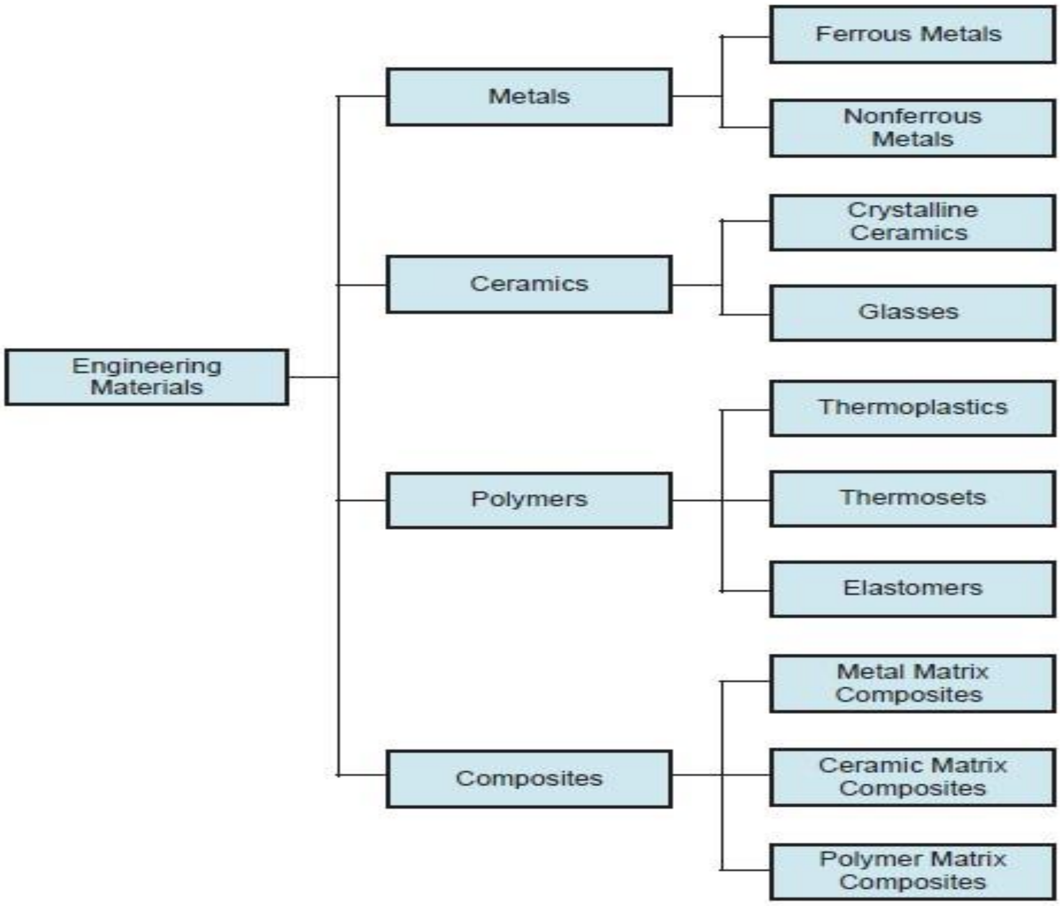


Figure 1.4: Classification of the four engineering materials

By Lect. Adwaa M. Al Nasrawee

Lecture No.2

Crystalline Structure

2.1 introduction

Atoms and molecules are used as building blocks for the more macroscopic structure of matter that is considered here and in the following section. When materials solidify from the molten state, they tend to close ranks and pack tightly, in many cases arranging themselves into a very orderly structure, and in other cases, not quite so orderly. Two fundamentally different material structures can be distinguished:(1) crystalline and (2) non-crystalline. Crystalline structures are examined in this section. Many materials forms into crystals on solidification from the molten or liquid state.

2.1 Fundamental Concepts of Crystalline Structures

A **crystalline structure** is one in which the atoms are located at regular and recurring positions in three dimensions. The pattern may be replicated millions of times within a given crystal. The structure can be viewed in the form of a unit cell, which is the basic geometric grouping of atoms that is repeated.

Lattice means a three-dimensional array of points coinciding with atom positions (or sphere centers). A group of one or more atoms, located in a particular way with respect to each other and associated with each lattice point, is known as the **basis**. We obtain a crystal structure by adding the lattice and basis (i.e., crystal structure = lattice + basis).

The **unit cell** is the subdivision of a lattice that still retains the overall characteristics of the entire lattice. Unit cells are shown in Figure 3.1*a*. Thus, the unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within. The most common types of unit cells are:

By Lect. Adwaa M. Al Nasrawee

- The Faced Centered Cubic (FCC),
- The Body-Centered Cubic (BCC) And
- The Hexagonal Close-Packed (HCP).

In the studying of the crystalline structures, we interest with four parameters:

1. a/R relationship.
2. No. of atoms per unit cell.
3. Coordination number (CN): the number of nearest- neighbor or touching atoms that surround specific atom.
4. Atomic packing factor (APF): it is also called packing efficiency, and represents the fraction of atoms volume in a unit cell.

Table 3.1 presents the crystal structures for the common metals. Three relatively simple crystal structures are found for most of the common metals: face centered cubic, body-centered cubic, and hexagonal close-packed.

Table 2.1 Crystal structures for the common metals (at room temperature).

Body-Centered Cubic (BCC)	Face-Centered Cubic (FCC)	Hexagonal Close-Packed (HCP)
Chromium (Cr) Iron (Fe) Molybdenum (Mo) Tantalum (Ta) Tungsten (W)	Aluminum (Al) Copper (Cu) Gold (Au) Lead (Pb) Silver (Ag) Nickel (Ni)	Magnesium (Mg) Titanium (Ti) Zinc (Zn)

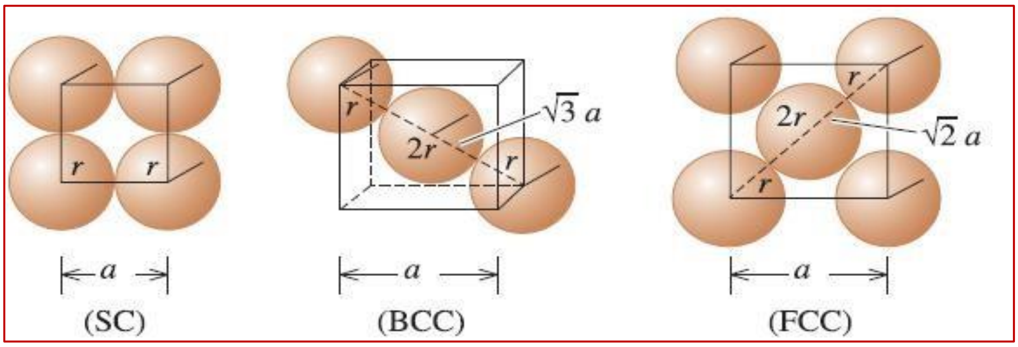


Figure 2.1 The relationships between the atomic radius and the lattice parameter in cubic systems.

2.2.1 The Face-Centered Cubic Crystal Structure

The crystal structure found for many metals has a unit cell of cubic geometry, with atoms located at each of the corners and the centers of all the cube faces. It is aptly called the **face-centered cubic (FCC)** crystal structure. Some of the familiar metals having this crystal structure are **copper, aluminum, silver, and gold** (see also Table 2.2).

Figure 3.1*a* shows a hard sphere model for the FCC unit cell, whereas in Figure 3.1*b* the atom centers are represented by small circles to provide a better perspective of atom positions. The aggregate of atoms in Figure 3.1*c* represents a section of crystal consisting of many FCC unit cells.

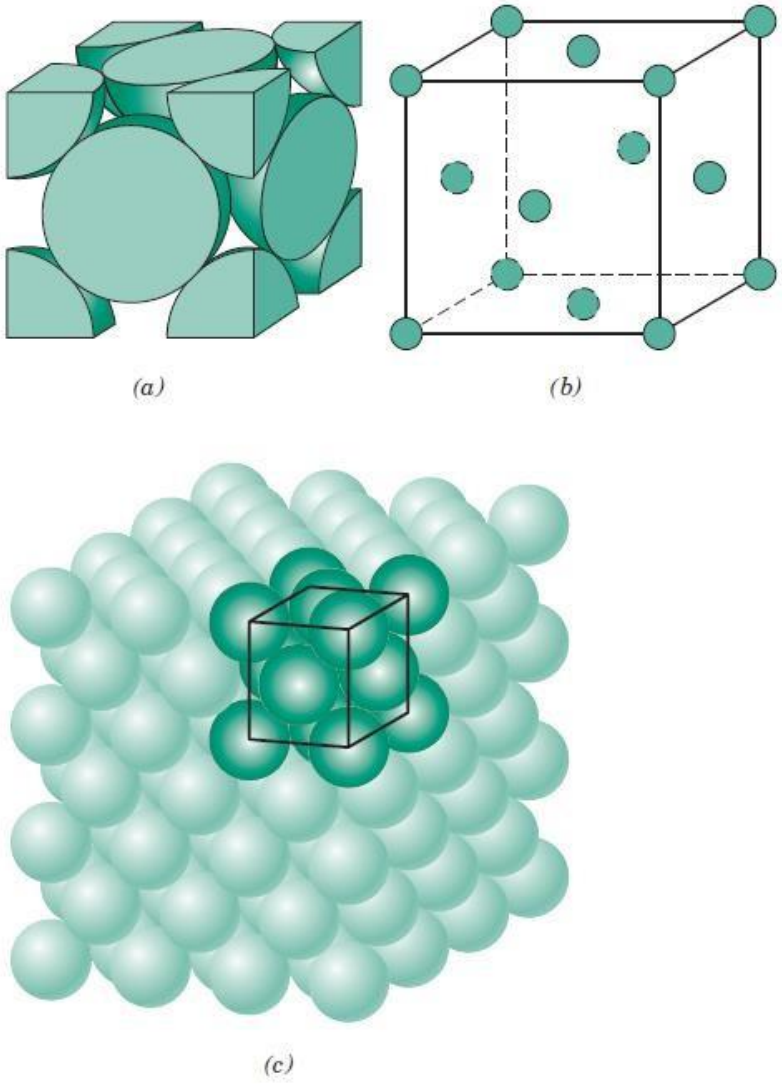


Figure 2.2 For the face-centered cubic crystal structure, (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms.

These spheres or ion cores touch one another across a face diagonal; the cube edge length a and the atomic radius (R) are related through

$$a=2R\sqrt{2}$$

For the FCC crystal structure, each corner atom is shared among eight-unit cells, whereas a face-centered atom belongs to only two. Therefore, one-eighth of each of the eight corner atoms and one-half of each of the six face atoms, or a total of four whole atoms, may be assigned to a given unit cell. This is depicted in Figure 2.3.

Two other important characteristics of a crystal structure are the **coordination number** and the **atomic packing factor (APF).** For metals, each atom has the same number of nearest-neighbor or touching atoms, which is the coordination number.

For face-centered cubic, the coordination number is 12. This may be confirmed by examination of Figure 3.3. the front face atom has four corner nearest-neighbor atoms surrounding it, four face atoms that are in contact from behind, and four other equivalent face atoms residing in the next unit cell to the front, which is not shown.

The APF is the sum of the sphere volumes of all atoms within a unit cell (assuming the atomic hard sphere model) divided by the unit cell volume—that is

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

For the FCC structure, the atomic packing factor is 0.74, which is the maximum packing possible for spheres all having the same diameter.

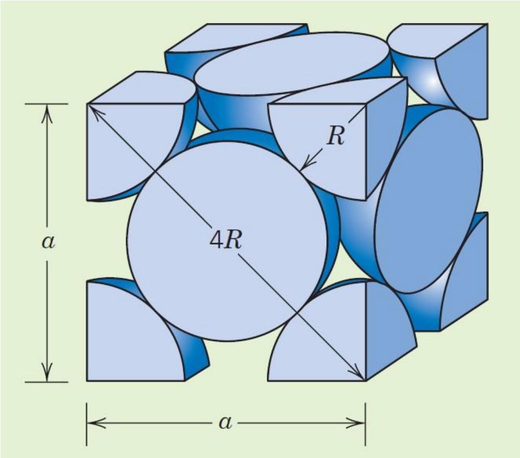


Figure 2.3 FCC unit cell illustrated.

2.2.2 The Body-Centered Cubic Crystal Structure

Another common metallic crystal structure also has a cubic unit cell with atoms located at all eight corners and a single atom at the cube center. This is called a **body-centered cubic (BCC)** crystal structure. A collection of spheres depicting this crystal structure is shown in Figure 3.4*c*, whereas Figures 3.4*a* and 3.4*b* are diagrams of BCC unit cells with the atoms represented by hard sphere and reduced-sphere models, respectively. Center and corner atoms touch one another along cube diagonals, and unit cell length *a* and atomic radius (*R)* are related through

$$a = \frac{4R}{\sqrt{3}}$$

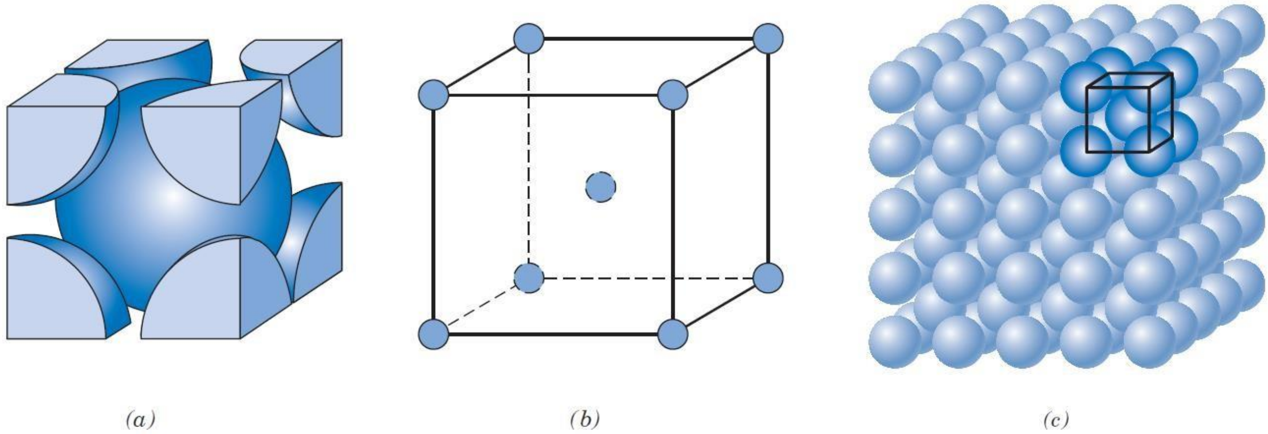


Figure 2.4 For the body-centered cubic crystal structure, (*a*) a hard sphere unit cell representation, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms.

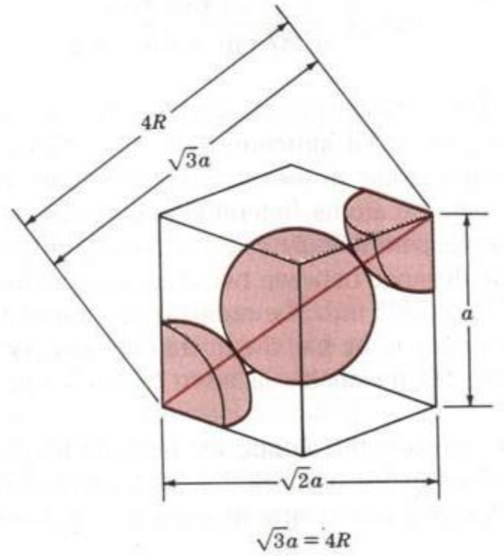
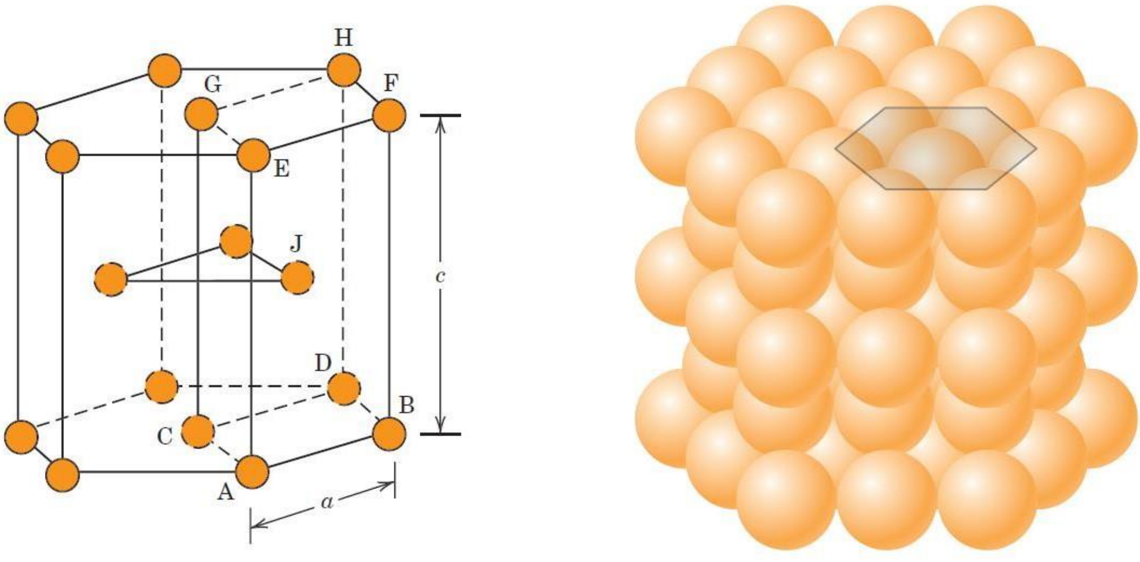


Figure 2.4 (d)

Two atoms are associated with each BCC unit cell: the equivalent of one atom from the eight corners, each of which is shared among eight-unit cells, and the single center atom, which is wholly contained within its cell. In addition, corner and center atom positions are equivalent. The coordination number for the BCC crystal structure is 8; each center atom has as nearest neighbors its eight corner atoms. Since the coordination number is less for BCC than FCC, so also is the atomic packing factor for BCC is 0.68 versus 0.74. Some of the familiar metals having this crystal structure are Cr, α-Fe, Mo and other shown in table (2.1).

2.2.2 The Hexagonal Close-Packed Crystal Structure

Not all metals have unit cells with cubic symmetry; the final common metallic crystal structure to be discussed has a unit cell that is hexagonal. Figure 2.5*a* shows a reduced-sphere unit cell for this structure, which is termed **hexagonal close-packed (HCP);** an assemblage of several HCP unit cells is presented in Figure 3.5*b*.The top and bottom faces of the unit cell consist of six atoms that form regular hexagons and surround a single atom in the center. Another plane that provides three additional atoms to the unit cell is situated between the top and bottom planes. The atoms in this midplane have as nearest neighbors' atoms in both of the adjacent two planes. The equivalent of six atoms is contained in each unit cell; one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all 3 midplane interior atoms. If a and c represent, respectively, the short and long unit cell dimensions of Figure 3.5*a*, the c/a ratio should be 1.633; however, for some HCP metals this ratio deviates from the ideal value.



(a) (b)

Figure 2.5 For the hexagonal close-packed crystal structure, (*a*) a reduced-sphere unit cell and (*b*) an aggregate of many atoms.

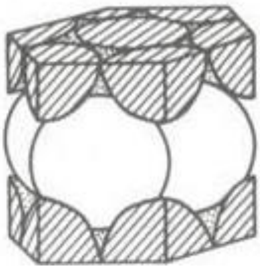


Figure 2.5 (c)

The coordination number and the atomic packing factor for the HCP crystal structure is the same as for FCC: 12 and 0.74, respectively. The HCP metals include **cadmium, magnesium, titanium, and zinc**; some of these are listed in Table 3.1.

$$\frac{c}{a} = 1.633 \quad , r = \frac{a}{2}$$

so the volume of the basic atoms is :

$$V_b = 6\left[\frac{4}{3}\Pi\left(\frac{a}{2}\right)^3\right] = \Pi a^3$$

and the volume of the unit cell is :

$$V_u = \frac{3\sqrt{3}}{2} a^2 . c = \frac{3\sqrt{3}}{2} \times 1.633 \quad a^3$$

$$A.P.F. = \frac{\Pi a^3}{\frac{3\sqrt{3}}{2} \times 1.633\ a^3} = 0.74$$

2.3 Density Computation

The theoretical density of a material can be calculated using the properties of the crystal structure. The general formula is:

Density $\rho = \frac{n A}{V_C N_A}$

where

n = number of atoms associated with each unit cell

A = atomic weight

V_C = volume of the unit cell

N_A = Avogadro's number (6.022×10^{23} atoms/mol)

Example 2.1

Determine the density of BCC iron, which has a lattice parameter of 0.2866 nm and an atomic weight of 55.847 g/mol

Solution

For a BCC cell,

Atoms/cell = 2

$a = 0.2866$ nm $= 2.866\times10^{-8}$ cm

Atomic mass of iron = 55.847 g/mol

Volume of unit cell = $a^3 = (2.866\times10^{-8}\text{cm})^3 = 23.54\times10^{-24}$ cm^3/cell

Avogadro's number N_A = (6.022×10^{23} atoms/mol)

Density $\rho = \frac{n A}{V_C N_A}$

$$\rho = \frac{(2)\times(55.847)}{(23.54\times10^{-24})(6.022\times10^{23})} = 7.882 \text{ g/cm}^3$$

The measured density is 7.870 g/cm^3. The slight discrepancy between the theoretical and measured densities is a consequence of defects in the material.

By Lect. Adwaa M. Al Nasrawee

Example 2.2

Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density.

Solution

For a FCC cell,

Atoms/cell = 4

Atomic weight for copper = 63.5 g/mol

Since, for FCC unit cells, $a = 4r/\sqrt{2}$

Volume of unit cell = $a^3 = (4r/\sqrt{2})^3 = (4 \times 1.28 \times 10^{-8}/\sqrt{2})^3$

$= 47.45 \times 10^{-24}$ cm^3/cell

$$\rho = \frac{nA}{V_C N_A}$$

$$\rho = \frac{(4) \times (63.5)}{(47.45 \times 10^{-24})\,(6.022 \times 10^{23})} = 8.89 \text{ g/cm}^3$$

By Lect. Adwaa M. Al Nasrawee

Lecture No.3

Imperfections in Solids

3.1 Introduction:

The arrangement of the atoms or ions in engineered materials contains imperfections or defects. These defects often have a profound effect on the properties of materials. Consequently, it is important to have a knowledge about the types of imperfections that exist and the roles they play in affecting the behavior of materials.

In this chapter, it has been introducing the three basic types of imperfections: point defects, line defects (or dislocations), and surface defects.

3.2 Point Defects:

Point defects are disruptions in atomic or ionic arrangements in a crystal structure. The Point defects involve: (a) vacancy, (b) interstitial atom, (c) small substitutional atom and (d) large substitutional atom as shown in fig. 3.1.

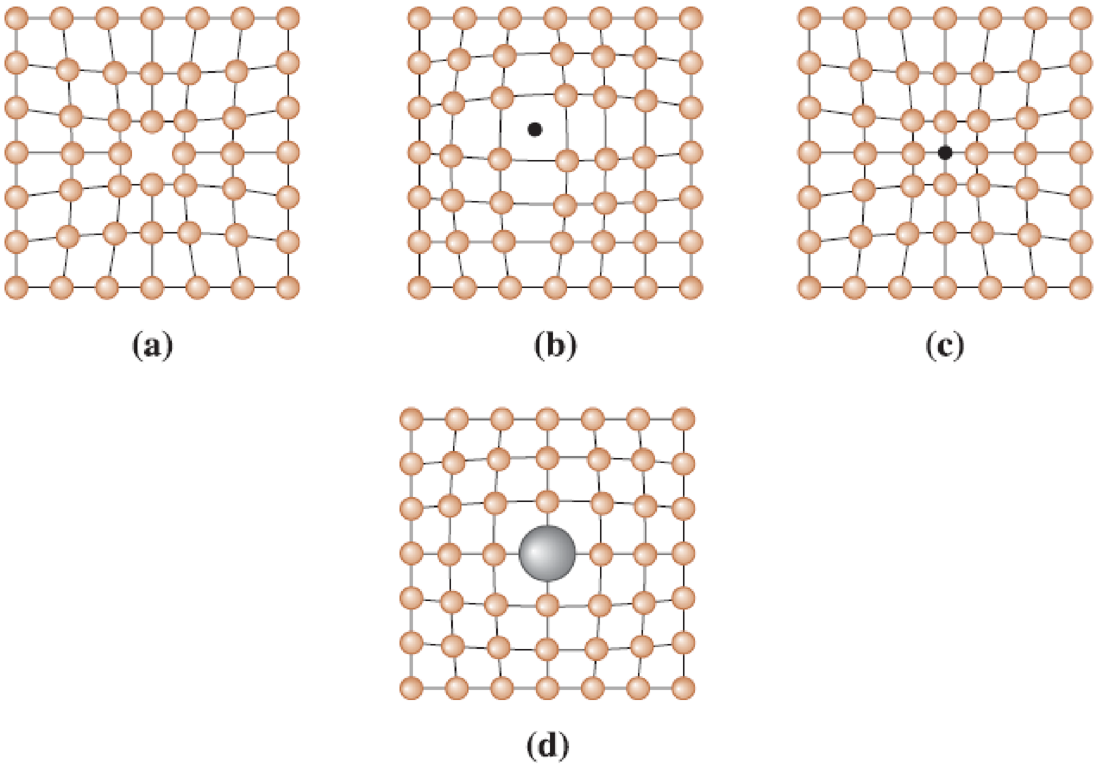


Figure 3.1 Point defects: (a) vacancy, (b) interstitial atom, (c) small substitutional atom and (d) large substitutional atom.

3. 2.1 Vacancies

Vacancies the simplest of the point defects is a **vacancy**. A vacancy is produced when an atom or an ion is missing from its normal site in the crystal structure, as in Figure 3.1(a). All crystalline materials have vacancy defects. The necessity of the existence of vacancies is explained using principles of thermodynamics; the presence of vacancies increases the entropy (i.e., the randomness) of the crystal. Vacancies are introduced into metals and alloys during solidification, at high temperatures.

The equilibrium number of vacancies for a given quantity of material depends on and increases with temperature according to

$$n_v = n \exp\left(\frac{-Q_v}{RT}\right) \qquad (3.1)$$

where:

n_v: is the number of vacancies per cm^3;

n: is the number of atoms per cm^3;

Q_v: is the energy required for the formation of a vacancy, in Cal/mol or Joules/mol;

R: is the gas constant, $1.987 \frac{cal}{mol-K}$ or $8.31 \frac{Joules}{mol-K}$; and

T: is the temperature in degrees Kelvin.

Example 3.1

Calculate the concentration of vacancies in copper at 25°C. What temperature will be needed to heat treat copper such that the concentration of vacancies produced will be 1000 times more than the equilibrium concentration of vacancies at room temperature? Assume that 20,000 Cal are required to produce a mole of vacancies in copper. The lattice parameter of FCC copper is 0.36151 nm.

Solution

The number of copper atoms, or lattice points, per cm^3 is:

$$n = \frac{4 \text{ atoms/cell}}{(3.6151 \times 10^{-8}\text{ cm})^3} = 8.47\times10^{22} \text{ copper atom/cm}^3$$

$$\text{At } 25°\text{C}, T = 25+273 = 298 \text{ K}:$$

$$n_v = n \exp\left(\frac{-Q_v}{RT}\right)$$

$$= (8.47\times 10^{22}\,\frac{atom}{cm^3})\exp\left(\frac{-20{,}000\,\frac{cal}{mol}}{1.987\,\frac{cal}{mol-K}\times 289\,K}\right)$$

$$= 1.815 \times 10^{8}\ \text{vacancies/cm}^3$$

The concentration of vacancies at heat treatment is 1000 times higher than this number, or $n_v = 1.815\times10^{11}$ vacancies/cm^3.

The copper must be heating to a temperature at which this number of vacancies forms:

$$n_v = 1.815\times10^{11} = n\exp\left(\frac{-Q_v}{RT}\right)$$

$$= (8.47 \times 10^{22})\exp(-20{,}000 / (1.987\times T))$$

$$\exp\left(\frac{-20{,}000}{1.987\ \times T}\right) = \frac{1.815\times10^{11}}{8.47\times10^{22}} = 0.214 \times 10^{-11}$$

$$\frac{-20{,}000}{1.987\,T} = \ln(0.214 \times 10^{-11}) = -26.87$$

$$T = \frac{20{,}000}{(1.987)\times(26.87)} = 375\ \text{K} = 102°\text{C}$$

Example 3.2

Determine the number of vacancies needed for a BCC iron crystal to have a density of 7.87 g/cm^3. The lattice parameter of BCC iron is 2.866×10^{-8} cm, and the atomic mass is 55.847 g/mol.

Solution

The iron with a density of 7.87 g/cm^3 can be produced by intentionally introducing vacancies into the crystal. Let's calculate the number of iron atoms and vacancies that would be present in each unit cell for the required density of 7.87 g/cm^3:

$$\rho = \frac{n\,A}{V_C\,N_A}$$

$$\rho = \frac{(X\ \text{atom/cell})\,(55.847\text{g/mol})}{(2.866\times10^{-8}\ \text{cm})^3\,(6.02\times10^{23}\ \text{atom/mol})} = 7.87\ \text{g/cm}^3$$

$$X\ \text{atoms/ cell} = \frac{(7.87)(2.866\times10^{-8})^3\,(6.02\times10^{23})}{55.847} = 1.9971$$

There should be 2.00 – 1.9971 = 0.0029 vacancies per unit cell. The number of vacancies per cm^3 is:

$$\text{Vacancies/ cm}^3 = \frac{0.0029\ \text{vacancies/cell}}{(2.866 \times 10^{-8}\ \text{cm})^3} = 1.23 \times 10^{20}$$

That introduction of vacancies has been assuming does not change the lattice constant.

3.2.2 Interstitial Defects:

An interstitial defect is formed when an extra atom or ion is inserted into the crystal structure at a normally unoccupied position, as in Figure 3.1(b). For example, carbon atoms are intentionally added to iron to produce steel. Unlike vacancies, once introduced, the number of interstitial atoms or ions in the structure remains nearly constant, even when the temperature is changed.

3.2.2.1 Self-Interstitial:

Self-interstitial defects are interstitial defects which contain only atoms which are the same as those already present in the lattice. A self-interstitial is an atom from the crystal that is crowded into an interstitial site, a small void space that under ordinary circumstances is not occupied. This kind of defect is also represented in Figure 3.2. In metals, a self-interstitial introduces relatively large distortions in the surrounding lattice because the atom is substantially larger than the interstitial position in which it is situated.

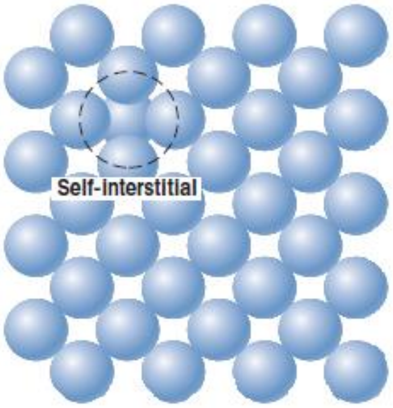


Figure 3.2 Two-dimensional representations of a self-interstitial.

3.2.2.2 Substitutional Defects:

A substitutional defect is introduced when one atom or ion is replaced by a different type of atom or ion as in Figure 3.1(c) and (d). The substitutional atoms or ions occupy the normal lattice sites. Substitutional atoms or ions may either be larger than the normal atoms or ions in the crystal structure, in which case the surrounding interatomic spacings are reduced, or smaller causing the surrounding atoms to have larger interatomic spacings. In either case, the substitutional defects alter the interatomic distances in the surrounding crystal. Again, the substitutional defect can be introduced either as an impurity or as a deliberate alloying addition.

Examples of substitutional defects include the copper and nickel alloy; copper atoms will occupy crystallographic sites where nickel atoms would normally be present. The substitutional atoms will often increase the strength of the metallic material.

3.3 Dislocations – Linear Defects

A *dislocation* is a linear or one-dimensional defects around which some of the atoms are misaligned in perfect crystal. They are introduced typically into the crystal during solidification of the material or when the material is deformed permanently. Dislocations are most significant in metals and alloys since they provide a mechanism for plastic deformation, which is the cumulative effect of slip of numerous dislocations. **Plastic deformation** refers to irreversible deformation or change in shape that occurs when the force or stress that caused it is removed. This is because the applied stress causes dislocation motion that in turn causes permanent deformation. Significance of dislocations can be summarized into:

1. The mechanical properties of a metal or alloy can be controlled by interfering with the movement of dislocations.
2. Dislocations also influence electronic and optical properties of materials. For example. There are three types of dislocations: the edge dislocation, the screw dislocation, and the mixed dislocation.

3.3.1Edge Dislocations:

The edge dislocation is represented in Figure 3.3: an extra portion of a plane of atoms, or half-plane, the edge of which terminates within the crystal. The bottom edge of this inserted plane represents the edge dislocation. This is sometimes termed the **dislocation line** which is perpendicular to the plane of the page. Sometimes the edge dislocation in Figure 3.4 is represented by the symbol ⊥ which also indicates the position of the dislocation line. An edge dislocation may also be formed by an extra half-plane of atoms that is included in the bottom portion of the crystal; its designation is a **T**.

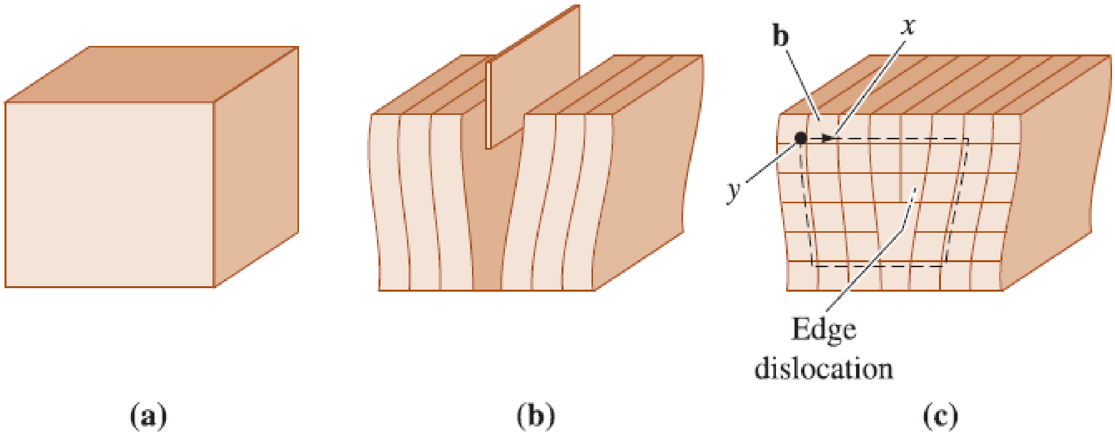


Figure 3.3 The perfect crystal in (a) is cut and an extra plane of atoms is inserted (b). The bottom edge of the extra plane is an edge dislocation (c). A Burgers vector **b** is required to close a loop of equal atom spacings around the edge dislocation.

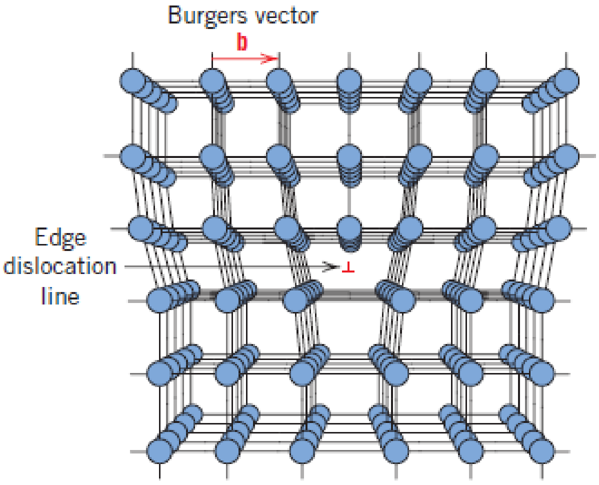


Figure 3.4 The atom positions around an edge dislocation.

3.3.2 Screw Dislocation

The screw dislocation is formed by a shear stress that is applied to produce the distortion shown in Figure 3.5 *a*: the upper front region of the crystal is shifted one atomic distance to the right relative to the bottom portion. The atomic distortion associated with a screw dislocation is linear and along a dislocation line, line *AB* in Figure 3.6*b*. Sometimes the symbol ↻ is used to designate a screw dislocation.

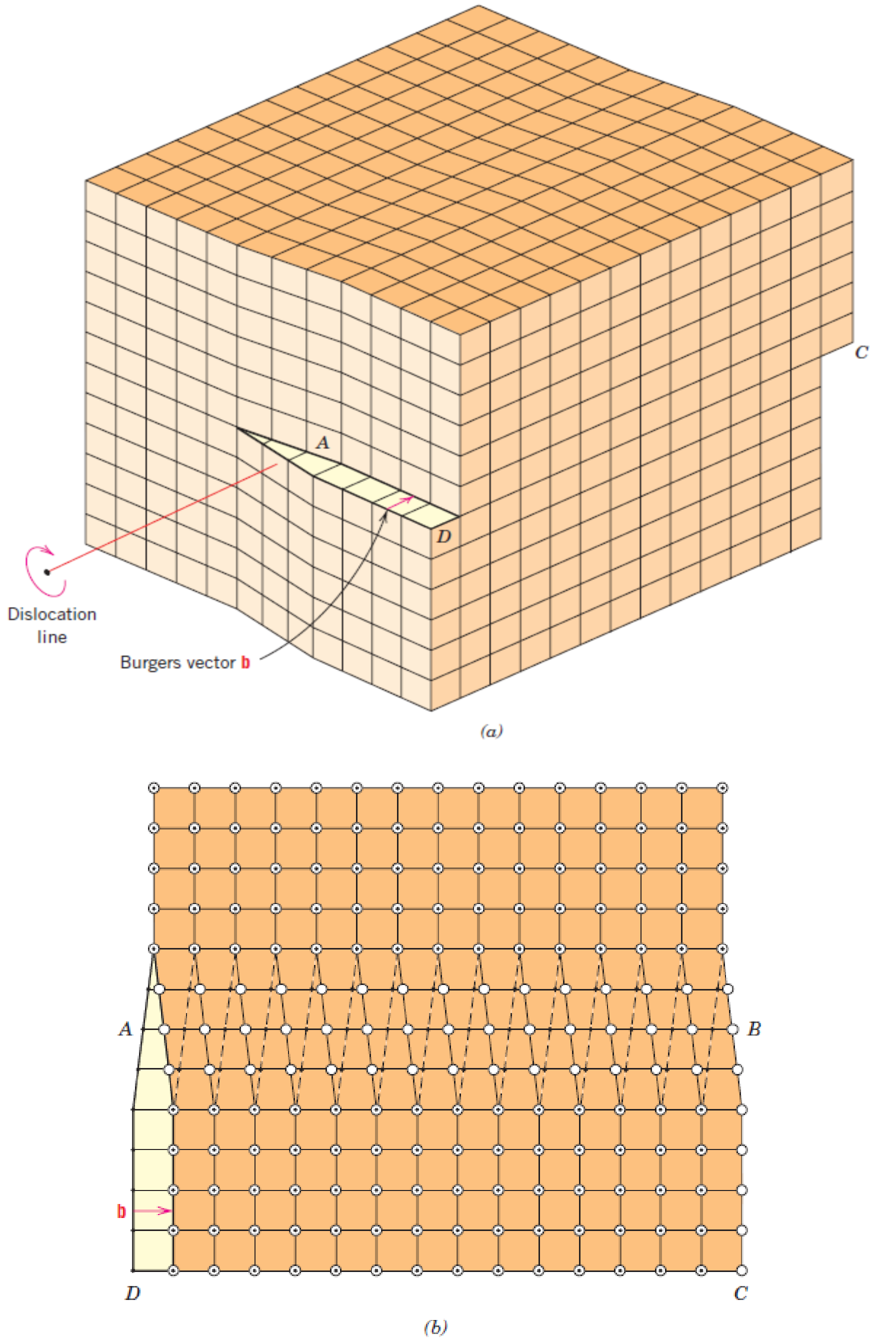
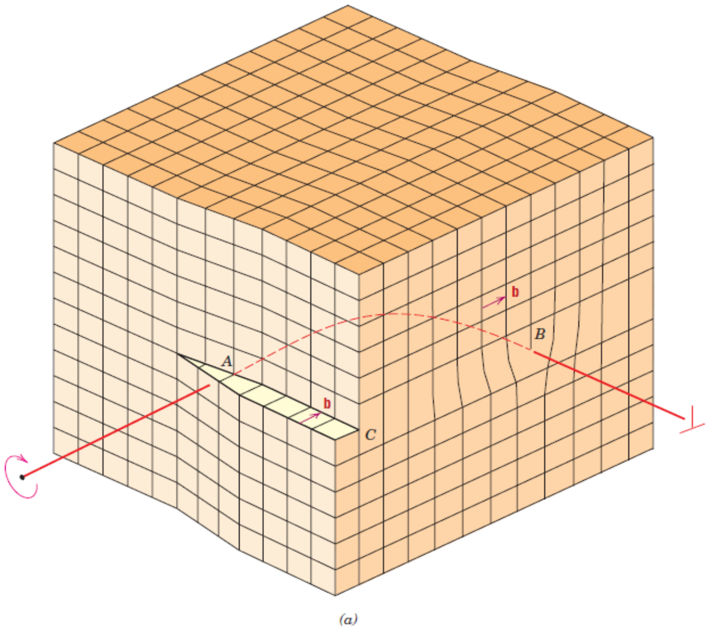


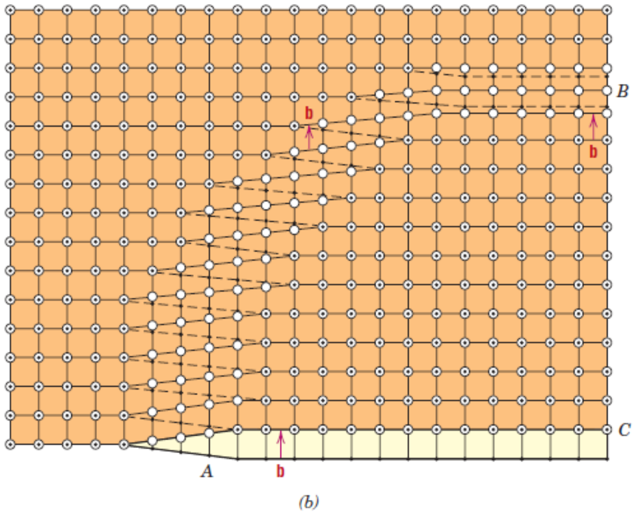
Figure 3.5 (*a*) A screw dislocation within a crystal. (*b*) The screw dislocation in (*a*) as viewed from above. The dislocation line extends along line *AB*.

3.3.3 Mixed Dislocations

Most dislocations found in crystalline materials are probably neither pure edge nor pure screw, but exhibit components of both types with a transition region between them; these are termed **mixed dislocations.** All three dislocation types are represented schematically in Figure 3.6



(*a*) Schematic representation of a dislocation that has edge, screw, and mixed character.



(*b*) Top view, where open circles denote atom positions above the slip plane, and solid circles, atom positions below.

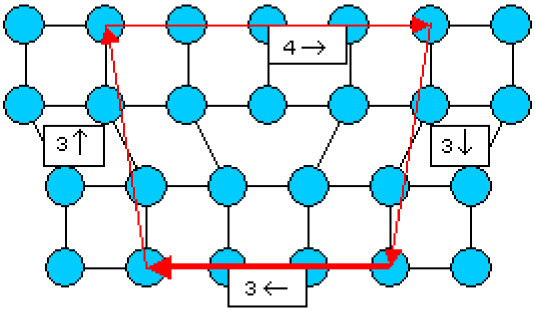
Figure 3.6 At point *A*, the dislocation is pure screw, while at point *B*, it is pure edge. For regions in between where there is curvature in the dislocation line, the character is mixed edge and screw.

3.4 Burger's vector

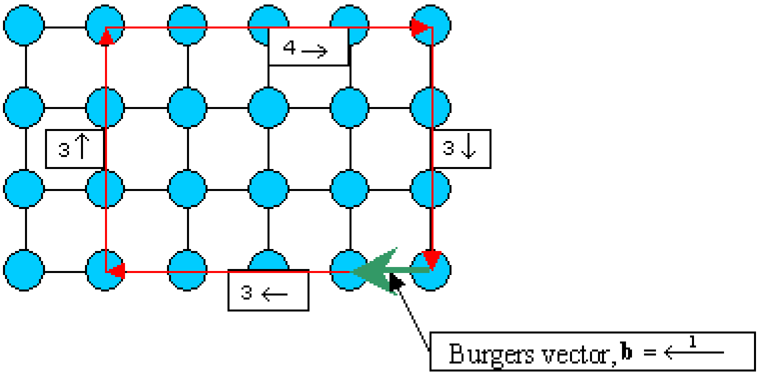
Burger's vector, the magnitude and direction of the lattice distortion associated with a dislocation is expressed in terms of a **Burgers vector,** denoted by a **b.** Burgers vectors are indicated in Figures 3.4 and 3.5 for edge and screw dislocations, respectively. Furthermore, the nature of a dislocation (i.e., edge, screw, or mixed) is defined by the relative orientations of dislocation line and Burger's vector. For an edge, they are perpendicular (Figure 3.4), whereas for a screw, they are parallel (Figure 3.5); they are neither perpendicular nor parallel for a mixed dislocation.

The Burgers vector of a dislocation is a crystal vector, specified by Miller indices, that quantifies the difference between the distorted lattice around the dislocation and the perfect lattice. Equivalently, the Burgers vector denotes the direction and magnitude of the atomic displacement that occurs when a dislocation moves. To determine the Burgers vector of a dislocation in a two-dimensional primitive square lattice, proceed as follows:

Trace around the end of the dislocation plane to form a closed loop. Record the number of lattice vectors travelled along each side of the loop (shown here by the numbers in the boxes):



In a perfect lattice, trace out the same path, moving the same number of lattice vectors along each direction as before. This loop will not be complete, and the closure failure is the Burgers vector:



3.4 Surface Defects

Surface defects are boundaries that have two dimensions and normally separate regions of the materials that have different crystal structures and/or crystallographic orientations. These imperfections include external surfaces, grain boundaries and twin boundaries.

3.4.1 External Surfaces

One of the most obvious boundaries is the external surface, along which the crystal structure terminates. Each atom at the surface no longer has the proper coordination number, and is therefore in a higher energy state than the atom at interior positions. The bonds of these surface atoms are disrupted give rise to a surface energy. The exterior surface may also be very rough, may contain tiny notches, and may be much more reactive than the bulk of the material.

3.4.2 Grain Boundaries

The microstructure of many engineered ceramic and metallic materials consists of many grains. A **grain** is a crystalline portion of the material within which the arrangement of the atoms is nearly identical. However, the orientation of the atom arrangement, or crystal structure, is different for each adjoining grain (Figure 3.7). The atoms are bonded less regularly along a grain boundary and, consequently, there is an interfacial or grain boundary energy similar to the surface energy just described. Grain boundaries are more chemically reactive than the grains themselves as a consequence of this boundary energy. Furthermore, impurity atoms often preferentially segregate along these boundaries because of their higher energy state. The total interfacial energy is lower in large or coarse-grained materials than in finegrained ones, because there is less total boundary area in the former. One method of controlling the properties of a material is by controlling the grain size. By reducing the grain size, the number of grains is increase and, hence, increase the amount of grain boundary area.

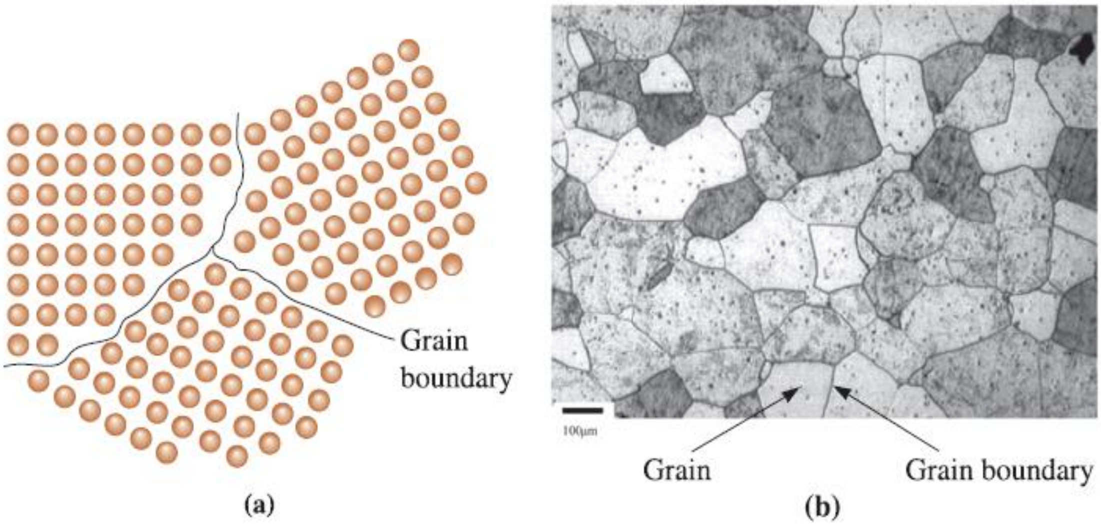


Figure 3.7 (a) The atoms near the boundaries of the three grains do not have an equilibrium spacing or arrangement. (b) Grains and grain boundaries in a stainless-steel sample.

Lecture No.4

Solidification of Metals and Alloys

4.1 Introduction

Solidification involves the transformation of the molten metal back into the solid state. The solidification process differs depending on whether the metal is a pure element or an alloy.

4.2 Cooling Curve for Pure Metal and Alloy

A cooling curve shows how the temperature of a material (in this case, a pure metal) changes with time (Figure 4.1). The liquid is poured into a mold at pouring temperature, point *A*. The difference between the pouring temperature and the freezing temperature is the superheat. The specific heat is extracted by the mold until the liquid reaches the freezing temperature (point *B*). The slope of the cooling curve before solidification begins is the cooling rate $\frac{\Delta T}{\Delta t}$. Solidification proceeds isothermally at the melting temperature (point *B* to *C*) as the latent heat given off from continued solidification is balanced by the heat lost by cooling. This region between points *B* and *C*, where the temperature is constant, is known as the **thermal arrest**. A thermal arrest, is produced because of the evolution of the latent heat of fusion balances the heat being lost because of cooling. At point *C*, solidification is complete and the solid casting cools from point *C* to room temperature.

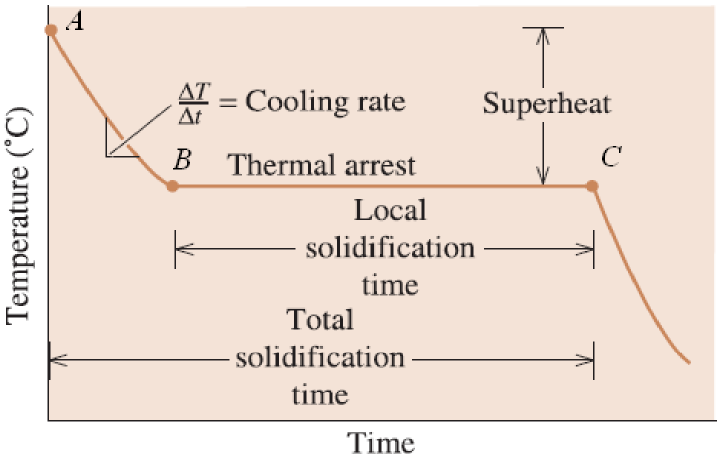


Figure 4.1: Cooling curve for a pure metal. Solidification begins at the melting temperature.

A pure metal solidifies at a constant temperature equal to its freezing point, which is the same as its melting point. The melting points of pure metals are well known. The process occurs over time as shown in the plot of Figure 4.1, called a cooling curve. The actual freezing takes time, called **the local solidification time** in casting, during which the metal's latent heat of fusion is released into the surrounding mold. **The total solidification time** is the time taken between pouring and complete solidification.

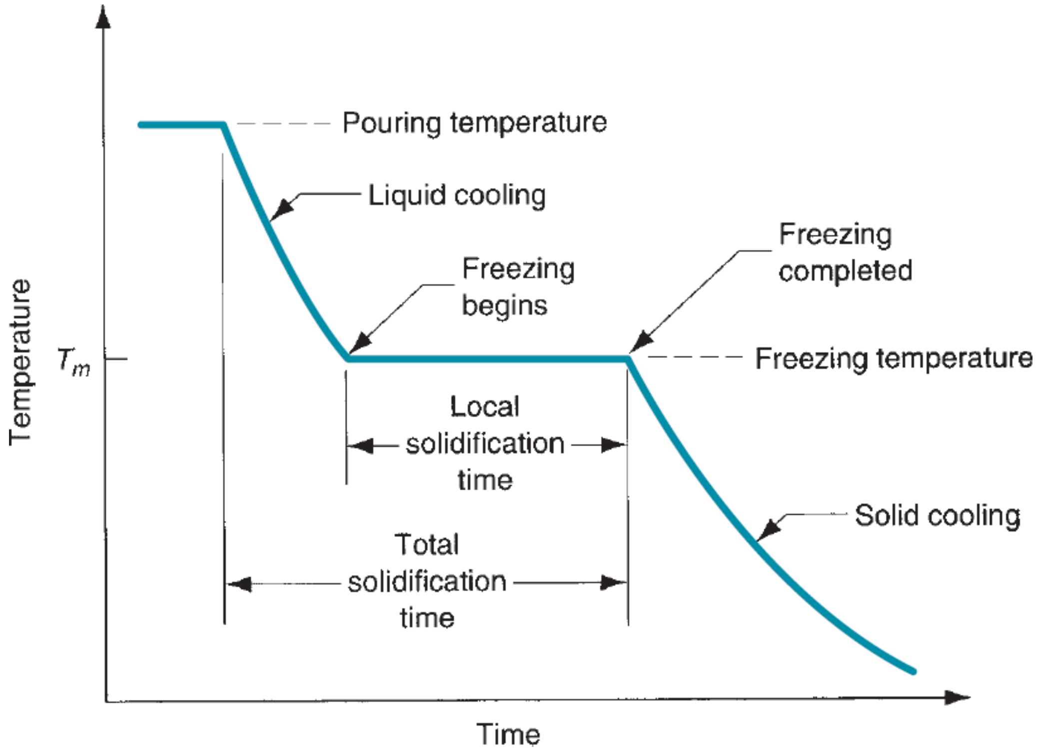
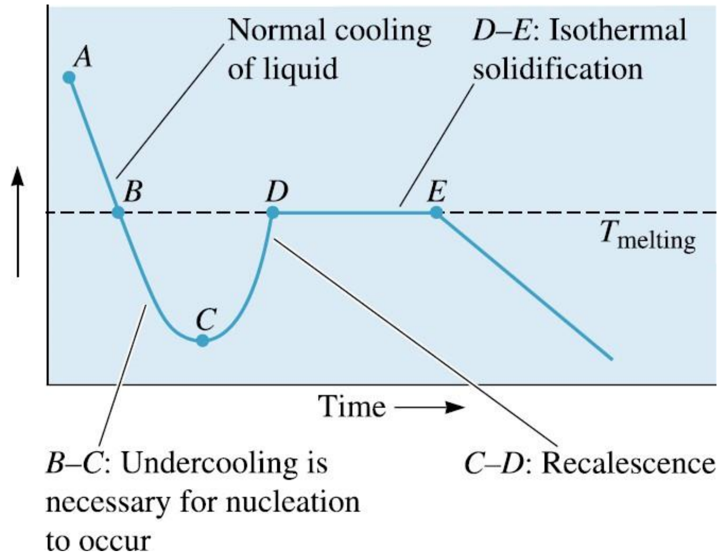


Figure 4.2: Cooling curve for a pure metal during casting.

After the casting has completely solidified, cooling continues at a rate indicated by the downward slope of the cooling curve.



Cooling curve for a pure metal that has not been well inoculated. Liquid cools as specific heat is removed (between points A and B). Undercooling is thus necessary (between points B and C). As the nucleation begins (point C), latent heat of fusion is released causing an increase in the temperature of the liquid. This process is known as recalescence (point C to point D). Metal continues to solidify at a constant temperature ($T_{melting}$). At point E, solidification is complete. Solid casting continues to cool from the point.

Because of the chilling action of the mold wall, a thin skin of solid metal is initially formed at the interface immediately after pouring. Thickness of the skin increases to form a shell around the molten metal as solidification progresses inward toward the center of the cavity. The rate at which freezing proceeds depends on heat transfer into the mold, as well as the thermal properties of the metal.

It is of interest to examine the metallic grain formation and growth during this solidification process. The metal which forms the initial skin has been rapidly cooled by the extraction of heat through the mold wall. This cooling action causes the grains in the skin to be fine and randomly oriented. As cooling continues, further grain formation and growth occur in a direction away from the heat transfer. Since the heat transfer is through the skin and mold wall, the grains grow inwardly as needles or spines of solid metal. As these spines enlarge, lateral branches form, and as these branches grow, further branches form at right angles to the first branches. This type of grain growth is referred to as dendritic growth, and it occurs not only in the freezing of pure metals but alloys as well. These treelike structures are gradually filled-in during freezing, as additional metal is continually deposited onto the dendrites until complete solidification has occurred. The grains resulting from this dendritic growth take on a preferred orientation, tending to be coarse, columnar grains aligned toward the center of the casting.

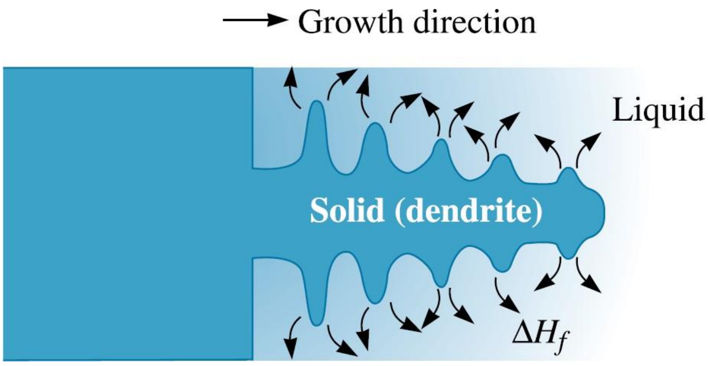


Figure 4.3: Dendritic Segregation.

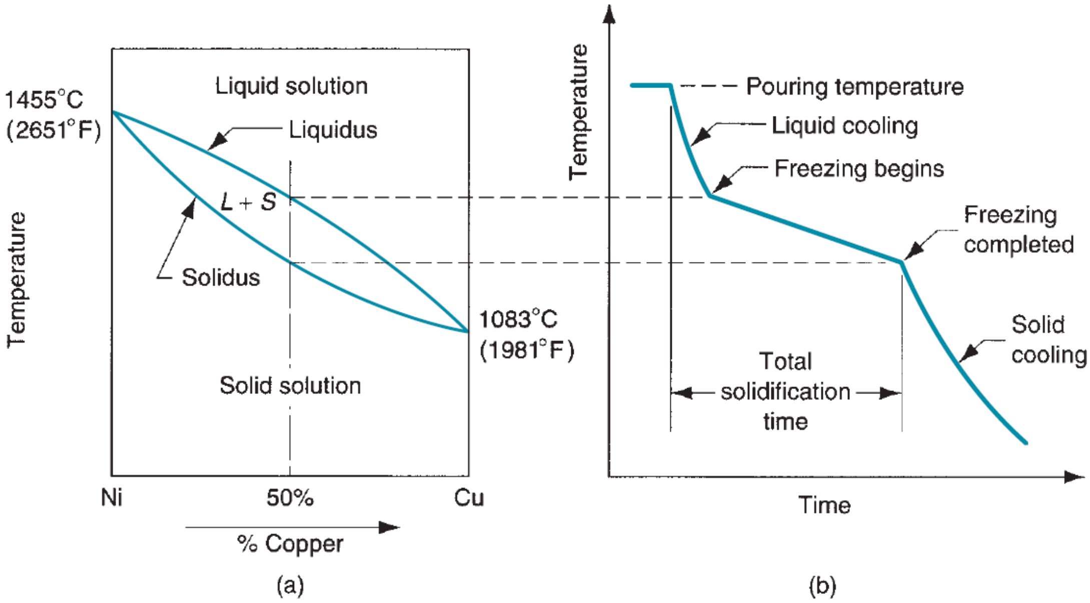


Figure 4.4: (A) Phase diagram for a copper– nickel alloy system and (b) associated cooling curve for a 50%Ni–50%Cu composition during casting.

Solidification of an alloy can be explained with reference to Figure 4.4, which shows the phase diagram for a particular alloy system and the cooling curve for a given composition. As temperature drops, freezing begins at the temperature indicated by the liquids and is completed when the solidus are reached. The start of freezing is similar to that of the pure metal. A thin skin is formed at them old wall due to the large temperature gradient at this surface. Freezing then progresses as before through the formation of dendrites that grow away from the walls. However, owing to the temperature spread between the liquids and solidus, the nature of the dendritic growth is such that an advancing zone is formed in which both liquid and solid metal coexist. The solid portions are the dendrite structures that have formed sufficiently to trap small islands of liquid metal in the matrix.

4.3 Structure of ingots

In manufacturing components by casting, molten metals are often poured into molds and permitted to solidify. The mold produces a finished shape, known as a casting. In other cases, the mold produces a simple shape, called an ingot. An ingot usually requires extensive plastic deformation before a finished product is created. A macrostructure, sometimes referred to as the ingot structure, consists of as many as three parts (Figure 4.5). to describe the structure of a material at a macroscopic scale. Hence, the term ‘‘ingot structure’’ may be more appropriate.

Chill Zone: The chill zone is a narrow band of randomly oriented grains at the surface of the casting. The metal at the mold wall is the first to cool to the freezing temperature.

Columnar Zone: The columnar zone contains elongated grains oriented in a particular crystallographic direction. As heat is removed from the casting by the mold material, the grains in the chill zone grow in the direction opposite the heat flow, or from the coldest toward the hottest areas of the casting. This tendency usually means that the grains grow perpendicular to the mold wall.

Equiaxed Zone: Although the solid may continue to grow in a columnar manner until all of the liquid has solidified, an equiaxed zone frequently forms in the center of the casting or ingot. These grains grow as relatively round, or equiaxed, grains with a random orientation, and they stop the growth of the columnar grains. The formation of the equiaxed zone is a nucleation controlled process and causes that portion of the casting to display isotropic behavior.

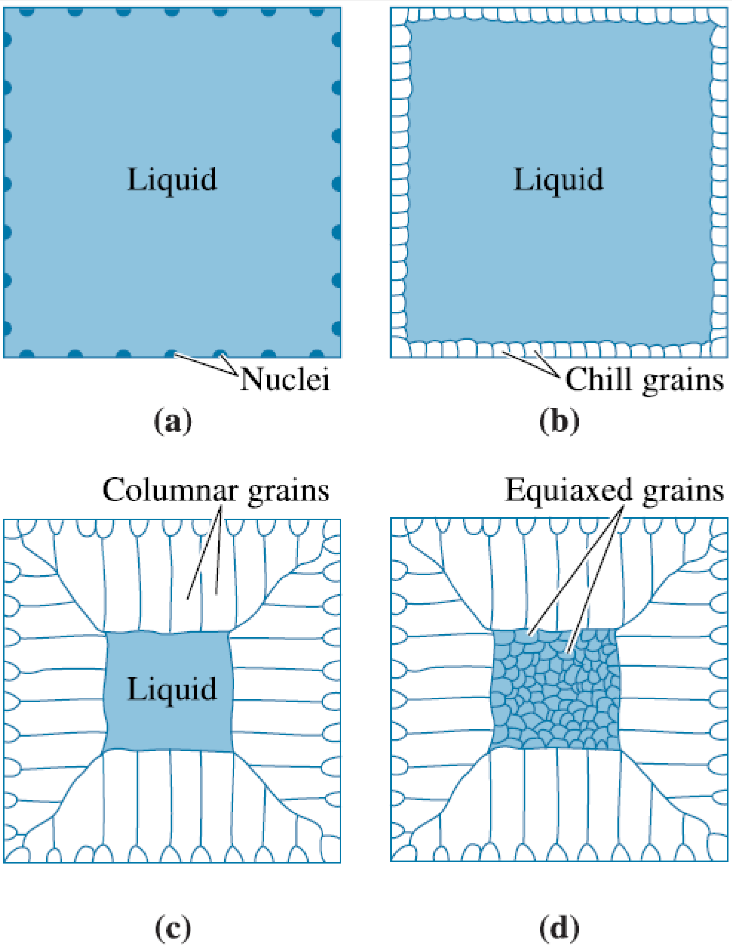


Figure 4.5: Development of the ingot structure of a casting during solidification: (a) Nucleation begins, (b) the chill zone forms, (c) preferred growth produces the columnar zone, and (d) additional nucleation creates the equiaxed zone.

Materials of Materials

Lecture.5 & 6

Thermal equilibrium diagrams

By

Lect. Adwaa M. Al Nasrawee

5.1 Introduction

- The understanding of phase diagrams for alloy systems is extremely important because there is a strong correlation between microstructure and mechanical properties.
- The development of microstructure of an alloy is related to the characteristics of its phase diagram.
- In addition, phase diagrams provide valuable information about melting, casting, crystallization, and other phenomena.

5.2 Definitions & Basic Concepts

- **Solvent** represents the element or compound that is present in the greatest amount.
- **Solute** is used to denote an element or compound present in a minor concentration.
- **Alloys** are combinations or mixtures of elements. Metals are alloyed to improve on properties of pure metals such as hardness, strength, corrosion resistance, etc. Alloys may behave differently when combined, some mix easily while others will only be soluble to a limited extent. Thermal Equilibrium diagrams seek to interpret how alloys combine.

- **Equilibrium diagram** illustrating the relationship between the composition, temperature, and structure, or state, of any alloy in a series, because there is a strong correlation between microstructure and mechanical properties of alloy.

5.3 Solid Solution

Solid solution alloy is a phase, where two or more elements are completely soluble in each other in the solid state. There are two types of solid solution:

- Substitutional solid solution, or
- Interstitial solid solution. (e.g. Copper-nickel alloy is a solid solution).

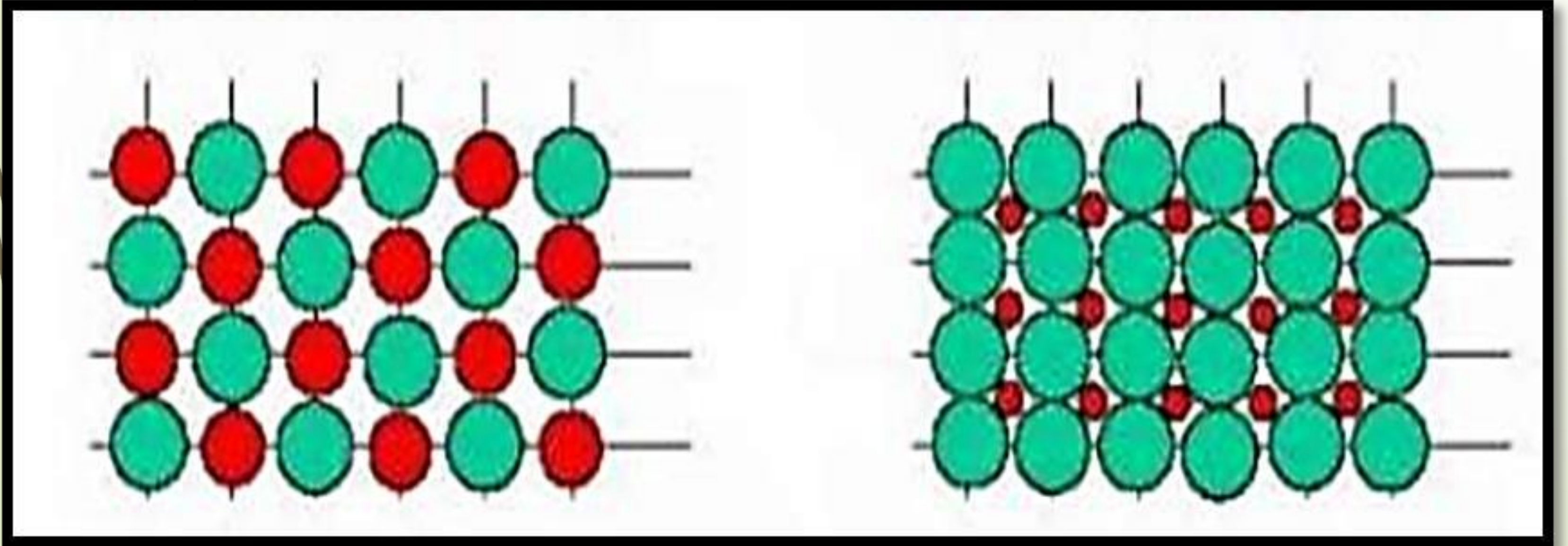


Figure 5.1: The two main types of solid solution: (a) a substitutional solid solution, (b) an interstitial solid solution.

5.4 Compounds

- A compound contains atoms of more than one element in a fixed proportion to each other. For example, water always has two times more hydrogen atoms than it does oxygen. Moreover, the atoms in a compound are joined together by bonds. The atoms have a definite relationship to each other in terms of how they are arranged in space.
- Compounds can be chemically broken down into simpler substances (For example, water can be separated into two elements, hydrogen and oxygen).

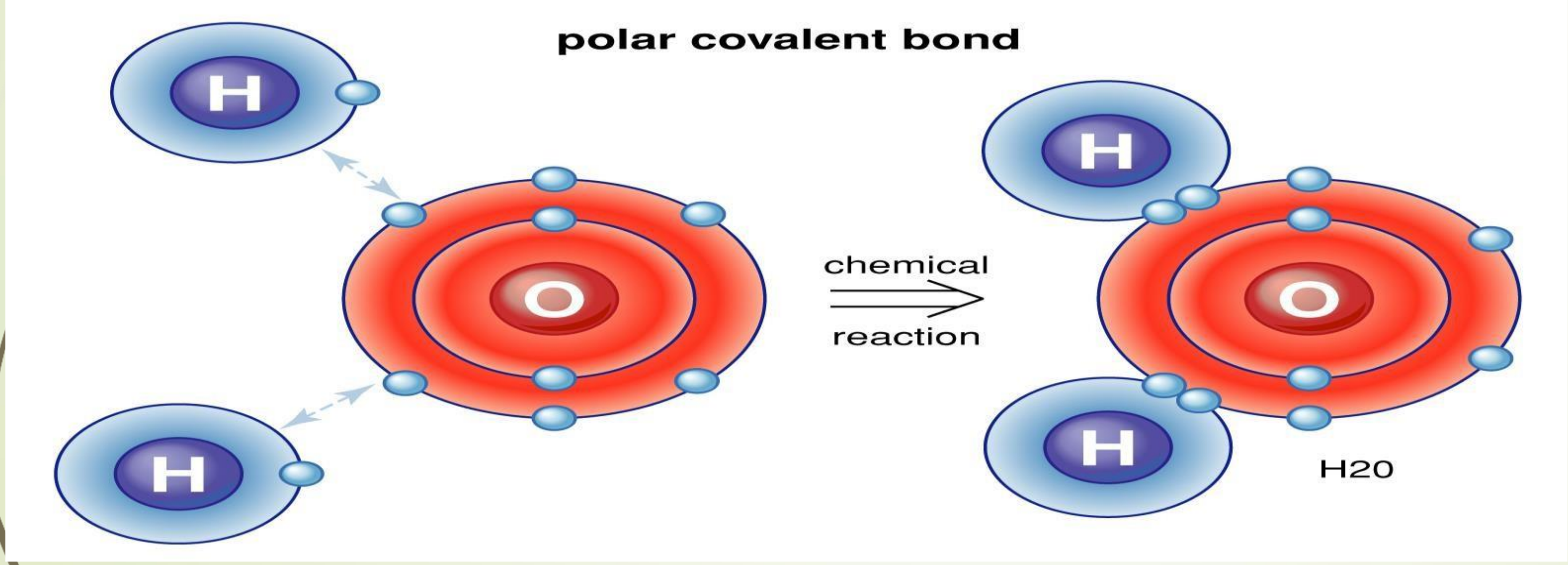


Figure 5.2: The formation of water molecules

5.5 Mechanical mixture

- A mechanical mixture is one that can be separated through mechanical means, such as a magnet or a centrifuge.
- Mechanical mixtures are not chemically bonded. While mechanical mixtures may be attracted to each other, there is no permanent gain or loss of electrons; they do not form different molecules.
- Examples of a mechanical mixture are water with microscopic particles in it is a mechanical mixture, as these particles can be removed through filtration. Oil floating on water is a mechanical mixture because oil and water do not combine.

Figure 5.3: The mechanical mixture of water and oil

5.6 Solubility limit

- For many alloy systems and at some specific temperature, there is a maximum concentration of solute atoms that may dissolve in the solvent to form a solid solution; this is called a **solubility limit.**
- Consider the sugar–water ($C_{12}H_{22}O_{11}$–H_2O) system. Initially, as sugar is added to water, a sugar– water solution or syrup forms.
- As more sugar is introduced, the solution becomes saturated with sugar and sugar simply settle to the bottom of the container.
- Thus, the system now consists of two separate substances: a sugar–water syrup liquid solution and solid crystals of undissolved sugar.

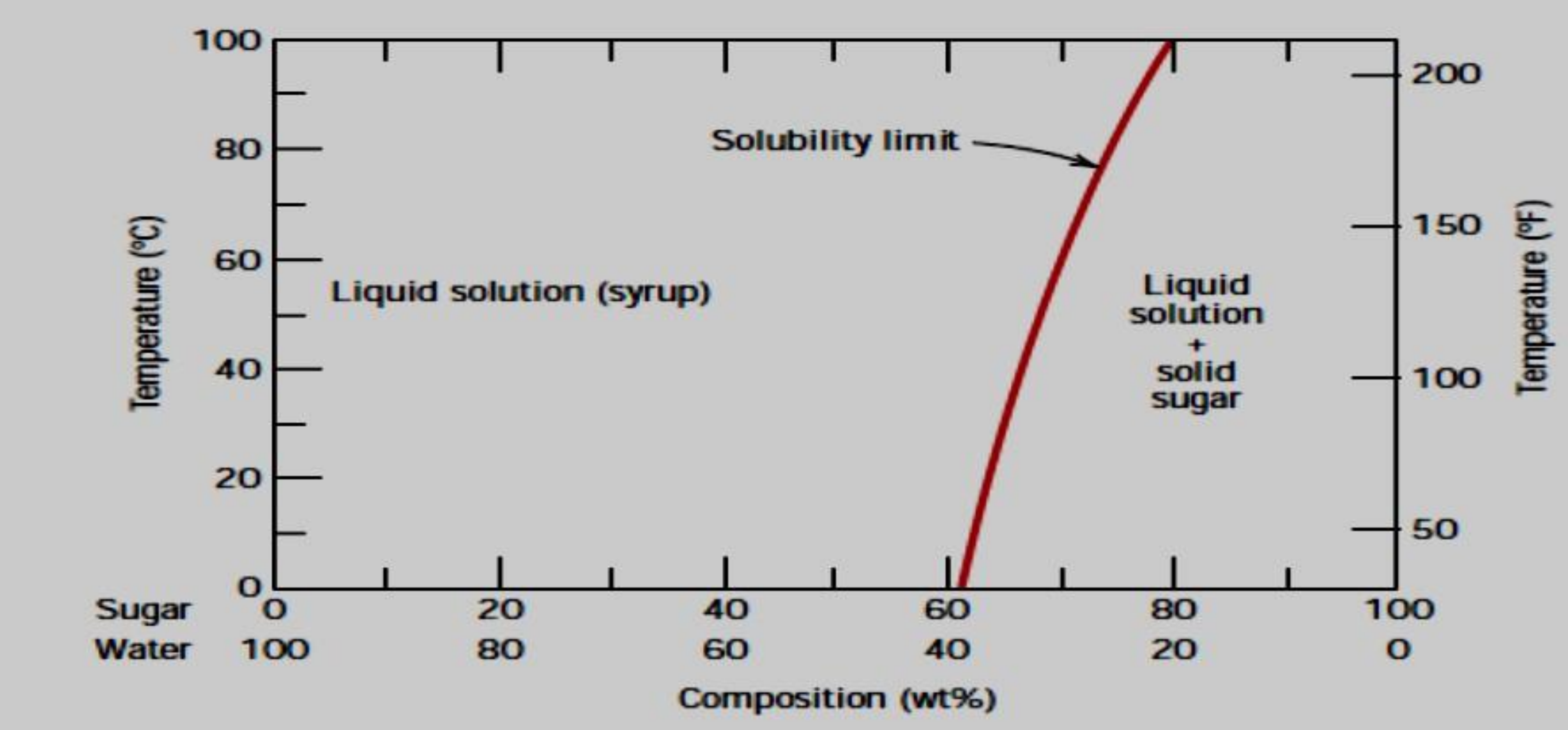


Figure 5.4: The solubility of sugar ($C_{12}H_{22}O_{11}$) in a sugar–water syrup.

5.7 Phases

- Also critical to the understanding of phase diagrams is the concept of a **phase.**
- A phase may be defined as a homogeneous portion of a system that has uniform physical and chemical characteristics.
- Every pure material is considered to be a phase; so also, is every solid, liquid, and gaseous solution.
- For example, the sugar–water syrup solution just discussed is one phase, and solid sugar is another.
- A single-phase system is called **homogeneous**, systems with two or more phases are **mixtures** or **heterogeneous** systems.

5.8 Binary Phase Diagrams

Binary phase diagram is a temperature-composition map which indicates the equilibrium phases present at a given temperature and composition. There are three different types of binary equilibrium diagrams:

1. The two metals are completely soluble in each other in the solid state (binary isomorphous system).
2. The two metals are partially soluble in each other in the solid state (binary eutectic system).
3. The two metals are completely insoluble in each other in the solid state.

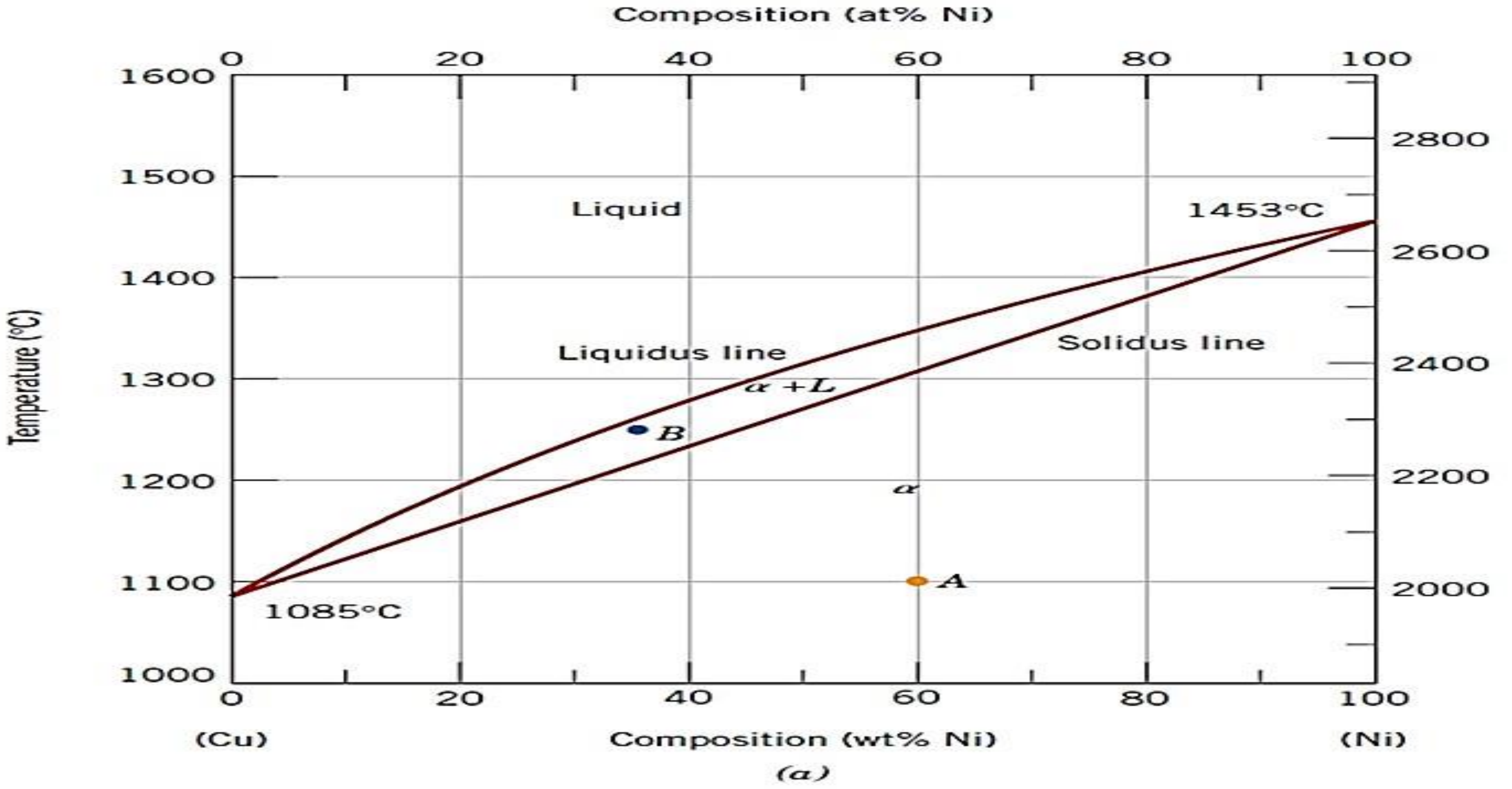
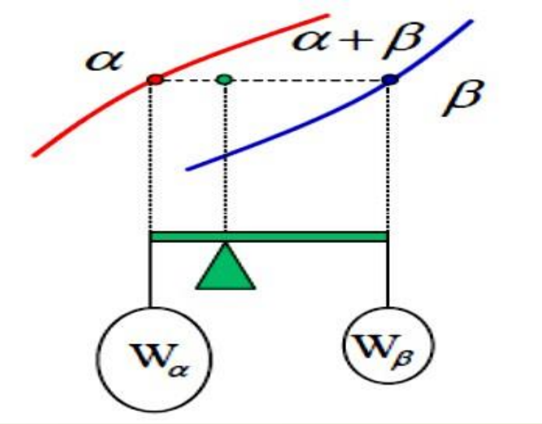


Figure 5.5: Copper-Nickel phase equilibrium diagram (binary isomorphous system).

Three different phase regions on this diagram:

1. Liquid L is a homogeneous liquid solution composed of both copper and nickel.
2. The α phase is a substitutional solid solution consisting of both Cu and Ni atoms, and having an FCC crystal structure.
3. Two-phase α + L region at equilibrium.

5.9 Determination of phase amount (Lever Rule)



Lastly, we are interested in the relative amounts of each phase present in the alloy. These amounts are normally expressed as weight percent (wt %).

1. Locate composition and temperature in diagram.
2. In two phase regions draw the tie line or isotherm.
3. Fraction of a phase is determined by taking the length of the tie line to the phase boundary for the other phase, and dividing by the total length of tie line.

- The sum of their mass fractions must be equal to unity

$$W_\alpha + W_L = 1$$

- The mass of one of the components that is present in both of the phases must be
- equal to the mass of that component in the total alloy

$$W_\alpha C_\alpha + W_L C_L = C_0$$

$$W_L = \frac{C_\alpha - C_0}{C_\alpha - C_L}$$

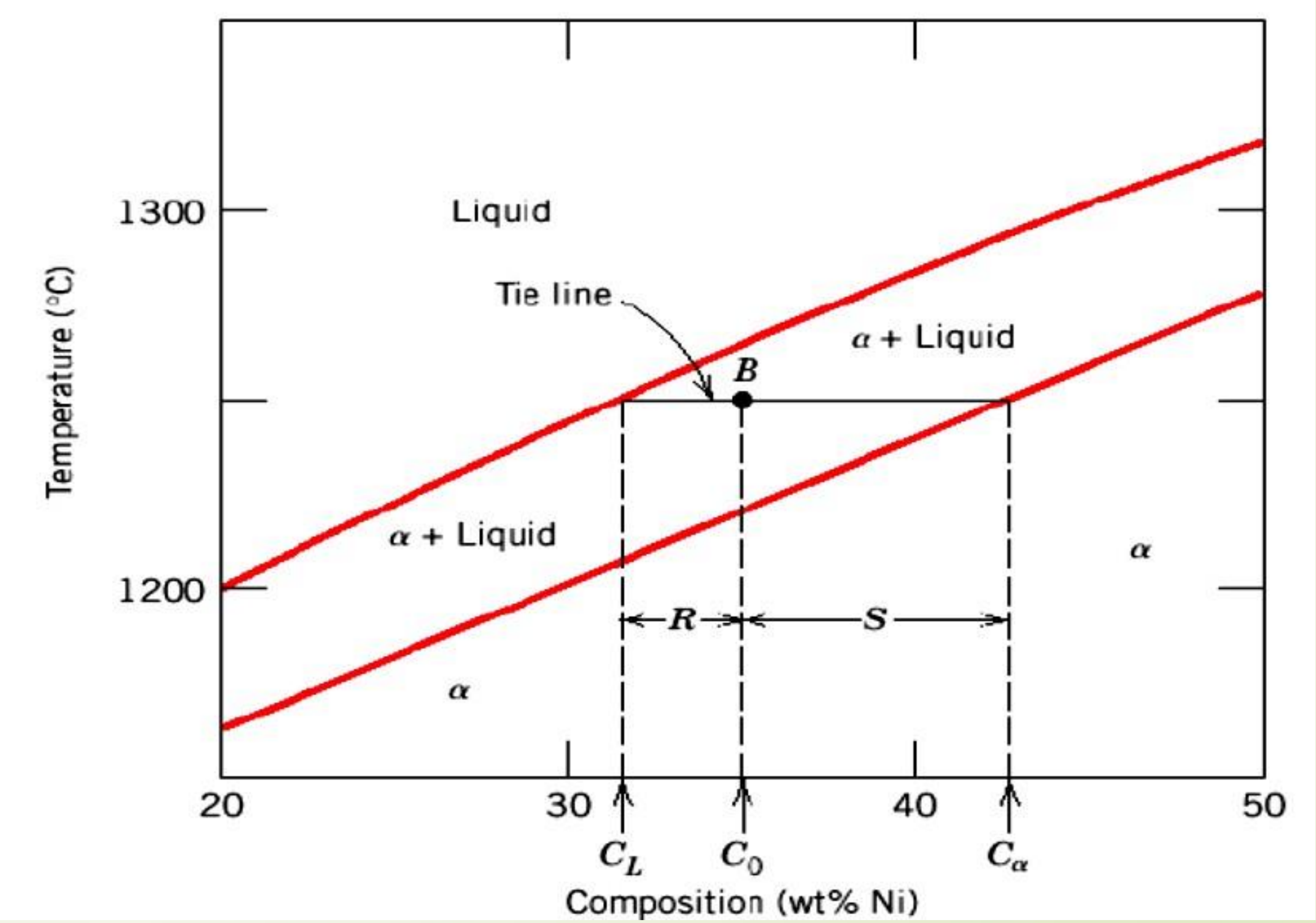
$$W_\alpha = \frac{C_0 - C_L}{C_\alpha - C_L}$$

$C_o = 35$ wt. %, $C_L = 31.5$ wt. %, $C_\alpha = 42.5$ wt. %

Mass fractions:

$$W_L = S / (R+S) = (C_\alpha - C_o) / (C_\alpha - C_L) = 0.68$$

$$W_\alpha = R / (R+S) = (C_o - C_L) / (C_\alpha - C_L) = 0.32$$



Ex/ For figure above, Calculate the amount of each phase present in 1 kg of a 50 wt.% Ni- 50 wt.% Cu alloy at a) 1400°C b) 1300°C c) 1200°C.

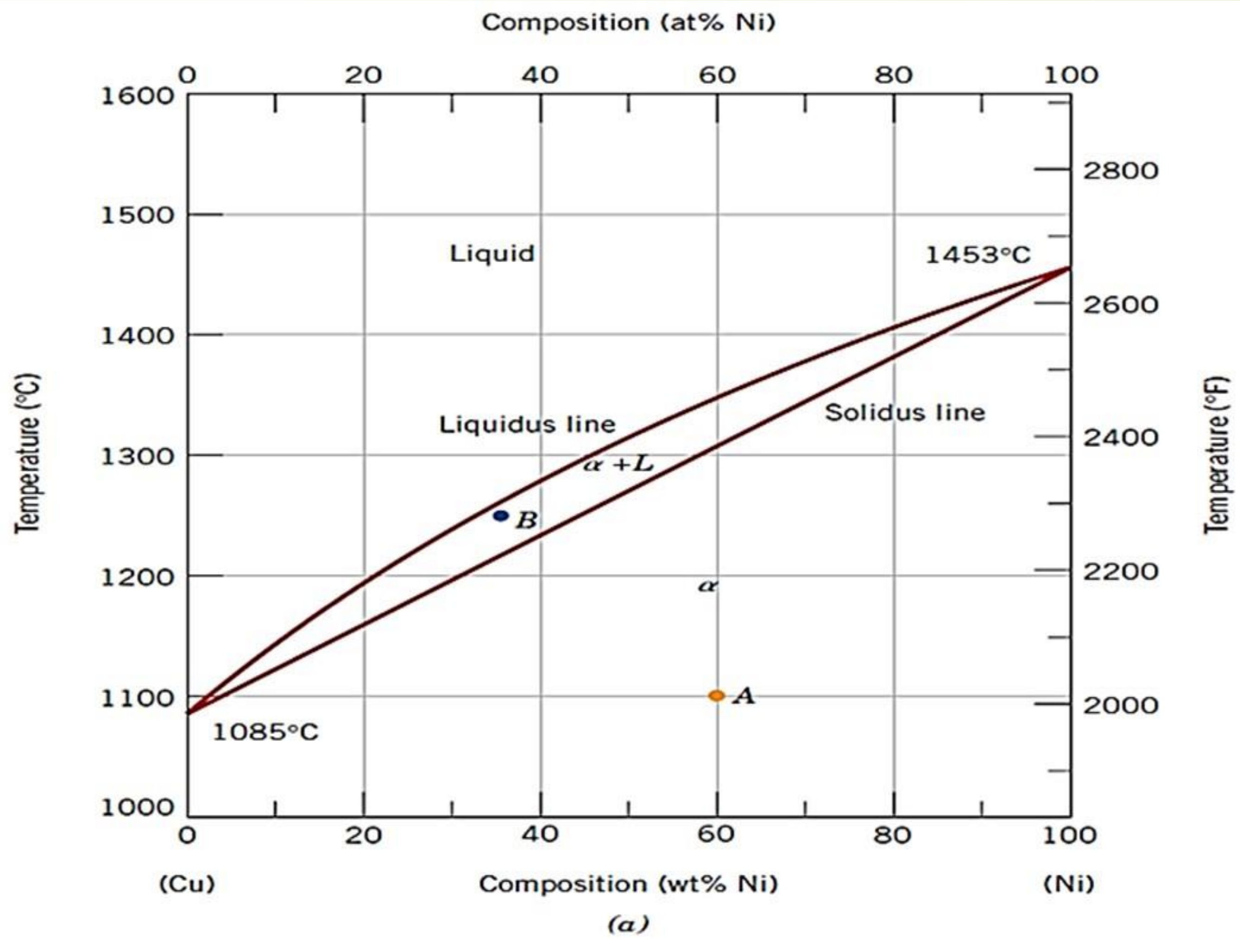
Sol/

a. At 1400°C, we are in the liquid (L) region of the phase diagram. Therefore, we have 1 kg of liquid (L).

b. At 1300°C, we are in the solid + liquid (α+L) region of the phase diagram. Here we must use the lever rule to calculate the mass fraction of each phase.

$$W_L = \frac{60-50}{60-45} \times 100 = 67\% \quad , \quad W_\alpha = \frac{50-45}{60-45} \times 100 = 33\%$$

a. At 1200°C, we are in the solid (α) region of the phase diagram. Therefore, we have 1 kg of solid (α).



5.10 **Binary Eutectic system (**partially soluble in each other in the solid state)

- Another type of common and relatively simple phase diagram found for binary alloys is shown in Figure 8.3 for the copper–silver system;
- this is known as a binary eutectic phase diagram. A number of features of this phase diagram are important and worth noting.
- **First of all**, three single-phase regions are found on the diagram

$$L(C_E) \underset{\text{heating}}{\overset{\text{cooling}}{\rightleftharpoons}} \alpha(C_{\alpha E}) + \beta(C_{\beta E})$$

- **α, β**, and liquid. The **α** phase is a solid solution rich in copper; it has silver as the solute component and an FCC crystal structure.
- The **β** phase solid solution also has an FCC structure, but copper is the solute.
- The **α** and **β** phases are considered to include pure copper and pure silver, respectively.

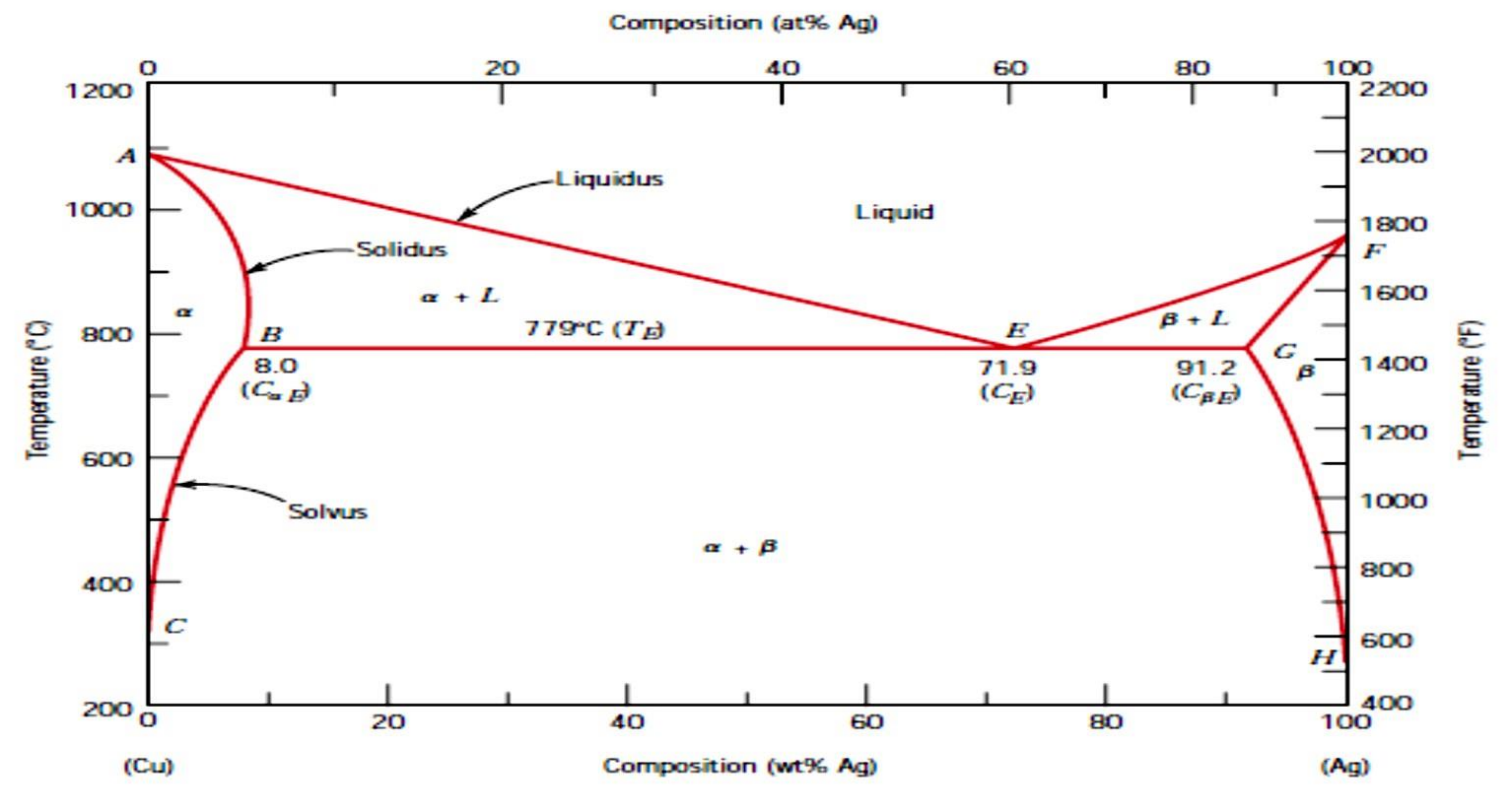


Figure 12.6 The copper–silver phase diagram.

Ex/ For the lead–tin alloy calculates the relative amount of each phase present in terms of mass fraction at150 ^{0}C.

Sol/

(a) Since the alloy consists of two phases, it is necessary to employ

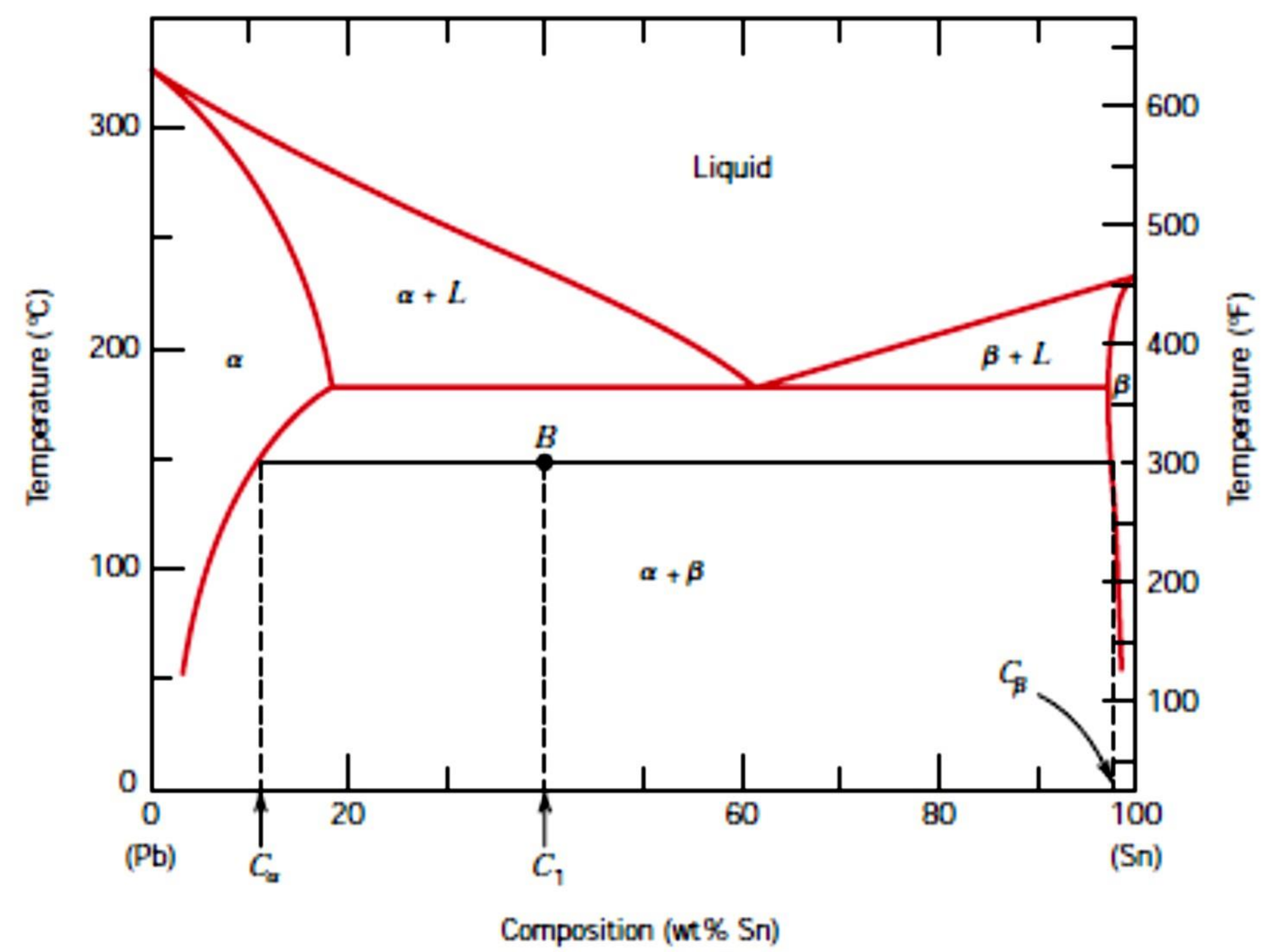
(b) the lever rules. If *C*1 denotes the overall alloy

(c) composition, mass fractions may

(d) be computed by subtracting compositions, in terms of weight percent tin, as follows:

$$W_\alpha = \frac{C_\beta - C_1}{C_\beta - C_\alpha} = \frac{98 - 40}{98 - 10} = 0.66$$

$$W_\beta = \frac{C_1 - C_\alpha}{C_\beta - C_\alpha} = \frac{40 - 10}{98 - 10} = 0.34$$



5.11 Binary Eutectoid system

- In addition to the eutectic, other invariant points involving three different phases are found for some alloy systems.
- One of these occurs for the copper–zinc system at 560 0C (1040 0F) and 74 wt% Zn–26 wt% Cu.
- Upon cooling, a solid δ phase transforms into two other solid phases (γ and e) according to the reaction the reverse reaction occurs upon heating. It is called a eutectoid (or eutectic like) reaction.

$$\delta \underset{\text{heating}}{\overset{\text{cooling}}{\rightleftharpoons}} \gamma + \epsilon$$

5.12 Binary peritectic system

- The **peritectic reaction** is yet another invariant reaction involving three phases at equilibrium.
- With this reaction, upon heating, one solid phase transforms into a liquid phase and another solid phase.
- A peritectic exists for the copper–zinc system (Figure 8.7, point *P*) at 598^0C (1108^0F) and 78.6 wt% Zn–21.4 wt% Cu; this reaction is as follows:

$$\delta + L \underset{\text{heating}}{\overset{\text{cooling}}{\rightleftharpoons}} \epsilon$$

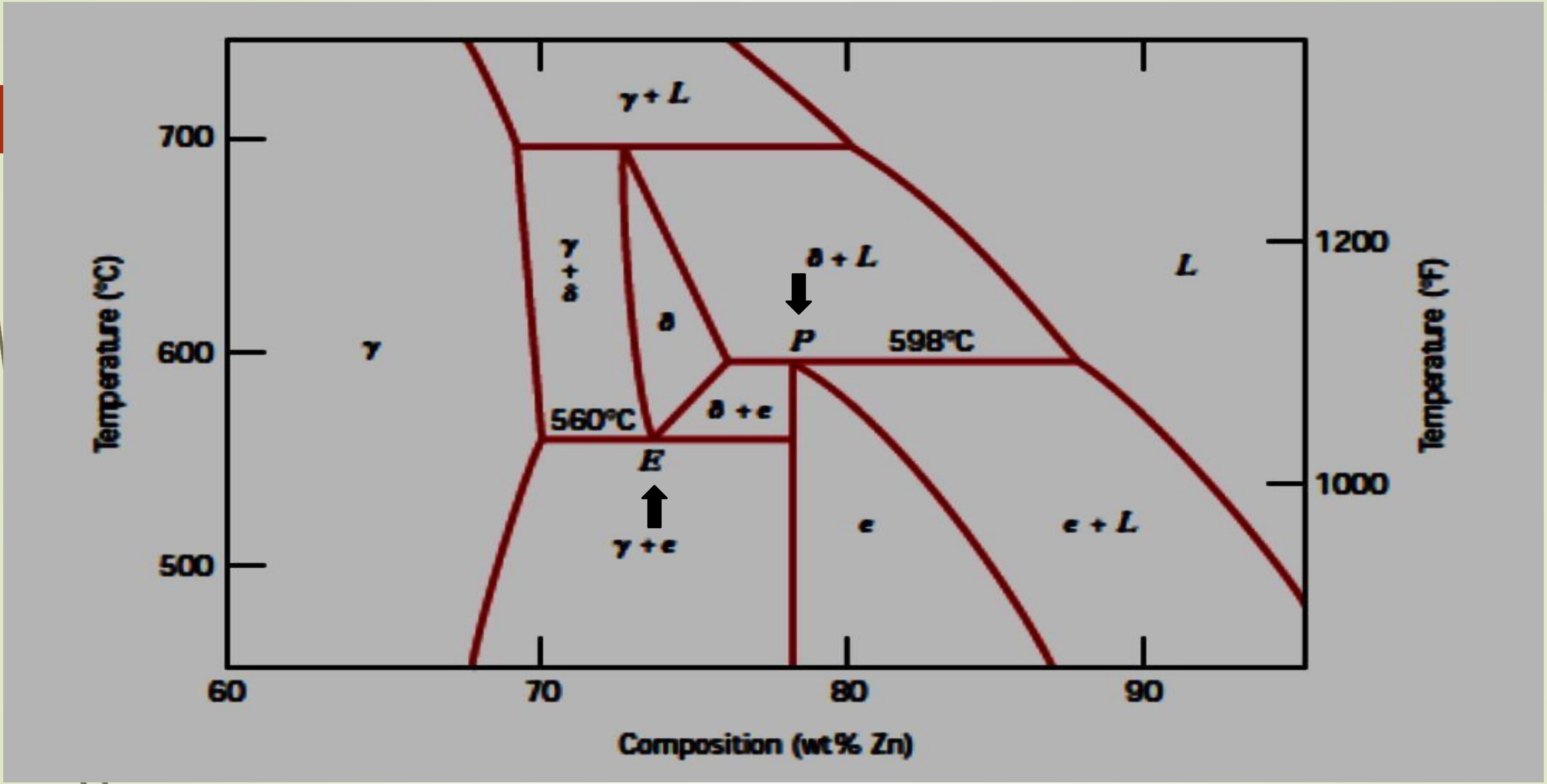
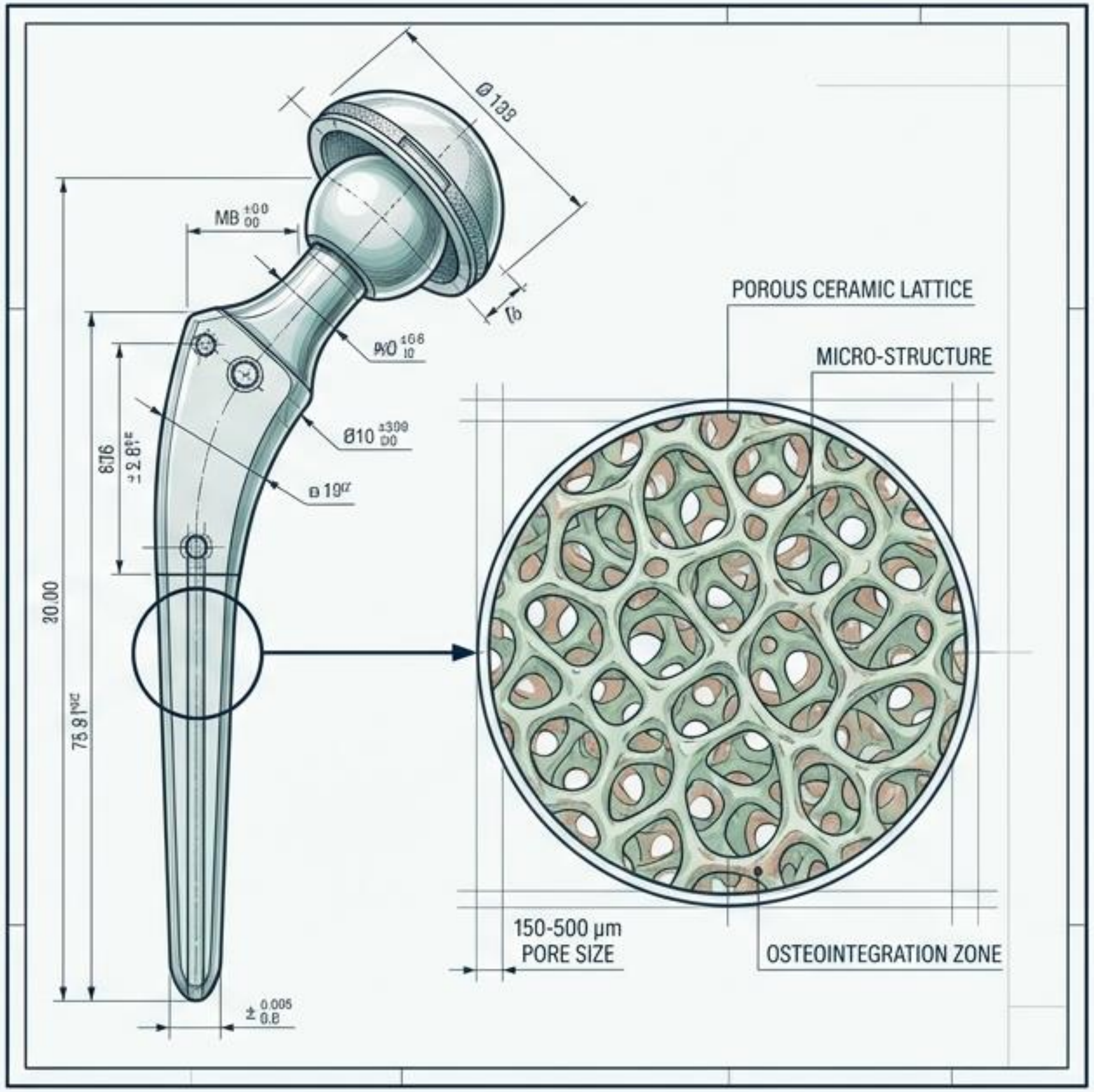


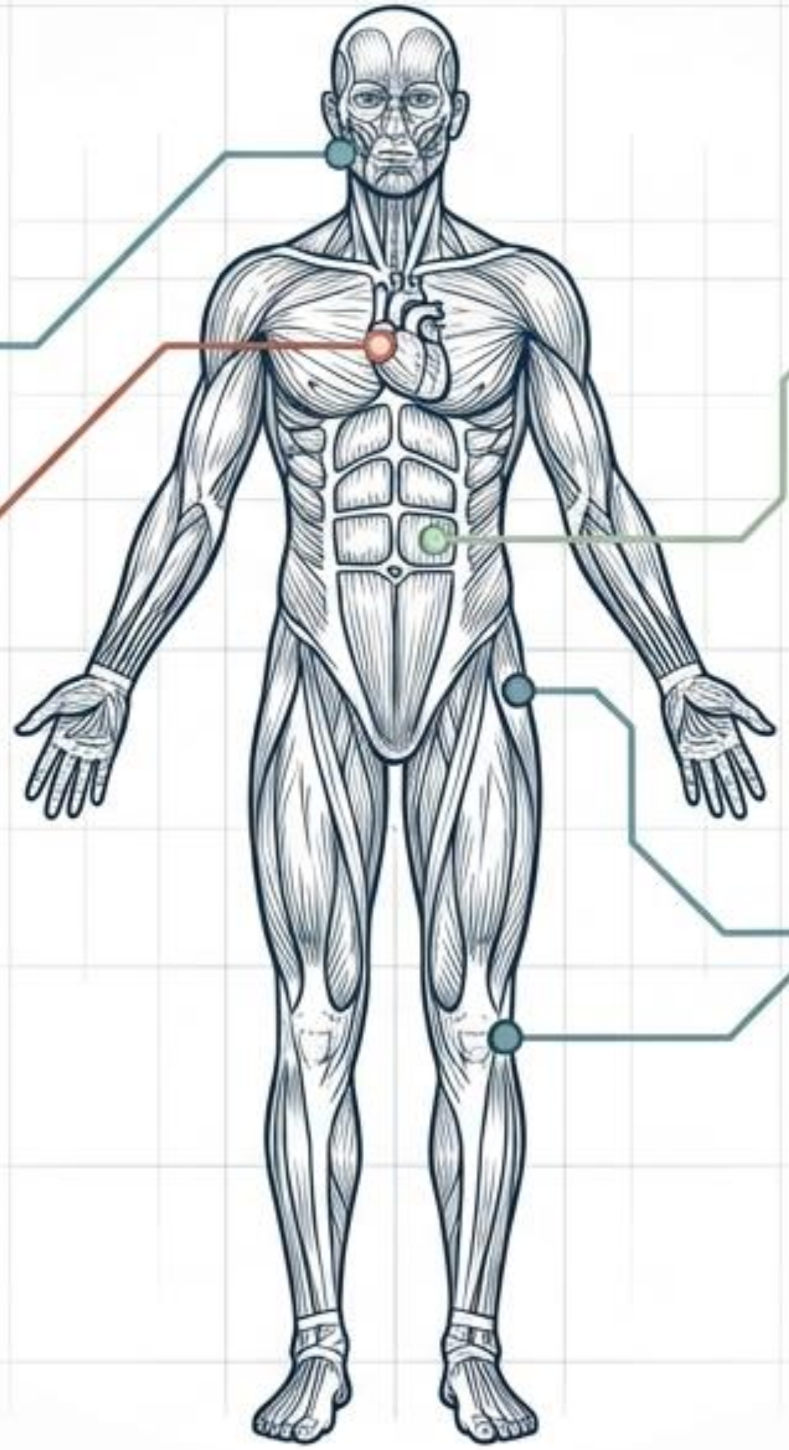
Figure 5.7 A region of the copper–zinc phase diagram that has been enlarged to show eutectoid and peritectic invariant points, labeled ***E*** (560^0C, 74 wt% Zn) and ***P*** (598^0C, 78.6 wt% Zn), respectively.

Bioceramics in Orthopedic and Prosthetic Applications

Lecturer:
Lect. Adwaa M. Al Nasrawee



Clinical Scope: Beyond Skeletal Reconstruction



Maxillofacial & Dental

Dental implants and jaw bone maintenance/reconstruction.

Cardiovascular System

Carbon-based coatings for prosthetic heart valves, utilized specifically for their thrombo-resistant (anti-clotting) behavior in blood-contacting devices.

Structural Spine

Spinal fusion devices and structural bone fillers.

Orthopedic Joints

Wear-resistant bearing surfaces for hip and knee prostheses.

The Tissue Response Spectrum

Bio-Integration Continuum

Rejection → **Encapsulation** → **Integration** → **Replacement**

Toxic

Surrounding tissue dies upon contact. Unsuitable for implantation.

Bioinert

Nontoxic but inactive. Elicits fibrous capsule formation.

Fixation Mode: Morphological (cementing, press-fit, surface irregularities).

Examples: Alumina, Zirconia.

Bioactive

Forms a **direct interfacial chemical bond** with living bone.

Fixation Mode: Bioactive fixation.

Examples: Hydroxyapatite, Bioactive glass.

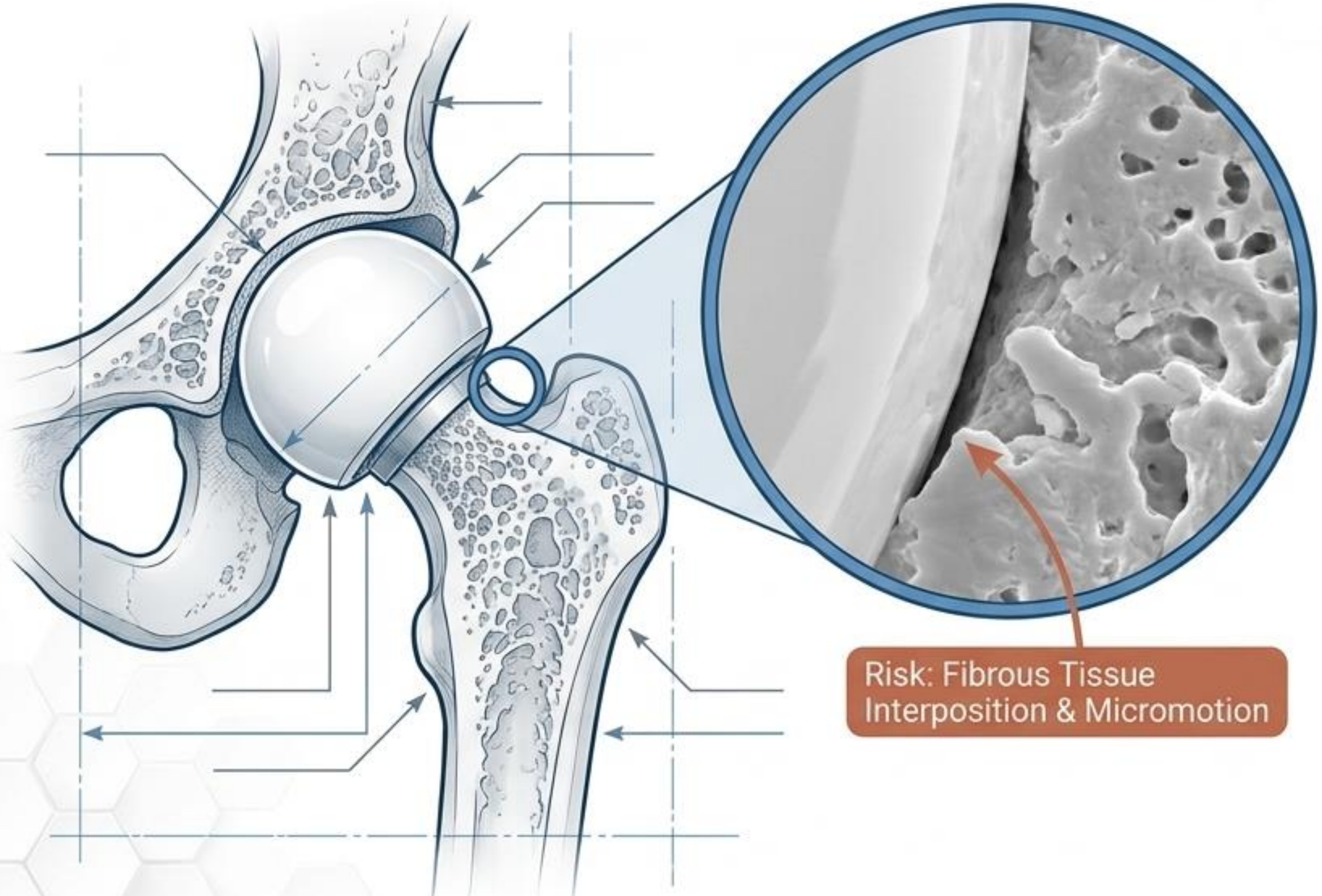
Resorbable

Gradually dissolves as host tissue replaces it.

Fixation Mode: Temporary support.

Examples: Calcium sulphate, Tricalcium phosphate.

Bioinert Ceramics: The Artificial Joint Specialists



Risk: Fibrous Tissue Interposition & Micromotion

Alumina (Al2O3)

High-density, high-purity. Exceptional hardness, low wear, and excellent corrosion resistance. Used in femoral heads, knee components, and bone screws.

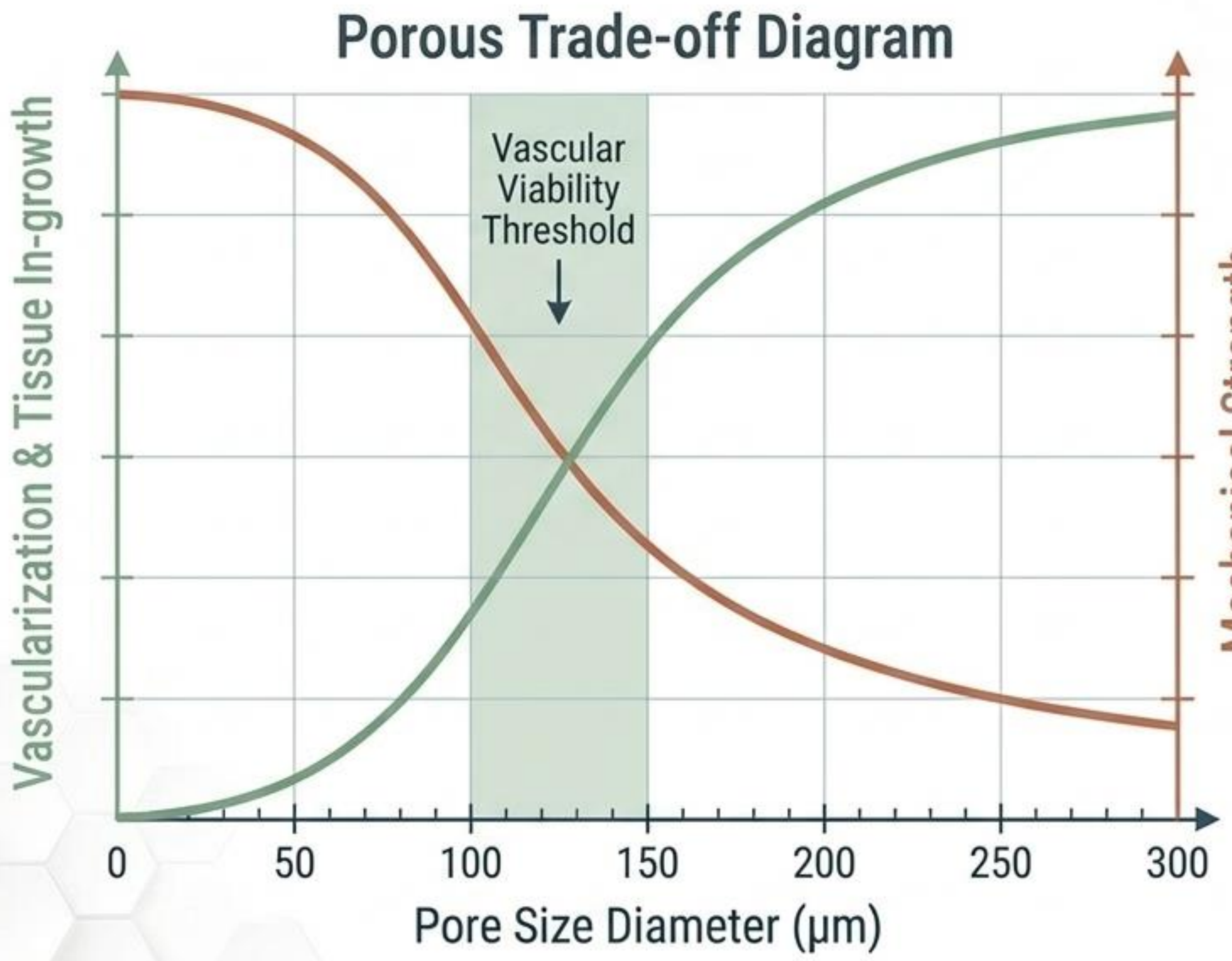
Zirconia (ZrO2)

Offers higher strength and fracture toughness than traditional ceramics. Requires careful design to ensure long-term phase stability.

Warning Panel

Limitation: Because bioinert ceramics lack a direct chemical bond with bone, fixation relies entirely on geometry. This creates a susceptibility to micromotion and fibrous capsule formation, which can compromise long-term implant stability.

The Geometry of Biological Fixation



Biological Fixation

Interconnected pores allow direct bone in-growth, creating mechanical interlocking (ideal for cementless prostheses).

The Vascular Rule

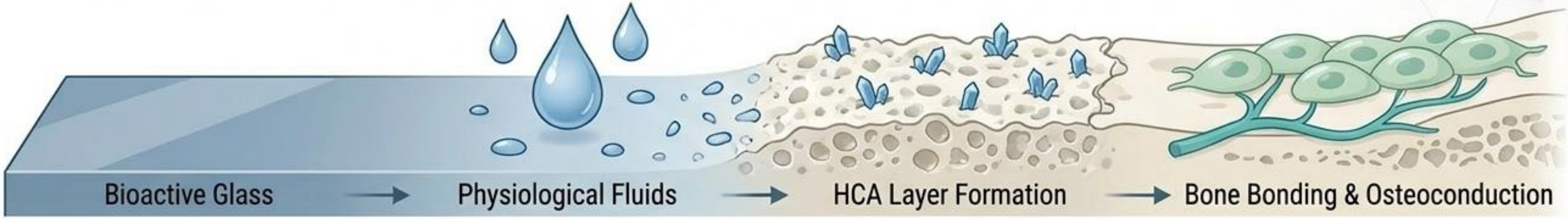
Pore diameters must exceed 100-150 µm. Smaller pores fail to develop adequate vascular tissue, leading to inflammation and reduced stability if micromotion occurs.

Application Constraint

Due to the inverse relationship between porosity and strength, these materials are restricted to coatings, scaffolds, and lower-load applications rather than standalone load-bearing joints.

Bioactive Chemistry and Interfacial Bonding

1. Implantation of bioactive material
2. Reaction with physiological fluids
3. Formation of Hydroxycarbonate Apatite (HCA) layer resembling natural bone mineral
4. Direct cellular adhesion and proliferation of osteogenic cells



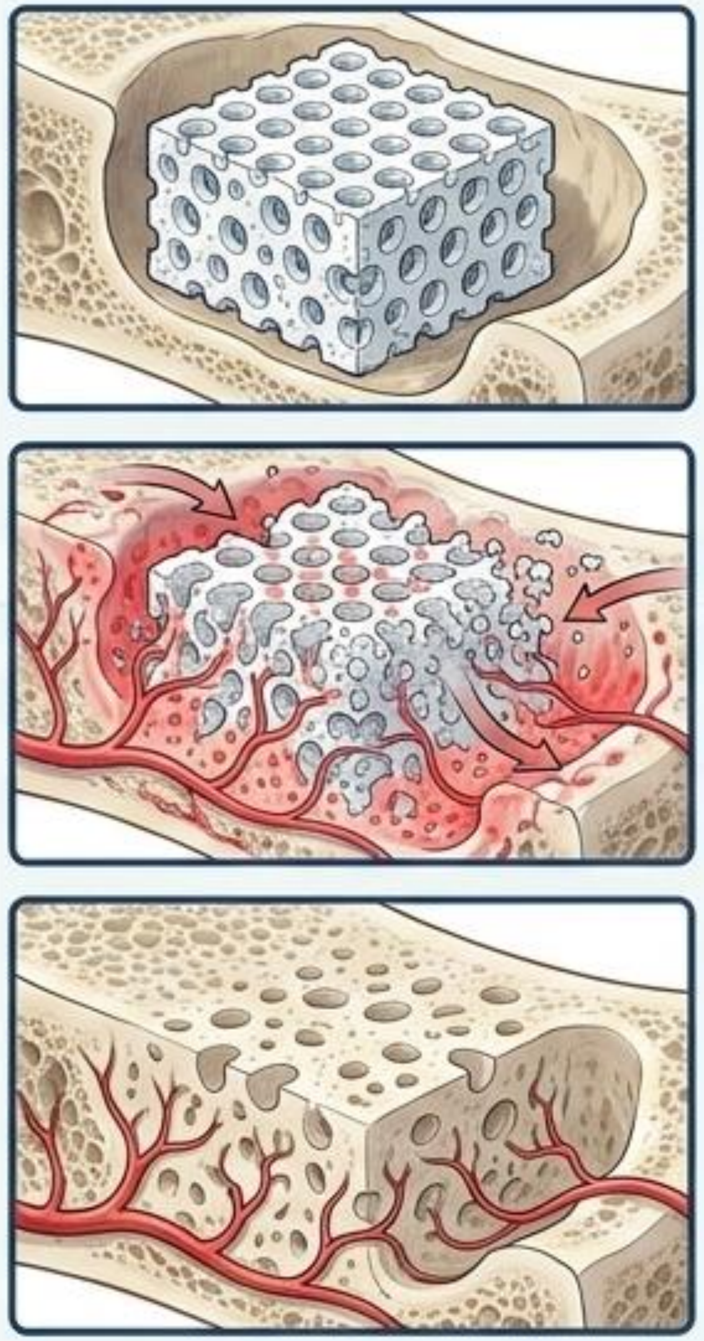
Representative Bioactive Compositions (mol%)

Component	45S5 Bioglass	A/W Glass-Ceramic	KGC Ceravital
SiO_2	45	34.2	46.2
CaO	24.5	44.9	20.2
$Ca(PO_3)_2$	–	0.5	–
MgO	–	4.6	2.9
Na_2O	24.5	–	4.8

Component	45S5 Bioglass	A/W Glass-Ceramic	KGC
CaF_2	45	34.2	25.5
P_2O_5	6	16.3	4.8

45S5 Bioglass is utilized for defect repair, jaw maintenance, and periodontal applications (high bioactivity, low load).

Resorption Dynamics and Synthetic Grafting Standards



Principle: Resorption rate must match tissue repair rate.

7 Essential Requirements for Grafting Materials

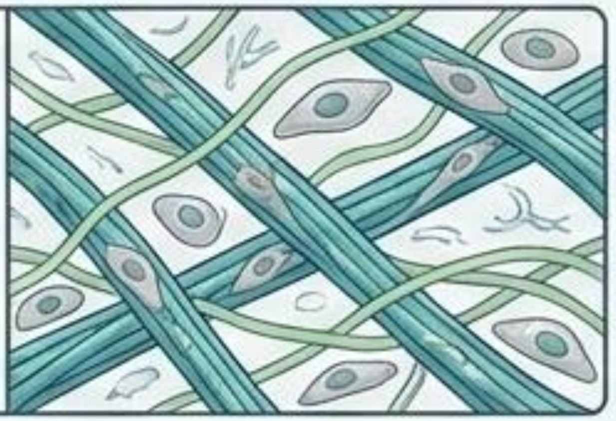
1. Fully biocompatible (non-toxic, non-allergic, non-carcinogenic, non-inflammatory).
2. Capable of stimulating bone induction.
3. Fully resorbable following bone replacement.
4. Radio-opaque (for radiographic tracking).
5. Capable of withstanding clinical sterilization.
6. Cost-effective and stable across temperature/humidity variations.
7. Features sufficient porosity to facilitate bone conduction and growth.

Material Note: Key systems include dicalcium phosphate, tricalcium phosphate, and hydroxyapatite. Utilized as fillers and graft extenders, not bulk load-bearing parts.

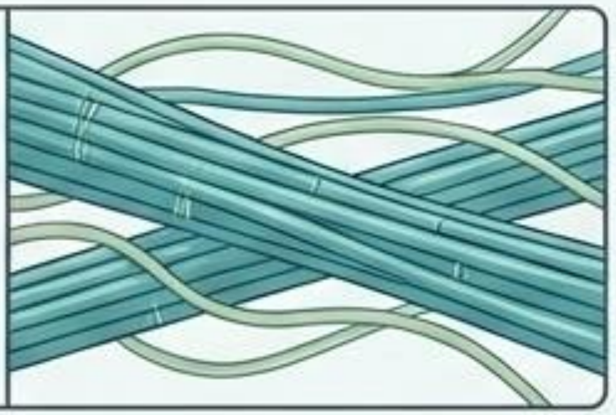
The Biological Baseline: Natural Composites

Structural Sidebar

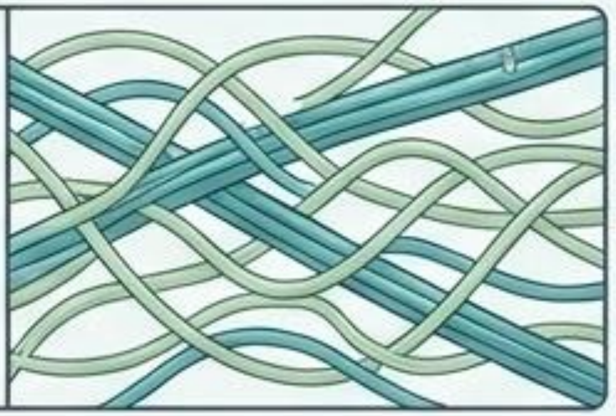
Macroscale soft and hard tissues are organic composites: complex arrays of elastic (elastin) and non-elastic (collagen) fibers suspended suspended in a cellular matrix.



Tendons: Low elastin. Transfers muscle movement directly to bone.



Ligaments: High elastin. Allows inter-bone movement while preventing joint dislocation.



	Tissue / Material	Tensile Strength (MPa)	Ultimate Elongation %
1.	Tendon (Low elastin)	53	9.4
2.	Skin (High elastin)	7.6	78.0
3.	Pure Elastin	1	100
4.	Pure Collagen	50-100	10

Synthetic biomaterials aim to replicate these dynamic mechanical properties to ensure physiological compatibility.

Mechanical Limitations vs. Engineering Interventions

The Ceramic Deficit

Inherent Brittleness

Susceptibility to slow crack growth

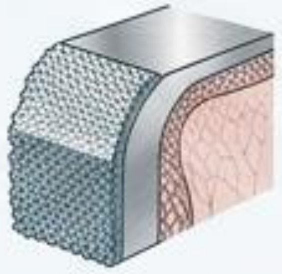
Vulnerability to cyclic fatigue under load

Uncertain clinical lifetime under complex stress conditions

The Engineering Interventions

Solution 1: Composites

Embedding reinforcing phases within a matrix to increase flexural strength, increase strain to failure, decrease elastic modulus, and mimic natural bone. (e.g., A/W glass-ceramic ceramic reinforced with tetragonal zirconia achieves 700 MPa bending strength and 4 MPa·m1/2 fracture toughness).



Solution 2: Coatings

Applying bioactive surfaces to high-strength metallic substrates to combine mechanical reliability with biological fixation.

The Bioceramic Composite Matrix

Type 1 (Nearly Inert)

Matrix	Reinforcing Phase
Polyethylene or Poly(methyl methacrylate)	Carbon fiber
Carbon	Epoxy resin
SiC	Alumina / Stainless steel

Type 3 (Bioactive)

Matrix	Reinforcing Phase
Bioglass	Stainless steel or Titanium fibers
Collagen or Polyethylene	HA
Poly(methyl methacrylate)	A/W glass-ceramic
Toughened ZrO2	Phosphate-silicate-apatite glass fiber

Type 2 (Porous Ingrowth)

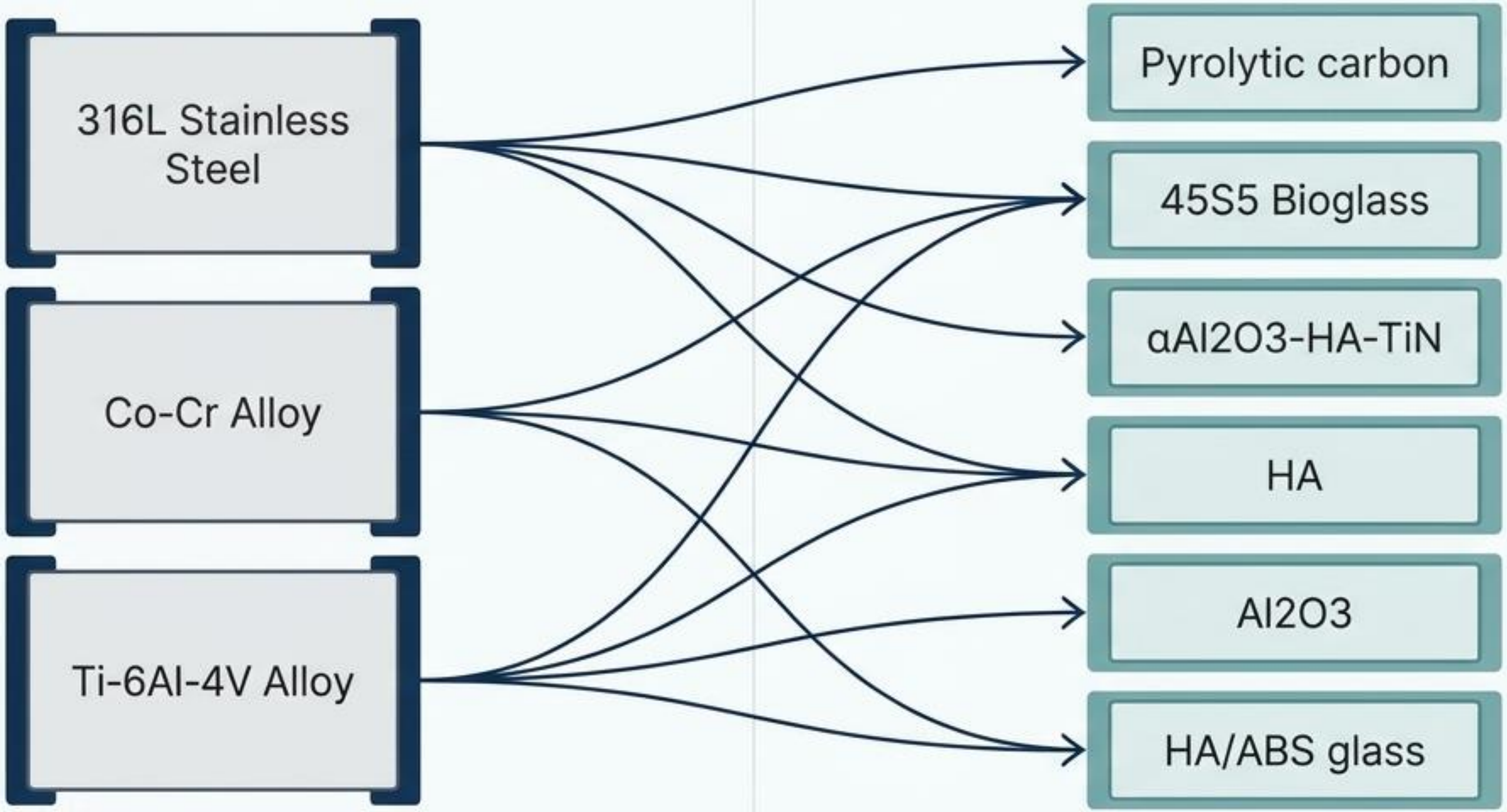
Matrix	Reinforcing Phase
Coral HA yoniopora	(Standalone / Unreinforced)
DL polylactic acid	(Standalone / Unreinforced)

Type 4 (Resorbable)

Matrix	Reinforcing Phase
Poly hydroxy buturate, or PLA/PGA	HA
PLA/PGA	PLA/PGA fibers

HA = Hydroxyapatite | PLA = Polylactic acid | PGA = Polyglycolic acid

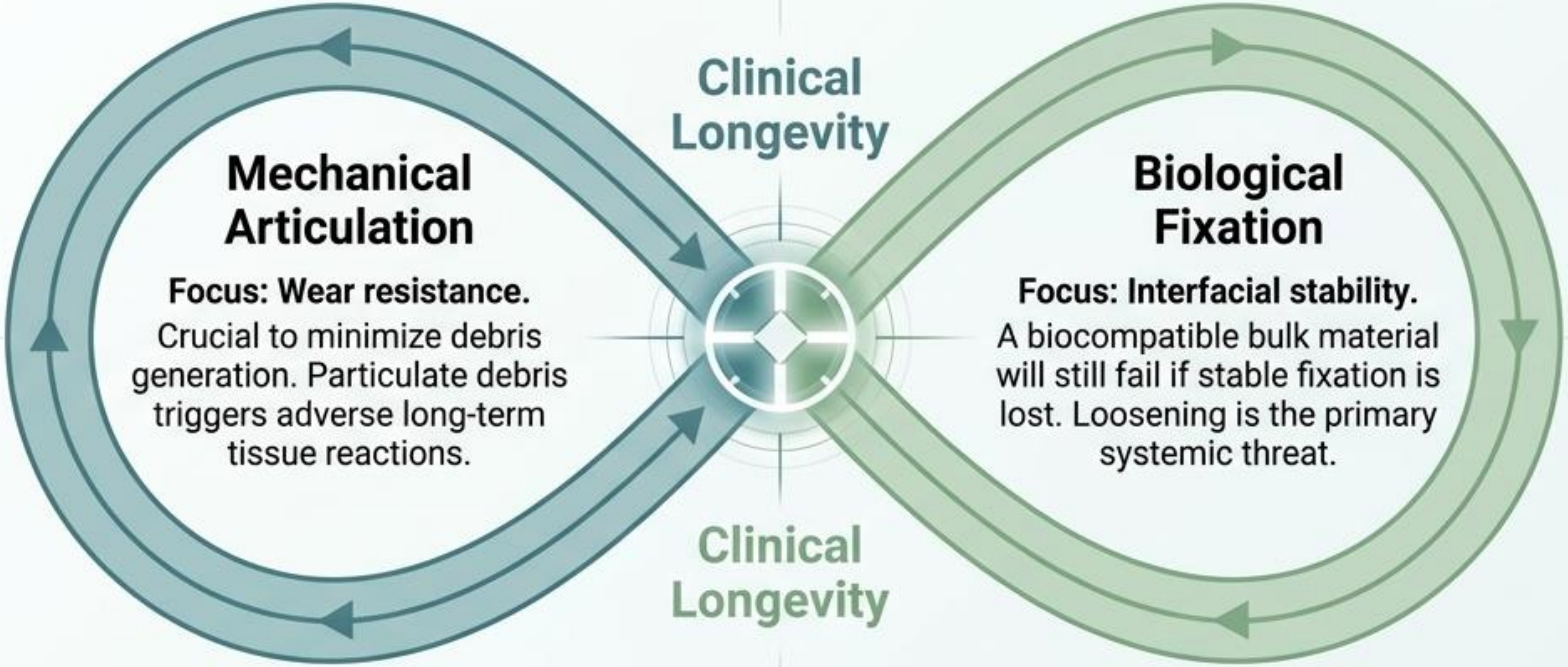
Substrate-Coating Architecture



Process Sidebar

Plasma spray coating is the preferred clinical method for applying Hydroxyapatite (HA) to porous metal surfaces, successfully combining high-strength mechanical support with bioactive implant fixation.

System Integration: Designing for Clinical Longevity



Clinical Longevity

Mechanical Articulation

Focus: Wear resistance.
Crucial to minimize debris generation. Particulate debris triggers adverse long-term tissue reactions.

Biological Fixation

Focus: Interfacial stability.
A biocompatible bulk material will still fail if stable fixation is lost. Loosening is the primary systemic threat.

Clinical Longevity

Synthesis Panel

There is no single universal bioceramic. Prosthetic design is a deliberate optimization exercise: prioritizing extreme wear resistance (Bioinert Alumina/Zirconia), vascular porosity (>100μm structures), direct bone bonding (HCA-forming Bioactive glass), or controlled temporary healing support (Resorbable Calcium Phosphates) based on specific clinical loading demands.

Academic Assessment & Synthesis

1. Why are alumina and zirconia important in artificial joint prostheses?
2. What is the difference between morphological fixation and biological fixation?
3. Why is pore size important in porous ceramics?
4. How does bioactive glass bond to bone?
5. Why are resorbable ceramics more suitable for temporary bone substitution than for major articulating prosthetic parts?

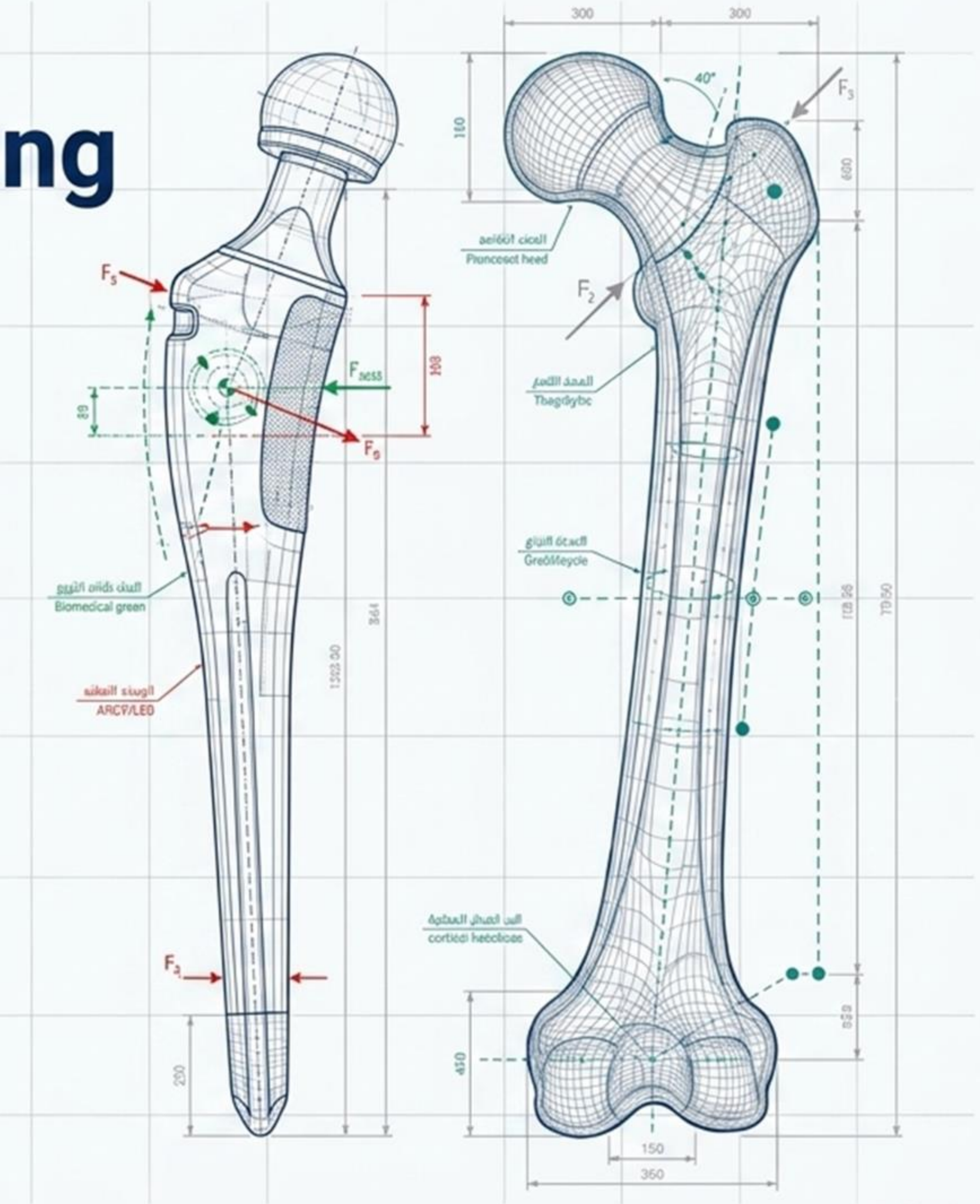
End of Module

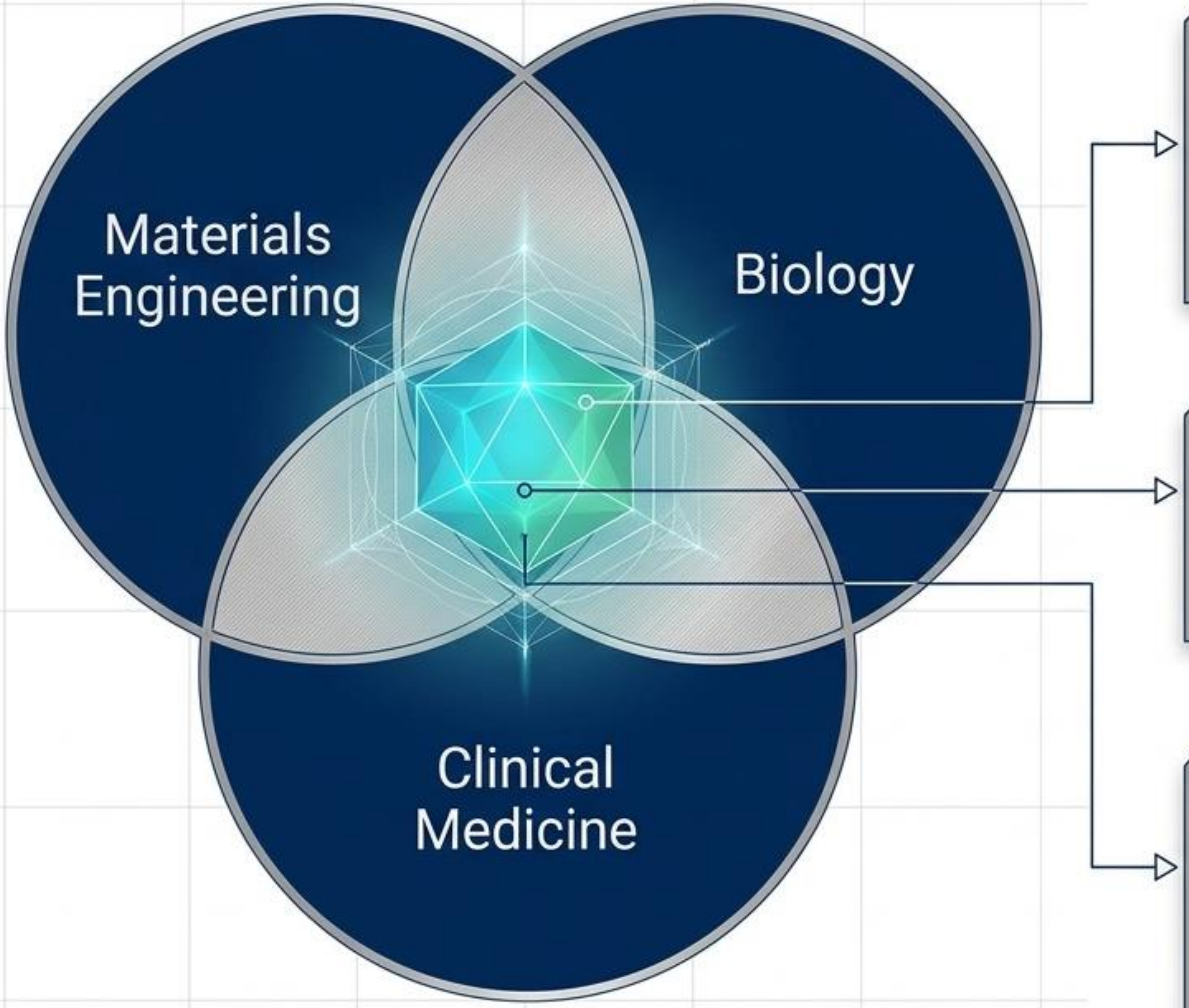
Bioceramics in Orthopedic and Prosthetic Applications

Biomaterials Engineering in Prosthetics: Mechanical Analysis of Metal Alloys and Clinical Applications

Dedicated to Students of Prosthetic and Medical Equipment Techniques

By Lect. Adwaa M. Al Nasrawee





Biomaterial

An engineered or synthetic material designed to interact with biological systems for a medical purpose (replacement, repair, or support of body functions).

Biological Material

A natural material produced by a biological system, such as bone and collagen.

Biocompatibility

The ability of a material to perform its desired function effectively within the body without eliciting any harmful local or systemic response, allergy, or immune rejection.

Medical Material Selection Methodology (Engineering Decision)

Phase 1: Medical Problem Analysis

Precise description of the missing or damaged function.

Phase 2: Bio-Environment Characterization

Studying the body's effect on the material (like corrosion in a saline environment) and the material's effect on the body.

Phase 3: Lifespan Determination

Defining the period of use: Is it a temporary implant (weeks for fracture healing) or permanent (years for an artificial joint)?

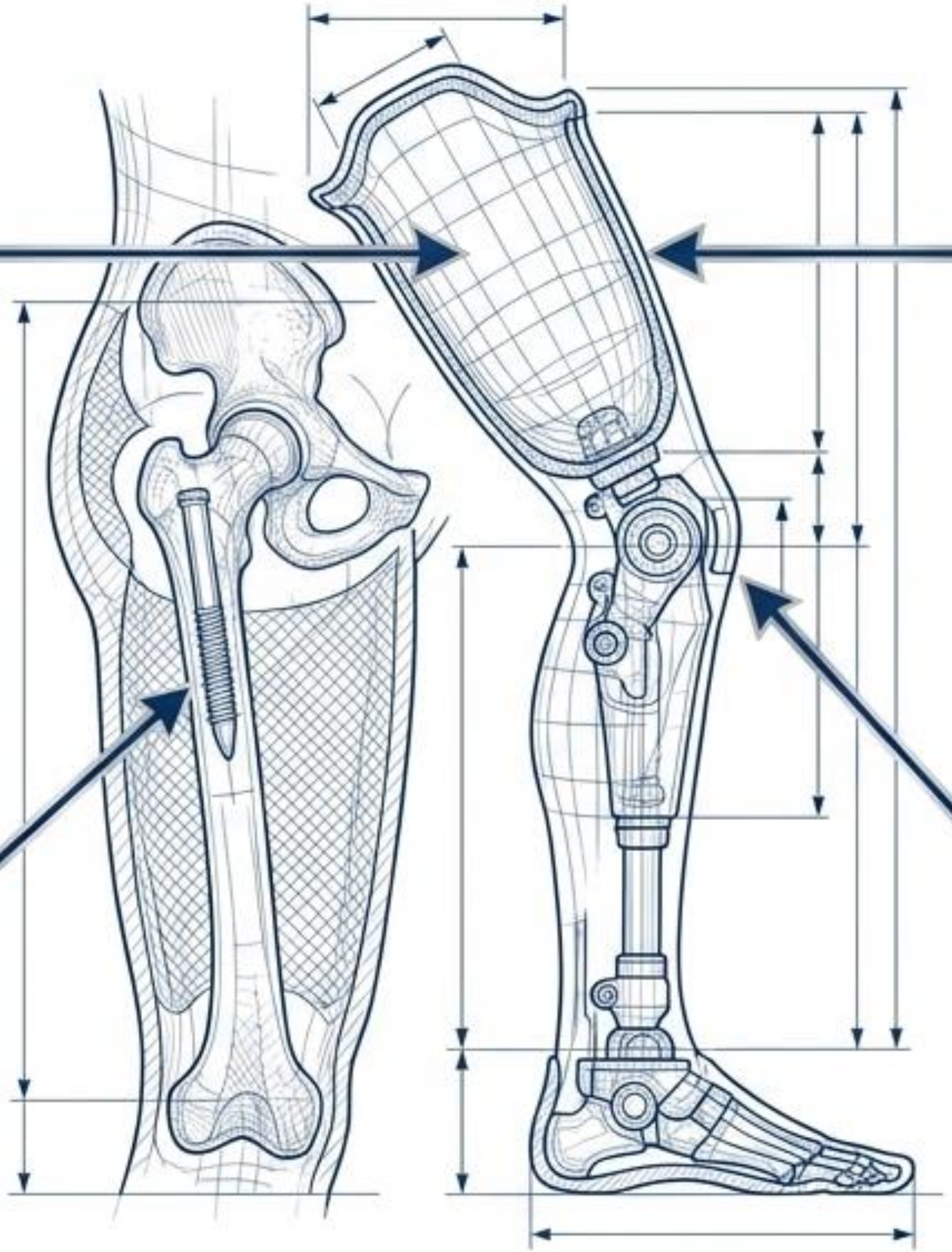
Phase 4: Toxicology (Safety Evaluation)

Comprehensive understanding of safe human use standards and cellular toxicity.

Phase 5: Final Engineering Decision

Choosing the optimal material based on the intersection between mechanical properties and clinical requirements.

Prosthetic Architecture



Liner

Made of medical silicone or polyurethane.

High elasticity and safe skin contact.

(Duration: 12-24 hours daily).

Osseointegration Implant

Titanium alloys.

Direct and safe bonding with the bone.
(Duration: 3-12 months for permanent bonding).

Socket

Carbon fiber or thermoplastic.

Provides lightweight characteristics and structural rigidity.

(Duration: Months to years).

Knee Joint

A blend of aluminum, titanium, and steel.

Mechanically precise to withstand movement and stress.

(Lifespan: 10-15 years).

Metals as Biomaterials:
The Driving Force and Engineering Challenges

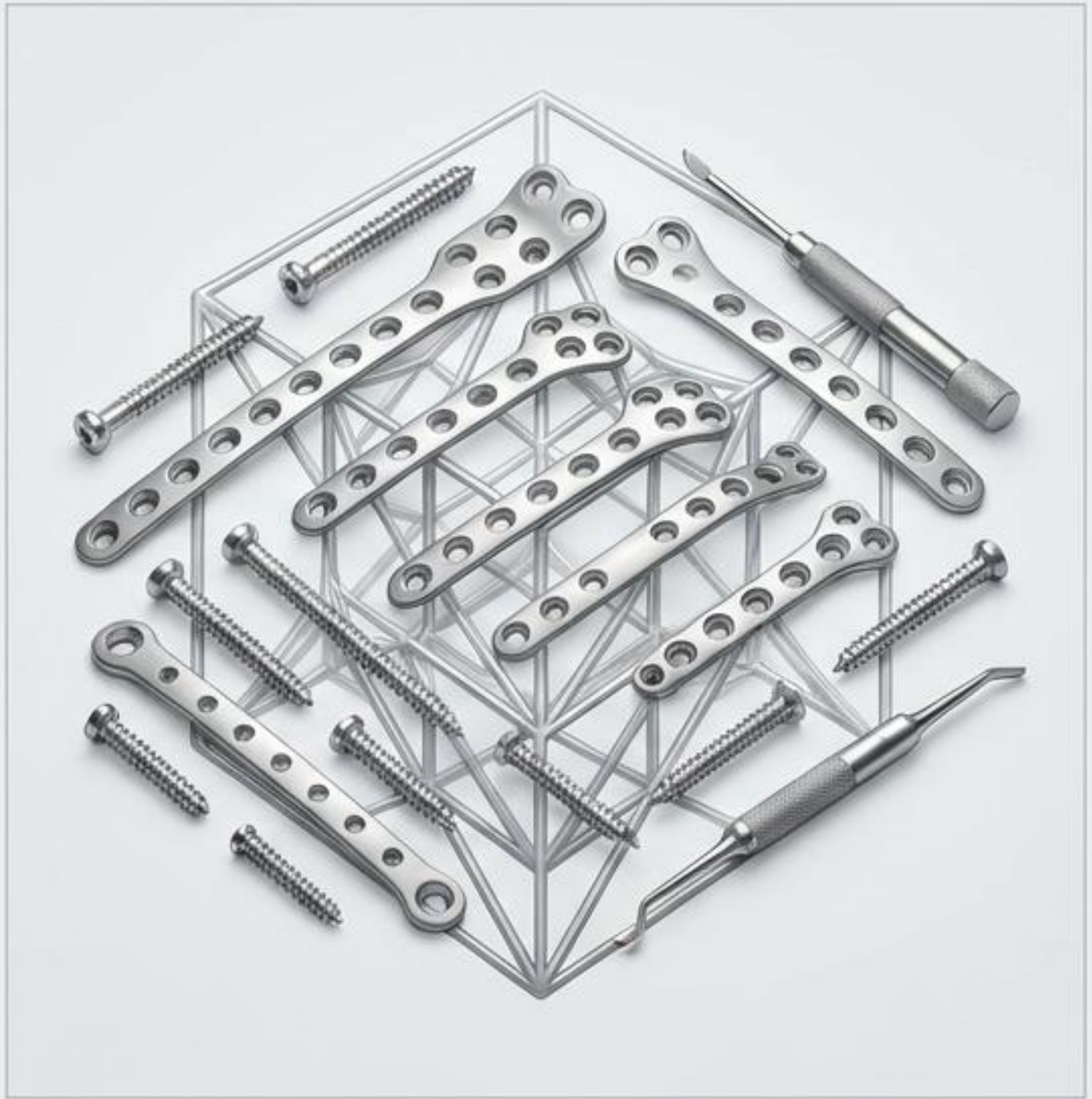
The Drawbacks
(What we engineer around)

- Very High Modulus (of elasticity) compared to bone.
- Susceptibility to chemical corrosion in the physiological environment.
- Potential for metal ion sensitivity (cellular toxicity).
- High specific density (heavy weight).

The Advantages
(Why we rely on them?)

- Exceptional hardness and resistance to fatigue and impact.
- High wear resistance.
- Ease of engineering fabrication and sterilization.
- Some possess ‘shape memory’ properties.

316L Stainless Steel



Core Composition (Why 316L?)

- **Chromium (17-20%):** To form a protective layer.
- **Nickel (12-14%):** To stabilize the Face-Centered Cubic (FCC) crystalline structure at room temperature.
- **Molybdenum (2-4%):** To prevent pitting corrosion in a saline environment.
- **Carbon (Max 0.03%):** The 'L' stands for Low Carbon to enhance corrosion resistance.

Optimal Application

Temporary Implants like bone plates and fracture fixation screws.

Engineering Limitation

Potential for corrosion when subjected to high stress and oxygen depletion over long periods (e.g., under the heads of fixation screws).

Cobalt-Chromium Alloys (Co-Cr): Absolute Strength

Approved Types

- **Cast (CoCrMo):** Used in dentistry and artificial joints.
- **Wrought (CoNiCrMo):** Designated for joint stems that bear exceptionally heavy loads.

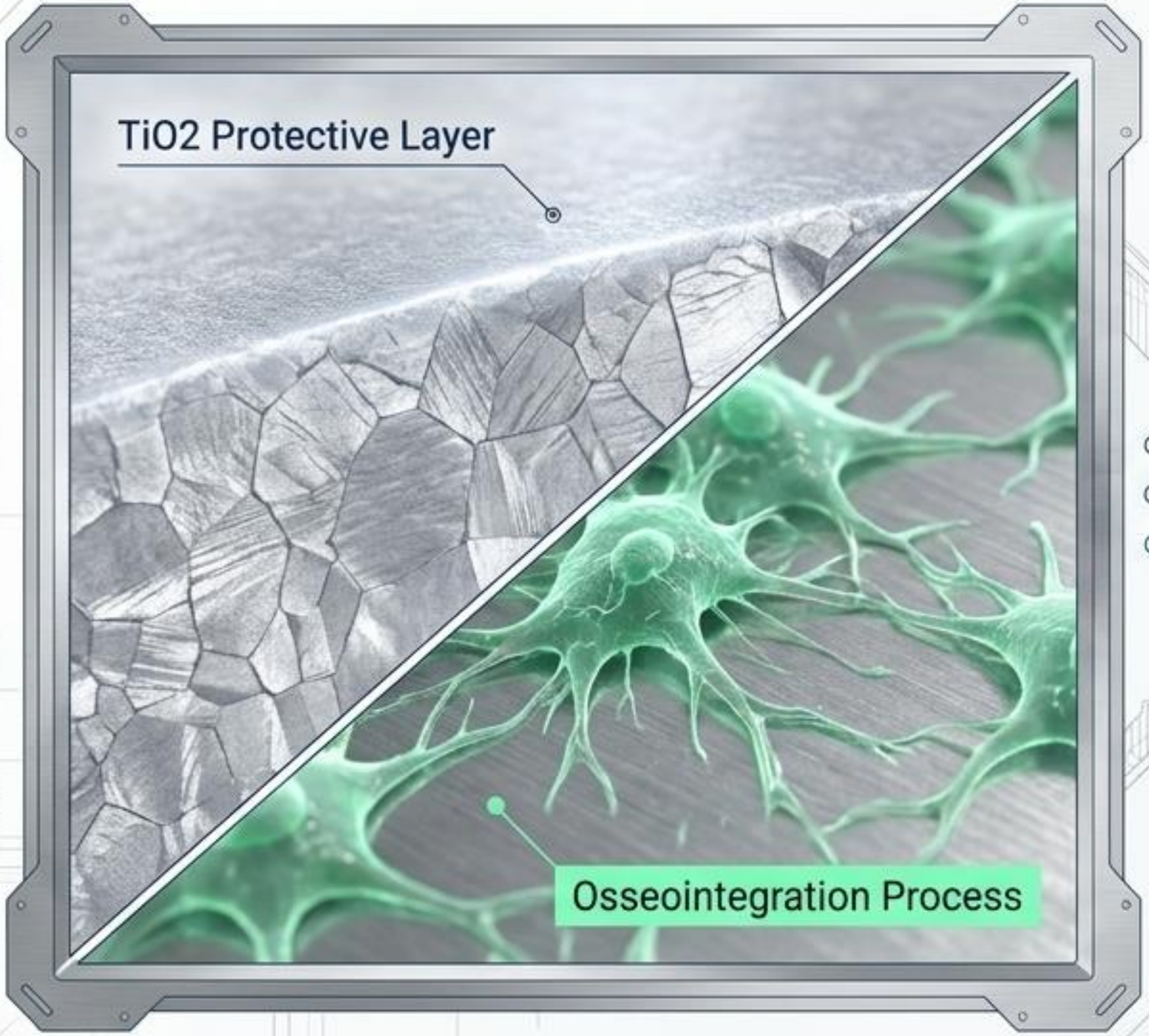
Mechanical Properties

Possesses the highest levels of strength and wear resistance among all medical alloys.

Manufacturing & Clinical Challenges

- Corrosion byproducts can be more toxic than steel (may cause allergic reactions to cobalt or chromium ions).
- Considered one of the hardest metals to fabricate engineering-wise.

Titanium and its Alloys:
The Gold Standard for Permanent Implants



Chemical Engineering (Ti-6Al-4V)

Addition of Aluminum (Alpha phase stabilizer) and Vanadium (Beta phase stabilizer).
Result: An alloy stronger than pure titanium with exceptional lightness.

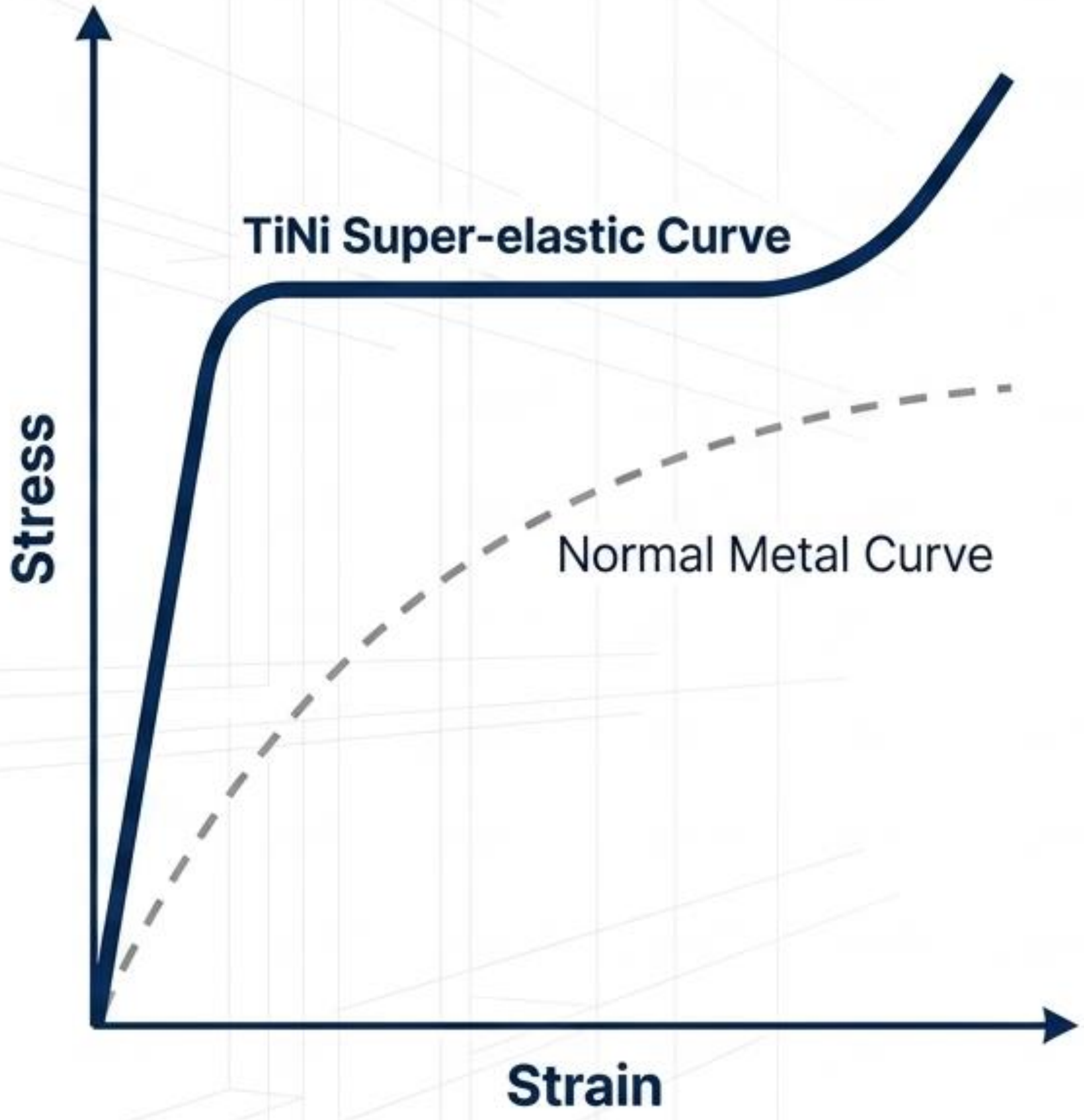
Biological Superiority

- Superior corrosion resistance due to the formation of a protective layer (TiO2).
- Osseointegration: A unique ability to directly and actively bond with living bone tissue.

Point of Weakness (Friction)

Very poor wear resistance. Therefore, it is prohibited for use in the articulating surfaces of moving joints unless subjected to advanced surface treatments (Ion Implantation).

Nitinol (TiNi): Shape Memory Alloys



Shape Memory Effect (SME)

The alloy's ability to recover its original geometric shape after plastic deformation, simply by raising its temperature (relies on Martensitic transformation).

Super-elasticity

A unique mechanical response where Stress does not increase with Strain in the traditional metallic way; it acts like a super-elastic spring.

Advanced Applications

Vascular stents, orthodontic wires, and cranial clamps.

The Major Challenge: Stress Shielding

15 - 30 GPa — Cortical Bone

~ 116 GPa — Titanium Alloys

~ 190 GPa — Stainless Steel

210 - 253 GPa — Cobalt-Chrome Alloys

Closest to bone

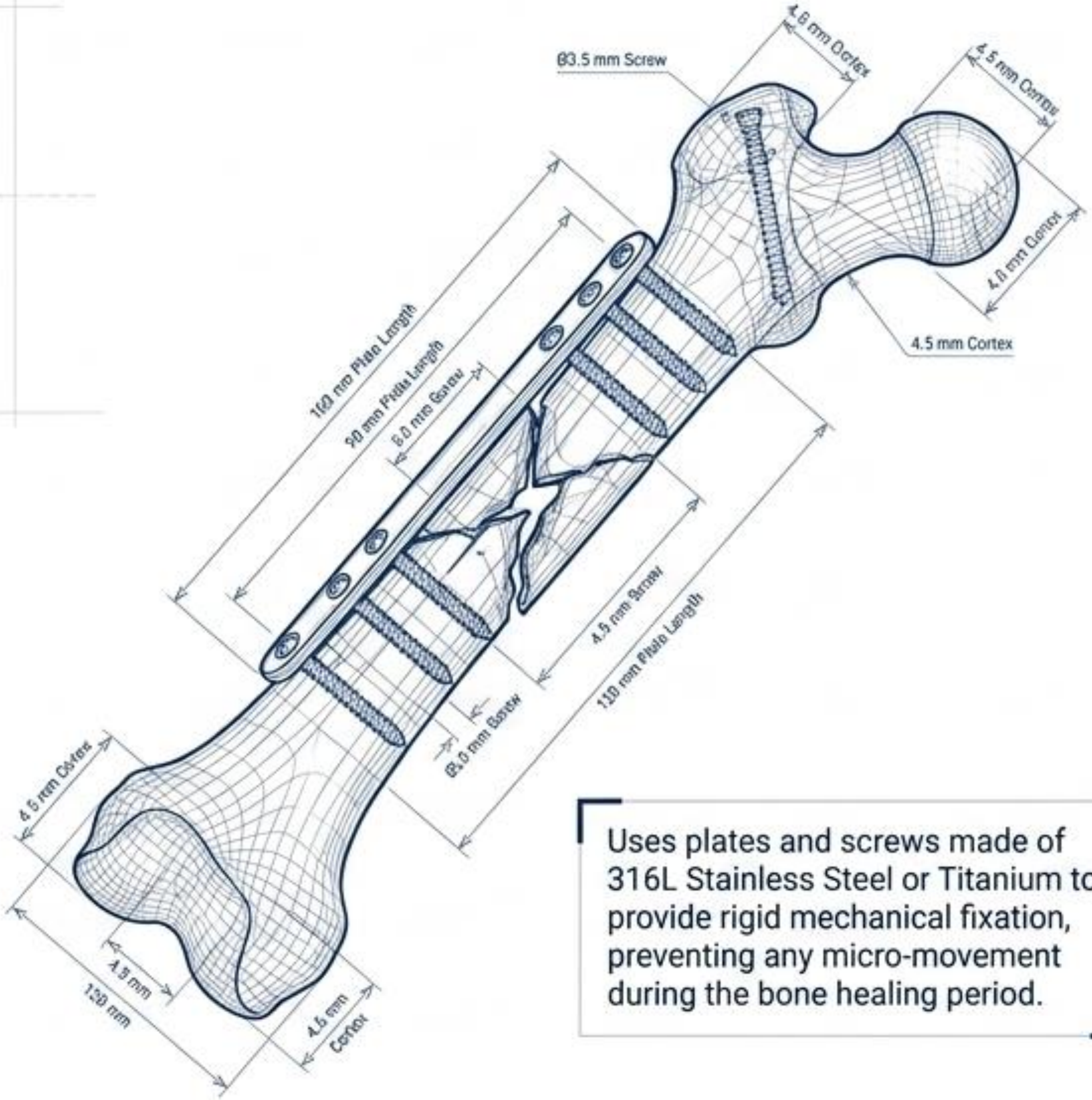
Huge Elasticity Mismatch

The Problem (Bold): When the metal's modulus of elasticity is much higher than the bone's**, the metal bears the entire mechanical load**, leading to **the atrophy and weakening of the bone** surrounding the implant.

Clinical Conclusion (Bold): Titanium possesses a lower modulus of elasticity among solid metals, which minimizes stress shielding and makes it the primary engineering choice for permanent implants inside the bone.

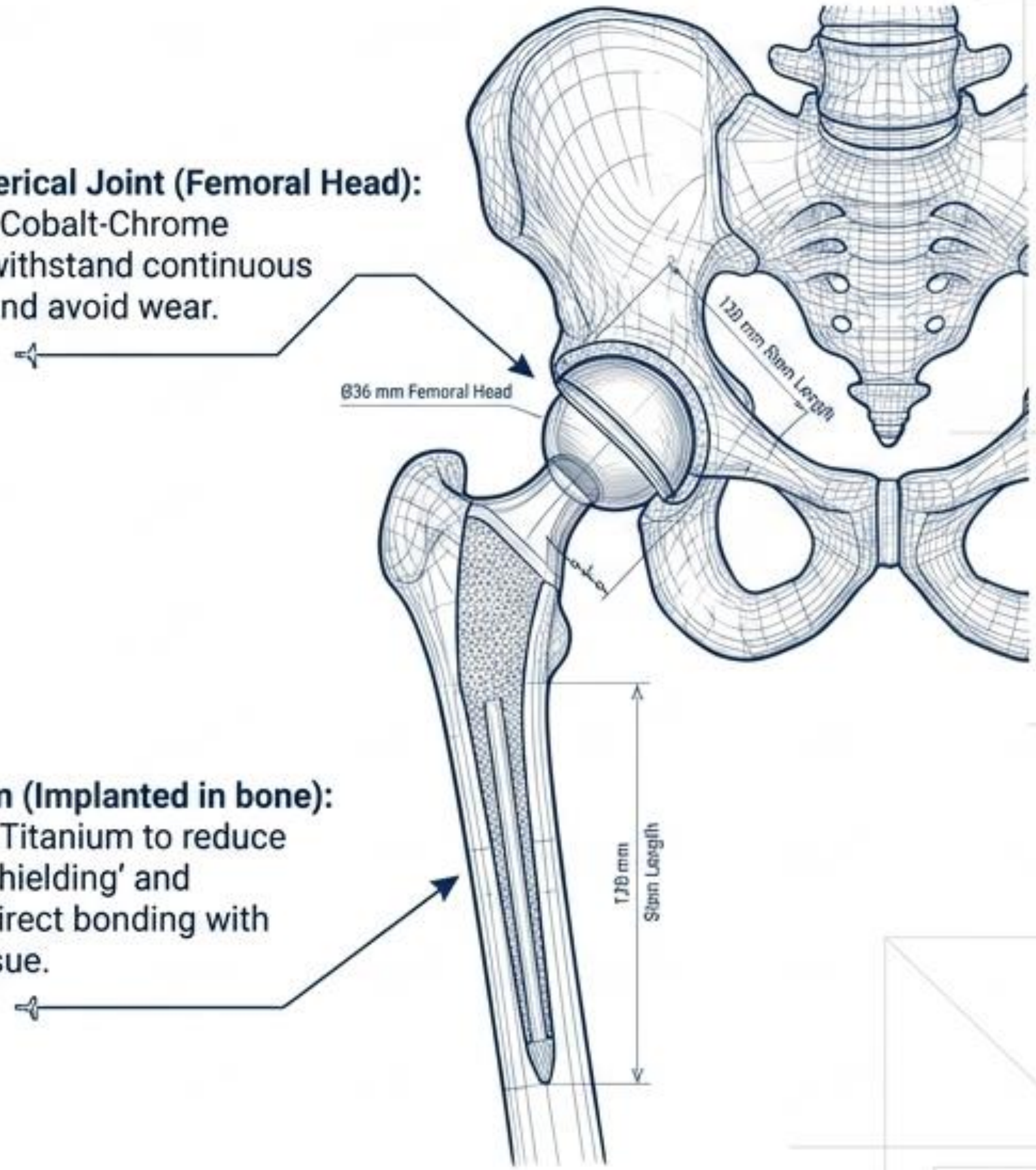
Mechanical Integration in Hard Tissue Replacement

Fracture Fixation (Osteo-synthesis): Rigid structural support



Uses plates and screws made of 316L Stainless Steel or Titanium to provide rigid mechanical fixation, preventing any micro-movement during the bone healing period.

Joint Replacement (Total Hip Replacement): Hybrid application



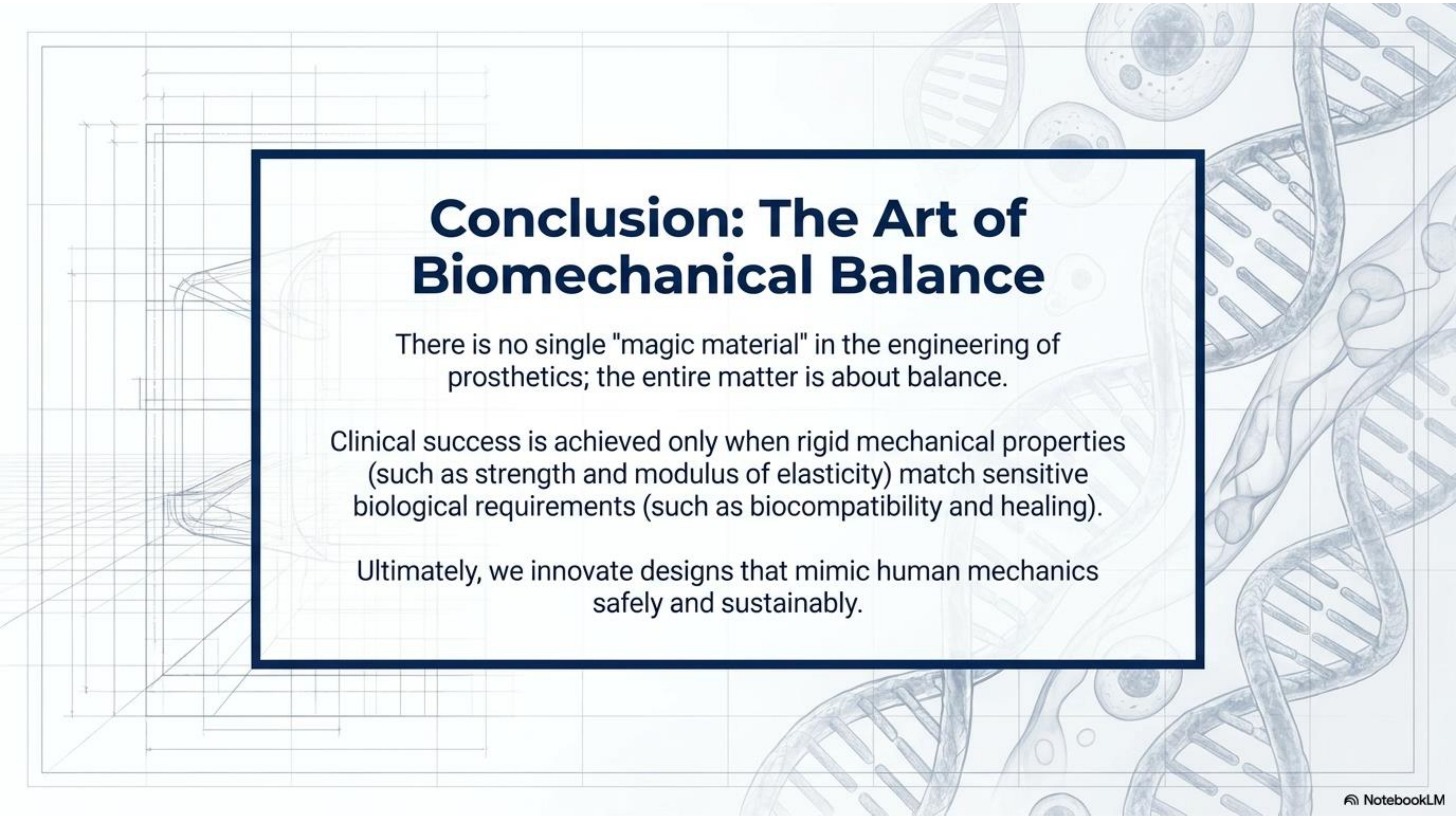
The Spherical Joint (Femoral Head): Made of Cobalt-Chrome alloy to withstand continuous friction and avoid wear.

The Stem (Implanted in bone): Made of Titanium to reduce 'Stress Shielding' and ensure direct bonding with bone tissue.

NotebookLM

Engineering Evaluation Matrix for Medical Metal Alloys

Property / Application	316L Stainless Steel	Cobalt-Chrome	Titanium	Nitinol
Wear Resistance	🟡 Moderate	🟢 Excellent	🔴 Poor	⚪ Not Applicable
Chemical Corrosion Resistance	🟡 Moderate	🟢 Excellent	🟢 Excellent	🟢 Excellent
Biocompatibility	🟢 Good	🟡 Moderate (Potential Toxicity)	🟢 Excellent (Osseointegration)	🟢 Excellent
Fabrication Difficulty	🟢 Low	🔴 Very High	🟡 High	🟡 High
Primary Application	Temporary fixation (screws/plates)	Moving joint surfaces	Permanent implants and stems	Vascular stents and orthodontics



Conclusion: The Art of Biomechanical Balance

There is no single "magic material" in the engineering of prosthetics; the entire matter is about balance.

Clinical success is achieved only when rigid mechanical properties (such as strength and modulus of elasticity) match sensitive biological requirements (such as biocompatibility and healing).

Ultimately, we innovate designs that mimic human mechanics safely and sustainably.

Q1: What are the essential medical and functional requirements to consider when selecting a material for prosthetic limbs?

Q2: Describe the main medical and prosthetic applications of: a)316L Stainless Steel, b) Cobalt-Chrome, c) Titanium, and d) Nitinol, and explain why each material is suitable for its specific application.

Q3: Explain the shape memory effect in Nitinol (TiNi). Then, with the aid of a drawing, show the difference between the super-elastic curve of Nitinol and the curve of a normal metal.