LECTURE NOTES ON

INTRODUCTION TO PHYSICAL METALLURGY AND ENGINEERING

MATERIALS

4th SEMESTER

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INTRODUCTION TO PHYSICAL METALLURGY

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Introduction

What is physical metallurgy?

- Evolution of structures in solid as it from liquid
- Effect of alloy elements/ impurities on the transformation processes
- Effect of processing techniques on evolution of structure
- Structure property relation.

Objectives

- At some point of time or the other an engineering problem involves issues related to material selection.
- □ Understanding the behavior of materials, particularly structure-property correlation, will help selecting suitable materials for a particular application.
- □ To provide a basic understanding of the underlying principles that determines the evolution the evolution of structures in metals and alloys during their processing and its relation with their properties & performance in service.

The Materials Tetrahedron

- A materials scientist has to consider four 'intertwined' concepts, which are schematically shown as the 'Materials Tetrahedron'.
 - ➤ When a certain performance is expected from a component (and hence the material constituting the same), the 'expectation' is put forth as a set of properties.
 - □ The material is synthesized and further made into a component by a set of processing methods (casting, forming, welding, powder metallurgy etc.).
 - > The structure (at various <u>length scales</u>) is determined by this processing.
 - The structure in turn determines the properties, which will dictate the performance of the component.

Hence each of these aspects is dependent on the others.



The broad goal of Metallurgy & Materials Engineering iss to umdenstand and 'Engineer' this Tetrahedron

A General Classification

- □ The broad scientific and technological segments of Metallurgy & Materials Science are shown in the diagram below.
- □ To gain a comprehensive understanding of Metallurgy, all these aspects have to be studied.



A Broad Overview

- □ Based on state (phase) a given material can be Gas, Liquid or Solid
- Based on structure (arrangement of atoms/molecules/ions) materials can be Crystalline, Quasicrystalline or Amorphous.
- □ Based on Band Structure we can classify materials into Metals, Semiconductors and Insulators.
- Based on the size of the entity in question we can Nanocrystals, Nanoquasicrystals etc.

Let us consider the common types of Engineering Materials.



Classification of materials based on form of usage



*Note: this use of the word 'lattice' should not be confused with the use of the word in connection with crystallography.

Common materials : with various 'viewpoints'



Classes of property

Economic	Price and Availability, Recyclability					
General Physical	Density					
Mechanical	Modulus, Yield and Tensile strength, Hardness, Fracture strength, Fatigue strength, Creep strength, Damping					
Thermal	Thermal conductivity, Specific Heat					
Electric & Magnetic	Resistivity, Dielectric constant, Magnetic permeability					
Environmental interactions	Oxidation, corrosion and wear					
Production	Ease of manufacturer, joining, finishing					
Aesthetic (Appearance)	Colour, Texture, Feel.					

Length scales in metallurgy



Length scales in metallurgy

Let us start with a cursory look at the lengthscales involved in Materials Science



Questions?

- 1. What is Physical Metallurgy?
- 2. Give the broad classification of Materials?
- 3. Define Metal, Ceramic and Composite.
- 4. Define Macrostructure and Microstructure?
- 5. What is Grain and Grain boundary?
- 6. Give some of important properties of materials.
- 7. What is composite?
- 8. What is Bio-materials?
- 9. What is smart materials?
- 10. Give some of the types of advanced materials and its applications.





Introduction

- □ In order to understand the structure of materials and its correlation to property, we have to start form the basic element of matter The Atom
- An atom consists of a nucleus composed of protons and neutrons and electrons which encircle the nucleus.
- \square Protons and electrons have same and opposite charge of 1.6 x10⁻¹⁹ C.
- Atomic number (Z) = Number protons = number of electrons
- □ Atomic mass (A) = proton mass + neutron mass
- □ Isotopes are the same element having different atomic masses. Number of protons in isotopes remains same while number of neutrons varies.
- Atomic mass unit (amu) = 1/12 mass of Carbon 12 (¹²C)
- \square 1 mol of substance contains 6.023 x 10²³ (Avogadro's number) atoms or molecules.
- Atomic weight = 1 amu/atom (or molecule) = 1 g/mol = Wt. of 6.023 x 10^{23} atoms or molecules.
 - □ For example, atomic weight of copper is 63.54 amu/atom or 63.54 g/mole

Role of atomic structure in materials

- As we know, common to all materials is that they are composed of **atoms**.
- □ The properties (whether mechanical, electrical, chemical etc) of all solid materials are dependent upon the relative positions of the atoms in the solid (in other words the atomic structure of the material) and their mutual interaction i.e. the nature of the bonding (whether e.g. covalent, ionic, metallic, van der Waals).
- □ There are examples of where the atom-atom interactions is strongly reflected in the atomic structure. An example is diamond. Here the carbon-carbon interactions lead to a very directional covalent bond called a sp³ bond which has tetrahedral symmetry this leads to an open structure as shown below.





Role of atomic structure in materials

- □ Of course carbon can also take the form of graphite. Here the carbon atoms are arranged in a rather different structure and graphite has very different properties to diamond!
- □ In other solid systems (for example many of the metallic elements) the atomic structure is dictated by how well we can 'pack' the atoms into 3D space 'packing efficiency' this leads to dense close-packed structures as we will also discuss in *crystal structure* chapter.
- □ So it is vital that to understand the properties of material, and to improve those properties for example by adding or removing atoms, we need to know the material's atomic structure.



As Richard Feynman said....!

As Richard Feynman sa

"It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are..."

Atomic Interaction

- □ When two neutral atoms are brought close to each other, they experience attractive and or repulsive force.
- Attractive force is due to electrostatic attraction between electrons of one atom and the nucleus of the other.
- □ Repulsive force arises due to repulsion between electrons and nuclei of the atoms.
- \Box The net force, F_N (Fig) acting on the atoms is the summation of attractive and repulsive forces.
- □ The distance, at which the attraction and repulsion forces are equal and the net force is zero, is the equilibrium interatomic distance, r_o . The atoms have lowest energy at this position.

❑ Attraction is predominant above r_o and repulsion is dominant below r_o.



The quantum mechanic principles as discussed before allow determination of electron configuration i.e. the manner in which electron states are occupied in a given atom. Σ



Electron configuration based on quantum numbers. Total number of electrons in a shell is $2n^2$ or $\sum_{l=1}^{n-1} 2(2l+1)$

 $\overline{l}=0$

The manner or sequence of filling of electron orbital's is decided a by a set of two principles / rules:



☐ Madelung's rule

- □ Aufbau principle (German meaning is *building up*) : it states that lower energy states will be filled up first.
- □ Madelung's rule : Orbitals fill in the order of increasing (n+l). 4s (n+l = 4+0 = 4) will be filled before 3d (n+l=3+2=5) and 5s (n+l=5+0=5)
- □ For orbital with same values of (n+*l*), the one with lower 'n' will be filled first. 3d will be filled before 4p.





Based on the foregoing discussion, it is now possible to find the electron configuration for a given atom.

35

□ For example, sodium Na¹¹₂₃ has 11 electrons – the configuration is shown in the first figure. The second picture shows the Bohr configuration. Na 11 electrons – the configuration is shown in the second picture shows the Bohr configuration.

Valence electrons

23

15

2p



- □ The electrons in the outer most shell are known as valence electrons. Na has one valence electron (the 3s electron). These electrons are responsible for chemical reaction and atomic bonding.
- □ Look at the electron configuration of inert gases (He, Ne, Ar, Kr, Xe) in the previous table. Their valence electron cell is completely filled unlike any other element.



- Note that the configuration of higher atomic number elements can be expressed by the previous inert element configuration.
- □ It is the tendency of every element to attain the lowest energy stable configuration that forms the basis of chemical reactions and atomic bonding.

Atomic number	Symbol	Electron configuration	Atomic number	Symbol	Electron configuration	Atomic number	Symbol	Electron configuration
1	Н	1s1	21	Sc	$[Ar]4s^23d^1$	41	Nb	[Kr]5s ¹ 4d ⁴
2	He	$1s^{2}$	22	Ti	$[Ar]4s^23d^2$	42	Mo	[Kr]5s14d5
3	Li	[He]2s ¹	23	V	$[Ar]4s^23d^3$	43	Tc	[Kr]5s ² 4d ⁵
4	Be	$[He]2s^2$	24	Cr	$[Ar]4s^{1}3d^{5}$	44	Ru	[Kr]5s14d7
5	В	[He]2s ² 2p ¹	25	Mn	$[\mathrm{Ar}]4s^23d^5$	45	Rh	[Kr]5s14d8
6	С	$[He] 2s^2 2p^2$	26	Fe	$[Ar]4s^23d^6$	46	Pd	[Kr]4d10
7	Ν	[He]2s ² 2p ³	27	Co	$[Ar]4s^23d^7$	47	Ag	[Kr]5s14d10
8	0	[He]2s ² 2p ⁴	28	Ni	$[Ar]4s^23d^8$	48	Cd	[Kr]5s ² 4d ¹⁰
9	F	[He]2s ² 2p ⁵	29	Cu	$[Ar]4s^{1}3d^{10}$	49	In	[Kr]5s ² 4d ¹⁰ 5p ¹
10	Ne	[He]2s ² 2p ⁶	30	Zn	$[Ar]4s^23d^{10}$	50	Sn	[Kr]5s ² 4d ¹⁰ 5p ²
11	Na	[Ne]3s1	31	Ga	$[Ar]4s^23d^{10}4p^1$	51	Sb	[Kr]5s ² 4d ¹⁰ 5p ³
12	Mg	[Ne]3s ²	32	Ge	$[Ar]4s^23d^{10}4p^2$	52	Te	[Kr]5s ² 4d ¹⁰ 5p ⁴
13	Al	[Ne]3s ² 3p ¹	33	As	$[Ar]4s^23d^{10}4p^3$	53	I	[Kr]5s ² 4d ¹⁰ 5p ⁵
14	Si	$[Ne]3s^23p^2$	34	Se	$[Ar]4s^23d^{10}4p^4$	54	Xe	[Kr]5s ² 4d ¹⁰ 5p ⁶
15	Р	[Ne]3s ² 3p ³	35	Br	$[Ar]4s^23d^{10}4p^5$	55	Cs	[Xe]6s ¹
16	S	[Ne]3s ² 3p ⁴	36	Kr	$[Ar]4s^23d^{10}4p^6$	56	Ba	[Xe]6s ²
17	Cl	[Ne]3s ² 3p ⁵	37	Rb	[Kr]5s ¹	57	La	[Xe]6s ² 5d ¹
18	Ar	[Ne]3s ² 3p ⁶	38	Sr	[Kr]5s ²	58	Ce	[Xe]6s ² 4f ¹ 5d ¹
19	K	[Ar]4s ¹	39	Y	$[Kr]5s^24d^1$	59	Pr	[Xe]6s ² 4f ³
20	Ca	$[Ar]4s^2$	40	Zr	$[Kr]5s^24d^2$	60	Nd	[Xe]6s ² 4f ⁴

Electron Configuration of Elements

Ionization Potential, Electron Affinity, Electronegativity

- □ If sufficient energy is supplied, an electron in the outer orbital can break away completely from the atom and become free. The energy required to remove an electron in this manner is known as the Ionization potential.
- □ When the extra electron is attracted from infinity to the outer orbital of the neutral atom, is known as the electron affinity of the atom.
- ☐ The tendency of an atom to attract electrons to itself during the formation of bonds with other atoms is measured by the electronegativity of the atom.



Let us start by looking at the relative sizes of some ions in the periodic table

Values are: Pauling-Ahrens Radii in Å

Concept of Thermal Expansion

- □ The length of a bond is defined as the center-to-center distance of the bonding atoms. Strong bonds pull the bonding atoms closer together and so have smaller bond lengths as compared to weak bonds.
- □ Primary bonds have lengths in the range 1-2 Å (0.1-0.2 nm). Secondary bond lengths are larger, in the range 2-5Å (0.2-0.5 nm)
- Some ambiguity in this definition arises if the element in question, exhibits different crystal forms.
- □ For example, the diameter of the iron atom is 2.48 Å when it is surrounded by eight neighbours in the BCC crystal and 2.54Å when it has 12 nearest neighbours in the FCC crystal.



Concept of Thermal Expansion

As the temperature of the system is raised to T_1 , and then further to T_2 , the solid becomes consistent with the higher temperatures by having the ions gain energy, and vibrate with increased amplitudes. Therefore, as shown in Figure(below), at T_1 , when the energy is E_1 , the ions are able to vibrate between the positions "A" and "B". Similarly, at T_2 , when the energy is E_2 , the ions are able to vibrate between the positions "C" and "D".



Effect of increasing temperature on the vibration of the ions and hence on the inter-ionic separation. The system is raised to temperature T_1 , and then further to T_2 . At T_1 , when the energy is E_1 , the ions are able to vibrate between the positions "A" and "B". Similarly, at T_2 , when the energy is E_2 , the ions are able to vibrate between the positions "C" and "D".

Concept of Thermal Expansion

- □ It is important to note from the Figure (previous slide) that, the midpoint between "A" and "B", which represents the mean inter-ionic distance at T_1 , is r_1 which is greater than r_0 . This is a direct result of the fact that the solid curve in Figure, is asymmetric.
- □ It is therefore important to note that thermal expansion occurs as a direct result of the fact that the 'E Vs R' curve is asymmetric.
- □ It is also important to note that while the general approach used here can be extended to many systems, the exact shape of the resultant curve obtained will depend on the details of the specific system. In some cases, such as ceramic materials, the resultant curve will have a very deep and narrow trough, such materials will have a very low coefficient of thermal expansion. In other cases, the resultant curve will have a shallow and wide trough, which will cause the material to display a high coefficient of thermal expansion.



Atomic Bonding

- □ The mechanisms of bonding between the atoms are based on the foregoing discussion on electrostatic inter- atomic interaction.
- □ The types of bond and bond strength are determined by the electronic structures of the atoms involved.
- □ The valence electrons take part in bonding. The atoms involved acquire, loose or share valence electrons to achieve the lowest energy or stable configuration of noble gases.
- □ Atomic bonding can be broadly classified as i) primary bonding ii) secondary bonding



Majority of the engineering materials consist of one of these bonds. Many properties of the materials depend on the specific kind of bond and the bond energy.

Ionic Bond

- □ Ionic bonds are generally found in compounds composed of metal and non-metal and arise out of electrostatic attraction between oppositely charged atoms (ions).
- □ Number of electron in outer shell is 1 in Na and 7 in Cl. Therefore, Na will tend to reject one electron to get stable configuration of Ne and Cl will accept one electron to obtain Ar configuration.
- □ The columbic attraction between Na+ and Cl[−] ions thus formed will make an ionic bond to produce NaCl.



 Na^+

 \Box Some other examples are CaF₂, CsCl, MgO, Al₂O₃



Covalent Bond

- □ In this type of bonding, atoms share their valence electrons to get a stable configuration.
- ☐ Methane (CH₄): Four hydrogen atoms share their valence electrons with one carbon atom and the carbon atom in turn shares one valence electron with each of the four hydrogen atoms. In the process both H and C atoms get stable configuration and form a covalent bond.





- Covalent bonds are formed between atoms of similar electro negativity.
- □ C atoms in diamond are covalently bonded to each other.
- □ Si also has valency of four and forms SiC through covalent bonding with C atoms.

Metallic Bond

□ In metals the valence electrons are not really bound to one particular atom, instead they form a sea or cloud of valence electrons which are shared by all the atoms. The remaining electrons and the nuclei form what is called the ion core which is positively charged. The metallic bond arises out of the columbic attraction between these two oppositely charged species – the electron cloud and the ion cores.



Electron cloud distribution in various kinds of bonding



Characteristics of primary bonds

- □ Ionic and covalent bonds posses high bond energy : 450-1000 KJ/mole
- □ High bond strength in ionic and covalent solids results in high melting point, high strength and hardness. e.g. diamond
- As the electrons are tightly bound to the atoms they are generally poor conductors of heat and electricity.
- Are brittle in nature
- □ Most of the ceramics consist of covalent (SiC) or ionic bonds (Al_2O_3) or a mix of both and hence, exhibit all the properties described above.
- □ Metallic bonds on the other hand provide good thermal and electrical conductivities as the valence electrons are free to move.
- □ The metallic bond energy is 68 kJ/mol (Hg) on the lower side and 850 kJ/mol (W, tungsten) on the higher side.
- □ Bond strength increases with atomic number as more electrons are available to form the bonds with the ion cores. As a result melting point, hardness and strength increases with atomic number.
- □ Metals are ductile as the free moving electrons provides agility to the bonds and allows plastic deformation.

Vanderwaals bonding

- □ Vanderwaals bonding between molecules or atoms arise due to weak attraction forces between dipoles.
- ☐ The natural oscillation of atoms leading to momentary break down of charge symmetry can generate temporary dipoles.



Dipoles can induce dipoles and attraction between opposites ends of the dipoles leads to weak bonding.



 \Box An ion can also induce a dipole (+

□ Some molecules like HCl have permanent dipoles due to asymmetrical arrangement of +ve and –ve charges.

$$\delta^+$$
 (H - CI) $\delta^ \delta^+$ (H - CI) δ^-

Vanderwaals bonding

- □ Van der Waals bonding is much weaker compared to primary bonds. Bond energy lies in the range of 2 10 kJ/mol
- □ Molecules in liquid and gas are held by weak Vanderwaals forces.
- □ The atomic layers in graphite are held together by weak vanderwaals bonds. Therefore, the layers can move easily over each other and this imparts the lubricating property graphite is known for.


Hydrogen bonding

- Hydrogen bond is a type of secondary bond found in molecules containing hydrogen as a constituent.
- □ The bond originates from electrostatic interaction between hydrogen and another atom of high electro-negativity such as fluorine or oxygen.
- \Box The strength of hydrogen bonds is in the range of 10 50 kJ/mol.
- □ Water molecules, for example, are connected by hydrogen bonds (dashed lines in the picture).



Mixed bonding

Many materials have a mixed bonding characteristics, between covalent and ionic bonding. Examples are as below.

• Oxides:	% ionic bonding	$\sim 70\%$
Nitrides:	% ionic bonding	$\sim 40\%$
Carbides:	% ionic bonding	~ 15~20%

Metallic-covalent Mixed Bonding: The transition metals are an example where s,p,d-bonding orbital's lead to high melting points.

Binding Energies of Bonds

Bond Type	Energy (eV)	Energy (kJ/mole)	Energy (kJ/mole)
Ionic	~5-15 (strong)	~500-1000	NaCl: 640
Covalent	~1-10 (strong)	~100-1000	Diamond: ~710
Metallic	~0.5-8.5 (strong)	~50-850	Fe: 406
Hydrogen	~0.05-1.5	~5-155	H ₂ O: 51
Van der Walls	~0.01-0.5	~1-50	Ar:7.7

Questions?

- 1. Define atom, electron, proton and neutron
- 2. What is Pauli's exclusion principle.
- 3. Define a solid. Glass is not considered as true solid
- 4. Why are noble gases inert?
- 5. Briefly explain the primary bonds in solids.
- 6. How do secondary bonds form? What is hydrogen bond?
- 7. Why is graphite lubricating?
- 8. Why are ceramics hard and brittle? Why are they not conductive?
- 9. How many atoms are there in 1 g of copper?
- 10. Why are some elements known as transition elements
- 11. Why is Tungsten (74) much stronger than Aluminium (13) though both are metallic?
- 12. Explain the arrangement of the elements in the periodic table





M.C. Esher : Art with Science



Every periodic pattern (and hence a Crystal) has a unique lattice associate with it.



Why study crystal structures?

- When we look around much of what we see is non-crystalline (organic things like wood, paper, sand; concrete walls, etc. → some of the things may have some crystalline parts!).
- □ But, many of the common 'inorganic' materials are 'usually'' crystalline: = Matalar Cu Zu E Cu Zu allows
 - □ Metals: Cu, Zn, Fe, Cu-Zn alloys
 - □ Semiconductors: Si, Ge, GaAs
 - \Box Ceramics: Alumina (Al₂O₃), Zirconia (Zr₂O₃), SiC, SrTiO₃
- Also, the usual form of crystalline materials (say a Cu wire or a piece of alumina) is polycrystalline and special care has to be taken to produce single crystals
- □ Polymeric materials are *usually* not 'fully' crystalline
- The crystal structure directly influences the properties of the material

Why study crystallography?

- Gives a terse (concise) representation of a large assemblage of species
- Gives the 'first view' towards understanding of the properties of the crystal

* Many of the materials which are usually crystalline can also be obtained in an amorphous form

Platonic Solids

- □ In 387B.C. scientist called "PLATO" most famous student of Socrates thought that whole universe is made up of five solids. Whole universe is periodic arrangement of five solids named as Platonic Solids.
 - Tetrahedron 4 faces Fire
 - Hexahedron 6 *faces Earth*
 - Octahedron 8 faces Air
 - Dodecahedron 12 faces GOD
 - Icosahedron 20 faces Water

He had a some philosophical thought; in the universe we have 5 elements made up of these five solids

- □ In icosahedron, we will get best packing as for we concerned. But only problem is, if we try to translate it in 3D we can't get continuous structure, without any voids left. This voids in crystallography is called *frustation*.
- ☐ Long back people thought, it is not possible to have solids with Icosahedron packing; but it is possible when Quasicrystals are discovered in 1984. (Al-Mn)







How to define a Crystal?

Crystal

A 3D translationally periodic arrangement of atoms in a space is called a crystal.

Lattice

A 3D translationally periodic arrangement of points in a space is called a crystal.



What is the relation between the two ?

$$Crystal = Lattice + Motif$$

Motif or Basis:

typically an atom or a group of atoms associated with each lattice point

Lattice > The underlying periodicity of the crystal

Basis > Entity associated with each lattice points

Lattice ➤ how to repeat Motif ➤ what to repeat

Lattice

Translationally periodic arrangement of points

Crystal

Translationally periodic arrangement of motifs

What is the relation between the two ?

Crystal = Lattice (Where to repeat)+Motif (What to repeat)



Motifs are associated with lattice points \rightarrow they need NOT *sit* physically at the lattice point



Put arrow marks pointing up and down alternately on the points:



What we get is a crystal of lattice parameter 'a' and not 'a/2'! \rightarrow as this lattice parameter is a measure of the repeat distance!



Why study symmetry..?

- Crystals are an important class of materials.
- Crystals (and in fact quasicrystals) are defined based on symmetry.
- Symmetry helps reduce the *'infinite'* amount of information required to describe a crystal into a finite *(preferably small)* amount of information.
- □ In crystallography (the language of describing crystals) when we talk of Symmetry; the natural question which arises is: *Symmetry of What?*
- The symmetry under consideration could be of one the following entities:

 \succ Lattice \succ Crystal \succ Motif \succ Unit cell

Symmetry can be defined as, if an object is brought into self-coincidence after some operation it said to possess symmetry with respect to that operation.



Translation

- The translation symmetry operator (t) moves an point or an object by a displacement t or a distance t.
- A periodic array of points or objects is said to posses translational symmetry.
- Translational symmetry could be in 2D or 3D (or in general nD).
- □ If we have translational symmetry in a pattern then instead of describing the entire pattern we can describe the 'repeat unit' and the translation vector(s).



Rotation Axis

- Rotation axis rotates a general point (and hence entire space) around the axis by a certain angle
- On repeated operation (rotation) the 'starting' point leaves a set of 'identity-points' before coming into coincidence with itself.
- As we are interested mainly with crystals, we are interested in those rotations axes which are compatible with translational symmetry → these are the (1), 2, 3, 4, 6 – fold axis.
- □ If an object come into self-coincidence through smallest non-zero rotation angle of θ then it is said to have an n-fold rotation axis where:

$$n = \frac{360^0}{\theta}$$



Rotational Symmetry



The rotations compatible with translational symmetry are [1, 2, 3, 4, 6]

Crystals can *only* have 1, 2, 3, 4 or 6 fold symmetry

Examples of Rotational Symmetry



Mirror and Inversion

- □ The left hand of a human being cannot be superimposed on the right hand by mere translations and rotations
- The left hand is related to the right hand by a mirror symmetry operation (m)
- The right hand is called the *enantiomorphic form* of the left hand
- Another operator which takes objects to enantiomorphic forms is the inversion operator (i)



Reflection (or mirror symmetry)



Unit Cells (UC)

- An unit cell (also sometimes causally referred to as a cell) is a representative unit of the structure
 - ✓ Instead of drawing the whole structure I can draw a representative part and specify the repetition pattern
- □ If the structure under considerations is a <u>crystal</u>, then the unit cell will also contain atoms (or ions or molecules etc.)
- □ The dimension of the unit cell will match the dimension of the structure; If the lattice is 1D the unit cell will be 1D, if the crystal is 3D then the unit cell will be 3D, if the lattice is <u>nD</u> the unit cell will be nD.
- □ If the lattice points are *only* at the corners, the cell is **primitive**.
- □ If there are lattice points in the cell other than the corners, the cell is **non-primitive**.

3D Unit Cell

- □ In order to define translations in 3-D space, we need 3 non-coplanar vectors
- Conventionally, the fundamental translation vector is taken from one lattice point to the next in the chosen direction
- □ With the help of these three vectors, it is possible to construct a parallelopiped called a UNIT CELL



Crystal Structures (or) 14 Bravais Lattices

A	A Symmetry based concept							
	Crystal System	Lattice Parameters	Bravais Lattices		es			
			Р	Ι	F	С		
1	Cubic	$(a = b = c, \alpha = \beta = \gamma = 90^{\circ})$	4	*	*			
2	Tetragonal	$(a = b \neq c, \alpha = \beta = \gamma = 90^{\circ})$	4	*				
3	Orthorhombic	$(a \neq b \neq c, \alpha = \beta = \gamma = 90^{\circ})$	4	*	*	4		
4	Hexagonal	$(a = b \neq c, \alpha = \beta = 90^{\circ}, \gamma = 120^{\circ})$	4					
5	Trigonal	$(a = b = c, \alpha = \beta = \gamma \neq 90^{\circ})$	•					
6	Monoclinic	$(a \neq b \neq c, \alpha = \gamma = 90^{\circ} \neq \beta)$	4			4		
7	Triclinic	$(a \neq b \neq c, \alpha \neq \beta \neq \gamma)$	•					

Р	Primitive
Ι	Body Centred
F	Face Centred
С	End Centred

Bravais Lattice: various viewpoints

- A lattice is a set of points constructed by translating a single point in discrete steps by a set of basis vectors.
- □ In three dimensions, there are 14 unique **Bravais** lattices (distinct from one another) in three dimensions. All crystalline materials recognized till now fit in one of these arrangements.
- □ In geometry and crystallography, a **Bravais lattice** is an infinite set of points generated by a set of discrete translation operations.
- A Bravais lattice looks exactly the same no matter from which point in the lattice one views it. An important property of a lattice
- Bravais concluded that there are only 14 possible Space Lattices (with Unit Cells to represent them). These belong to 7 Crystal systems.
- > There are 14 Bravais Lattices which are the Space Group symmetries of lattices





• Elements with Tetragonal structure \rightarrow In, Sn







$$a = b \neq c$$

$$\alpha = \beta = 90^{\circ}, \gamma = 120^{\circ}$$



A single unit cell (marked in blue) along with a 3-unit cells forming a hexagonal prism

• Elements with Hexagonal structure \rightarrow Be, Cd, Co, Ti, Zn

Note: there is only one type of hexagonal lattice *(the primitive one)* What about the HCP? (Does it not have an additional atom somewhere in the middle?)







Elements with Trigonal structure
→ As, B, Bi, Hg, Sb, Sm





• Elements with Monoclinic structure \rightarrow P, Pu, Po

			Р	Ι	F	С
7	Triclinic	Parallelepiped (general)	4			







MILLER INDICES



From the law of rational indices developed by French Physicist and mineralogist Abbé René Just Haüy and popularized by William Hallowes Miller

Miller Indices

- □ Miller indices are used to specify directions and planes.
- □ These directions and planes could be in <u>lattices</u> or in <u>crystals</u>.
- □ The number of indices will match with the dimension of the lattice or the crystal: in 1D there will be 1 index and 2D there will be two indices etc.
- □ Some aspects of Miller indices, especially those for planes, are not intuitively understood and hence some time has to be spent to familiarize oneself with the notation.



Miller Indices for directions in 2D



Miller indices for directions in 3D

- \Box A vector **r** passing from the origin to a lattice point can be written as
- **a** $\mathbf{r} = \mathbf{r}_1 \, \mathbf{a} + \mathbf{r}_2 \, \mathbf{b} + \mathbf{r}_3 \, \mathbf{c}$
- $\Box \text{ Where, } \mathbf{a}, \mathbf{b}, \mathbf{c} \rightarrow \text{basic vectors}$

$$r = r_1 \vec{a} + r_2 \vec{b} + r_3 \vec{c}$$

- Basis vectors are unit lattice translation vectors which define the coordinate axis *(as in the figure below).*
- Note their length is not 1 unit! (like for the basis vectors of a coordinate axis).


Possible coordinates in 3D



If you have confusion while selecting origin in negative indices refer this figure

Important directions in 3D represented by Miller Indices (cubic lattice)



Procedure as before:

- (Coordinates of the final point coordinates of the initial point)
- Reduce to smallest integer values

Family of directions

□ A set of directions related by symmetry operations of the lattice or the crystal is called a family of directions

A family of directions is represented (Miller Index notation) as: <u v w>

Index	Members in family for cubic lattice					
<100>	[100	[100],[100],[010],[010],[001],[001]				
<110>	[110	[110],[110],[110],[110],[101],[101],[101],[101],[011],[
<111>	[11]	[111],[111],[111],[111],[111],[111],[111],[111],[111]				
Sym	bol	Alternate	the 'negative (opposite di	res'		

Symbol	Alternate symbol			(0]
[]		\rightarrow	Particular direction	
<>	[[]]	\rightarrow	Family of directions	

Miller Indices for Planes



- \Box Find intercepts along axes $\rightarrow 2 \ 3 \ 1$
- □ Take reciprocal* $\rightarrow 1/2 \ 1/3 \ 1$
- \Box Convert to smallest integers in the same ratio \rightarrow 3 2 6
- \Box Enclose in parenthesis \rightarrow (326)

*The reciprocal procedure avoids the intercept of ∞ for a plane parallel to an axis, by making it 0

Important Planes in 3D represented by Miller Indices (cubic lattice)





Summary on planes and directions

- $\Box \text{ Unknown direction} \rightarrow [\text{uvw}]$
- $\Box \text{ Unknown plane} \rightarrow (\text{hkl})$
- □ Double digit indices should be separated by commas \rightarrow (12,22,3)

□ In cubic lattices/crystals [hkl] \perp (hkl)

Interplanar spacing (d_{hkl}) in cubic lattice (& crystals)

$$d_{hkl}^{cubic\ lattice} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

	Symbol		Alternate symbols		
Direction	[]	[uvw]		\rightarrow	Particular direction
	<>	<uvw></uvw>	[[]]	\rightarrow	Family of directions
Plane	()	(hkl)		\rightarrow	Particular plane
	{ }	{hkl}	(())	\rightarrow	Family of planes

Directions L Planes

- **Cubic system:** (hkl) \perp [hkl]
- □ Tetragonal system: only special planes are \perp to the direction with same indices: [100] \perp (100), [010] \perp (010), [001] \perp (001), [110] \perp (110) ([101] not \perp (101))
- Orthorhombic system: $[100] \perp (100), [010] \perp (010), [001] \perp (001)$
- □ Hexagonal system: $[0001] \perp (0001)$ (this is for a general c/a ratio; for a Hexagonal crystal with the special c/a ratio = $\sqrt{(3/2)}$ the cubic rule is followed)
- □ Monoclinic system: $[010] \perp (010)$
- **Characterization** Other than these a general [hkl] is NOT \perp (hkl)

Coordination Number

Coordination number is defined as the total number of nearest neighboring atoms

Simple cubic

The coordination number of simple cubic crystal is '6' It is shown in figure. In this figure we are considered one corner and drawn 3 lines connecting to six points.

Body Centered cubic

The coordination number of BCC crystal is 8. The body centered atom is in contact with all the eight corner atoms. Each corner atom is shared by eight unit cells and hence, each of these atoms is in touch with eight body centered atoms.



Coordination Number

Face Centered cubic

In the FCC lattice each atom is in contact with 12 neighbor atoms. FCC coordination number Z = 12. For example, the face centered atom in the front face is in contact with four corner atoms and four other facecentered atoms behind it (two sides, top and bottom) and is also touching four facecentered atoms of the unit cell in front of it.





Hexagonal close pack structure

In Hexagonal lattice Z = 12. The center atom of the top face is in touch with six corner atoms, three atoms of the mid layer and other three atoms of the mid layer of the unit cell above it.



Average number of atoms per unit cell

		Position of atoms	Effective number of atoms
1	SC	8 Corners	$= [8 \times (1/8)] = 1$
2	BCC	8 Corners + 1 body centre	= [1 (for corners)] + [1 (BC)] = 2
3	FCC	8 Corners + 6 face centres	= $[1 (for corners)] + [6 \times (1/2)] = 4$
4	НСР	 12 corners (6 bottom+6 top) + 2 atoms at face centers + 3 atoms in the interior 	= $[12 \times (1/6)] + [2 \times (1/2)] + [3$ (interior)] = 6

Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell. *Volumeofatoms*

 $APF = \frac{Volume of atoms}{Volume of unit cell}$

Simple Cubic

In a simple cubic structures, the atoms are assumed to be placed in such a way that any two adjacent atoms touch each other. If 'a' is the lattice parameter of simple cubic structure and 'r' the radius of atoms. From the figure it is clear that Atomic radius $(r) = a_2^{a_2}$



Body Centered Cubic

In body centered cubic structures the center atom touches the corner atoms as shown in Figure



Face Centered Cubic

From this figure; first we can calculate atomic radius:

$$(4r)^{2} = a^{2} + a^{2} \rightarrow 16r^{2} = 2a^{2} \rightarrow r^{2} = \frac{2a^{2}}{16}$$

$$r = a^{2} - \frac{a}{4} = \frac{4r}{a} = -34r = 2a$$

$$4 = 2 - \frac{2}{\sqrt{2}} = \frac{2}{\sqrt{2}} = \frac{2}{\sqrt{2}} = \sqrt{2}$$



$$APF = \frac{4 \times \frac{4}{3} \prod r^{3} + 4 \times \frac{4}{3} \prod \left(\frac{a}{2 \times 2}\right)^{3}}{a^{3}} = \frac{16 \times 2}{\sqrt{3} \times 64a^{3}} = 0.74$$

 $APF_{FCC} = 0.74(or)74\%$

- Directions and planes in hexagonal lattices and crystals are designated by the 4-index Miller-Bravais notation
- □ In the four index notation:
 - \succ the first three indices are a symmetrically related set on the basal plane

 \succ the third index is a *redundant one* (which can be derived from the first two) and is introduced to make sure that members of a family of directions or planes have a set of numbers which are identical

> the fourth index represents the 'c' axis (\perp to the basal plane)

□ Hence the first three indices in a hexagonal lattice can be permuted to get the different members of a family; while, the fourth index is kept separate. Related to 'l' index a_3

Related to 'i' index

Related to 'k' index

Related to 'h' index



In general three indices point is denoted as miller indices i.e., (h k l). But hexagonal crystals we are using 4 indices point is denoted by miller-bravais indices i.e., (h k i l)The use of the 4 index notation is to bring out the equivalence between crystallographically equivalent planes and directions.







Hexagonal crystals → Miller-Bravais Indices : DIRECTIONS

Drawing the $[11\overline{2}0]$ direction

- Trace a path along the basis vectors as required by the direction. In the current example move (1) Junit along a_1 , 1) unit along a_2 and -2 units along a_3 .)
- Directions are projected onto the basis vectors to determine the components and hence the Miller-Bravais indices can be determined as in the table.



Drawing the $[10\overline{1}0]$ direction



Hexagonal crystals → Miller-Bravais Indices : DIRECTIONS



Ρ

<u>c</u> 2

30

Hexagonal Close Packed Structure



The distance between any neighboring atoms is 'a' from the figure 'AB' = a

$$AY = AB\cos 30^0 = \frac{a \cdot 3}{2} \qquad \sqrt{}$$

From the figure 'Ax' is orthocenter; so,

$$Ax = \frac{2}{3}AY = \frac{2}{3} \times \frac{a}{2} = \frac{3}{\sqrt{2}} = \frac{3}{\sqrt{2}}$$



Hexagonal Close Packed Structure

Consider ΔAPx

$$(AP)^{2} = (Ax)^{2} + (xP)^{2}$$

$$a^{2} = -\frac{1}{3} + -\frac{1}{4} \rightarrow a^{2} - -\frac{1}{3} = \frac{c^{2}}{4} \rightarrow \frac{c^{2}}{4} = \frac{2a^{2}}{3}$$

$$\frac{c^2}{a^2} = \frac{8}{3} \to \frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$





In cubic a=b=c, so volume is a^3 but in this case, it is H.C.P so here a=b \neq c

Volume of unitcell = Area of base of hexagonal × Height

Hexagonal Close Packed Structure

Volume of unitcell = Area of base of hexagonal × Height

Volumeofuitcell=6×*areaof*AOB×*c* $Volume of unit cell = 6 \times \frac{1}{2} \times OB \times AY \times c$ $Volume of unit cell = 6 \times \frac{1}{2} \times a \times \frac{a\sqrt{3}}{2} \times c = ca^2 \frac{3\sqrt{3}}{2}$ $APF = \frac{\frac{6 \times \frac{4}{3} \prod r^{3}}{ca^{2} \frac{3\sqrt{3}}{2}}}{\frac{6 \times \prod r^{3}}{2} = \frac{6 \times \prod r^{3}}{6 \times \prod r^{3}}} = \frac{2 \prod a}{ca^{2} \frac{3\sqrt{3}}{2}} = 0.74$ $APF = \frac{\frac{3}{2} \sum_{a} \frac{3\sqrt{3}}{2}}{ca^{2} \frac{3\sqrt{3}}{2}} = \frac{2 \prod a}{cx^{3} \sqrt{3}} = 0.74$ $APF_{HCP} = 0.74(or)74\%$

Summary on PACKING FRACTION / Efficiency

Packing Fraction $= \frac{\text{Volume occupied by atoms}}{\text{Volume of Cell}}$

	SC*	BCC*	ССР	DC	НСР
Relation between atomic radius (r) and lattice parameter (a)	a = 2r	$\sqrt{3}a = 4r$	$\sqrt{2}a = 4r$	$\frac{\sqrt{3}}{4}a = 2r$	$a = 2r$ $c = 4r\sqrt{\frac{2}{3}}$
Atoms / cell	1	2	4	8	2
Lattice points / cell	1	2	4	4	1
No. of nearest neighbours	6	8	12	4	12
Packing fraction	$\frac{\pi}{6}$	$\frac{\sqrt{3\pi}}{8}$	$\frac{\sqrt{2\pi}}{6}$	$\frac{\sqrt{3}\pi}{16}$	$\frac{\sqrt{2\pi}}{6}$
	~ 0.52	~ 0.68	~ 0.74	~ 0.34	~ 0.74

* Crystal formed by monoatomic decoration of the lattice

Density

- □ The usual density is mass/volume
- In materials science various other kinds of density and occupation ratios are defined. These include:
 - Linear density: mass/length [kg/m]

atoms/length [/m] or number/length

length occupied/length [m/m]

Planar(Areal) density: mass/area [kg/m²]

atoms/area [/m²] *or number/area*

- area occupied/area [m²/m²]
- Volume density: mass/volume [kg/m³]

atoms/volume [/m³] *or number/volume* volume occupied/volume [m³/m³]

- □ The volume occupied/volume of space $[m^3/m^3]$ is also called the packing fraction
- □ In this context other important quantities include:
 - \blacktriangleright Length/area [m/m²] \rightarrow e.g. length of dislocation lines per unit area of interface (interfacial dislocations)
 - > Length/volume $[m/m^3] \rightarrow e.g.$ length of dislocation lines per unit volume of material
 - Area/volume $[m^2/m^3] \rightarrow e.g.$ grain boundary area per unit volume of material
- □ The 'useful' way to write these quantities is to NOT factor out the common terms: i.e. write [m/m³] '*as it is* ' and *not as* [1/m²]

Linear density

Linear density (LD) is the number of atoms per unit length along a particular direction



<110> directions in the FCC lattice have 2 atoms ($1/2 \ge 2$ corner atoms + 1 center atom) and the length is

$$LD_{[110]} = \frac{2}{2a} = \frac{2}{\frac{a}{\sqrt{2}}} - \frac{\sqrt{2}}{\sqrt{2}}$$

This is the most densely packed direction in the FCC lattice

Planar(Areal) density

Planar density (PD) refers to density of atomic packing on a particular plane.



Theoretical (Volume) density

Theoretical density calculation from crystal structure

Theoretical density
$$\rho = \frac{nA}{V_C N_A}$$
 n = number of atoms in the unit cell
A = atomic weight
 $V_C = Volume of unitcell$
 $N_A = Avogadro's number (6.023 × 10^{23})$

Calculate the theoretical density of Aluminum (Al)

Given : Al is FCC structure; Lattice parameter is 4.05A⁰; n=4; Atomic weight of Al is 26.98 g/mol

$$\rho = \frac{4 \times 26.98}{(4.05 \times 10^{-8})^3 \times 6.023 \times 10^{23}} = 2.697g / cc$$

CCP=FCCClosed Packed Structures : FCCCCP=F

Start with a row of atoms (close packed in 1D)



Make a 2D hexagonal close packed array (the A layer)



 $Monatomic\ decoration\ of\ FCC\ lattice$

- This is a close packed layer with close packed directions (like <110> directions represented using cubic indices)
- As we shall see this becomes the {111} plane in the FCC crystal

There is only one way of doing so!

To build the next layer \rightarrow leading to the 3D structure, there are 2 stable positions where atoms can be put \rightarrow called the B and C positions. If atoms are put in the B position than we cannot put atoms in the C position (no space!)





Closed Packed Structures : FCC

Putting atoms in the B position in the II layer and in C positions in the III layer we get a stacking sequence \rightarrow ABC ABC ABC.... > The CCP (FCC) crystal











Closed Packed Structures : HCP

An alternate packing (<u>one amongst an infinite possibilities</u>) is where in the III layer coincides with the I layer \rightarrow giving rise to a AB AB AB ... packing \rightarrow The Hexagonal Close Packed Crystal (*this arrangement is close packed only for ideal c/a ratio; i.e. for 'hard sphere' packing*)

As before we make a 2D hexagonal close packed array (the A layer)



- This is a close packed layer with close packed directions (like <1120> directions)
- As we shall see this becomes the {0001} plane in the HCP crystal

Metals which adopt HCP structure Mg, Zn, Ti, Co, Be, Cd, Zr, Y, Sc, Tc, Ru, Gd, Tb, Dy, Ho, Er, Tm, Lu, Hf, Re, Os, Tl



Structure-Property Correlation

- Aluminum (Al) is ductile while iron (Fe) and magnesium (Mg) are not. This can be explained from their crystal structures.
- □ Al is FCC where as Fe is BCC and Mg is HCP.
- Plastic deformation in metals takes place mainly by a process called slip. Slip can broadly be visualized as sliding of crystal planes over one another. Slip occurs on most densely packed planes in the most closely packed directions lying on that plane.
- □ The slip plane and the direction together is called a Slip system
- □ In FCC, {111} planes are close-packed and there are four unique {111} planes. Each of these planes contains three closely packed <110> directions. Therefore, there are 4 x 3 = 12 slip systems
- □ In HCP, the basal plane, (0001) is the close-packed and it contains three <11 $\overline{2}$ 0> directions. Hence, number of slip system = 1 x 3 = 3
- □ Slip in more number of slip systems allows greater plastic deformation before fracture imparting ductility to FCC materials.
- Close-packed planes are also planes with greatest interplanar spacing and this allows slip to take place easily on these planes.
- BCC structure on the other hand has 48 possible slip systems. However, there is no close-packed plane. Hence, plastic deformation before fracture is not significant. Slip might occur in {110}, {112} and {123} planes in the <111> directions.

Questions?

- 1. What is unit cell? What is lattice parameter?
- 2. What is Bravais lattice? How are the Bravais lattices obtained from the primitive cell? How many types of Bravais lattices are there?
- 3. Draw two adjacent FCC unit cells and join the top and bottom face centers of each cell. Also join these four face centers to the nearest common corners.
 - i. What is the unitcell outlined by this procedure?
 - ii. Is it in the Bravais list?
- 4. Show that packing efficiency of FCC is 74% and that of BCC is 68%.
- 5. Show that the ideal c/a ratio in a hexagonal unit cell is 1.633 and calculate the packing efficiency.
- 6. What is miller index? How is it obtained?
- 7. Draw the planes $(1^{-1}0), (1^{-2}1), (2^{-3}4), (1^{-1}2)$ and directions $[11\overline{1}], [123], [120], [1^{-1}21]$ in a cubic unit cell.
- 8. If the lattice parameter of Alpha iron is 286 pm, what is its atomic radius?
- 9. Lattice constant of Al is 4.05 Å. What is the atomic radius of Al?
- 10. What is the difference between atomic structure and crystal structure?

Questions?

- 11. Why it is necessary to include a fourth miller index in the hexagonal system?
- 12. Convert the directions [112], [1 3], [110], [111], to four indices in a hexagonal lattice.
- 13. A metal has a density of 10.22 $\overline{g2}/cc$, atomic weight of 95.94 and atomic radius of 0.136 nm. Is it BCC or FCC?
- Calculate the volume of the unit cell of Zn crystal. a and c of Zn are 266.5 pm and 494.7 pm respectively.
- 15. Some hypothetical metal has the simple cubic crystal structure. If its atomic weight is 74.5 g/mol and the atomic radius is 0.145 nm, compute its density.
- 16. Calculate the planar density of {110} planes in α -Fe (BCC) crystal. a = 0.287 nm.
- 17. Calculate the linear density of [110] direction in a Cu crystal. a = 0.361 nm.
- 18. What are the miller indices of a plane that intersects the X axis at 2 and the Y axis at $\frac{1}{2}$ and is parallel to the z axis? The structure is cubic.
- 19. Copper has FCC crystal structure and the unit cell with a lattice constant of 0.361 nm. What is the inter-planar spacing of d111 planes?
Questions?

20. Determine the indices for the directions and plane shown in the following hexagonal unit cell:



INTRODUCTION

Mechanical metallurgy is the area of knowledge which deals with the behavior and response of metals to applied forces.

It will mean different things to different persons

- Mechanical properties of metals or mechanical testing
- The plastic working and shaping of metals
- Theoretical aspects of the field, which merge with metal physics and physical metallurgy
- Mechanical metallurgy is closely allied with applied mathematics and applied mechanics

Mechanical metallurgy is the area of metallurgy which is concerned primarily with the response of metals to forces or loads.

It is necessary to know something about the limiting values which can be withstood without failure.

- A *continuous body* is one which does not contain voids or empty spaces of any kind.
- A body is *homogeneous* if it has identical properties at all points.
- A body is considered to be *isotropic* with respect to some property when that property does not vary with direction or orientation.
- A property which varies with orientation with respect to some system of axes is said to be *anisotropic*.

ELASTIC AND PLASTIC BEHAVIOR

- The recovery of the original dimensions of a deformed body when the load is removed is known as *elastic behavior*.
- The limiting load beyond which the material no longer behaves elastically is the *elastic limit*.
- If the elastic limit is exceeded, the body will experience a permanent set or deformation when the load is removed. A body which is permanently deformed is said to have undergone *plastic deformation*.

Hooke's law

- For most materials, as long as the load does not exceed the elastic limit, the deformation is proportional to the load. This relationship is known as Hooke's law; it is more frequently stated as 5.
- However, it does not necessarily follow that all materials which behave elastically will have a linear stress-strain relationship. Rubber is an example of a material with a nonlinear stress-strain relationship that still satisfies the definition of an elastic material.

AVERAGE STRESS AND STRAIN

A load *P* is applied to one end of the bar, and the gage length undergoes a slight increase in length and decrease in diameter. The distance between the gage marks has increased by an amount δ , called the deformation.

The *average linear strain e* is the ratio of the change in length to the original length.



Figure I-I Cylindrical bar subjected to axial load.

$$e = \frac{\delta}{L_0} = \frac{\Delta L}{L_0} = \frac{L - L_a}{L_0}$$

Strain is a **dimensionless** quantity.

The external load *P* is balanced by the internal resisting force σ . *dA*, where σ is the stress normal to the cutting plane and *A* is the cross-sectional area of the bar. The equilibrium equation is



Figure 1-2 Free-body diagram for Fig. 1-1.

The elastic limit Hooke's law can be considered valid, so that the average stress is proportional to the average strain,

$$\frac{o}{e} = E = Constan$$

The constant *E* is the *modulus of elasticity*, or *Young's modulus*.

TENSILE DEFORMATION OF DUCTILE METAL

The data obtained from the tension test are generally plotted as a stress-strain diagram.

- It shows a typical stress-strain curve for a metal such as aluminum or copper.
- The initial linear portion of the curve **O**A is the elastic region within which Hooke's law is obeyed.
- Point *A* is the elastic limit, defined as the greatest stress that the metal can withstand without experiencing a permanent strain when the load is removed.

- The determination of the elastic limit is quite tedious, not at all routine, and dependent on the sensitivity of the strain-measuring instrument.
- For these reasons it is often replaced by the *proportional limit*, point A'.
- The proportional limit is the stress at which the stress-strain curve deviates from linearity.
- The slope of the stress-strain curve in this region is the modulus of elasticity.
- For engineering purposes the limit of usable elastic behavior is described by the *yield strength*, point **B**.
- The yield strength is defined as the stress which will produce a small amount of permanent deformation, generally equal to a strain of 0.002. This permanent strain, or offset, is **OC**.



Figure 1-3 Typical tension stress-strain curve.

- Plastic deformation begins when the elastic limit is exceeded.
- As the plastic deformation of the specimen increases, the metal becomes stronger (strain hardening) so that the load required extending the specimen increases with further straining.
- Eventually the load reaches a maximum value. The maximum load divided by the original area of the specimen is the *ultimate tensile strength*.
- For a ductile metal the diameter of the specimen begins to decrease rapidly beyond maximum load, so that the load required continuing deformation drops off until the specimen fractures.

DUCTILE Vs BRITTLE BEHAVIOR

Brittle Materials: A completely brittle material would fracture almost at the elastic limit

Ductile Materials: A brittle metal, such as white cast iron, shows some slight measure of plasticity before fracture



Figure 1-4 (a) Stress-strain curve for completely brittle material (ideal behavior); (b) stress-strain curve for brittle metal with slight amount of ductility.

- Adequate ductility is an important engineering consideration, because it allows the material to redistribute localized stresses.
- It is important to note that brittleness is not an absolute property of a metal.
- A metal such as tungsten, which is brittle at room temperature, is ductile at an elevated temperature.
- A metal which is brittle in tension may be ductile under hydrostatic compression.
- Furthermore, a metal which is ductile in tension at room temperature can become brittle in the presence of notches, low temperature, high rates of loading, or embrittling agents such as hydrogen.

CONCEPT OF STRAIN AND THE TYPES OF STRAIN

The average linear strain (engineering strain) was defined as the ratio of the change in length to the original length of the same dimension.

$$e = \frac{\delta}{L_0} = \frac{\Delta L}{L_0} = \frac{L - L_a}{L_0}$$

Where e = average linear strain

 δ = deformation

Rather than referring the change in length to the original gage length, it often is more useful to define the strain as the change in linear dimension divided by the instantaneous value of the dimension. The above equation defines the *natural* or *true strain*.

Not only will the elastic deformation of a body result in a change in length of a linear element in the body, but it may also result in a change in the initial angle between any two lines. The angular change in a right angle is known as *shear strain*.



Figure 1-7 Shear strain.

Poisson's ratio: While a tensile force in the x direction produces an extension along that axis, it also produces a contraction in the transverse y and z directions. The transverse strain has been found by experience to be a constant fraction of the strain in the longitudinal direction. This is known as **Poisson's ratio**, denoted by the symbol P.

• For most metals the values of v are close to 0.33.

Material	Modulus of elasticity, GPa	Shear modulus, GPa	Poisson's ratio	
Aluminum alloys	72.4	27.5	0.31	
Copper	110	41.4	0.33	
Steel (plain carbon and low-alloy)	200	75.8	0.33	
Stainless steel (18-8)	193	65.6	0.28	
Titanium	117	44.8	0.31	
Tungsten	400	157	0.27	

Table 2-t Typical room-temperature values of elastic constants for isotropic materials

ELEMENTS OF THE THEORY OF PLASTICITY

- The theory of plasticity deals with the behavior of materials at strains where Hooke's law is no longer valid.
- Elastic deformation depends only on the initial and final states of stress and strain.
- The plastic strain depends on the loading path by which the final state is achieved.
- Moreover, in plastic deformation there is no easily measured constant relating stress to strain as with Young's modulus for elastic deformation.
- The phenomenon of **strain hardening** is difficult to accommodate within the theory of plasticity without introducing considerable mathematical complexity.
- Also, several aspects of real material behavior, such as plastic anisotropy, elastic hysteresis, and the Bauschinger effect cannot be treated easily by plasticity theory.

THE FLOW CURVE

The stress-strain curve obtained by uniaxial loading, as in the ordinary tension test, is of fundamental interest in plasticity when the curve is plotted in terms of true stress and true strain.

- A true stress-strain curve is frequently called a *flow curve* because it gives the stress required to cause the metal to flow plastically to any given strain.
- Many attempts have been made to fit mathematical equations to this curve.
- The most common is a power expression of the form

$$\sigma = K\varepsilon^n$$

- Were *K* is the stress at $\varepsilon = 1.0$ and *n*, the strain-hardening coefficient, is the slope of a log-log plot of above Eq.
- This equation can be valid only from the beginning of plastic flow to the maximum load at which the specimen begins to neck down.



(a) Rigid ideal plastic material

(b) ideal plastic material (c) piecewise linear (strain-hardening) material

TRUE STRESS AND TRUE STRAIN

STRESS

Stress, σ , is defined as the intensity of force at a point:

$\sigma = \partial F / \partial A \text{ as } \partial A \to 0.$

If the state of stress is the same everywhere in a body,

$\sigma = F/A.$

A *normal stress* (compressive or tensile) is one in which the force is normal to the area on which it acts. With a *shear stress*, the force is parallel to the area on which it acts.

Two subscripts are required to define a stress. The first subscript denotes the normal to the plane on which the force acts and the second subscript identifies the direction of the force.* For example, a tensile stress in the *x*-direction is denoted by σ_{xx} , indicating that the force is in the *x*-direction and it acts on a plane normal to *x*. For a shear stress, σ_{xy} , a force in the *y*-direction acts on a plane normal to *x*.

Because stresses involve both forces and areas, they are not vector quantities. Nine components of stress are needed to describe a state of stressfully at a point, as shown in Figure 1.1. The stress component $\sigma_{yy} = F_y/A_y$

describes the tensile stress in the y-direction. The stress component $\sigma_{zy} = F_y/A_z$ is the shear stress caused by a shear force in the y-direction acting on a plane normal to z. Repeated subscripts denote normal stresses (e.g., σ_{xx} , σ_{yy} , ...) whereas mixed subscripts denote shear stresses (e.g., σ_{xy} , σ_{zx} , ...). In *tensor* notation the state of stress is expressed as

$$\sigma_{ij} = \begin{bmatrix} \sigma_{xx} & \sigma_{yx} & \sigma_{zx} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{zy} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix},$$

Where *i* and *j* are iterated over *x*, *y*, and *z*. Except where tensor notation is required, it is often simpler to use a single subscript for a normal stress and to denote a shear stress by τ ; for **Example**,

$$\sigma_x \equiv \sigma_{xx}$$
 and $\tau_{xy} \equiv \sigma_{xy}$



Figure 1.1. The nine components of stress acting on an infinitesimal element. The normal stress components are σ_{XX} , σ_{YY} , and σ_{ZZ} . The shear stress components are σ_{yZ} , σ_{ZX} , σ_{XY} , σ_{ZY} , σ_{XZ} , and σ_{YX} .



Figure 1.2. Stresses acting on an area, *A'*, under a normal force, *F_Y*. The normal stress $\sigma_{y'y'} = F_{y'}/A_{y'} = F_{y}\cos\theta/(A_{y}/\cos\theta) = \sigma_{yy}\cos^2\theta$. The shear stress $\tau_{y'x'} = F_{x}/A_{y'} = F_{y}\sin\theta/(A_{yx}/\cos\theta) = \sigma_{yy}\cos\theta\sin\theta$.

STRAINS

An infinitesimal normal strain is defined by the change of length, L, of a line:

$$\mathrm{d}\varepsilon = \mathrm{d}L/L$$
.

Integrating from the initial length, *L*o, to the current length, *L*,

$$\varepsilon = \int \mathrm{d}L/L = \ln(L/L_{\rm o}).$$

This finite form is called *true strain* (or *natural strain*, *logarithmic strain*). Alternatively, *engineering* or *nominal strain*, *e*, is defined as

$$e = \Delta L/L_{o}$$
.

If the strains are small, then engineering and true strains are nearly equal. Expressing $\varepsilon = \ln(L/L_0) = \ln(1 + e)$ as a series expansion, $\varepsilon = e - e^{2/2} + e^{3/3!} - \cdot$, so as $e \to 0$, $\varepsilon \to e$. This is illustrated in the following example.

Example problem: Calculate the ratio e/ε for several values of e.

Solution: $e/\varepsilon = e/\ln(1 + e)$. Evaluating:

For e = 0.001, $e/\varepsilon = 1.0005$; For e = 0.01, $e/\varepsilon = 1.005$; For e = 0.02, $e/\varepsilon = 1.010$; For e = 0.05, $e/\varepsilon = 1.025$; For e = 0.10, $e/\varepsilon = 1.049$; For e = 0.20, $e/\varepsilon = 1.097$; For e = 0.50, $e/\varepsilon = 1.233$.

Note that the difference between *e* and ε is less than 1% for *e* < 0.02. There are several reasons that true strains are more convenient than engineering strains.

- 1. True strains for equivalent amounts of deformation in tension and compression are equal except for sign.
- 2. True strains are additive. For a deformation consisting of several steps, the overall strain is the sum of the strains in each step.

3. The volume change is related to the sum of the three normal strains. For constant volume, $\varepsilon x + \varepsilon y + \varepsilon z = 0$. These statements are not true for engineering strains, as illustrated in the following examples.

STRESS - STRAIN CURVES



Figure . Typical engineering stress- strain curve for a ductile material



Figure. The low-strain region of the stress-strain curve for a ductile material



Figure Inhomogeneous yielding of low carbon steel



Figure Inhomogeneous yielding of a linear polymer



Figure After a maximum on the stress-strain curve, deformation localizes to form a neck.

TRUE STRESS AND STRAIN

TENSION TEST:

The true stress is defined as

$$\sigma = F/A$$

Where, A is the instantaneous cross-sectional area corresponding to the force F. Before necking begins, the true strain is given by

$$\varepsilon = \ln(L/L_{\rm o}).$$

The engineering stress is defined as the force divided by the original area, $s=F/A_0$, and the engineering strain is defined as the change in length divided by the original length, $e=\Delta L/L_0$. As long as the deformation is uniform along the gauge length, the true stress and true strain can be calculated from the engineering quantities. With constant volume,

 $LA=L_0 A_0$, so that

$$A_{\rm o}/A = L/L_{\rm o}$$

and thus Ao/A=1+e Rewriting above Equation as $\sigma = (F/Ao)(Ao/A)$ and substituting Ao/A=1+e and s=F/Ao,

$$\sigma = s(1+e)$$

Substitution of $L/L_0 = 1 + e$ into Equation (3.5) gives

$$\varepsilon = \ln(1 + e)$$

COMPRESSION TEST:

The shape of the engineering stress-strain curve in compression can be predicted from the true stress-strain curve in tension, assuming that absolute values of true stress in tension and compression are the same at the same absolute strain values. Equations (3.7) and (3.8) apply, but it must be remembered that both the stress and strain are negative in compression,

$$e_{\text{comp}} = \exp(\varepsilon) - 1$$

 $s_{\text{comp}} = \sigma/(1+e)$



Figure Comparison of engineering and true stress-strain curves. Before necking, a point on the true stressstrain curve (σ - ε) can be constructed from a point on the engineering stress-strain curve (s-e) with Equations (3.7) and (3.8). After necking, the cross-sectional area at the neck must be measured to find the true stress and strain.



Figure Stress–strain relations in compression for a ductile material. Each point σ , ε on the true stress–true strain curve corresponds to a point *s*, *e* on the engineering stress–strain curve. The arrows connect these points.

• The engineering stress-strain curve does not give a true indication of the deformation characteristics of a material because it is based entirely on the original dimensions of the specimen, and these dimensions change continuously during the test.

$$e = \frac{\Delta L}{L_0} = \frac{1}{L_0} \int_{L_0}^{L} dL$$

- This definition of strain is satisfactory for elastic strains where ΔL is very small.
- However, in plastic deformation the strains are frequently large, and during the extension the gage length changes considerably.
- Ludwik first proposed the definition of true strain, or natural strain, ε, which obviates this difficulty.
- In this definition of strain the change in length is referred ·to the instantaneous gage length, rather than to the original gage length.

$$\varepsilon = \sum \frac{L_1 - L_0}{L_0} + \frac{L_{2-L_1}}{L_1} + \frac{L_3 - L_2}{L_2} + \cdots$$

Or,

$$\varepsilon = \int_{L_0}^{L} \frac{dL}{L} = ln \frac{L}{L_0}$$

• The relationship between true strain and conventional linear strain follows from previous relationship.

$$e = \frac{\Delta L}{L_0} = \frac{L - L_0}{L_0} = \frac{L}{L_0} - 1$$
$$e + 1 = \frac{L}{L_0}$$
$$\varepsilon = \ln \frac{L}{L_0} = \ln (e + 1)$$

• Values of true strain and conventional linear strain are given for comparison:

True strain ε	0.01	0.10	0.20	0.50	1.0	4.0
. Conventional strain e	0.01	0.105	0.22	0.65	1.72	53.6

- *True stress* is the load at any instant divided by the cross-sectional area over which it acts.
- The *engineering stress*, or conventional stress, is the load divided by the original area.
- True stress will be denoted by the familiar symbol σ , while engineering stress will be denoted by s.

True stress
$$\sigma = \frac{P}{A}$$
Engineering stress $S = \frac{P}{A_0}$

The true stress may be determined from the engineering stress as follows:

$$\sigma = \frac{P}{A} = \frac{P}{A_0} \times \frac{A_0}{A}$$

But, by the constancy-of-volume relationships

$$\frac{A_0}{A} = \frac{L}{L_0} = e + 1$$

From above eq.:

$$\sigma = \frac{P}{A_0} \times \frac{A_0}{A} = S(e+1)$$

HYDROSTATIC AND DEVIATOR COMPONENTS OF STRESS

• The total stress tensor can be divided into a hydrostatic or mean stress tensor am, which involves only pure tension or compression, and a deviator stress tensor $\sigma'_{l,l}$, which represents the shear stresses in the total state of stress (Fig. 2-18).



Figure 2-18 Resolution of total stress into hydrostatic stress and stress deviator

- The hydrostatic component of the stress tensor produces **only elastic volume changes** and **does not cause plastic deformation**.
- Experiment shows that the yield stress of metals is independent of hydrostatic stress, although the fracture strain is strongly influenced by hydrostatic stress.
- Because the stress deviator involves the shearing stresses, it is important in causing plastic deformation
- We shall see that the stress deviator is useful in formulating theories of yielding. The hydrostatic or mean stress is given by

$$\sigma_m = \frac{\sigma_{kk}}{3} = \frac{\sigma_x + \sigma_y + \sigma_z}{3} = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3}$$

The decomposition of the stress tensor is given by

$$\sigma_{ij} = \sigma_{ij}' + \frac{1}{3}\delta_{ij}\sigma_{kk}$$

Therefore,

$$\sigma_{ij}' = \sigma_{ij} - \sigma_m \delta_{ij}$$

$$\sigma_{ij}' = \begin{vmatrix} \frac{2\sigma_x - \sigma_y - \sigma_z}{3} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \frac{2\sigma_y - \sigma_z - \sigma_x}{3} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \frac{2\sigma_z - \sigma_x - \sigma_y}{3} \end{vmatrix}$$

ELASTIC STRESS-STRAIN RELATIONS

- Equations of this nature are called **constitutive equations**. In this chapter we shall consider only constitutive equations for elastic solids. Moreover, initially we shall only consider isotropic elastic solids.
- The elastic stress is linearly related to elastic strain by means of the modulus of elasticity (Hooke's law).

$$\sigma_x = E \varepsilon_x$$

Where E is the modulus of elasticity in tension or compression

Poisson's ratio

- While a tensile force in the x direction produces an extension along that axis, it also produces a contraction in the transverse y and z directions.
- The transverse strain has been found by experience to be a constant fraction of the strain in the longitudinal direction. This is known as **Poisson's ratio**, denoted by the symbol γ

$$\epsilon_y = \epsilon_z = -\nu \epsilon_x = -\frac{\nu \sigma_x}{E}$$

• Only the absolute value of v is used in calculations. For **most metals** the values of v are close to **0.33**.

Stress-strain relations for a 3D state of stress

• The elastic stresses are small and the material is isotropic, we can assume that normal stress ox does not produce shear strain on the x, y, or z planes and that a shear stress t does not produce normal strains on the x, y, or z planes.

Thus,

Stress	Strain in the x direction	Strain in the y direction	Strain in the z direction	
σχ	$\varepsilon_x = \frac{\sigma_x}{E}$	$\epsilon_y = -\frac{\nu \sigma_x}{E}$	$\epsilon_x = -\frac{\nu \sigma_x}{E}$	
σ _y .	$\epsilon_x = -\frac{\nu \sigma_y}{E}$	$\epsilon_y = \frac{\sigma_y}{E}$	$\varepsilon_z = -\frac{\nu \sigma_y}{E}$	
$\sigma_{\tilde{c}}$	$\epsilon_x = -\frac{\nu \sigma_z}{E}$	$\epsilon_y = -\frac{\nu \sigma_z}{E}$	$\epsilon_z = \frac{\sigma_z}{E}$	

By superposition of the components of strain in the x, y, and z directions

$$\epsilon_{x} = \frac{1}{E} \left[\sigma_{x} - \nu (\sigma_{y} + \sigma_{z}) \right]$$
$$\epsilon_{y} = \frac{1}{E} \left[\sigma_{y} - \nu (\sigma_{z} + \sigma_{x}) \right]$$
$$\epsilon_{z} = \frac{1}{E} \left[\sigma_{z} - \nu (\sigma_{x} + \sigma_{y}) \right]$$

The shearing stresses acting on the unit cube produce shearing strains

$$\tau_{xy} = G\gamma_{xy}$$
 $\tau_{yz} = G\gamma_{yz}$ $\tau_{xz} = G\gamma_{xz}$

- The proportionality constant G is the modulus of elasticity in shear, or the modulus of rigidity. Values of G are usually determined from a torsion test.
- Still another elastic constant is the bulk modulus or the volumetric modulus of elasticity K. *The bulk modulus is the ratio of the hydrostatic pressure to the dilatation that it produces.*

$$K = \frac{\sigma_m}{\Delta} = \frac{-p}{\Delta} = \frac{1}{\beta}$$

• Where -p is the hydrostatic pressure and $\frac{1}{\beta}$ is the compressibility.

Many useful relationships may be derived between the elastic constants E, G, $\mathcal{Y}K$. For example, if we add up the three equations

$$\varepsilon_x + \varepsilon_y + \varepsilon_z = \frac{1-2\nu}{E}(\sigma_x + \sigma_y + \sigma_z)$$

The term on the left is the volume strain Δ , and the term on the right is $3\sigma_m$.

$$\Delta = \frac{1-2\nu}{E} 3\sigma_m$$

Or

$$K=\frac{\sigma_m}{\Delta}=\frac{E}{3(1-2\nu)}$$

Another important relationship is the expression relating E, G, and γ

$$G=\frac{E}{2(1+\nu)}$$

Many other relationships can be developed between these four isotropic elastic constants. **For example,**

$$E = \frac{9K}{1 + 3K/G} \qquad \nu = \frac{1 - 2G/3K}{2 + 2G/3K}$$
$$G = \frac{3(1 - 2\nu)K}{2(1 + \nu)} \qquad K = \frac{E}{9 - 3E/G}$$

STRAIN ENERGY

- The *elastic strain energy* U is the energy expended by the action of external forces in deforming an elastic body.
- Essentially all the work performed during elastic deformation is stored as elastic energy, and this energy is recovered on the release of the applied forces.
- Energy (or work) is equal to a force multiplied by the distance over which it acts.
- In the deformation of an elastic body, the force and deformation increase linearly from initial values of zero so that the average energy is equal to one-half of their product.
- This is also equal to the area under the load-deformation curve.

$$U = \frac{1}{2}P\delta$$

For an elemental cube that is subjected to only a tensile stress along the x axis, the elastic strain energy is given by

$$dU = \frac{1}{2}P \, du = \frac{1}{2}(\sigma_x A)(\varepsilon_x \, dx)$$
$$= \frac{1}{2}(\sigma_x \varepsilon_x)(A \, dx)$$

The strain energy per unit volume or strain energy density U₀ is given by

$$U_0 = \frac{1}{2}\sigma_x \varepsilon_x = \frac{1}{2}\frac{\sigma_x^2}{E} = \frac{1}{2}\varepsilon_x^2 E$$

By the same type of reasoning, the strain energy per unit volume of an element subjected to pure shear is given by

$$U_0 = \frac{1}{2}\tau_{xy}\gamma_{xy} = \frac{1}{2}\frac{\tau_{xy}^2}{G} = \frac{1}{2}\gamma_{xy}^2G$$

CONTINUUM MECHANICS

It should be recognized that the equations describing the state of stress or strain in a body are applicable to any solid continuum, whether it be an elastic or plastic solid or a viscous fluid. Indeed, this body of knowledge is often called *continuum mechanics*. The equations relating stress and strain are called *constitutive equations* because they depend on the material behavior.

For example,

- In a thin plate loaded in the plane of the plate there will be no stress acting perpendicular to the surface of the plate. The stress system will consist of two normal stresses σ_x and σ_y and a shear stress τ_{xy} . A stress condition in which the stresses are zero in one of the primary directions is called *plane stress*.
- ★ For any state of stress it is always possible to define a new coordinate system which has axes perpendicular to the planes on which the maximum normal stresses act and on which no shearing stresses act. These planes are called the *principal planes*, and the stresses normal to these planes are the *principal stresses*. For two-dimensional plane stress there will be two principal stresses and₂ which occur at angles that are 90° apart (Fig. 2-4). For the general case of stress in three dimensions there will be three principal stresses_{$\sigma_1} and . \sigma_3$ </sub>
- According to convention, a1 is the algebraically greatest principal stress, while is the algebraically smallest stress.
- The directions of the principal stresses are the principal axes 1, 2, and 3. Although in general the principal axes 1, 2, and 3 do not coincide with the Cartesian-coordinate axes x, y, z, for many situations that are encountered in practice the two systems of axes coincide because of symmetry of loading and deformation.
- The specification of the principal stresses and their direction provides a convenient way of describing the state of stress at a point.

State of Stress in Three Dimensions

- The general three-dimensional state of stress consists of three unequal principal stresses acting at a point. This is called a tri-axial state of stress.
- If two of the three principal stresses are equal, the state of stress is known as cylindrical,
- While if all three principal stresses are equal, the state of stress is said to be hydrostatic or spherical.
- The determination of the principal stresses for a three-dimensional state of stress in terms of the stresses acting on an arbitrary Cartesian-coordinate system is an extension of the method described in Sec. 2-3 for the two-dimensional case.
- Figure 2-7 represents an elemental free body similar to that shown in Fig. 2-1 with a diagonal plane JKL of area A. The plane JKL is assumed to be a principal plane cutting through the unit cube; σ is the principal stress acting normal to the plane JKL.
- Let *l*, *m*, *n* be the direction cosines of σ , that is, the cosines of the angles between σ and the x, y, and z axes. Since the free body in Fig. 2-7, must be in equilibrium, the forces acting on each of its faces must balance.

The components of σ along each of the axes are S_x , S_y and S_z

$$S_x = \sigma l,$$
 $S_y = \sigma m$ $S_z = \sigma n$

Area KOL = AI

Area JOK = Am

Area JOL = An

Taking the summation of the forces in the x direction results in

$$\sigma Al - \sigma_x Al - \tau_{yx} Am - \tau_{zx} An = 0$$

This reduces to,

$$(\sigma - \sigma_x)l - \tau_{yx}m - \tau_{zx} = 0$$

Summing the forces along the other two axes results in

$$-\tau_{yx}l + (\sigma - \sigma_y)m - \tau_{zy}n = 0$$

$$-\tau_{xz} - \tau_{yz} + (\sigma - \sigma_z)n = 0$$

Equations (2-13) are three homogeneous linear equations in terms of /, m, and n. The only nontrivial solution can be obtained by setting the determinant of the coefficients of l, m, and n equal to zero, since l, w, and n cannot all be zero.

$$\begin{vmatrix} \sigma - \sigma_x & -\tau_{yx} & -\tau_{zx} \\ -\tau_{xy} & \sigma - \sigma_y & -\tau_{zy} \\ -\tau_{xz} & -\tau_{yz} & \sigma - \sigma_z \end{vmatrix} = 0$$

Solution of the determinant results in a cubic equation in σ .

$$\sigma^{3} - (\sigma_{x} + \sigma_{y} + \sigma_{z})\sigma^{2} + (\sigma_{x}\sigma_{y} + \sigma_{y}\sigma_{z} + \sigma_{x}\sigma_{z} - \tau_{xy}^{2} - \tau_{yz}^{2} - \tau_{xz}^{2})\sigma - (\sigma_{x}\sigma_{y}\sigma_{z} + 2\tau_{xy}\tau_{yz}\tau_{xz} - \sigma_{x}\tau_{yz}^{2} - \sigma_{y}\tau_{xz}^{2} - \sigma_{z}\tau_{xy}^{2}) = 0$$

The three roots of Eq. (2-14) are the three principal stresses $\sigma_1 \sigma_2$, and σ_3 To determine the direction, with respect to the original x, y, z axes, in which the principal stresses act, it is necessary to substitute, o, and o each in turn into the three equations of Eq. (2-13). The resulting equations must be solved simultaneously for 1, m, and n with the help of the auxiliary relationship $l^2 + m^2 + n^2 = 1$.

Note that there are three combinations of stress components in Eq. (2-14) that make up the coefficients of the cubic equation. Since the values of these Coefficients determine the principal stresses, they obviously do not vary with Changes in the coordinate axes. Therefore, they are invariant coefficients.

$$\sigma_x + \sigma_y + \sigma_z = I_1$$

$$\sigma_x \sigma_y + \sigma_y \sigma_z + \sigma_x \sigma_z - \tau_{xy}^2 - \tau_{yz}^2 - \tau_{xz}^2 = I_2$$

$$\sigma_x \sigma_y \sigma_z + 2\tau_{xy} \tau_{yz} \tau_{xz} - \sigma_x \tau_{yz}^2 - \sigma_y \tau_{xz}^2 - \sigma_z \tau_{xy}^2 = I_3$$

The first invariant of stress l_1 has been seen before for the two-dimensional state of stress. It states the useful relationship that the sum of the normal stresses for any orientation in the coordinate system is equal to the sum of the normal stresses for any other orientation.

For example

$$\sigma_x + \sigma_y + \sigma_z = \sigma_{x'} + \sigma_{y'} + \sigma_{z'} = \sigma_1 + \sigma_2 + \sigma_3$$

Stress Tensor

- Many aspects of the analysis of stress, such as the equations for the transformation of the stress components from one set of coordinate axes to another coordinate system or the existence of principal stresses, become simpler when it is realized that stress is a second-rank tensor quantity.
- Many of the techniques for manipulating second-rank tensors do not require a deep understanding of tensor calculus, so it is advantageous to learn something about the properties of tensors.
- We shall start with the consideration of the transformation of a vector (a first-rank tensor) from one coordinate system to another.

Consider the vector

$$\mathbf{S} = S_1 i_1 + S_2 i_2 + S_3 i_3$$

- When the unit vectors i₁, i₂, i₃ are in the directions S₁, S₂, S₃ (In accordance with convention and convenience in working with tensor quantities, the coordinate axes will be designated x₁, x₂, etc., where x₁ is equivalent to our previous designation x, x₂ is equivalent to the old y, etc.)
- > S₁, S₂, S₃ are the components of S referred to the axes x1, x2, x3. We now want to find the components of S referred to the x'_1, x'_2, x'_3 axes, Fig. 11. S is obtained by resolving S₁, S₂, S₃ along the new direction x'_1 .



Figure 2-9 Transformation of axes for a vector

$$S'_{1} = S_{1} \cos(x_{1}x'_{1}) + S_{2} \cos(x_{2}x'_{1}) + S_{3} \cos(x_{3}x'_{1})$$

Or,

Where a_{11} is the direction cosine between x'_1 and x_1 , a_{12} is the direction cosine between x'_1 and x_2 etc., similarly $S'_2 = a_{21}S_1 + a_{22}S_1 + a_{23}S_3$

$$S_3' = a_{31}S_1 + a_{32}S_2 + a_{33}S_3$$

We note that the leading suffix for each direction cosine in each equation is the same, so we could write these equations as

$$S'_{1} = \sum_{j=1}^{3} a_{1,j} S_{j}$$
, $S'_{2} = \sum_{j=1}^{3} a_{2,j} S_{j}$, $S'_{3} = \sum_{j=1}^{3} a_{3,j} S_{j}$

These three equations could be combined by writing

$$S_i' = \sum_{j=1}^3 a_{i,j} S_j (i = 1, 2, 3) = a_{i1} S_1 + a_{i2} S_2 + a_{i3} S_3$$

Still greater brevity is obtained by writing Eq. (2-23) in the Einstein suffix notation

$$S_i' = a_{ij}S_j$$

- The suffix notation is a very useful way of compactly expressing the systems of equations usually found in continuum mechanics. In Eq. (2-24) it is understood that when a suffix occurs twice in the same term (in this case the suffix j), it indicates summation with respect to that suffix. Unless otherwise indicated, the summation of the other index is from 1 to 3.
- > In the above example, I is a free suffix and it is understood that in the expanded form there is one equation for each value of i. The repeated index is called a dummy suffix. Its only purpose is to indicate summation. Exactly the same three equations would be produced if some other letter were used for the dummy suffix, for example, $S'_i = a_{ir}S_i$ would mean the same thing as Eq. (2-24).
- We saw in Sec. 2-5 that the complete determination of the state of stress at a point in a solid requires the specification of nine components of stress on the orthogonal faces of the element at the point. A vector quantity only requires the specification of three components. Obviously, stress is more complicated than a vector.
- Physical quantities that transform with coordinate axes in the manner of Eq. (2-18) are called tensors of the second rank.
- Stress, strain, and many other physical quantities are second-rank tensors. A scalar quantity, which remains unchanged with transformation of axes, requires only a single number for its specification. Scalars are tensors of zero rank.
- > Vector quantities require three components for their specification, so they are tensors of the first rank.
- The number of components required to specify a quantity is?, where n is the rank of the tensor. The elastic constant that relates stress with strain in an elastic solid is a fourth-rank tensor with 81 components in the general case.

Stress Tensor $\tau_{i,j}$ the stress (force per unit area) at a point in fluid needs nine components to be completely specified, since each component of the stress must be depend not only by the direction in which it acts but also the orientation of the surface upon which it is acting. The first index specifies the direction in which the stress component acts, and the second identifies the orientation of the surface upon which it is acting. The first index upon which it is acting. Therefore, the *i*th component of the force acting on a surface whose outward normal points in the *j*th direction is $\tau_{i,j}$



Figure 1: Shear stresses on an infinitesimal cube whose surface are parallel to the coordinate system.



Figure 2: Consider an infinitesimal body at rest with a surface PQR that is not perpendicular to any of the Cartesian axis. The unit normal vector to that surface is $\hat{n} = n_1 \hat{x}_1 + n_2 \hat{x}_2 + n_3 \hat{x}_3$. The area of the surface = A_0 , and the area of each surface perpendicular to X_i is $A_i = A_0 n_i$, for i = 1, 2, 3.

Newton's law:
$$\sum_{all \leq faces} F_i = (\text{volume force})_i \text{ for } i = 1, 2, 3$$

If δ is the typical dimension of the body : surface forces $\sim \delta^2$
; volume forces $\sim \delta^3$

An example of surface forces is the shear force and an example of volumetric forces is the gravity force. At equilibrium, the surface forces and volumetric forces are in balance. As the body gets smaller, the mass of the body goes to zero, which makes the volumetric forces equal to zero and leaving the sum of the surface forces equal zero. So, as $\delta \rightarrow 0$; $\sum_{all \ 4 \ faces} F_i = 0$ for i = 1, 2, 3.

FLOW CURVES IN DUCTILE MATERIALS:

- The true stress-strain curve for a typical ductile metal, such as aluminum, is illustrated in Fig. 3-l(a).
- Hooke's law is followed up to some yield stress σ_0 . (The value of σ_0 will depend upon the accuracy with which strain is measured.)
- Beyond σ_0 , the metal deforms plastically.
- Most metals strain-harden in this region, so that increases in strain require higher values of stress than the initial yield stress σ_0 .

- However, unlike the situation in the elastic region, the stress and strain are not related by any simple constant of proportionality. If the metal is strained to point A, when the load is released the total strain will immediately decrease from ε₁ to ε₂ by an amount σ₀/E.
- The strain decrease ϵ_1 is ϵ_2 the recoverable elastic strain. However, the strain remaining is not all permanent plastic strain.
- Depending upon the metal and the temperature, a small amount of the plastic strain $\epsilon_2 \epsilon_3$ will disappear with time. This is known as an elastic behavior. Generally the anelastic strain is neglected in mathematical theories of plasticity.



Figure 3-1 Typical true stress-strain curves for a ductile metal.

- Usually the stress-strain curve on unloading from a plastic strain will not be exactly linear and parallel to the elastic portion of the curve (Fig. 3-1(b)).
- Moreover, on reloading the curve will generally bend over as the stress approaches the original value of stress from which it was unloaded. With a little additional plastic strain the stress-strain curve becomes a continuation of what it would have been had no unloading taken place.
- The hysteresis behavior resulting from unloading and loading from a plastic strain is generally neglected in plasticity theories.
- If a specimen is deformed plastically beyond the yield stress in one direction, e.g., in tension, and then after unloading to zero stress it is reloaded in the opposite direction, e.g., in compression, it is found that the yield stress on reloading is less than the original yield stress.
- Referring to Fig. 3-1 (c), $\sigma_b < \sigma_a$. This dependence of the yield stress on loading path and direction is called the *Bauschinger effect*.
- The Bauschinger effect is commonly ignored in plasticity theory, and it is usual to assume that the yield stress in tension and compression are the same.

YIELDING CRITERIA FOR DUCTILE MATERIALS:

- The problem of deducing mathematical relationships for predicting the conditions at which plastic yielding begins when a material is subjected to any possible combination of stresses is an important consideration in the field of plasticity.
- The yielding criteria are essentially empirical relationships. However, a yield criterion must be consistent with a number of experimental observations, the chief of which is that pure hydrostatic pressure does not cause yielding in a continuous solid.
- As a result of this, the hydrostatic component of a complex state of stress does not influence the stress at which yielding occurs. Therefore, we look for the stress deviator to be involved with yielding. Moreover, for an isotropic material, the yield criterion must be independent of the choice of axes, i.e., it must be an invariant function.
- These considerations lead to the conclusion that the yield criteria must be some function of the invariants of the stress deviator. At present there are two generally accepted criteria for predicting the onset of yielding in ductile metals.
 - 1. Von Mises' or Distortion-Energy Criterion
 - 2. Maximum-Shear-Stress or Tresca Criterion

VON MISES' OR DISTORTION-ENERGY CRITERION:

Von Mises (1913) proposed that yielding would occur when the second invariant of the stress deviator J_2 exceeded some critical value.

$$J_2 = k^2$$

Where,

$$J_2 = \frac{1}{6} \left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right]$$

To evaluate the constant k and relate it to yielding in the tension test, we realize that at yielding in uniaxial tension $\sigma_1 = \sigma_0$, $\sigma_2 = \sigma_3 = 0$

$$\sigma_0^2 + \sigma_0^2 = 6k^2$$
$$\sigma_0 = \sqrt{3}k$$

$$\sigma_0 = \frac{1}{\sqrt{2}} \left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 \right]^{1/2}$$

Or, from Eq. (2-61)

$$\sigma_0 = \frac{1}{\sqrt{2}} \left[\left(\sigma_x - \sigma_y \right)^2 + \left(\sigma_y - \sigma_z \right)^2 + \left(\sigma_z - \sigma_x \right)^2 + \left(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{xz}^2 \right) \right]^{1/2}$$

Equation (3-12) or (3-13) predicts that yielding will occur when the differences of stresses on the right side of the equation exceed the yield stress in uniaxial tension σ_0 .

To identify the constant k in Eq. (3-10), consider the state of stress in pure shear, as is produced in a torsion test.

 $\sigma_1 = -\sigma_3 = \tau \, \sigma_2 = 0$

At yielding
$$\sigma_1^2 + \sigma_1^2 + 4 \sigma_1^2 = 6 k^2$$

 $\sigma_1 = k$

So that k represents the yield stress in pure shear (torsion). Therefore, the Von Mises' criterion predicts that the yield stress in torsion will be less than in uniaxial tension according to

$$k = \frac{1}{\sqrt{3}}\sigma_0 = 0.577\sigma_0$$

To summarized, note that the Von Mises' yield criterion implies that is not depend on any particular normal stress or shear stress, but instead, yielding depend on a function of all three values of principal shearing stress. Since the yield criterion is based on differences of normal stresses, $\sigma_1 - \sigma_2$, etc., the criterion is independent of the component of hydrostatic stress.

Since the von Mises' yield criterion involves squared terms, the result is independent of the sign of the individual stresses. This is an important advantage since it is not necessary to know which are the largest and smallest principal stresses in order to use this yield criterion.

MAXIMUM-SHEAR-STRESS OR TRESCA CRITERION

This yield criterion assumes that yielding occurs when the maximum shear stress reaches the value of the shear stress in the uniaxial-tension test. From Eq. (2-21), the maximum shear stress is given by

$$\tau_{max} = \frac{\sigma_1 - \sigma_3}{2}$$

Where al is the algebraically largest and o3 is the algebraically smallest principal stress

For uniaxial tension, $\sigma_1 = \sigma_0$, $\sigma_2 = \sigma_3 = 0$, and the shearing yield stress τ_0 is equal to $\sigma_0/2$. Substituting in Eq. (3-20),

$$\tau_{max} = \frac{\sigma_1 - \sigma_3}{2} = \tau_0 = \frac{\sigma_0}{2}$$

Therefore, the maximum-shear-stress criterion is given by

$$\sigma_1 - \sigma_3 = \sigma_0$$

For a state of pure shear, $\sigma_1 = -\sigma_3 = k, \sigma_2 = 0$, the maximum-shear-stress criterion predicts that yielding will occur when

$$\sigma_1 - \sigma_3 = 2k = \sigma_0$$
$$k = \frac{\sigma_0}{2}$$

So that the maximum-shear-stress criterion may be written

$$\sigma_1 - \sigma_3 = \sigma_1' - \sigma_3' = 2k$$

Note that the maximum shear stress criterion is lass complicated mathematically than the von Mises' criterion and for this reason it is often used in engineering design.

However, the maximum shear criterion does not take into consideration the intermediate principal stress.

It suffers from the major difficulty that it is necessary to know in advance which the maximum are and minimum principal stresses

Moreover, the general form of the maximum-shear-stress criterion, Eq. (3-23), is far more complicated than the von Mises' criterion, Eq (3-10), and for this reason the von Mises' criterion is preferred in most theoretical work.



Figure 3-5 Comparison of yield criteria for plane stress.

PLASTIC DEFORMATION OF SINGLE CRYSTALS

- Following the discovery of the diffraction of x-rays by metallic crystals by Von Laue in 1912 and the realization that metals were fundamentally composed of atoms arranged in specific geometric lattices there have been a great many investigations of the relationships between atomic structure and the plastic behavior of metals.
- The dislocation theory, which plays such an important part in modem concepts of plastic deformation.

CONCEPTS OF CRYSTAL GEOMETRY

- X-ray diffraction analysis shows that the atoms in a metal crystal are arranged in a regular, repeated three-dimensional pattern.
- The atom arrangement of metals is most simply portrayed by a crystal lattice in which the atoms are visualized as hard balls located at particular locations in a geometrical arrangement.
- The most elementary crystal structure is the **simple cubic lattice** (Fig. 4-1).
- This is the type of structure cell found for ionic crystals, such as NaCl and LiF.
- Three mutually perpendicular axes are arbitrarily placed through one of the comers of the cell.

- Crystallographic planes and directions will be specified with respect to these axes in terms of *Miller indices*.
- A crystallographic plane is specified in terms of the length of its intercepts on the three axes, measured from the origin of the coordinate axes.
- To simplify the crystallographic formulas, the reciprocals of these intercepts are used.
- They are reduced to a lowest common denominator to give the Miller indices (*hkl*) of the plane.



Figure 4-1 Simple cubic structure.

- For example, the plane *ABCD* in Fig. 4-1 is parallel to the x and z axes and intersects the y axis at one interatomic distance a_0 .
- Therefore, the indices of the plane are 1/00, 1/1, 1/00, or (hkl) = (010).
- Plane *EBCF* would be designated as the (100) plane, since the origin of the coordinate system can be moved to G because every point in a space lattice has the same arrangement of points as every other point.
- The bar over one of the integers indicates that the plane intersects one of the axes in a negative direction.
- There are six crystallographically equivalent planes of the type (100), anyone of which can have the indices (100), (010), (001), (100), (001) depending upon the choice of axes.
- The notation $\{100\}$ is used when they are to be considered as a group, or *family of planes*.
- Crystallographic directions are indicated by integers in brackets: *[uvw]*.
- Reciprocals are not used in determining directions. As an example, the direction of the line FD is obtained by moving out from the origin a distance a_0 along the x axis and moving an equal distance in the positive y direction.
- The indices of this direction are then [110].
- A family of crystallographically equivalent directions would be designated *<uvw>*.
- For the cubic lattice only, a direction is always perpendicular to the plane having the same indices.
- Many of the common metals have either a **body-centered cubic (bcc)** or **face-centered cubic (fcc)** crystal structure.

• Figure 4-2a shows a body-centered cubic structure cell with an atom at each corner and another atom at the body center of the cube.



- •
- Each corner atom is surrounded by eight adjacent atoms, as is the atom located at the center of the cell.
- Therefore, there are two atoms *per structure cell* for the body-centered cubic structure $\left(\frac{8}{3}+1\right)$.
- Typical metals which have this crystal structure are **alpha iron**, **columbium**, **tantalum**, **chromium**, **molybdenum**, **and tungsten**.
- Figure 4-2b shows the structure cell for a face-centered cubic crystal structure. In addition to an atom at each corner, there is an atom at the center of each of the cube faces.
- Since these latter atoms belong to two unit cells, there are four atoms per structure cell in the facecentered cubic structure $(\frac{8}{8} + \frac{6}{2})$.
- Aluminum, copper, gold, lead, silver, and nickel are common face centered cubic metals.

For cubic systems there is a set of simple relationships between a direction *[uvw]* and a plane *(hkl)* which are very useful.

- 1. [uvw] is normal to (hkl) when u = h; v = k; w = l. [111] is normal to (111).
- 2. [uvw] is parallel to (hkl), i.e., [uvw] lies in (hkl), when hu + kv + lw = 0. [112] is a direction in (111).
- 3. Two planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ are normal if $h_1h_2 + k_1k_2 + l_1l_2 = 0$. (001) is perpendicular to (100) and (010). (110) is perpendicular to (110).
- 4. Two directions $u_1v_1w_1$ and $u_2v_2w_2$ are normal if $u_1u_2 + v_1v_2 + w_1w_2 = 0$. [100] is perpendicular to [001]. [111] is perpendicular to [112].
- 5. Angles between planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ are given by

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\left[\sqrt{h_1^2 + k_1^2 + l_1^2}\right]\left[\sqrt{h_2^2 + k_2^2 + l_2^2}\right]}$$

• The third common metallic crystal structure is the hexagonal close-packed (hcp) structure (Fig. 4-3).

- In order to specify planes and directions in the hcp structure, it is convenient to use the Miller-Bravais system with four indices of the type (*hkil*).
- These indices are based on four axes; the three axes a_1 , a_2 , a_3 are 120^0 apart in the basal plane, and the vertical c axis is normal to the basal plane.
- The third index is related to the first two by the relation i = -(h + k).



Figure 4-3 Hexagonal close-packed structure.

The face-centered cubic and hexagonal close-packed structures can both be built up from a stacking of closepacked planes of spheres. Figure 4-4 shows that I there are two ways in which the spheres can be stacked.



Figure 4-4 Stacking of close-packed spheres.

- The first layer of spheres is arranged so that each sphere is surrounded by and just touching six other spheres.
- This corresponds to the solid circles in Fig. 4-4.
- A second layer of close-packed spheres can be placed over the bottom layer so that the centers of the atoms in the second plane cover one-half the number of valleys in the bottom layer (dashed circles in Fig. 4-4).

- There are two ways of adding spheres to give a third close-packed plane. Although the spheres in the third layer must fit into the valleys in the second plane, they may lie either over the valleys not covered in the first plane (the dots in Fig. 4-4) or directly above the atoms in the first plane (the crosses in Fig. 4-4).
- The first possibility results in a stacking sequence *ABCABC*.....which is found for the {111} planes of an **fcc structure**.
- The other possibility results in the stacking sequence *ABAB*.....which is found for the (0001) basal plane of the **hcp structure**.
- For the ideal hcp packing, the ratio $\frac{c}{a}$ is $\sqrt{\frac{8}{3}}$ r 1.633.

Table 4-1 shows that actual hcp metals deviate from the ideal $\frac{c}{a}$ ratio.

Table 4-1 Axial ratios of some hexagonal metals				
Metal	cia			
Be	1.567			
Ti	1.587			
Mg	1.623			
Ideal hcp	1.633			
Zn	1.856			
Cd	1.886			

- The fcc and hcp structures are both close-packed structures.
- 74 % of the volume of the unit cell is occupied by atoms, on a hard sphere model, in the fcc and hcp structures.
- This is contrasted with **68 %** packing for a bcc unit cell.
- 52 % of the volume occupied by atoms in the simple cubic unit cell.

LATTICE DEFECTS

- While the concept of the perfect lattice is adequate for explaining the *structure-insensitive* properties of metals.
- For a better understanding of the *structure-sensitive* properties it has been necessary to consider a number of types of lattice defects.

Structure-insensitive	Structure-sensitive
Elastic constants	Electrical Conductivity
Melting point	Semiconductor properties
Density	Yield stress
Specific heat	Fracture strength
Coefficient of thermal expansion	Creep strength

• The term *defect*, or *imperfection*, is generally used to describe any deviation from an orderly array of lattice points.

0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0
0	0		0	0	0	0	0	0	•	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0
	(a)	Figure Vacan purity	e 4-5 ey; (b atom.	Poin) in	t (terst	lefects. itial; ((a) c) im-		(c		

- □ Low-angle boundaries and grain boundaries are surface defects.
- When the deviation from the periodic arrangement of the lattice is localized to the vicinity of only a few atoms it is called a *point defect*, or *point imperfection*.
- However, if the defect extends through microscopic regions of the crystal, it is called a *lattice imperfection*.
- Lattice imperfections may be divided into *line defects* and *surface*, or *plane*, *defects*.
- The edge and screw dislocations that are discussed in this section are the common line defects encountered in metals.
- The *stacking fault* between two close-packed regions of the crystal that have alternate stacking sequences and twinned region of a crystal are other examples of **surface defects.**

POINT DEFECTS

- A *vacancy* or vacant lattice site exists when an atom is missing from a normal lattice position (Fig. 4-5a).
- In pure metals, small numbers of vacancies are created by thermal excitation, and these are thermodynamically stable at temperatures greater than absolute zero.
- At equilibrium, the fraction of lattices that are vacant at a given temperature is given approximately by the equation.

$$\frac{n}{N} = e^{-E_s/_{kT}}$$

- Where n is the number of vacant sites in N sites and E_s is the energy required to move an atom from the interior of a crystal to its surface.
- An atom that is trapped inside the crystal at a point intermediate between normal lattice positions is called an *interstitial atom*, or interstitialcy (Fig. 4-5b).
- The interstitial defect occurs in pure metals as a result of bombardment with high-energy nuclear particles (radiation damage), but it does not occur frequently as a result of thermal activation.

- The presence of an *impurity atom* at a lattice position (Fig. 4-5c) or at an interstitial position results in a local disturbance of the periodicity of the lattice, the same as for vacancies and interstitials.
- It is important to realize that no material is completely pure. Most commercially "pure" materials contain usually 0.01 to 1 percent impurities,
- While ultra purity materials, such as germanium and silicon crystals for transistors, contain purposely introduced foreign atoms on the order of one part in 10¹⁰.

LINE DEFECTS-DISLOCATIONS

- The most important two-dimensional, or line, defect is the *dislocation*.
- The dislocation is the defect responsible for the phenomenon of **slip**, by which most metals deform plastically.
- In Fig. 4-6, *AB* represents a dislocation lying in the slip plane, which is the plane of the paper. It is assumed that slip is advancing to the right. All the atoms above area C have been displaced one atomic distance in the slip direction; the atoms above *D* have not yet slipped. *AB* is then the boundary between the slipped and unslipped regions.
- In the absence of obstacles, a dislocation can move easily on the application of only a small force.
- This helps explain why real crystals deform much more readily than would be expected for a crystal with a perfect lattice.
- Not only are dislocations important for explaining the slip of crystals, but they are also intimately connected with nearly all other mechanical phenomena such as strain hardening, the yield point, creep, fatigue, and brittle fracture.
- The two basic types of dislocations are the edge dislocation and the screw dislocation.



Figure Edge dislocation produced by slip in a simple cubic lattice. Dislocation lies along *AD*, perpendicular to slip direction. Slip has occurred over area *ABCD*.

• Figure shows the slip that produces an edge dislocation for an element of crystal having a simple cubic lattice. Slip has occurred in the direction of the slip vector over the area *ABCD*. The boundary between the right-hand slipped part of the crystal and the left-hand part which has not yet slipped is the line *AD*, the edge dislocation.

- The amount of displacement is equal to the *Burgers vector* **b** of the dislocation. A defining characteristic of an **edge dislocation** is that its Burgers vector is always **perpendicular to the dislocation line**.
- There is one more vertical row of atoms above the slip plane than below it. The atomic arrangement results in a **compressive stress** above the slip plane and a **tensile stress** below the slip plane.
- An edge dislocation with the extra plane of atoms above the slip plane, as in Figure, by convention is called a *positive edge dislocation* and is frequently indicated by the symbol ⊥. If the extra plane of atoms lies below the slip plane, the dislocation is a **negative edge dislocation**, [¬].
- A pure edge dislocation can glide or slip in a direction perpendicular to its length. However, it may move vertically by a process known as *climb*, if diffusion of atoms or vacancies can take place at an appreciable rate.

Plastic Deformation of Single Crystals



Figure Atomic arrangement in a plane normal to an edge dislocation

- Although the exact arrangement of atoms along AD is not known, it is generally agreed that Fig. closely represents the atomic arrangement in a plane normal to the edge dislocation AD.
- The plane of the paper in this figure corresponds to a (100) plane in a simple cubic lattice and is equivalent to any plane parallel to the front face of previous Figure.
- Note that the lattice is distorted in the region of the dislocation. There is one more vertical row of atoms above the slip plane than below it. The atomic arrangement results in a compressive stress above the slip plane and a tensile stress below the slip plane.
- An edge dislocation with the extra plane of atoms above the slip plane, as in Fig., by convention is called a positive edge dislocation and is frequently indicated by the symbol[⊥]. If the extra plane of atoms lies below the slip plane, the dislocation is a negative edge dislocation, T.
- A pure edge dislocation can glide or slip in a direction perpendicular to its length. However, it may move vertically by a process known as climb, if diffusion of atoms or vacancies can take place at an appreciable rate.

- Consider Fig.. For the edge dislocation to move upward (positive direction of climb), it is necessary to remove the extra atom directly over the symbol⊥ or to add a vacancy to this spot.
- One such atom would have to be removed for every atomic spacing; which the dislocation climbs. Conversely, if the dislocation moved down, atoms would have to be added. Atoms could be removed from the extra plane of atoms by the extra atom interacting with a lattice vacancy.
- Atoms are added to the extra plane for negative climb by the diffusion of an atom from the surrounding crystal, creating a vacancy. Since movement by climb is diffusion controlled, motion is much slower than in glide and less likely except at high temperatures.



Figure Slip that produces a screw dislocation in a simple cubic lattice. Dislocation lies along AD, parallel to slip direction. Slip has occurred over the area ABCD.



Figure Atomic arrangement around the screw dislocation shown in previous Fig.. The plane of the figure is parallel to the slip plane. A BCD is the slipped area, and AD is the screw dislocation. Open circles represent atoms in the atomic plane just above the slip plane, and the solid circles are atoms in the plane just below the slip plane.

• The second basic type of dislocation is the screw, or Burgers, dislocation. Figure shows a simple example of a screw dislocation. The upper part of the crystal to the right of AD has moved relative to the lower part in the direction of the slip vector. No slip has taken place to the left of AD, and therefore AD is a dislocation line.
- Thus, the dislocation line is parallel to its Burgers vector, or slip vector, and by definition this must be a screw dislocation. Consider the trace of a circuit around the dislocation line, on the front face of the crystal.
- Starting at X and completing a counterclockwise circuit, we arrive at X', one atomic plane behind that containing X. In making this circuit we have traced the path of a right-handed screw.
- Every time a circuit is made around the dislocation line, the end point is displaced one plane parallel to the slip plane in the lattice. Therefore, the atomic planes are arranged around the dislocation in a spiral staircase or screw.
- The arrangement of atoms (in two dimensions) around a screw dislocation in a simple cubic lattice is shown in Fig.
- In this figure we are looking down on the slip plane in Fig.. The open circles represent atoms just above the slip plane, and the solid circles are atoms just below the slip plane. A screw dislocation does not have a preferred slip plane, as an edge dislocation has, and therefore the motion of a screw dislocation is less restricted than the motion of an edge dislocation. However, movement by climb is not possible with a screw dislocation.

DEFORMATION BY SLIP

- The usual method of plastic deformation in metals is by the sliding of blocks of the crystal over one another along definite crystallographic planes, called **slip planes**.
- As a very crude approximation, the slip, or glide of a crystal can be considered analogous to the distortion produced in a deck of cards when it is pushed from one end.



Figure 4-11 Schematic drawing of classical idea of slip.

Figure illustrates this classical picture of slip.

- In Fig. 4- 11a, a shear stress is applied to a metal cube with a top polished surface. Slip occurs when the shear stress exceeds a critical value.
- The atoms move an integral number of atomic distances along the slip plane, and a step is produced in the polished surface (Fig. 4-11b).

- When we view the polished surface from above with a microscope, the step shows up as a line, which we call a slip line. If the surface is then repolished after slip has occurred, so that the step is removed, the slip line will disappear (Fig. 4-11c).
- Because of the translational symmetry of a crystal lattice, the crystal structure is perfectly restored after slip has taken place provided that the deformation was uniform.
- Note that slip lines are due to changes in surface elevation and that the surface must be suitably prepared for microscopic observation prior to deformation if the slip lines are to be observed. Figure 4-12 shows straight slip lines in copper.



Figure 4-12 Straight slip lines in copper (500 ×). (Courtesy W. L. Phillips.)

The fine structure of slip lines has been studied at high magnification by means of the electron microscope. What appears as a line, or at best a narrow band at 1,500 diameters' magnification in the optical microscope can be resolved by the electron microscope as discrete slip lamellae at 20,000 diameters, shown schematically in Fig. 4-13.



Figure Schematic drawing of the line structure of a slip band, (a) Small deformation; (b) large deformation

- Slip occurs most readily in specific directions on certain crystallographic planes.
- Generally the slip plane is the plane of greatest atomic density (Table 4-2) and the slip direction is the closest-packed direction within the slip plane.
- The slip plane together with the slip direction establishes the slip system

Crystal structure	Plane	Atomic density, atoms per unit area	Distance between planes
Face-centered cubic	Octahedral (111) Cube (100)	$4/\sqrt{3} a_0^2$	$a_0/\sqrt{3}$
	Dodecahedral (110)	$\frac{2}{\sqrt{2}a_0^2}$	$\frac{u_0}{2}$
Body-centered cubic	Dodecahedral {110} Cube {100}	$\frac{2}{\sqrt{2}}a_0^2}{1/a_0^2}$	$a_0/\sqrt{2}$ $a_0/2$
Hexagonal close-packed	Octahedral {111} Basal {0001}	$\frac{1}{\sqrt{3}} \frac{a_0^2}{a_0^2}$ $\frac{2}{\sqrt{3}} \frac{a_0^2}{a_0^2}$	$a_0/2\sqrt{3}$

Table 4-2 Atomic density of low-index planes

HCP System

- In the **hexagonal close-packed metals**, the only plane with high atomic density is the basal plane (0001). The axes <1120> are the close-packed directions.
- For zinc, cadmium, magnesium, and cobalt slip occurs on the (0001) plane in the <1120> directions.1 since there is only one basal plane per unit cell and three <1120> directions.
- The hcp structure possesses three slip systems.
- The limited number of slip systems is the reason for the extreme orientation dependence and low ductility in hcp crystals.
- **Zirconium** and **titanium**, which have low **c/a ratios**, slip primarily on the prism and pyramidal planes in the <1120> direction.

FCC System

- In the **face-centered cubic** structure, the **{111}** octahedral planes and the <110> directions are the close-packed systems.
- There are eight {111} planes in the fcc unit cell. However, the planes at opposite faces of the octahedron are parallel to each other, so that there are only four sets of octahedral planes.
- Each {111} plane contains three <110> directions (the reverse directions being neglected).
- Therefore, the fcc lattice has 12 possible slip systems.

Example:

Determine the slip systems for slip on a (111) plane in a fee crystal and sketch the result.



Slip direction in fee is <110> type direction. Slip directions are most easily established from a sketch of the (111) plane.

To prove that these slip directions lie in the slip plane hu + kv + Iw - 0

(1)(1) + (1)(0) + (1)(-1) = 0(1)(-1) + (1)(1) + (1)(0) = 0(1)(0) + (1)(-1) + (1)(1) = 0

BCC System

- The bcc structure is not a close-packed structure like the fcc or hcp structures.
- Accordingly, there is **no one plane of predominant atomic density**, as (111) in the fcc structure and (0001) in the hcp structure.
- The {110} planes have the **highest atomic density in the bcc structure**, but they are **not greatly superior** in this respect to several other planes.
- However, in the **bcc structure the (111) direction** is just as **close-packed** as the (110) and (1120) directions in the fcc and hcp structures.
- Therefore, the **bcc metals** obey the general rule that **the slip direction is the close-packed direction**, but they differ from most **other metals by not having a definite single slip plane**.
- Slip in bcc metals is found to occur on the {110}, {112}, and {123} planes, while the slip direction is always the [111] direction.
- There are **48 possible slip systems**, but since the planes are not **so close-packed** as in the fcc structure, higher shearing stresses are usually required to cause slip.
- Slip lines in bcc metals have a wavy appearance.
- This is due to the fact that **slip occurs on several planes**, **{110}**, **{112}**, **{123}** but always in the **closepacked (111) direction** which is common to each of these planes.
- Dislocations can readily move from one type of plane to another by cross sip, giving rise to the irregular wavy slip bands.

Property at high temp:

- Certain metals show additional slip systems with increased temperature. Aluminum deforms on the {110} plane at elevated temperature, while in magnesium the {1011} pyramidal plane plays an important role in deformation by slip above 225 °C.
- In all cases the slip direction remains the same when the slip plane changes with temperature.

Slip in a perfect lattice

- If slip is assumed to occur by the translation of one plane of atoms over another, it is possible to make a reasonable estimate of the shear stress required for such a movement in a perfect lattice.
- Consider two planes of atoms subjected to a homogeneous shear stress (Fig. 4-14). The shear stress is assumed to act in the slip plane along the slip direction. The distance between atoms in the slip directions is b, and the spacing between adjacent lattice planes is a. The shear stress causes a displacement x in the slip direction between the pair of adjacent lattice planes.



Figure (a) Shear displacement of one plane of atoms over another atomic plane; (b) variation of shearing stress with displacement in slip direction.

- The shearing stress is initially zero when the two planes are in coincidence, and it is also zero when the two planes have moved one identity distance b, so that point 1 in the top plane is over point 2 on the bottom plane.
- The shearing stress is also zero when the atoms of the top plane are midway between those of the bottom plane, since this is a symmetry position.
- Between these positions each atom is attracted toward the nearest atom of the other row, so that the shearing stress is a periodic function of the displacement.

As a first approximation, the relationship between shear stress and displacement can be expressed by a sine function

$$\tau = \tau_m \sin \frac{2\pi x}{b}$$

Where τ_m the amplitude of the sine wave and b is is the period. At small values of displacement, Hooke's law should apply.

$$\tau = G\gamma = \frac{Gx}{a}$$

For small values of x/b, Eq. (4-2) can be written

$$\tau \approx \tau_m \frac{2\pi x}{b}$$

Combining Eqs. (4-3) and (4-4) provides an expression for the maximum shear stress at which slip should occur.

$$T_m = \frac{G}{2\pi} \frac{b}{a}$$

• As a rough approximation, **b** can be taken equal to **a**, with the result that the theoretical **shear strength of a perfect crystal is approximately equal to the shear modulus divided** $by2\pi$

- The shear modulus for metals is in the range 20 to 150 GPa. Therefore, Eq. (4-6) predicts that the theoretical shear stress will be in the range (3 to 30 GPa),
- While actual values of the shear stress required to produce, plastic deformation in metal single crystals are in the range 0.5 to 10 MPa.
- Even if more refined calculations are used to correct the sine-wave assumption, the value of τ_m cannot be made equal to the observed shear stress.
- Tyson, using a computer solution of the interatomic force equations, predicted $\tau_m = G/16$ for an fcc metal, G/8 for an NaCl structure, and G/4 for a covalently bonded diamond structure.
- Since the theoretical shear strength of metal crystals is at least 100 times greater than the observed shear strength, it must be concluded that a mechanism other than bodily shearing of planes of atoms is responsible for slip.
- In the next section it is shown that dislocations provide such a mechanism.

Slip by Dislocation Movement

- The concept of the dislocation was first introduced to explain the discrepancy between the observed and theoretical shear strengths of metals.
- For the dislocation concept to be valid it is necessary to show
- (1) that the motion of a dislocation through a crystal lattice requires a stress far smaller than the theoretical shear stress, and
- (2) That the movement of the dislocation produces a step, or slip band, at the free surface.
- In a perfect lattice all atoms above and below the slip plane are in minimum energy positions.
- When a shear stress is applied to the crystal, the same force opposing the movement acts on all the atoms. This is the model for slip presented in **Fig. 4-14**.

- When there is a dislocation in the crystal, the atoms well away from the dislocation are still in the minimum energy positions but at the dislocation only a small movement of the atoms is required.
- Referring to Fig. 4-15a, the extra plane of atoms at the edge dislocation initially is at 4.
- Under the action of the shear stress, a very small movement of atoms **to the right** will allow this **half plane** to line up with the **half plane 5**', at the same time cutting the half plane 5 from its neighbors below the slip plane.



Figure (a) Atom movements near dislocation in slip; (b) movement of an edge dislocation.

- By this process the edge dislocation line has moved from its initial position between planes 4' and 5' to a new position between planes 5' and 6'.
- Since the atoms around the dislocations are symmetrically placed on opposite sides of the extra half plane, equal and opposite forces oppose and assist the motion.
- Thus, in a first approximation there is no net force on the dislocation and the stress required to move the dislocation is zero.
- The continuation of this process under the stresses shown in Fig. 4-15 moves the dislocation to the right.
- When the extra half plane of atoms reaches a free surface (Fig. 4-15b), it results in a slip step of one Burgers vector, or one atomic distance for the simple cubic lattice.



Figure (a) Energy change from unslipped to slipped state; (b) stages in growth of slipped region.

- Slip by dislocation motion has been proposed by **Cottrell**. Consider that plastic deformation is the transition from an unslipped to a slipped state (Fig. 4-16(a). Since the process is opposed by an energy barrier △ fin order to facilitate the process it is logical to assume that the material will not all make the transition simultaneously.
- To minimize the energetic of the process, the slipped material will grow at the expense of the unslipped region by the advance of an interfacial region (Fig. 4-16b). The interfacial region is a *dislocation*.
- To minimize the energy for the transition, we expect the interface thickness *w* to be narrow.
- The distance *w* is the width of the dislocation.
- The smaller the width of the dislocation, the lower is the interfacial energy, but the wider the dislocation, the lower is the elastic energy of the crystal because then the atomic spacing in the Slip direction is closer to its equilibrium spacing.
- Thus, the equilibrium width of the dislocation is determined by a balance between these two opposing energy changes.

PEIERLS-NABARRO FORCE

Where **a** is

- The dislocation width is important because it determines the force required to move a dislocation through the crystal lattice.
- □ This force is called the **Peierls Nabarro force**. The **Peierls stress is the shear stress required to** move a dislocation through a crystal lattice in a particular direction.

$$\tau_p \approx \frac{2G}{1-\nu} e^{-2\pi w/b} \approx \frac{2G}{1-\nu} e^{-[2\pi a/(1-\nu)b]}$$

the distance between slip planes and **b**

is the distance between atoms in the slip direction.

- Note that the dislocation width appears in the exponential term in Eq. (4-7), so that the Peierls stress will be very sensitive to the atomic position at the core of a dislocation.
- These are not known with any high degree of accuracy and, since Eq. (4-7) was derived for the sinusoidal force-distance law that has only limited validity,
- The equation cannot be used for precise calculations. However, it is accurate enough to show that the stress needed to move a dislocation in a metal is quite low.
- In spite of these limitations, the Peierls equation has important conceptual value. It shows that materials with wide dislocations will require a low stress to move the dislocations.

CRITICAL RESOLVED SHEAR STRESS FOR SLIP

The extent of slip in a single crystal depends on

- 1. the magnitude of the shearing stress produced by external loads,
- 2. the geometry of the crystal structure,
- 3. and the orientation of the active slip planes with respect to the shearing stresses
- Slip begins when the shearing stress on the slip plane in the slip direction reaches a threshold value called the *critical resolved shear stress*.
- This value is really the single-crystal equivalent of the yield stress of an ordinary stress-strain curve.
- The value of the critical resolved shear stress depends mainly on composition and temperature.
- The fact that different tensile loads are required to produce slip in single crystals of different orientation can be rationalized by a critical resolved shear stress; this was first recognized by *Schmid*.
- To calculate the critical resolved shear stress from a single crystal tested in tension, it is necessary to know, from x-ray diffraction, the orientation with respect to the tensile axis of the plane on which slip first appears and the slip direction.



Figure Diagram for calculating critical resolved shear stress.

- Consider a cylindrical single crystal with cross-sectional area A.
- The angle between the normal to the slip plane and the tensile axis is ϕ and the angle which the slip direction makes with the tensile axis is λ
- The area of the slip plane inclined at the angle ϕ will be A /cos ϕ and the component of the axial load acting in the slip plane in the slip direction is Pcos λ

Therefore, the critical resolved shear stress is given by:

$$\tau_R = \frac{P\cos\lambda}{A/\cos\phi} = \frac{P}{A}\cos\phi\cos\lambda$$

• Equation (4-13) gives the shear stress resolved on the slip plane in the slip direction.

- This shear stress is a maximum when $\phi = \lambda = 45^\circ$, so that $\tau_R = \frac{1}{2}P/A$.
- If the tension axis is normal to the slip plane ($\lambda = 90^\circ$) or if it is parallel to the slip plane ($\phi = 90^\circ$), the resolved shear stress is zero.
- Slip will not occur for these extreme orientations since there is no shear stress on the slip plane.
- Crystals close to these orientations tend to fracture rather than slip.

Example:

Determine the tensile stress that is applied along the $[1\overline{1}0]$ axis of a silver crystal to cause slip on the $(1\overline{11})$ $[0\overline{11}]$ system. The critical resolved shear stress is 6 MPa.

The angle between tensile axis $[1\overline{1}0]$ and normal to $(1\overline{11})$ is

The angle between
$$\cos \phi = \frac{(1)(1) + (-1)(-1) + (0)(-1)}{\sqrt{(1)^2 + (-1)^2 + (0)^2}\sqrt{(1)^2 + (-1)^2 + (-1)^2}} = \frac{2}{\sqrt{2}\sqrt{3}} = \frac{2}{\sqrt{6}} \text{ tensile axis}$$
[1]D] and slip direction [0] 11] is
$$\cos \lambda = \frac{(1)(0) + (-1)(-1) + (0)(-1)}{\sqrt{2}\sqrt{(0)^2 + (-1)^2 + (-1)^2}} = \frac{1}{\sqrt{2}\sqrt{2}} = \frac{1}{2}$$

From Eq. (4-13)

$$\sigma = \frac{P}{A} = \frac{\tau_R}{\cos\phi\cos\lambda} = \frac{6}{2/\sqrt{6} \times \frac{1}{2}} = 6\sqrt{6} = 14.7 \text{ MPa}$$

Property of CRSS

- The importance of small amounts of impurities in increasing the critical resolved shear stress is shown by the data for silver and copper.
- Alloying-element additions have even a greater effect, as shown by the data for gold-silver alloys in Fig..



Figure Variation of critical resolved shear stress with composition in silver-gold-alloy single crystals.

• Note that a large increase in the resistance to slip is produced by **alloying gold and silver** even though these atoms are very much alike in size and electro negativity, and hence they form a solid solution over the complete range of composition.

- In solid solutions, where the solute atoms differ considerably in size from the solvent atoms, an even greater increase in critical resolved shear stress would be observed.
- The magnitude of the critical resolved shear stress of a crystal is determined by the interaction of its population of dislocations with each other and with defects such as vacancies, interstitials, and impurity atoms.
- This stress is, of course, greater than the stress required to move a single dislocation, but it is appreciably lower than the stress required to produce slip in a perfect lattice.
- On the basis of this reasoning, the critical resolved shear stress should decrease as the density of defects decreases, provided that the total number of imperfections is not zero.

SCHMID LAW:

- The ratio of the resolved shear stress to the axial stress is called the Schmid factor m. For a single crystal loaded in tension or compression along its axis, $\mathbf{m} = \cos \phi \cos \lambda$
- It is observed experimentally that a single crystal will slip when the resolved shear stress on the slip plane reaches a critical value. This behavior, known as **Schmid's law**, is best demonstrated with hcp metals where the limited number of slip systems allows large differences in orientation between the slip plane and the tensile axis.

Deformation of Single crystals

- Most studies of the mechanical properties of single crystals are made by subjecting the crystal to simple uniaxial tension.
- Therefore, the specimen is not permitted to deform freely by uniform glide on every slip plane along the gage length of the specimen, as is pictured in Fig. 4-20(a). Instead, the slip planes rotate toward the tensile axis since the tensile axis of the specimen remains fixed, as in Fig. 4-20b
- Since plastic low occurs by slip on certain planes in particular directions, the measured increase in length of the specimen for a given amount of slip will depend on the orientations of the slip plane and direction with the specimen axis.
- The fundamental measure of plastic strain in a single crystal is the crystallographic glide strain γ
- Glide strain is the relative displacement of two parallel slip planes separated at a unit distance. The equations relating glide strain with specimen extension can be derived from Fig.



Figure 4-20 (a) Tensile deformation of single crystal without constraint; (b) rotation of slip planes due to constraint.

- As the single crystal elongates, the slip direction rotates toward the tensile axis. For simplicity in Fig. 4-21, the glide elements are kept fixed and the tensile axis is rotated as the crystal elongates from L_0 to L_1 .
- The two cases are equivalent geometrically. Moreover, for simplicity the orientation of the slip plane is given by the angle χ between the axis of the glide ellipse and the tensile axis rather than the angle Φ between the normal to the glide ellipse (slip plane) and the tensile axis. With this selection of angles, = P/A sin χ cos Φ. From triangle ABB', using the law of sines, we can see that.



Figure Extension of a single crystal

From triangles ABC and AB'C

$$AC = L_0 \sin \chi_0 = L_1 \sin \chi_1$$

The glide strain is defined as the total amount of slip divided by the thickness of the glide packet

 $\lambda = \frac{BB'}{AC}$

Again, from the law of sines

$$BB' = \frac{L_1 \sin (\lambda_0 - \lambda_1)}{\sin \lambda_0}$$

Substitution in the expression for glide strain, and after considerable trigonometric manipulation, results in

$$\gamma = \frac{1}{\sin \chi_0} \left\langle \left[\left(\frac{L_1}{L_0} \right)^2 - \sin^2 \lambda_0 \right]^{1/2} - \cos \lambda_0 \right\rangle$$

- Thus, the glide shear strain may be determined from the initial orientation of the slip plane and slip direction (xo and X0) and the extension of the specimen L₁/L₀. This analysis assumes that slip occurs on only a single slip system.
- If the orientation of the glide elements can be determined during or after deformation, the glide strain may be determined from



Figure Typical single-crystal stress-strain curves

• The fundamental way to present single-crystal data is by plotting resolved shear stress vs. glide shear strain. Figure 4-22 shows that there are important differences between metals. Typically, fcc metals exhibit greater strain hardening than hcp metals.

Deformation of face-centered cubic crystals

- Because fee crystals have high symmetry and 12 potential slip systems, there is a wide choice of slip systems. The slip plane will not have to undergo much rotation before the resolved shear stress becomes high on another {111} <110> slip system.
- The initial operative slip system, the primary slip system, will be the one with the highest Schmid factor, $m = \sin \chi \cos \lambda$. The primary system will depend on the orientation of the crystal relative to the tensile stress axis.
- The relationship between the stress axis and the 12 possible slip systems is best shown on a stereographic projection (Fig. 4-23), where each of the unit triangles defines a region in which a particular slip system operates.
- There are four (111) poles ABCD representing the normals to the octahedral {111} slip planes. Slip directions are indicated I through IV.
- For a specimen axis at P, the slip system BIV will be operative. Φ_0 and λ_0 are given by the great circles through B-P-IV.
- We can use the stereographic plot to follow the rotation of the slip system toward the tensile axis. As the specimen elongates, λ decreases and Φ increases. However it is more convenient to consider that the slip system remains fixed and the specimen axis rotates.



Figure Standard (001) stereographic projection or a cubic crystal.

- As the specimen elongates, the specimen axis eventually reaches the [001]-[111] boundary at P'. Now the resolved shear stress is equal on the primary slip system and the conjugate slip system (111) [011]. At this point deformation proceeds on the two slip systems simultaneously to produce duplex slip or multiple slip.
- Under the microscope conjugate slip appears as another set of intersecting slip lines. The fact that slip can occur equally on both slip systems indicates that latent strain hardening must have occurred on the conjugate system when only the primary system was acting.

• The specimen axis rotates along the [001]-[111] boundary to the [112] pole, which is midway between the two operative slip directions [101] and [011]. When the specimen axis reaches [112] it stays at that orientation until the specimen necks down and fractures.



- Crystals whose axes lie at orientations along the boundaries of the stereographic triangle represent a special situation because the critical resolved shear stress will be the same on more than one slip system.
- Therefore, plastic deformation will begin on more than one slip plane and they will initially deform by duplex slip. Figure 4-24 shows the number of operative slip systems in a cubic crystal at these orientations.
- Deformation by duplex slip results in a high degree of strain hardening because of interaction between dislocations on two intersecting slip systems. This is shown in Fig. 4-22 where Mg and Zn deform on a single Figure 4-24 Operative slip systems along boundaries of stereographic triangle. slip system (because of the hcp geometry) while the stress-strain curves for Al and Cu are for crystals oriented for duplex slip.

Deformation by Twinning

- The second important mechanism by which metals deform is the process known as twinning.
- Twinning results when a portion of the crystal takes up an orientation that is related to the orientation of the rest of the untwinned lattice in a definite, symmetrical way.



Figure Classical picture of twinning

- The twinned portion of the crystal is a mirror image of the parent crystal. The plane of symmetry between the two portions is called *the twinning plane*.
- Figure 4-25 illustrates the classical atomic picture of twinning. Figure 4-25 a represents a section perpendicular to the surface in a cubic lattice with a low-index plane parallel to the paper and oriented at an angle to the plane of polish.
- The twinning plane is perpendicular to the paper.
- If a shear stress is applied, the crystal will twin about the twinning plane (Fig. 4-25b). The region to the right of the twinning plane is undeformed. To the left of this plane, the planes of atoms have sheared in such a way as to make the lattice a mirror image across the twin plane.
- In Fig. 4-256, open circles represent atoms which have not moved, dashed circles indicate the original positions in the lattice of atoms which change position, and solid circles are the initial positions of these atoms in the twinned region.
- Note that the twin is visible on the polished surface because of the change in elevation produced by the deformation and because of the difference in crystallographic orientation between the deformed and undeformed regions.

	Slip		Twinning
1.	The orientation of the crystal above and below	1.	While twinning results in an orientation
	the slip plane is the same after deformation as		difference across the twin plane.
	before.	2.	While in twinning the atom movements are
2.	Slip is usually considered to occur in discrete		much less than anatomic distance.
	multiples of the atomic spacing	3.	The twinned region of a crystal every atomic
3.	Slip occurs on relatively widely spread planes		plane is involved in the deformation.
4.	Slip appears as thin lines	4.	While twinning appears as a board lines or
5.	There is very little change in lattice		bands
	orientation and the steps are visible only on	5.	In twinning, there is a different lattice
	the surface of the crystal. If the steps are		orientation in the twinned region, removal of
	removed by polishing there will be no		the steps by surface polishing will not
	evidence that slip has taken place		destroy the evidence of twinning. Proper
			etching solutions, sensitive to the difference
			in orientation will reveal the twinned region

Difference between Slip & Twinning

- If the surface were polished down to section AA, the difference in elevation would be eliminated but the twin would still be visible after etching because it possesses a different orientation from the untwinned region.
- Twins may be produced by mechanical deformation or as the result of annealing following plastic deformation. The first type are known as mechanical twins; the latter are called annealing twins.

- Mechanical twins are produced in bcc or hcp metals under conditions of rapid rate of loading (shock loading) and decreased temperature.
- Face-centered cubic metals are not ordinarily considered to deform by mechanical twinning, although gold-silver alloys twin fairly readily when deformed at low temperature, and mechanical twins have been produced in copper by tensile deformation at 4 K and by shock loading.
- Twins can form in a time as short as a few microseconds, while for slip there is a delay time of several milliseconds before a slip band is formed. Under certain conditions, twins can be heard to form with a click or loud report [tin cry].
- If twinning occurs during a tensile test, it produces serrations in the stress-strain curve.
- However, twinning is not a dominant deformation mechanism in metals which possess many possible slip systems.
- Twinning generally occurs when the slip systems are restricted or when something increases the critical resolved shear stress so that the twinning stress is lower than the stress for slip.
- This explains the occurrence of twinning at low temperatures or high strain rates in bcc and fcc metals or in hcp meals at orientations which are unfavorable for basal slip.

Crystal structure	Typical examples	Twin plane	Twin direction
bcc	α-Fe, Ta	(112)	[111]
hcp	Zn, Cd, Mg, Ti	(1012)	[1011]
fee	Ag, Au, Cu	(111)	[112]
			04/02/2011

Table 4-5 Twin planes and twin directions

• Twinning is important in the overall deformation of metals with a low number of slip systems, such as the hcp meals.



Figure Microstructures of twins, (a) **Neumann bands in iron**; (b) **mechanical twins produced in zinc by polishing;** (c) **annealing twins in gold-silver alloy**.

- However, it should be understood that only a relatively small fraction of the total volume of a crystal is reoriented by twinning, and therefore hcp metals will, in general, possess less ductility than metals with a greater number of slip systems
- A process closely related to twinning is the formation of a martensite region. by a difusionless shear transformation. Although both processes produce a local region of new lattice orientation, the basic difference is that in a martensite plate the crystal structure is different from the parent crystal.
- The driving force for twinning is the applied shear stress, while in the martensite transformation; the diving force is the free energy difference between the parent crystal and the martensitic phase. This thermodynamic driving force may be assisted by the applied shear stress.

Stacking Faults

- The atomic arrangement on the (111) plane of an fee structure and the {0001} plane of an hcp structure could be obtained by the stacking of close-packed planes of spheres.
- For the fee structure, the stacking sequence of the planes of atoms is given by ABC ABC. For the hcp structure, the stacking sequence is given by AB AB AB.
- Errors, or faults, in the stacking sequence can be produced in most metals by plastic deformation. Slip on the {111} plane in an fcc lattice produces a deformation stacking fault by the process shown in Fig. 4-27b. Slip has occurred between an A and a B layer. The stacking sequence then becomes ABC AC AB.
- Comparison of this faulted stacking sequence (Fig. 4-27b) with the stacking sequence for an hcp structure without faults CACA (Fig. 4-27d) shows that the deformation stacking fault contains four layers of an hcp sequence. Therefore, the formation of a stacking fault in an fcc metal is equivalent to the formation of a thin hcp region.
- Another way in which a stacking fault could occur in an fcc metal is by the sequence² shown in Fig. 4-27c. The stacking sequence ABC ACB CA is called an extrinsic, or twin, stacking fault. The three layers ACB constitute the twin. Thus, stacking faults in fcc metals can also be considered as submicroscopic twins of nearly atomic thickness. The reason why mechanical twins of microscopically resolvable width are not formed readily when fcc metals are deformed is that the formation of stacking faults is so energetically favorable.





Figure Faulted structures, (a) fcc packing; (b) deformation fault in fee; (c) twin fault in fee; (d) hcp packing.

- The differences in the deformation behavior of fee metals are due to the differences in stacking-fault behavior. The creation of a region with hcp stacking CACA introduces a region with higher free energy than the fcc structure.
- A stacking fault in a fee metal, when viewed from dislocation theory, is an extended dislocation consisting of a thin hcp region bounded by partial dislocations (Fig. 4-28). The nearly parallel partial dislocations tend to repel each other, but this is counterbalanced by the surface tension of the stacking fault pulling them together.



Figure Schematic model of a stacking fault.

Table 4-6 Typical values of stacking-fault energy

Metal	Stacking-fault energy, mJ m ⁻² (= erg cm ⁻²)	
Brass	< 10	
303 stainless steel	8	
304 stainless steel	20	
310 stainless steel	45	
Silver	- 25	
Gold	~ 50	
Copper	~ 80 ·	
Nickel	~ 150	
Aluminum	~ 200	

• The lower the stacking-fault energy the greater the separation between the partial dislocations and the wider the stacking fault.1 Typical values for stacking fault energy (SFE) are given in Table 4-6. The data for the stainless steels illustrate that SFE is very sensitive to chemical composition.

- Stacking faults influence the plastic deformation in a number of ways. Metals with wide stacking faults (low SFE) strain-harden more rapidly, twin easily on annealing, and show a different temperature dependence of low stress than metals with narrow stacking faults.
- Metals with high SFE have a deformation substructure of dislocation tangles and cells, while low-SFE metals show a deformation substructure of banded, linear arrays of dislocations.

DEFORMATION BANDS AND KINK BANDS

- Inhomogeneous deformation of a crystal results in regions of different orientation called deformation bands.
- When slip occurs without restraint in a perfectly homogeneous fashion, the slip lines are removed by subsequent polishing of the surface. Deformation bands, however, can be observed even after repeated polishing and etching because they represent a region of different crystallographic orientation.
- The tendency for the formation of deformation bands is greater in polycrystalline specimens because the restraints imposed by the grain boundaries make it easy for orientation differences to arise in a grain during deformation.
- Deformation bands generally appear irregular in shape but are elongated in the direction of principal strain.
- Deformation bands have been observed in both fcc and bcc metals, but not in hcp metals.
- Consideration of the equation for critical resolved shear stress shows that it will be difficult to deform a hexagonal crystal when the basal plane is nearly parallel to the crystal axis.
- Orowan found that if a cadmium crystal of this orientation were loaded in compression, it would deform by a localized region of the crystal suddenly snapping into a tilted position with a sudden shortening of the crystal.



Figure 4-29 Kink band

- The **bucking**, or **kinking**, behavior is illustrated in Fig. 4-29. The horizontal lines represent basal planes, and the planes designated p are the **kink planes** at which **the orientation suddenly changes**.
- Distortion of the crystal is essentially confined to the kink band.

- Further study of kink bands by **Hess and Barrett** showed that they can be considered to be a simple type of deformation band.
- Kink bands have also been observed in zinc crystals tested in tension, where a non uniform distribution of slip can produce a bending moment which can cause kink formation.

STRAIN HARDENING OF SINGLE CRYSTALS

- One of the chief characteristics of the plastic deformation of metals is the fact that the shear stress required to produce slip continuously increases with increasing shear strain.
- The increase in the stress required to cause slip because of previous plastic deformation is known as **strain hardening**, **or work hardening**.
- An increase in low stress of over 100 percent from strain hardening is not unusual in single crystals of ductile metals,
- Strain hardening is caused by dislocations interacting with each other and with barriers which impede their motion through the crystal lattice.
- Hardening due to dislocation interaction is a complicated problem because it involves large groups of dislocations, and it is difficult to specify group behavior in a simple mathematical way.
- The dislocation density of a good annealed crystal is 10^5 to 10^6 cm⁻² (= 10^3 to 10^4 mm⁻²), while the observed dislocation density in cold-worked metal is 10^{10} to 10^{12} cm⁻² (= 10^8 to 10^{10} mm⁻²).
- One of the earliest dislocation concepts to explain strain hardening was the idea that dislocations pile up on slip planes at barriers in the crystal.
- The pile-ups produce a **back stress** which opposes the applied stress on the slip plane. The existence of a back stress was demonstrated experimentally by shear tests on zinc single crystals. Zinc crystals are ideal for crystal-plasticity experiments because they slip only on the basal plane, and hence complications due to duplex slip are easily avoided.



Shear strain γ

Figure 4-31 Effect of complete reversal of slip direction on stress-strain curve.

- In Fig. 4-31, the crystal is strained to point **O** unloaded, and then reloaded in the direction opposite to the original slip direction. Note that on reloading the crystal yields at a lower shear stress than when it was first loaded.
- This is because the **back stress** developed as a result of **dislocations piling up** at barriers during the first loading cycle is **aiding dislocation movement** when the direction **of slip is reversed**.
- Furthermore, when the slip direction is reversed, dislocations of opposite sign could be created at the same sources that produced the dislocations responsible for strain in the first slip direction. Since dislocations of opposite sign attract and annihilate each other, the net effect would be a further softening of the lattice.
- This explains the fact that the low curve in the reverse direction lies below the curve for continued low in the original direction. The lowering of the yield stress when deformation in one direction is followed by deformation in the opposite direction is called the Bauschinger effect.

SESSILE DISLOCATION

- The dislocation of low mobility that is produced by a dislocation reaction is called a **sessile dislocation**.
- Since **sessile dislocations** do not lie on the slip plane of low shear stress, they act as a barrier to dislocation motion until the stress is increased to a high enough level to break down the barrier.

LOMER-COTTRELL BARRIERS

• The most important dislocation reaction, which leads to the formation of sessile dislocations, is the formation of Lomer-Cottrell barriers in fee metals by slip on intersecting {111} planes.

DISLOCATION FOREST

• Another mechanism of strain hardening, in addition to that due to the back stress resulting from dislocation pile-ups at barriers, is believed to occur when dislocations moving in the slip plane cut through other dislocations intersecting the active slip plane. The dislocations threading through the active slip plane are often called a *dislocation forest*, and this strain-hardening process is referred to as *the intersection of a forest of dislocations*.

JOGS

• Figure 4-32a shows that dislocation intersection results in a small step or jog in the dislocation line. Jogs on a dislocation restrict its motion so that they contribute to strain hardening. Jogs are also formed by a screw dislocation cross slipping from the primary slip plane to another plane which contains the common slip direction (Fig. 4-32b)



Figure 4-32 Formation of a jog J {a} by a dislocation cutting through a screw dislocation as it glides from AB to A'B'\ (b) by part of a screw dislocation line AB cross slipping from the primary slip plane PQ into the plane

CROSS SLIP

• The phenomenon of cross slip is restricted to screw dislocations. Since the line of a screw dislocation and its Burgers vector are parallel, this does not define a specific plane as with an edge dislocation (where b is perpendicular to the dislocation line). To a screw dislocation, all directions around its axis look the same, and it can glide on any plane as long as it moves parallel to its original orientation.

STRESS - STRAIN CURVES FOR SINGLE CRYSTALS

• When the stress-strain curves for single crystals are plotted as resolved shear stress vs. shear strain, certain generalizations can be made for all fcc metals. Following the notation proposed by **Seeger**, the flow curve for pure-metal single crystals can be divided into three stages (Fig. 4-33).

STAGE – I

• The region of **easy glide** is a stage in which the crystal undergoes little strain hardening. During easy glide, the dislocations are able to move over **relatively large distances** without encountering barriers. The **low strain hardening** produced during this stage implies that most of the dislocations escape from the crystal at the surface. During easy glide, slip always occurs on only one slip system. For this reason, stage I slip is sometimes called laminar flow.



Figure 4-33 Generalized flow curve for fcc single crystals.

STAGE – II

- Stage II is a **nearly linear part of the flow curve** where strain hardening increases rapidly. In this stage, slip occurs on **more than one set of planes**.
- The length of the active slip lines decreases with increasing strain, which is consistent with the formation of a greater number of Lomer-Cottrell barriers with increasing strain.
- During stage II, the ratio of the strain-hardening coefficient (the slope of the curve) to the shear modulus is nearly independent of stress and temperature, and approximately independent of crystal orientation and purity.
- The fact that the slope of the flow curve in stage II is nearly independent of temperature agrees with the theory that assumes the chief strain-hardening mechanism to be piled-up groups of dislocations.

The average dislocation density in stage II correlates with resolved shear stress according to

$$\tau = \tau_0 + \alpha G b \rho^{1/2}$$

• Where τ_0 is the shear stress needed to move a dislocation in the absence of other dislocations and a is a numerical constant which varies from 0.3 to 0.6 for different fcc and bcc metals.

STAGE – III

- Stage III is a region of decreasing rate of strain hardening.
- The processes occurring during this stage are often called **dynamical recovery**.
- In this region of the flow curve, the stresses are high enough so that dislocations can take part in processes that are suppressed at lower stresses.
- **Cross slip** is believed to be the main process by which dislocations, piled up at obstacles during stage II, can escape and reduce the internal-strain field.

- The stress at which stage III begins, τ_3 , is strongly temperature-dependent.
- Also, the flow stress of a crystal strained into stage III is more temperature-dependent than if it had been strained only into stage II.
- This temperature dependence suggests that the intersection of forests of dislocations is the chief strainhardening mechanism in stage III.

Effect of Crystal Orientation on the flow curve of fcc single crystals

- Figure 4-34 shows that crystal orientation can have a very strong effect on the low curve of fcc single crystals.
- When the tensile axis is parallel to a <011> direction, one slip system is carrying appreciably more shear stress than any other and the low curve shows a relatively large region of easy glide.
- When the tensile axis is close to a <100> or <111> direction, the stress on several slip systems is not very different and the low curves show rapid rates of strain hardening.



Figure 4-34 Effect of specimen orientation on the shape of the flow curve for fcc single crystals.

DISLOCATION THEORY

Introduction

- A dislocation is the linear lattice defect that is responsible for nearly all aspects of the plastic deformation of metals.
- This chapter is intended to present a more complete treatment of dislocation theory. Techniques for observing dislocations in metals are discussed. The effect on dislocation behavior of considering real fcc, bcc, or hcp crystal structures are considered.
- The origin of dislocations and the mechanisms for their multiplication are discussed. Interaction of dislocations with other dislocations, vacancies, and foreign atoms is discussed in some detail.
- The object of this chapter is the presentation of the *basic geometric* and *mathematical relationships* which describe dislocation behavior.
- These relationships will be used to explain *mechanical behavior and strengthening mechanisms* in subsequent chapters of this book.

Observation of dislocations

- The concept of the dislocation was proposed independently by Taylor, Orowan, and Polanyi1 in 1934, but the idea lay relatively undeveloped until the end of World War II. There followed a period of approximately 10 years in which the theory of dislocation behavior was developed extensively and applied to practically every aspect of the plastic deformation of metals.
- Practically all the experimental techniques for detecting dislocations utilize the strain field around a dislocation to increase its effective size. These experimental techniques can be roughly classified into *two categories*, those *involving chemical reactions* with the dislocation, and those utilizing the *physical changes at the site of a dislocation*.
- Chemical methods include etch-pit techniques and precipitation techniques. Methods based on the physical structure at a dislocation site include transmission electron microscopy of thin films and x-ray diffraction techniques.
- The simplest chemical technique is the use of an etchant which forms a pit at the point where a dislocation intersects the surface. Etch pits are formed at dislocation sites because the strain field surrounding the dislocation causes preferential chemical attack.
- Figure 5-1 shows the excellent resolution obtainable from etch-pit studies on alpha brass. Pits only 500 0 A (= 50 nm) apart have been resolved. In the region of heavy slip shown in this electron micrograph the *dislocation density is 10¹⁰ cm⁻² (= 10⁸ mm⁻²)*.
- A similar method of detecting dislocations is to form a visible precipitate along the dislocation lines. Usually a small amount of impurity is added to form the precipitate after suitable heat treatment. The procedure is called *"decoration"* of dislocations.



Figure 5-1 Etch pits on slip bands in alpha brass crystals (5,000 X).

- This technique was first used by Hedges and Mitchell1 to decorate dislocations in AgBr with photolytic silver. It has since been used with many other ionic crystals,2 such as AgCl, NaCl, KCl, and CaF2. With these optically transparent crystals this technique has the advantage that it shows the internal structure of the dislocation lines.
- Figure 5-2 shows a hexagonal network of dislocations in a NaCl crystal which was made visible by decoration.



Figure 5-2 Hexagonal network of dislocations in NaCl detected by a decoration technique.

• The most powerful method available today for the detection of dislocations in metals is *transmission electron microscopy of thin foils*. Thin sheet, less than 1 mm thick, is thinned after deformation by electro polishing to a thickness of about 1,000 A (= 100 nm). At this thickness the specimen is transparent to electrons in the electron microscope.

- In *conventional transmission electron microscopy, individual dislocation lines can be observed because the intensity of the diffracted electron beam* is altered by the strain field of the dislocation.
- The width of the diffraction image of a dislocation in a thin foil is about 100 A (= 10 nm), so that this technique can be used at dislocation densities up to about 10^{11} cm⁻² (= 10^9 mm⁻²).
- By means of this technique it has been possible to observe dislocation networks (Fig. 5-3), stacking faults, dislocation pile-up at grain boundaries (Fig.6-1), Lomer-Cottrell barriers, and many other structural features of dislocation theory.



Figure 5-3 Dislocation network in cold-worked aluminum (32,500 X).

- However, this technique is not without disadvantages. Since only a miniscule volume of material is examined with thin films, great care must be exerted to obtain a representative sample. It is possible to alter the defect structure during sectioning and polishing to a thin film, and dislocation structures may relax in a very thin foil.
- The greatest defect of transmission electron microscopy is that it is not very effective in detecting longrange stresses, nor does it give very much information about slip line lengths or surface step heights.
- The dislocation structure of a crystal can be detected by x-ray microscopy. The most common techniques are the Berg-Barrett reflection method.

Burgers vector and the dislocation loop

- The Burgers vector b is the vector which defines the magnitude and direction of slip. Therefore, it is the most characteristic feature of a dislocation.
- It has already been shown that for a pure edge dislocation the Burgers vector is perpendicular to the dislocation line, while for a pure screw dislocation the Burgers vector is parallel to the dislocation line.



Figure 5-4 (a) Macroscopic deformation of a cube produced by glide of an edge dislocation. (b) Macroscopic deformation of a cube produced by glide of a screw dislocation. Note that the end result is identical for both situations. '

- The macroscopic slip produced by the motion of an edge dislocation is shown in Fig. 5-4a and by a screw dislocation in Fig. 5-4b.
- For an edge dislocation the dislocation line moves parallel to the slip direction while the screw dislocation moves at right angles to it.

	Type of d	lislocation
Dislocation property	Edge	Screw
Relationship between dislocation line and b	perpendicular	parallel
Slip direction	parallel to b	parallel to b
Direction of dislocation line movement relative to b (slip direction)	parallel	perpendicular
Process by which dislocation may leave slip plane	climb	cross-slip

Table 5-1 Geometric properties of dislocations

- Actually, dislocations in real crystals are rarely straight lines and rarely lie in a single plane. In general, a dislocation will be partly edge and partly screw in character.
- For example, in *Fig. 5-5*, the dislocation loop is pure screw at point A and pure edge at point B, while along most of its length it has mixed edge and screw components. Note, however, that the Burgers vector is the same along the entire dislocation loop.



Figure 5-5 Dislocation loop lying in a slip plane (schematic).

- A convenient way of defining the *Burgers vector* of a *dislocation is with a Burgers circuit*. Consider the positive edge dislocation shown in Fig. 5-6a. If we *start at a lattice point and imagine a clockwise path traced* from atom to atom an equal distance in each direction, we find that *at the finish of the path the circuit does not close*.
- *The closure failure from finish to start is the Burgers vector b of the dislocation*. (If we had made the Burgers circuit around the dislocation in the anticlockwise direction, the direction of the Burgers vector would have been in the opposite sense.)
- Moreover, if we traverse a *Burgers circuit about the screw dislocation* shown in Fig. 5-6b, we would find the closure error pointing out of the front face of the crystal. This is a right-handed screw dislocation since in traversing the circuit around the dislocation line; we advance the helix one atomic plane into the crystal.



Figure 5-6 Burgers circuits, (a) Around positive edge dislocation; (b) around a right-handed dislocation.

- The process of *cross slip* illustrated in Fig. 5-7, will serve as an example of dislocation loops. In Fig. 5-7a a small loop of dislocation line with $b = a_0/2[101]$ is moving on a (111) plane in an fcc crystal.
- The dislocation loop is pure positive edge at w and pure negative edge at y. At x the dislocation is a right-handed screw while at z the dislocation loop is a pure left-handed screw dislocation. At some stage (Fig. 5-lb), the shear stress causing expansion of the loop tends to move the dislocation on the intersecting (111) plane.



Figure 5-7 Cross slip in a face-centered cubic crystal

- Since the dislocation is pure screw at z, it is free to move on this plane. In Fig. 5-7c the loop has expanded on the second plane, while in Fig. 5-7d *double cross slip* has taken place as the loop glides back onto the original (111) plane.
- Note that during the glide of the dislocation on the cross-slip plane only the screw component of the loop has moved.
- Because a dislocation *represents the boundary between the slipped and unslipped region of a crystal*, topographic considerations require that it either must be a closed loop or else must end at the free surface of a crystal or at a grain boundary.
- In general, a *dislocation line cannot end inside of a crystal*. The *exception is at a node*, where *three or four dislocation lines meet*. At a node two dislocations with Burgers vectors b₁ and b₂ combine to produce a resultant dislocation b₃. *The vector b₃ is given by the vector sum of b₁ and b₂*.
- A dislocation with a Burgers vector equal to one lattice spacing is said to be a dislocation of unit strength. Because of energy considerations dislocations with strengths larger than unity are generally unstable and dissociate into two or more dislocations of lower strength.
- The criterion for deciding whether or not dissociation will occur is base on the fact that the strain energy of a dislocation is proportional to the square of its Burgers vector.

- Therefore, the dissociation reaction $b_1 \rightarrow b_2 + b_3$ will occur when $b_1 > b_2^2 + b_3^2$ but not if $b_1 < b_2^2 + b_3^2$
- In adding Burgers vectors, each of the corresponding components is added separately. Thus $b_1 + b_2 = a_0[110] + a_0[211] = a_0[321]$. In adding or subtracting components common unit vectors must be used. Thus $a_0/3[112] + a_0/6[11-1]$ must be expressed as $a_0/6[224] + a_0/6[11-1]] = a_0/6[333] = a_0/2[111]$.

Example

Determine whether the dislocation dissociation reaction is feasible.

$$b_1 = b_2 + b_3$$
$$\frac{a}{2} [0\overline{1}1] = \frac{a}{6} [1\overline{2}1] + \frac{a}{6} [\overline{11}2]$$

Since this is a vector equation the x, y, and z components of the right-hand side of the equation must equal the x, y, and z components of the left side (original dislocation).

x components:	$0 = \frac{1}{6} - \frac{1}{6}$
y components:	$-\frac{1}{2} = -\frac{2}{6} - \frac{1}{6} = -\frac{1}{2}$
z components:	$\frac{1}{2} = \frac{1}{6} + \frac{2}{6} = \frac{1}{2}$

For the dissociation to be energetically favorable

$$b_1^2 > b_2^2 + b_3^2$$

$$b_1 = \frac{a}{2} \left[0 + (-1)^2 + (1)^2 \right]^{1/2} = \frac{\sqrt{2}a}{2} \qquad b_1^2 = \frac{a^2}{2}$$

$$b_2 = \frac{a}{6} \left[(1)^2 + (-2)^2 + (1)^2 \right]^{1/2} = \frac{\sqrt{6}a}{6} \qquad b_2^2 = \frac{a^2}{6}$$

$$b_3 = \frac{a}{6} \left[(-1)^2 + (-1)^2 + (2)^2 \right]^{1/2} = \frac{\sqrt{6}a}{6} \qquad b_3^2 = \frac{a^2}{6}$$

 $\therefore b_1^2 > b_2^2 + b_3^2$ and (i e dislocation reaction is feasible.

- A dislocation of unit strength, or unit dislocation, has a minimum energy when its Burgers vector is parallel to a direction of closest atomic packing in the lattice. This agrees with the experimental observation that crystals always slip in the close-packed directions.
- A unit dislocation of this type is also said to be a *perfect dislocation* because translation equal to one Burgers vector produces an identity translation.
- A unit dislocation parallel to the slip direction cannot dissociate further unless it becomes an *imperfect dislocation*, where a translation of one Burgers vector does not result in an identity translation

FORCES ON DISLOCATIONS

- When an external force of sufficient magnitude is applied to a crystal, the dislocations move and produce slip. Thus, there is force acting on a dislocation line which tends to drive it forward
- Figure 5-15 shows a dislocation line moving in the direction of its Burgers vector under the influence of a uniform shear stress τ. An element of the dislocation line ds is displaced in the direction of slip normal to ds by an amount dl The area swept out by the line element is then ds dl
- This corresponds to an average displacement of the crystal above the slip plane to the crystal below the slip plane of an amount (dsdl/A)b, where A is the area of the slip plane. The applied force creating the shear stress is τA . The work done when the increment of slip occurs is

$$dW = \tau A \left(\frac{ds \, dl}{A} \right) b$$

The force on a dislocation is always defined as a force F per unit length of dislocation line. Since F = dW/dl and remembering that this is a force per unit length {ds}, we have



Figure 5-15 Force acting on a dislocation line

FORCES BETWEEN DISLOCATIONS

- Dislocations of opposite sign on the same slip plane will attract each other, run together, and annihilate each other.
- This can be seen readily for the case of an edge dislocation (Fig. 4-8) where the superposition of a positive and negative dislocation on the same slip plane would eliminate the extra plane of atoms and therefore the dislocation would disappear.
- Conversely, dislocations of like sign on the same slip plane will repel each other.
- We can understand this by considering the energy changes. For two dislocations separated at a large distance, the elastic strain energy for the combined situations will be

$$2\cdot\frac{Gb^2}{4\pi(1-\nu)}\ln\frac{r_1}{r_0}$$

• When the two dislocations are very close together the configuration can be approximated by a single dislocation of strength 2b. For this case, the elastic strain energy will be

$$\frac{G(2b)^2}{4\pi(1-\nu)}\ln\left(\frac{r_1}{r_0}\right)$$

DISLOCATION CLIMB

- An edge dislocation can glide only in the slip plane containing the dislocation line and its Burgers vector. However, under certain conditions an edge dislocation can move out of the slip plane onto a parallel plane directly above or below the slip plane. This is the process of dislocation climb.
- This type of movement is termed neoconservative, as compared with conservative movement when a dislocation glides in its slip plane.



Figure 5-18 (a) Diffusion of vacancy to edge dislocation; (b) dislocation climbs up one lattice spacing.

- Dislocation climb occurs by the diffusion of vacancies or interstitials to or away from the site of the dislocation. Since climb is diffusion-controlled, it is thermally activated and occurs more readily at elevated temperature. In *positive climb* atoms are removed from the extra half plane of atoms at a positive edge dislocation so that this extra half plane moves up one atom spacing.
- In negative climb a row of atoms is added below the extra half plane so that the dislocation line moves down one atom spacing.

INTERSECTION OF DISLOCATIONS

- The intersection of two dislocations produces a sharp break, a few atom spacings in length, in the dislocation line. These breaks can be of two types.
- A *jog* is a sharp break in the dislocation moving it out of the slip plane.
- A *kink* is a sharp break in the dislocation line which remains in the slip plane.

MULTIPLICATION OF DISLOCATIONS

- One of the original stumbling blocks in the development of dislocation theory was the formulation of a reasonable mechanism by which sources originally present in the metal could produce new dislocations by the process of slip.
- Moreover, if there were no source generating dislocations, cold-work should decrease, rather than increase, the density of dislocations in a single crystal. Thus, there must be a method of generating dislocations or of multiplying the number initially present to produce the high dislocation density found in cold-worked metal. The scheme by which dislocations could be generated from existing dislocations was proposed by Frank and Read1 and is commonly called a *Frank-Read source*.
- Consider a dislocation line DD' lying in a slip plane (Fig. 5-26(3). The plane of the figure is the slip plane. The dislocation line leaves the slip plane at points D and D', so that it is immobilized at these points. This could occur if D and D' were nodes where the dislocation in the plane of the paper intersects dislocations in other slip planes, or the anchoring could be caused by impurity atoms
- The maximum value of shear stress is required when the dislocation bulge becomes a semicircle so that R has the minimum value 1/2 (Fig. 5-26b).
- Beyond this point R will increase and the dislocation loop will continue to expand under a decreasing stress (Fig. 5-26c). When the loop reaches Fig. 5-26d, the segments at m and n will meet and annihilate each other to form a large loop and a new dislocation (Fig. 5-26e).



Figure 5-26 Schematic representation of the operation of a Frank-Read source.

- The stage shown in Fig. 5-26d can best be understood if we assume that the original pinned length DD' has a screw orientation. Then segments m and n are in edge orientation but of opposite sign, so that annihilation will occur. Once the loop moves into the stage shown in Fig. 5-26c, the loop can continue to expand under increased shear stress and the pinned segment DD' is in a position to repeat the process.
- This process can be repeated over and over again at a single source, each time producing a dislocation loop which produces slip of one Burgers vector along the slip plane.
- However, once the source is initiated it does not continue indefinitely. The back stress produced by the dislocations piling up along the slip plane (see Sec. 5-16) opposes the applied stress and when this equals the critical stress given by Eq. (5-30), the source ceases to operate.
STRENGTHENING MECHANISMS

Different types of strengthening mechanisms

- 1. Fine grain size is often desired for high strength
- 2. Large additions of solute atoms are added to increase strength
- 3. Bring about new phase relationships
- 4. Fine-particles may be added to increase strength
- 5. Phase transformations may be utilized to increase strength

GRAIN BOUNDARIES AND DEFORMATION

- The crystallographic orientation changes abruptly in passing from one grain to the next across the grain boundary.
- The ordinary high-angle grain boundary represents a region of random misfit between the adjoining crystal lattices. As the difference in orientation between the grains on each side of the boundary decreases, the state of order in the boundary increases.
- For the limiting case of a low-angle boundary where the orientation difference across the boundary may be less than 1° (see Sec. 6-4), the boundary is composed of a regular array of dislocations.
- Figure 6-la schematically illustrates the structure at a high-angle grain boundary. Note the unorganized structure, with a few atoms belonging to both grains, while most belong to neither. Those atoms that belong to both grains are called coincidence sites
- This grain boundary structure contains grain-boundary dislocations (Fig. 6-1b). These are not mobile dislocations producing extensive slip; rather, their chief role is that they group together within the boundary to form a step or grain-boundary ledge.



Figure 6-1 (a) Schematic atomic model of a grain boundary; (b) dislocation model of a rain boundary.

- High-angle grain boundaries are boundaries of rather high surface energy. For example, a grain boundary in copper has an interfacial surface energy of about, 600 mJ m⁻², while the energy of a twin boundary is only about 25 mJ m⁻².
- Von Mises showed that for a crystal to undergo a general change of shape by slip requires the operation of five independent slip systems.

- This arises from the fact that an arbitrary deformation is specified by the six components of the strain tensor, but because of the requirement of constant volume ($\Delta V = 0 = \epsilon_{11} + \epsilon_{22} + \epsilon_{33}$), there are only five independent strain components.
- Crystals which do not possess five independent slip systems are never ductile in polycrystalline form, although small plastic elongation may be obtained if there is twinning or a favorable preferred orientation.
- Cubic metals easily satisfy this requirement, which accounts for their general high ductility. Hexagonal close-packed and other low-symmetry metals do not satisfy this requirement and have low ductility at room temperature in polycrystalline form.
- Polycrystalline Zn and Mg become ductile at some elevated temperature at which non basal slip can become operative and increase the number of slip systems to at least five.
- At temperatures above about one-half of the melting point, deformation can occur by sliding along the grain boundaries. Grain-boundary sliding becomes more prominent with increased temperature and decreasing strain rate, as in creep.
- A rough way of distinguishing when grain-boundary sliding becomes prominent is with the equicohesive temperature. Above this temperature the grain boundary region is weaker than the grain interior and strength increases with increasing grain size. Below the equicohesive temperature the grain-boundary region is stronger than the grain interior and strength increases with decreasing grain size (increasing grain-boundary area).
- The strengthening mechanisms discussed in this chapter are those which impede the conservative motion of dislocations. Generally speaking they are operative at temperatures below about 0.5T_m, where Tm is the melting temperature in degrees Kelvin. High temperature deformation of metals is considered in Chapter 13.

STRENGTHENING FROM GRAIN BOUNDARIES

- Direct evidence for the mechanical strengthening of grain boundaries is provided by experiments1 on bicrystals in which the orientation difference between a longitudinal grain boundary was varied in a systematic manner.
- The yield stress of the bicrystals increased linearly with increasing misorientation across the grain boundary, and extrapolation to zero misorientation angle gave a value close to that of the yield stress of a single crystal.
- These results imply that a simple grain boundary has little inherent strength and that the strengthening due to grain boundaries results from mutual interference to slip within the grains.
- Several attempts have been made to calculate the stress-strain curve for a polycrystal from stress-strain curves for single crystals. In Chap. 4 we saw that the resolved shear stress in a single crystal was given by

$$\tau = \sigma \sin \chi \cos \lambda = \frac{\sigma}{M}$$

• Where M is an orientation factor (the reciprocal of the Schmid factor). For a polycrystal the orientation factor M varies from grain to grain and it is necessary to determine some average orientation factor M. The best estimate for an FCC lattice is M = 3.1, obtained by G. I. Taylor1 based on the use of the von Mises compatibility condition and assuming that all grains undergo the same deformation as the overall deformation.

HALL-PETCH RELATION

A general relationship between yield stress (and other mechanical properties) and grain size was proposed by Hall and greatly extended by Fetch.

Where,

$$\sigma_0 = \sigma_i + k D^{-1/2}$$

 σ_0 = the yield stress

 σ_i = the "friction stress," representing the overall resistance of the crystal lattice to dislocation movement K=the "locking parameter," which measures the relative hardening contribution of the grain boundaries D = grain diameter

- The Hall-Petch equation was originally based on yield-point measurements in low-carbon steel.
- It has been found to express the grain-size dependence of the low stress at any plastic strain out to ductile fracture and also to express the variation of brittle fracture stress with grain size and the dependence of fatigue strength on grain size.1
- The Hall-Petch equation also has been found to apply not only to grain boundaries but to other kinds of boundaries such as ferrite-Cementite in pearlite, mechanical twins, and martensite plates.
- The original dislocation model for the Hall-Petch equation was based on the concept that grain boundaries act as barriers to dislocation motion.
- Consider a dislocation source at the center of a grain D which sends out dislocations to pile-up at the grain boundary.
- The stress at the tip of this pile-up must exceed some critical shear stress τ_c to continue slip past the grain-boundary barrier. From Eq. (5-38) we have

$$\tau_c = n\tau_s = \frac{\pi\tau_s^2 D}{4Gb}$$

• The resolved shear stress τ_s required to overcome the barrier can be taken equal to the applied stress less the friction stress to overcome lattice resistance to dislocation motion τ_i ,

$$\tau_s = \tau - \tau_i$$

Therefore,

$$\tau_c = \frac{\pi (\tau - \tau_i)^2 D}{4Gb}$$
$$\tau = \tau_i + \left(\frac{\tau_c 4Gb}{\pi D}\right)^{1/2} = \tau_i + k' D^{-1/2}$$

Expressing (6-9) in terms of normal stresses, results in Eq. (6-6)

- The factor *k* is the slope of the straight line that is obtained when σ_0 is plotted against $D^{-1/2}$
- Many physical interpretations have been ascribed to the term, which is roughly independent of temperature.
- The term σ_i is the intercept along the ordinate in a plot of $\sigma_0 \mbox{ vs } D^{-l/2}$
- It is interpreted as the friction stress needed to move unlocked dislocations along the slip plane. This term depends strongly on temperature, strain, and alloy (impurity) content.
- While the Hall-Petch equation is a very general relationship, it must be used with some caution. For example, if Eq. (6-6) were extrapolated to the smallest grain size imaginable (approximately 4 nm), it would predict strength levels close to the theoretical shear strength.
- Such an extrapolation is in error because the equations for the stresses in a pile-up on which Eq. (6-6) is based were derived for large pile-ups containing more than 50 dislocations. For small pile-ups other equations must be considered.
- The growing realization of the importance of grain boundaries as dislocation sources has cast considerable doubt on the dislocation pile-up model for the Hall-Petch equation. A more general model proposed by Li2 avoids the description of the stresses at grain boundaries and instead concentrates on the influence of grain size on the dislocation density, and hence, on the yield or low stress. The low stress is given in terms of dislocation density by

$$\sigma_0 = \sigma_i + \alpha G b \rho^{1/2}$$

• Where a, has the same meaning as in Eq. (6-6), a is a numerical constant generally between 0.3 and 0.6, and p is the dislocation density. The justification for this equation was given in Sec. 4-14. The tie-in with grain size is based on the experimental observation that p is an inverse function of the grain size. Thus $\rho = 1/D$

$$\sigma_0 = \sigma_i + \alpha G b D^{-1/2} = \sigma_i + k' D^{-1/2}$$

LOW-ANGLE GRAIN BOUNDARIES

• Perhaps the most general method of producing a substructure network is by introducing a small amount of deformation (from about 1 to 10 percent pre strain) and following this with an annealing treatment to rearrange the dislocations into sub grain boundaries. The amount of deformation and temperature must be low enough to prevent the formation of new grains by recrystallization. This process has been called recrystallization in situ, or *polygonization*



Figure 6-6 Movement of dislocations to produce polygonization (schematic).

- The term polygonization was used originally to describe the situation that occurs when a single crystal is bent to a relatively small radius of curvature and then annealed. Bending results in the introduction of an excess number of dislocations of one sign. These dislocations are distributed along the bent-glide planes as shown in Fig. 6-6a. When the crystal is heated, the dislocations group themselves into the lower-energy configuration of a low-angle boundary by dislocation climb. The resulting structure is a polygon like network of low-angle grain boundaries (Fig. 6-6/)).
- The effect of a substructure of low-angle grain boundaries on the stress-strain curve of 1020 steel is shown in Fig. 6-7. Note that the material that was cold-reduced and annealed, so as to produce a substructure, has a higher yield point and tensile strength than both the annealed material and the material which as only cold-reduced. Moreover, the ductility of the material containing a substructure is almost as good as the ductility of the annealed steel.



Figure 6-7 Effect of a substructure of low-angle grain boundaries on the stress-strain curve of SAE 1020 steel. (After E. R. Parker and J. Washburn, "Impurities and Imperfections," p. 155, American Society for Metals, Metals Park, Ohio, 1955. By permission of the publishers.)

YIELD-POINT PHENOMENON

- Many metals, particularly low-carbon steel, show a localized, heterogeneous type of transition from elastic to plastic deformation which produces a yield point in the stress-strain curve. Rather than having a flow curve with a gradual transition from elastic to plastic behavior, such as was shown in Fig. 3-1, metals with a yield point have a low curve or, what is equivalent, a load-elongation diagram similar Fig. 6-8.
- The load increases steadily with elastic strain, drops suddenly, fluctuates about some approximately constant value of load, and then rises with further strain. The load at which the sudden drop occurs is called the *upper yield Point*. The constant load is called the *lower yield point*, and the elongation which occurs at constant load is called the yield-point elongation.
- The deformation occurring throughout the yield-point elongation is heterogeneous. At the upper yield point a discrete band of deformed metal, often readily visible with the eye, appears at a stress concentration such as a fillet, and coincident with the formation of the band the load drops to the lower yield point. The band then propagates along the length of the specimen, causing the yield-point elongation.
- In the usual case several bands will form at several points of stress concentration. These bands are generally at approximately 45° to the tensile axis. They are usually called *Luders bands, Hartmann lines, or stretcher strains*, and this type of deformation is sometimes referred to as the *Piobert efect*.
- The yield-point phenomenon was found originally in low-carbon steel. A pronounced upper and lower yield point and a yield-point elongation of over 10 percent can be obtained with this material under proper conditions.
- More recently the yield point has come to be accepted as a general phenomenon, since it has been observed in a number of other metals and alloys. In addition to iron and steel, yield points have been observed in polycrystalline molybdenum, titanium, and aluminum alloys and in single crystals of iron, cadmium, zinc, alpha and beta brass, and aluminum.
- Usually the yield point can be associated with small amounts of interstitial or substitutional impuities. For example, it has been shown1 that almost complete removal of carbon and nitrogen from low carbon steel by wet-hydrogen treatment will remove the yield point. However, only about 0.001 percent of either of these elements is required for a reappearance of the yield point.
- A number of experimental factors affect the attainment of a sharp upper yield point. A sharp upper yield point is promoted by the use of an elastically rigid (hard) testing machine, very careful axial alignment of the specimen, the use of specimens free from stress concentrations, high rate of loading, and, frequently, testing at subambient temperatures.



Liengenen

Figure 6-8 Typical yield-point behavior.

- If the stress to operate the sources is high, then the initial yield stress is high. The explanation of the yield-point phenomenon in terms of dislocation behavior arose originally from the idea that the dislocation sources were locked or pinned by solute atom interactions (Sec. 5-15).
- The explanation of this behavior was one of the early triumphs of dislocation theory. Carbon or nitrogen atoms in iron readily diffuse to the position of minimum energy just below the extra plane of atoms in a positive edge dislocation. The elastic interaction is so strong that the impurity atmosphere becomes completely saturated and condenses into a row of atoms along the core of the dislocation.
- Pinning can arise from the solute-dislocation inter- action or by precipitation of fine carbides or nitrides along the dislocation. The yield point occurs as a result of unlocking the dislocations by a high stress, or for case of strong pinning, by creating new dislocations at the points of stress concentration.

STRAIN AGING

- Strain aging is a type of behavior, usually associated with the yield-point phenomenon, in which the strength of a metal is increased and the ductility is decreased on heating at a relatively low temperature after cold-working. This behavior can best be illustrated by considering Fig. 6-9, which schematically describes the effect of strain aging on the low curve of a low-carbon steel.
- Region A of Fig. 6-9 shows the stress-strain curve for a low-carbon steel strained plastically through the yield-point elongation to a strain corresponding to point X.
- The specimen is then unloaded and retested without appreciable delay or any heat treatment (region B). Note that on reloading the yield point does not occur, since the dislocations have been torn away from the atmosphere of carbon and nitrogen atoms.

- Consider now that the specimen is strained to point Y and unloaded. If it is reloaded after aging for several days at room temperature or several hours at an aging temperature like 400 K, the yield point will reappear.
- Moreover, the yield point will be increased by the aging treatment from Y to Z. The reappearance of the yield point is due to the diffusion of carbon and nitrogen atoms to the dislocations during the aging period to form new atmospheres of interstitials anchoring the dislocations.
- Support for this mechanism is found in the fact that the activation energy for the return of the yield point on aging is in good agreement with the activation energy for the diffusion of carbon in alpha iron.



Figure 6-9 Stress-strain curves for low-carbon steel showing strain aging. Region A, original material strained through yield point. Region B, immediately retested after reaching point X. Region C, reappearance and increase in yield point after aging at 400 K ($\approx 130^{0}$ C)



Figure 6-10 Portevin-LeChatelier effect in iron (schematic).

• Nitrogen plays a more important role in the strain aging of iron than carbon because it has a higher solubility and diffusion coefficient and produces less complete precipitation during slow cooling. From a practical standpoint it is important to eliminate strain aging in deep-drawing steel because the reap pearance of the yield point can lead to difficulties with surface markings or "stretcher strains" due to the localized heterogeneous deformation.

- To control strain aging, it is usually desirable to lower the amount of carbon and nitrogen in solution by adding elements which will take part of the interstitials out of solution by forming stable carbides or nitrides. Aluminum, vanadium, titanium, columbium, and boron have been added for this purpose.
- The occurrence of strain aging is a fairly general phenomenon in metals. In addition to the return of the yield point and an increase in the yield stress after aging, strain aging also produces a decrease in ductility and a low value of strain-rate sensitivity Strain aging also is associated with the occurrence of serrations in the stress-strain curve (discontinuous or repeated yielding). This dynamic strain-aging behavior (Fig. 6-10) is called the *Portevin-LeChatelier effect*.
- The solute atoms are able to diffuse in the specimen at a rate faster than the speed of the dislocations so as to catch and lock them. Therefore, the load must increase and when the dislocations are torn away from the solute atoms there is a load drop. This process occurs many times, causing the serrations in the stress-strain curve.
- For plain carbon steel discontinuous yielding occurs in the temperature region of 500 to 650 K. This temperature region is known as the blue brittle region because steel heated in this temperature region shows a decreased tensile ductility and decreased notched-impact resistance. This temperature range is also the region in which steels show a minimum in strain-rate sensitivity and a maximum in the rate of strain aging.
- The phenomenon of strain aging should be distinguished from a process known as quench aging, which occurs in low-carbon steels. Quench aging is a type of true precipitation hardening that occurs on quenching from the temperature of maximum solubility of carbon and nitrogen in ferrite. Subsequent aging at room temperature, or somewhat above, produces an increase in hardness and yield stress, as in the age hardening of aluminum alloys. Plastic deformation is not necessary to produce quench aging.

SOLID-SOLUTION STRENGTHENING

- The introduction of solute atoms into solid solution in the solvent-atom lattice invariably produces an alloy which is stronger than the pure metal.
- There are two types of solid solutions. If the solute and solvent atoms are roughly similar in size, the solute atoms will occupy lattice points in the crystal lattice of the solvent atoms. This is called substitutional solid solution.
- If the solute atoms are much smaller than the solvent atoms, they occupy interstitial positions in the solvent lattice. Carbon, nitrogen, oxygen, hydrogen, and boron are the elements which commonly form interstitial solid solutions.
- The factors which control the tendency for the formation of substitutional solid solutions have been uncovered chiefly through the work of Hume-Rothery.
- If the sizes of the two atoms, as approximately indicated by the lattice parameter, differ by less than 15 percent, the size factor is favorable for solid-solution formation. When the size factor is greater than 15 percent, the extent of solid solubility is usually restricted to less than 1 percent.

- Metals which do not have a strong chemical affinity for each other tend to form solid solutions, while metals which are far apart on the electromotive series tend to form intermetallic compounds.
- The relative valence of the solute and solvent also is important. The solubility of a metal with higher valence in a solvent of lower valence is more extensive than for the reverse situation. For example, zinc is much more soluble in copper than is copper in zinc.
- This relative-valence effect can be rationalized to a certain extent in terms of the electron-atom ratio.1 For certain solvent metals, the limit of solubility occurs at approximately the same value of electron-atom ratio for solute atoms of different valence.
- Finally, for complete solid solubility over the entire range of composition the solute and solvent atoms must have the same crystal structure.



Figure 6-12 Effect of solute alloy additions on stress strain curve.

Solute atoms can interact with dislocations by the following mechanisms:

- 1. Elastic interaction
- 2. Modulus interaction
- 3. Stacking-fault interaction
- 4. Electrical interaction
- 5. Short-range order interaction
- 6. Long-range order interaction

STRENGTHENING FROM FINE PARTICLES

• Small second-phase particles distributed in a ductile matrix are a common source of alloy strengthening. In dispersion hardening the hard particles are mixed with matrix powder and consolidated and processed by powder metallurgy techniques. However, very many alloy systems can be strengthened by precipitation reactions in the solid state.

- Precipitation hardening, or age hardening, is produced by solution treating and quenching an alloy in which a second phase is in solid solution at the elevated temperature but precipitates upon quenching and aging at a lower temperature.
- The age-hardening aluminum alloys and copper-beryllium alloys are common examples. For precipitation hardening to occur, the second phase must be soluble at an elevated temperature but must exhibit decreasing solubility with decreasing temperature. By contrast, the second phase in dispersion-hardening systems has very little solubility in the matrix, even at elevated temperatures.

FIBER STRENGTHENING

- Materials of high strength, and especially high strength-to-weight ratio, can be produced by incorporating fine fibers in a ductile matrix.
- The fibers must have high strength and high elastic modulus while the matrix must be ductile and nonreactive with the fibers. Because of their very high strength, whiskers of materials such as Al203 have been used with good results, but most fiber- strengthened materials use fibers of boron or graphite or metal wires such as tungsten.
- The fibers may be long and continuous, or they may be discontinuous. Metals and polymers have been used as matrix materials. Glass-fiber-reinforced polymers are the most common fiber-strengthened materials. Fiber-reinforced materials are an important group of materials generally known as composite materials.

MARTENSITE STRENGTHENING

- The transformation of austenite to martensite by diffusion less shear-type transformation in quenching of steel is one of the most common strengthening processes used in engineering materials.
- Although martensitic transformations occur in a number of metallurgical systems, only the alloys based on iron and carbon show such a pronounced strengthening effect.
- Figure 6-26 shows how the hardness of martensite varies with carbon content and compares this degree of strengthening with that achieved in dispersed aggregates of iron and cementite.
- The high strength of martensite implies that there are many strong barriers to dislocation motion in this structure. The complexity of the system allows for considerable controversy and hardening mechanisms abound, but it appears that there are *two main contributions* to the high strength of martensite.
- The conventional martensite has a plate structure with a unique habit plane and an internal structure of parallel twins each about 0.1 µm thick within the plates.
- The other type of martensite structure is a block martensite containing a high dislocation density of 10⁹ to 10¹⁰ mm⁻², comparable to that in a highly deformed metal. Thus, part of the high strength of martensite arises from the effective barriers to slip provided by the ine twin structure or the high dislocation density.

• The second important contribution to the strength of martensite comes from the carbon atoms. Figure 6-26 shows that the hardness of martensite is very sensitive to carbon content below 0.4 percent. On rapidly transforming from austenite to ferrite in the quench, the solubility of carbon in iron is greatly reduced. The carbon atoms strain the ferrite lattice and this strain can be relieved by redistribution of carbon atoms by diffusion at room temperature.



Figure 6-26 Hardness of various transformation products in steel.

COLD-WORKED STRUCTURE

• Plastic deformation which is carried out in a temperature region and over a time interval such that the strain hardening is not relieved is called cold-work.



Figure 6-28 (a) Deformed to 10 percent strain. Beginning of cell formation with dislocation tangles; (b) deformed to 50 percent strain. Equilibrium cell size with heavy dislocation density in cell walls (schematic)

- Plastic deformation produces an increase in the number of dislocations, which by virtue of their interaction results in a higher state of internal stress. An annealed metal contains about 10⁴ to 10⁶ dislocations per mm², while a severely plastically deformed metal contains about 10¹⁰ mm⁻².
- Strain hardening or cold work can be readily detected by x-ray diffraction, although detailed analysis of the x-ray patterns in terms of the structure of the cold-worked state is not usually possible.

STRAIN HARDENING

- Strain hardening or cold-working is an important industrial process that is used to harden metals or alloys that do not respond to heat treatment.
- The rate of strain hardening can be gaged from the slope of the low curve.
- Generally, the rate of strain hardening is lower for hcp metals than for cubic metals. Increasing temperature also lowers the rate of strain hardening.
- For alloys strengthened by solid-solution additions the rate of strain hardening may be either increased or decreased compared with the behavior for the pure metal.
- However, the final strength of a cold-worked solid-solution alloy is almost always greater than that of the pure metal cold-worked to the same extent.



Figure 6-29 Variation of tensile properties with amount of cold-work.

- Figure 6-29 shows the typical variation of strength and ductility parameters with increasing amount of cold-work. Since in most cold-working processes one or two dimensions of the metal are reduced at the expense of an increase in the other dimensions, cold-work produces elongation of the grains in the principal direction of working.
- Severe deformation produces a reorientation of the grains into a preferred orientation (Sec. 6-17). In addition to the changes in tensile properties shown in Fig. 6-29, cold-working produces changes in other physical properties.

• A high rate of strain hardening implies mutual obstruction of dislocations gliding on intersecting systems. This can come about (1) through interaction of the stress fields of the dislocations, (2) through interactions which produce sessile locks, and (3) through the interpenetration of one slip system by another (like cutting trees in a forest) which results in the formation of dislocation jogs.

ANNEALING OF COLD-WORKED METAL

- The cold-worked state is a condition of higher internal energy than the undeformed metal. Although the cold worked dislocation cell structure is mechanically stable, it is not thermodynamically stable.
- With increasing temperature the cold-worked state becomes more and more unstable. Eventually the metal softens and reverts to a strain-free condition.
- The overall process by which this occurs is known as annealing. Annealing is very important commercially because it restores the ductility to a metal that has been severely strain-hardened.
- Therefore, by interposing annealing operations after severe deformation it is possible to deform most metals to a very great extent.
- The process of annealing can be divided into three fairly distinct processes: recovery, recrystallization, and grain growth.
- Figure 6-30 will help to distinguish between these processes. Recovery is usually defined as the restoration of the physical properties of the cold-worked metal without any observable change in microstructure.



Figure 6-30 Schematic drawing indicating recovery, recrystallization, and grain growth and chief property changes in each, region.

• Electrical conductivity increases rapidly toward the annealed value during recovery, and lattice strain, as measured with x-rays, is appreciably reduced. The properties that are most affected by recovery are those which are sensitive to point defects.

• The strength properties, which are controlled by dislocations, are not affected at recovery temperatures. An exception to this is single crystals of hep metals which have deformed on only one set of planes (easy glide)



Figure 6-31 Changes in microstructure of cold-worked 70-30 brass with annealing, (a) Cold-worked 40 percent; (b) 440oC, 15 min; (c) 5750C, 15 min (150X)

- Recrystallization is the replacement of the cold-worked structure by a new set of strain-free grains.
- Recrystallization is readily detected by metallographic methods and is evidenced by a decrease in hardness or strength and an increase in ductility. The density of dislocations decreases considerably on recrystallization, and all effects of strain hardening are eliminated.
- The stored energy of cold-work is the driving force for both recovery and recrystallization. If the new strain-free grains are heated at a temperature greater than that required to cause recrystallization, there will be a progressive increase in grain size.
- The driving force for grain growth is the decrease in free energy resulting from a decreased grainboundary area due to an increase in grain size.
- Figure 6-31 shows the progression from a cold-worked microstructure to a fine recrystallized grain structure, and finally to a larger grain size by grain growth.

□ Six main variables influence recrystallization behavior. They are

- (1) Amount of prior deformation,
- (2) Temperature,
- (3) Time,
- (4) Initial grain size,
- (5) Composition,
- (6) Amount of recovery or polygonization prior to the start of recrystallization.
- Because the temperature at which recrystallization occurs depends on the above variables, it is not a fixed temperature in the sense of a melting temperature.

- For practical considerations a recrystallization temperature can be defined as the temperature at which a given alloy in a highly cold-worked state completely recrystallizes in 1 h.
- Because the driving force for grain growth is appreciably lower than the driving force for recrystallization, at a temperature at which recrystallization occurs readily grain growth will occur slowly. However, grain growth is strongly temperature-dependent, and a grain-coarsening region will soon be reached in which the grains increase in size very rapidly.

The relationship of the above variables to the recrystallization process can be summarized as follows:

- 1. A minimum amount of deformation is needed to cause recrystallization.
- 2. The smaller the degree of deformation, the higher the temperature required to cause recrystallization.

3. Increasing the annealing time decreases the recrystallization temperature. However, temperature is far more important than time. Doubling the annealing time is approximately equivalent to increasing the annealing temperature 10oC.

4. The initial grain size depends chiefly on the degree of deformation and to a lesser extent on the annealing temperature. The greater the degree of deformation, and the lower the annealing temperature, the smaller the recrystallized grain size.

5. The larger the original grain size, the greater the amount of cold-work required to produce an equivalent recrystallization temperature.

6. The recrystallization temperature decreases with increasing purity of the metal. Solid-solution alloying additions always raise the recrystallization temperature.

7. The amount of deformation required to produce equivalent recrystallization behavior increases with increased temperature of working.

8. For a given reduction in cross section, different metalworking processes, such as rolling, drawing, etc., produce somewhat different effective deformations. Therefore, identical recrystallization behavior may not be obtained.

Fe-C Diagram

Fe-Carbon Diagram





δ-ferrite – Solid solution of carbon in iron. Maximum concentration of carbon in δ-ferrite is 0.09% at 2719 °F (1493°C) – temperature of the peritectic transformation. The crystal structure of δ-ferrite is BCC (cubic body centered).



Austenite – interstitial solid solution of carbon in γ -iron. Austenite has FCC (cubic face centered) crystal structure, permitting high solubility of carbon – up to 2.06% at 2097 °F (1147 °C). Austenite does not exist below 1333 °F (727°C) and maximum carbon concentration at this temperature is 0.83%.



★ α-ferrite – solid solution of carbon in α-iron. α-ferrite has BCC crystal structure and low solubility of carbon – up to 0.25% at 1333 °F (727°C). α-ferrite exists at room temperature.









Temperature \Rightarrow Alloys, containing from 2.06% to γ = Austenite a = Ferrite 6.67% of carbon, experience eutectic 8 = Delta iron transformation at (1130 °C). The M = Cementite 1539 eutectic concentration of carbon is 1492 4.3%. CM begins 1400 to solidiffy Primary In practice only hypoeutectic alloys austenite begins to are used. These alloys (carbon and solidify content from 2.06% to 4.3%) are L + FeaC 2066⁰ F called *cast iron*. When temperature 1130 of an alloy from this range reaches FesC Austentite (1130 °C), it contains primary ledeburite and 910 FeyC cementite austenite crystals and some amount Cementite Austenite and of the liquid phase. The latter to pearlite A1.2.3 **Iedeburite** decomposes by eutectic mechanism Cementite, pearlite to a fine mixture of austenite and and transformed Fe₃C ledeburite cementite, called ledeburite. Magnetic change of Fe₃C - 210 10.008% 4.3. 6.67. 0.83% 1% 0.50 2% 3%. 5% 6% 65% 4% -Hypo-eutectoid ----- Hyper-eutectoid Cast Iron Steel

760

723



CRITICAL TEMPERATURE

✤ Upper critical temperature (point)
A₃ is the temperature, below which ferrite starts to form as a result of ejection from austenite in the hypoeutectoid alloys.

\diamond Upper critical temperature (point) A_{CM} is the temperature, below which cementite starts to form as a result of ejection from austenite in the hypereutectoid alloys.

* Lower critical temperature (point) A_1 is the temperature of the austenite-topearlite eutectoid transformation. Below this temperature austenite does not exist.







 γ = Austenite

emperatur

PHASE COMPOSITIONS OF THE IRON-CARBON ALLOYS AT ROOM <u>TEMPERATURE</u>

Hypoeutectoid steels (carbon content from 0 to 0.83%) consist of primary proeutectoid) ferrite (according to the curve A3) and pearlite.

Eutectoid steel (carbon content 0.83%) entirely consists of pearlite.

Hypereutectoid steels (carbon content from 0.83 to 2.06%) consist of primary (proeutectoid) cementite (according to the curve ACM) and pearlite.

Cast irons (carbon content from 2.06% to 4.3%) consist of proeutectoid cementite C2 ejected from austenite according to the curve ACM, pearlite and transformed ledeburite (ledeburite in which austenite transformed to pearlite.)



PHASES OF IRON



Alpha"Ferrite", BCC IronRoom Temperature



Gamma"Austenite", FCC IronElevated Temperatures



These are <u>PHASES</u> of iron. <u>Adding carbon</u> changes the phase transformation temperature.

MICROSTRUCTURE OF AUSTENITE



MICROSTRUCTURE OF PEARLITE



Photomicrographs of (a) coarse pearlite and (b) fine pearlite. 3000X

MICROSTRUCTURE OF MARTENSITE



IRON-CARBON (Fe-C) PHASE DIAGRAM (EXAMPLE 1)

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EXAMPLE 1

 An alloy of eutectoid composition (0.83 wt% C) as it is cooled down from a temperature within the γ-phase region (e.g., at 800 °C).

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- Initially the alloy is composed entirely of the austenitic phase having a composition of 0.83 wt% C
- As the alloy is cooled, no changes will occur until the eutectoid temperature (727 °C).
- Upon crossing this temperature to point B, the austenite transforms according to:

Eutectoid (B):

 $\gamma (0.83 \text{ wt\% C}) \Rightarrow \alpha (0.025 \text{ wt\% C}) + \text{Fe}_3\text{C} (6.7 \text{ wt\% C})$

EXAMPLE 1 (cont.)

- The microstructure for this eutectoid steel is slowly cooled through the eutectoid temperature consists of alternating layers or lamellar of the two phases (α and Fe₃C) that form simultaneously during the transformation.
- Point B is called **pearlite**.
- Mechanically, pearlite has properties intermediate between the soft, ductile ferrite and the hard, brittle cementite.

EXAMPLE 1 (cont.)

The alternating α and Fe₃C layers in pearlite form as such for the same reason that the eutectic structure forms because the composition of austenite (0.83 %wt C) is different from either of ferrite (0.025 wt% C) and cementite (6.70 wt% C), and the phase transformation requires that there be a redistribution of the carbon by diffusion.

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 Subsequent cooling of the pearlite from point B will produce relatively insignificant microstructural changes.



EXAMPLE 2 (cont.)

- Within the $\alpha + \gamma$ region, most of the α particles will form along the original γ grain boundaries.
- The particles will grow larger just above the eutectoid line. As the temperature is lowered below T_e , all the γ phase will transform to pearlite according to:

$$\gamma \Rightarrow \alpha + Fe_3C$$

- There will be virtually no change in the α phase that existed just above the T_e.
- This α that is formed above T_e is called **proeutectoid** (pro=pre=before eutectoid) ferrite.

EXAMPLE 2 (cont.)

- The ferrite that is present in the pearlite is called eutectoid ferrite.
- As a result, two microconstituents are present in the last micrograph (the one below T_e): proeutectoid ferrite and pearlite





MICROSTRUCTURE OF HYPO-EUTECTOID

Hypo-eutectoid Composition (0.38 wt% C)









Example: Phase Equilibria

For a 99.6 wt% Fe-0.40 wt% C at a temperature just below the eutectoid, determine the following

- a) composition of Fe₃C and ferrite (α)
- b) the amount of carbide (cementite) in grams that forms per 100 g of steel
- c) the amount of pearlite and proeutectoid ferrite (α)





TTT DIAGRAM

T (Time) T(Temperature) T(Transformation) diagram is a plot of temperature versus the logarithm of time for a steel alloy of definite composition. It is used to determine when transformations begin and end for an isothermal (constant temperature) heat treatment of a previously austenitized alloy. When austenite is cooled slowly to a temperature below LCT (Lower Critical Temperature), the structure that is formed is Pearlite. As the cooling rate increases, the pearlite transformation temperature gets lower. The microstructure of the material is significantly altered as the cooling rate increases. By heating and cooling a series of samples, the history of the austenite transformation may be recorded. TTT diagram indicates when a specific transformation starts and ends and it also shows what percentage of transformation of austenite at a particular temperature is achieved.





<u>AUSTENITE</u>

Austenite is stable at temperatures above LCT but unstable below LCT. Left curve indicates the start of a transformation and right curve represents the finish of a transformation. The area between the two curves indicates the transformation of austenite to different types of crystal structures. (Austenite to pearlite, austenite to martensite, austenite to bainite transformation.) Isothermal Transform Diagram shows that γ to transformation (a) is rapid! at speed of sound; (b) the percentage of transformation depends on Temperature only.



FIGURE 10.13 The complete isothermal transformation diagram for an iron–carbon alloy of eutectoid composition: A, austenite; B, bainite; M, martensite; P, pearlite. As indicated when is cooled to temperatures below LCT, it transforms to other crystal structures due to its unstable nature. A specific cooling rate may be chosen so that the transformation of austenite can be 50 %, 100 % etc. If the cooling rate is very slow such as annealing process, the cooling curve passes through the entire transformation area and the end product of this the cooling process becomes 100% Pearlite. In other words, when slow cooling is applied, all the Austenite will transform to Pearlite. If the cooling curve passes through the middle of the transformation area, the end product is 50 % Austenite and 50 % Pearlite, which means that at certain cooling rates we can retain part of the Austenite, without transforming it into Pearlite.

Upper half of TTT Diagram(Austenite-Pearlite Transformation Area)



If a cooling rate is very high, the cooling curve will remain on the left hand side of the Transformation Start curve. In this case all Austenite will transform to Martensite. If there is no interruption in cooling the end product will be martensite.

