Ministry of Higher Education and Scientific Research

University of RELIZANE

Faculty of Science and Technology

Department of Physics

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Handout

Properties of crystal defects

Courses and Exercises

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Intended for third-year Materials Physics students

بسم الله الرحمن الرحيم

Presentation

In this second-semester course of the academic year, we will study the module "Properties of Crystalline Defects" in the third-year Materials Physics program. This course has been designed to facilitate students' understanding and assimilation of the covered topics.

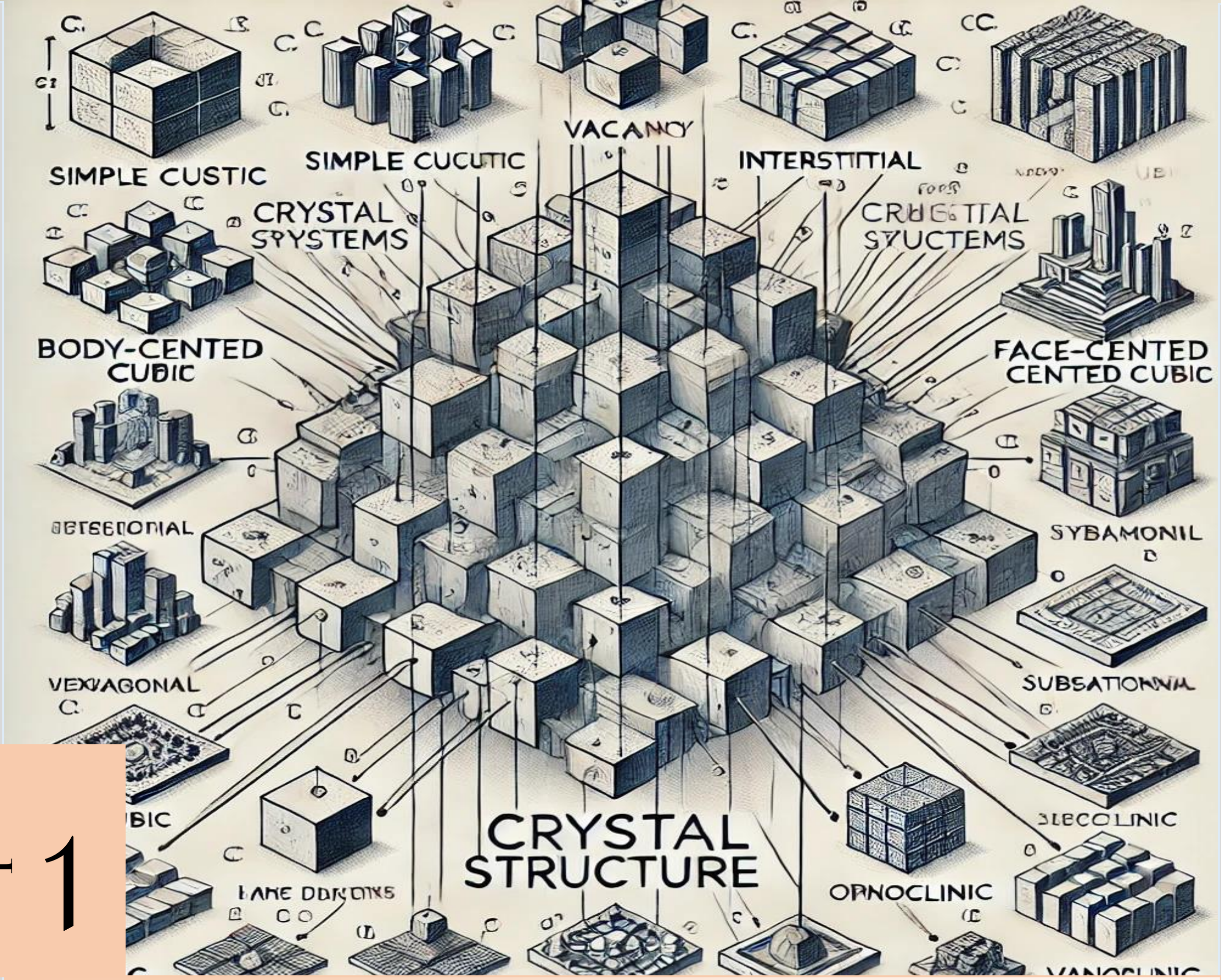
The module, in accordance with the LMD system, includes six main chapters:

- Review of Crystal Structure
- Point Defects
- Linear Defects (Dislocations)
- Two-Dimensional Defects
- Three-Dimensional Defects
- Factors Affecting Electrical Conductivity and Hardness of a Material

Therefore, I am open to receiving any feedback, critiques, or suggestions regarding the content or presentation of this manuscript.

content

Chapter 6 : *Factors Influencing the Electrical Conductivity and Hardness of a Material*



Chapter 1

The crystal structure

The crystal structure is formed by atoms that repeat periodically (regularly) in space under the effect of symmetry operations of the space group. The concept of this structure is essential in many fields of science and technology.

I. Crystal Structure

Crystalline solids are characterized by a **highly ordered, three-dimensional arrangement** of their atomic or molecular components. This repeating structural pattern, known as the **crystal lattice**, can be effectively represented by identifying its **smallest repeating unit**, called the **unit cell**. The unit cell serves as the fundamental building block of the crystal, and when replicated in all three spatial dimensions, it reconstructs the entire crystalline structure.

II. Visualizing Unit Cells in Two and Three Dimensions

The **simplest way** to visualize unit cells is in **two dimensions (figure 1)**, where they form a periodic grid-like structure. A given two-dimensional lattice can often be represented by multiple possible unit cells. However, **the most efficient unit cell is the smallest one that fully captures the periodic order** of the structure. An incorrectly chosen unit cell—one that does not preserve the symmetry and periodicity of the lattice—cannot adequately represent the crystal.

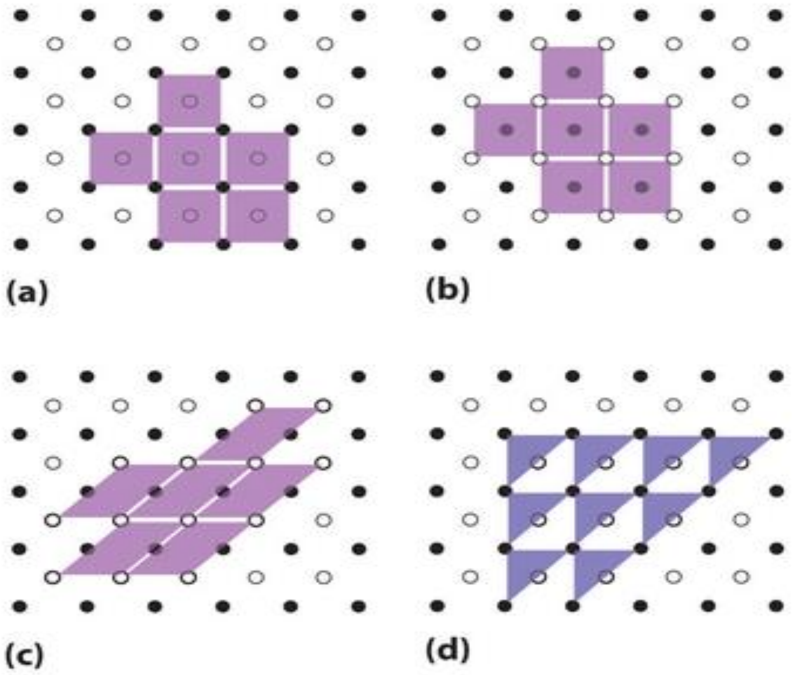


Figure 1. Unit Cells in Two Dimensions. (a–c) Three two-dimensional lattices illustrate the possible choices of the unit cell. (d) The triangle is not a valid unit cell because repeating it in space fills only half of the space in the pattern.

This concept extends into **three-dimensional lattices**, where unit cells can take various geometric forms, depending on the atomic arrangement and symmetry of the crystal. In **Figure 2**, a three-dimensional schematic illustrates how unit cells repeat in space to create a continuous crystal lattice. These unit cells are defined by **lattice parameters**—the edge lengths **(a, b, c)** and interaxial angles **(α, β, γ)**—which determine the overall structure of the crystal.

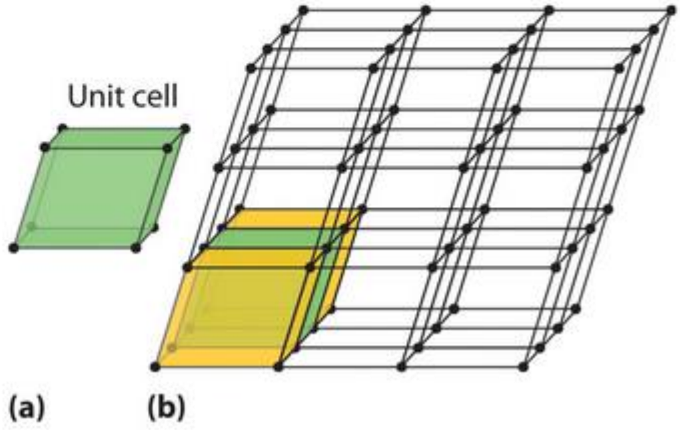


Figure 2. Unit Cells in Three Dimensions. These images show (a) a three-dimensional unit cell and (b) the resulting regular three-dimensional lattice.

III. The Unit Cell

There are seven fundamentally different kinds of unit cells, which differ in the relative lengths of the edges and the angles between them (Figure 3). Each unit cell has six sides, and each side is a parallelogram. We focus primarily on the cubic unit cells, in which all sides have the same length and all angles are 90°, but the concepts that we introduce also apply to substances whose unit cells are not cubic.

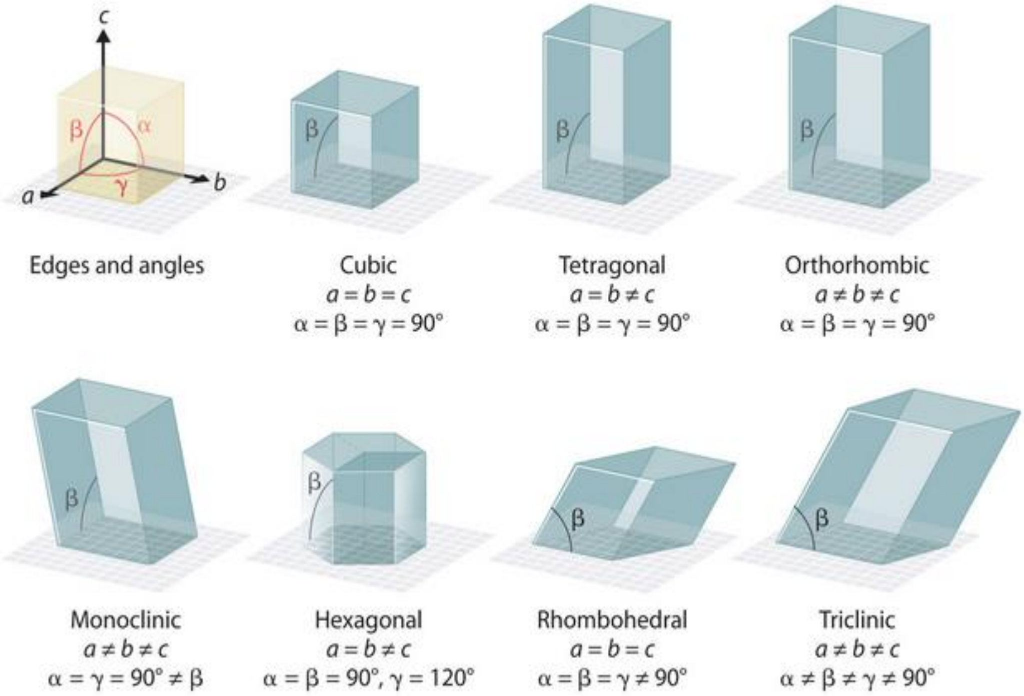
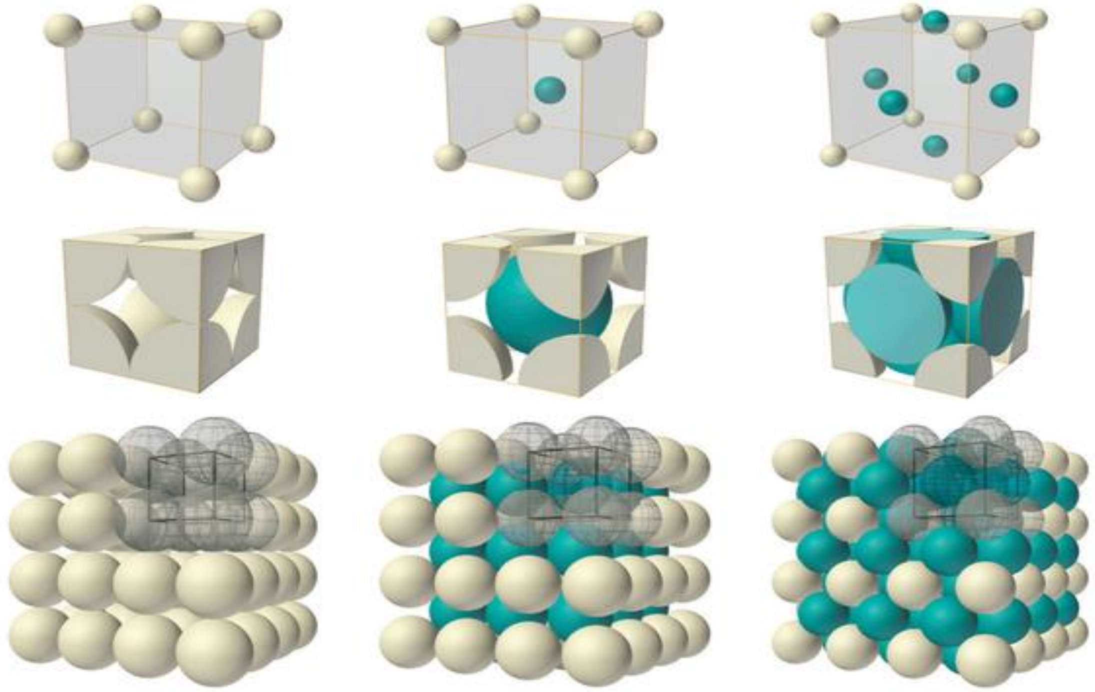


Figure 4. The General Features of the Seven Basic Unit Cells. The lengths of the edges of the unit cells are indicated by a, b, and c, and the angles are defined as follows: α, the angle between b and c; β, the angle between a and c; and γ, the angle between a and b

If the cubic unit cell consists of eight component atoms, molecules, or ions located at the corners of the cube, then it is called simple cubic (part (a) in Figure 5). If the unit cell also contains an identical component in the center of the cube, then it is body-centered cubic (bcc) (part (b) in Figure 5). If there are components in the center of each face in addition to those at the corners of the cube, then the unit cell is face-centered cubic (fcc) (part (c) in Figure 5)



(a) Simple cubic (b) Body-centered cubic (c) Face-centered cubic

Figure 5. The Three Kinds of Cubic Unit Cell.

As indicated in Figure 5, a solid consists of a large number of unit cells arrayed in three dimensions. Any intensive property of the bulk material, such as its density, must therefore also be related to its unit cell. Because density is the mass of substance per unit volume, we can calculate the density of the bulk material from the density of a single unit cell. To do this, we need to know the size of the unit cell (to obtain its volume), the molar mass of its components, and the number of components per unit cell. When we count atoms or ions in a unit cell, however, those lying on a face, an edge, or a corner contribute to more than one unit cell, as shown in Figure 5. For example, an atom that lies on a face of a unit cell is shared by two adjacent unit cells and is therefore counted as 12 atom per unit cell. Similarly, an atom that lies on the edge of a unit cell is shared by four adjacent unit cells, so it contributes 14 atom to each. An atom at a corner of a unit cell is shared by all eight adjacent unit cells and therefore contributes 18 atom to each.The statement that atoms lying on an edge or a corner of a unit cell count as 14 or 18 atom per unit cell, respectively, is true for all unit cells except the hexagonal one, in which three unit cells share each vertical edge and six share each corner (Figure 4), leading to values of 13 and 16 atom per unit cell, respectively, for atoms in these positions. In contrast, atoms that lie entirely within a unit cell, such as the atom in the center of a body-centered cubic unit cell, belong to only that one unit cell.

APPLICATION

Exercise 1 : Magnesium Oxide Crystal

Magnesium oxide (MgO) has a NaCl-type structure.

a. Draw the structure.

b. Show that this structure is consistent with the stoichiometric composition of MgO.

c. The edge length of the unit cell is 4.1×10^{-10} m. Calculate the density and packing efficiency (compacity).

d. Among the following compounds: KF, NaI, FeO, $MgCl_2$, which are likely to crystallize with the same structure?

Data: Molar mass of Mg = 24.3 g/mol

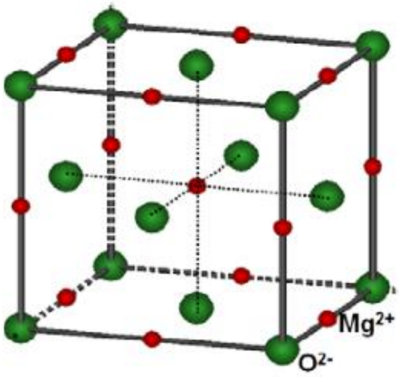
- Molar mass of O = 16.0 g/mol
- Ionic radii in nm (values likely provided in the problem)

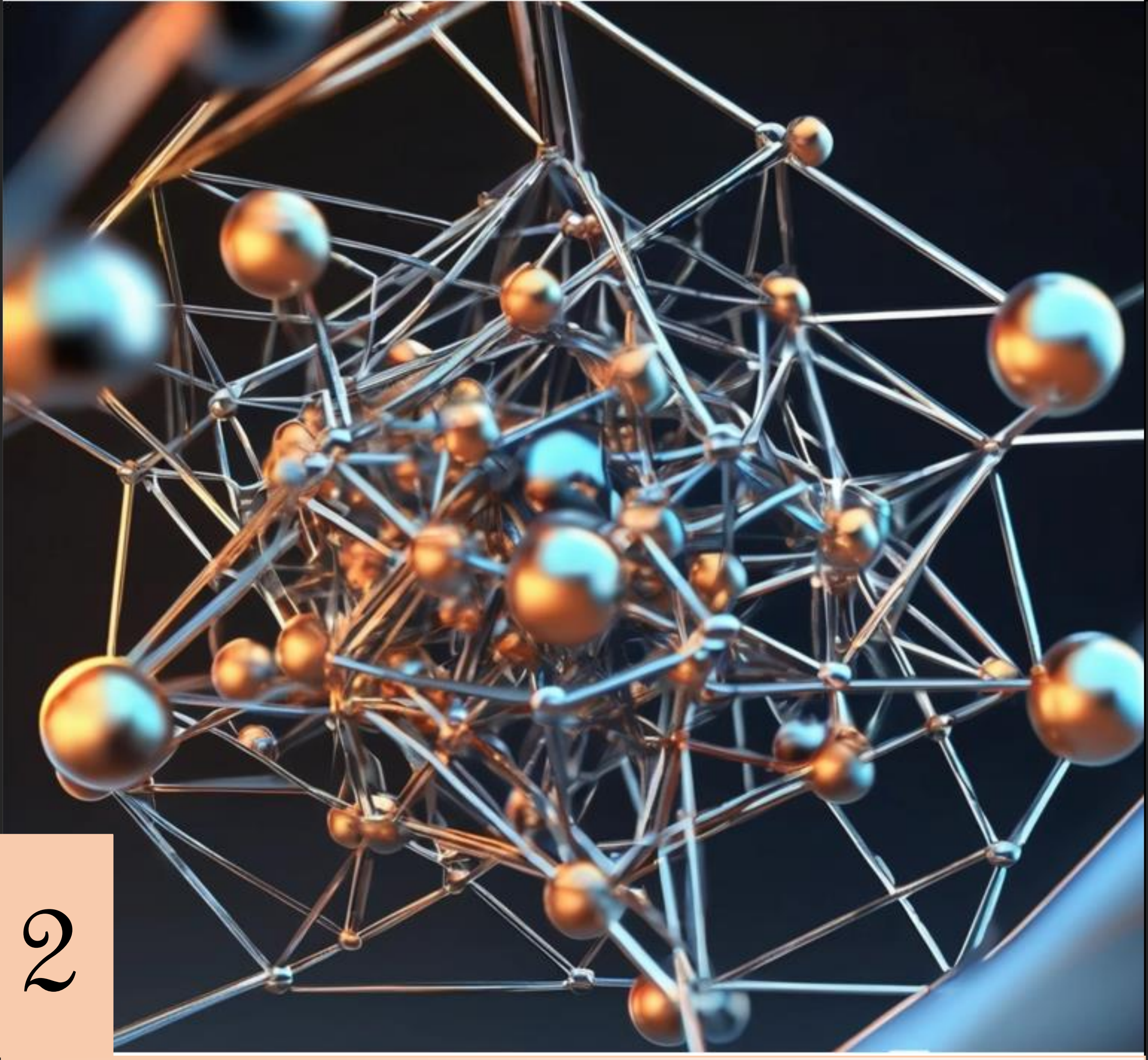
O^{2-}	Mg^{2+}	K^+	Fe^{2+}	F^-	Cl^-	Na^+	I^-
0.140	0.065	0.138	0.063	0.136	0.181	0.102	0.220

Solution

a. The O^{2-} ions are located at the corners of the cube and at the centers of the faces (forming an FCC structure). The Mg^{2+} ions occupy all the octahedral sites, i.e., the center of the cube and the midpoints of the edges.

b. the number of O^{2-} per unit cell : $Z(O^{2-})=4$ and the number of Mg^{2+} per unit cell $Z(Mg^{2+})=4\rightarrow$ in accordance with the stoichiometry





Chapter 2

Point Defects

Defects are microscopic regions of a crystal in which an atom is surrounded by close neighbors located at positions different from those observed in a perfect crystal. Generally, defects are divided into four categories according to their dimensionality. The following paragraphs review point (0D), linear (1D), planar (2D), and volume (3D) defects.

I. Stoichiometric Defect

In this kind of point defect, the ratio of positive and negative ions (Stoichiometric) and electrical neutrality of a solid is not disturbed. Sometimes it is also known as intrinsic or thermodynamic defects.

Fundamentally, they are of two types:

a. Vacancy defect: When an atom is not present at their lattice sites, then that lattice site is vacant and it creates a vacancy defect. Due to this, the density of a substance decreases [Figure 1].

Vacancies are a very important type of point defect because they facilitate the movement of atoms in the crystal (diffusion). Diffusion largely controls the behavior of materials at high temperatures (creep, heat treatments).

A non-ionic compound mainly shows vacancy and interstitial defects. An ionic compound shows the same in Frenkel and Schottky defect.

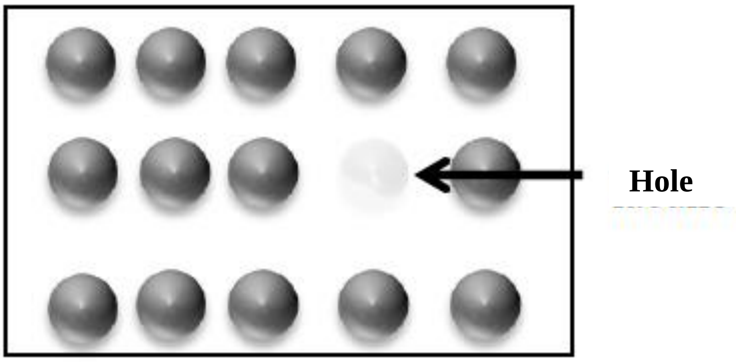


Figure 1: Hole in a network**.**

b. Interstitial defect: It is a defect in which an atom or molecule occupies the intermolecular spaces in crystals. In this defect, the density of the substance increases [Figure 2].

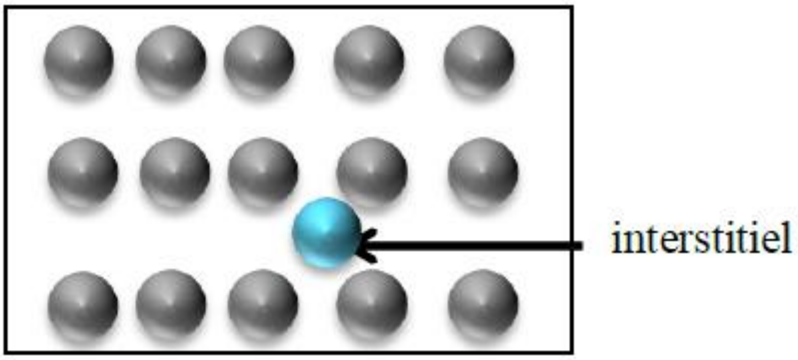


Figure 2: Interstitial atom in a lattice

c. **Substitution atoms:** When an atom occupies a site normally occupied by an atom of a different chemical nature, we speak of a substitutional impurity [Figure 3].

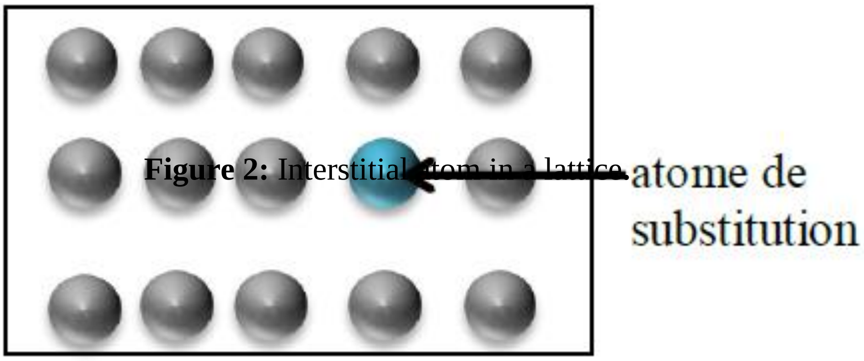


Figure 3: Substitution in a network

II. Point Defects in Ionic Solids

In monoatomic crystals (metals), point defects are created independently of each other. In ionic crystals, the creation of defects must preserve the electrical neutrality of the material. As a result, defects are created by pairs of opposite signs.

Schottky defects composed of an anionic gap and a cationic gap are distinguished by the Frenkel defects consisting of a set consisting of a gap (cationic or anionic) and an interstitial ion (anion or cation).

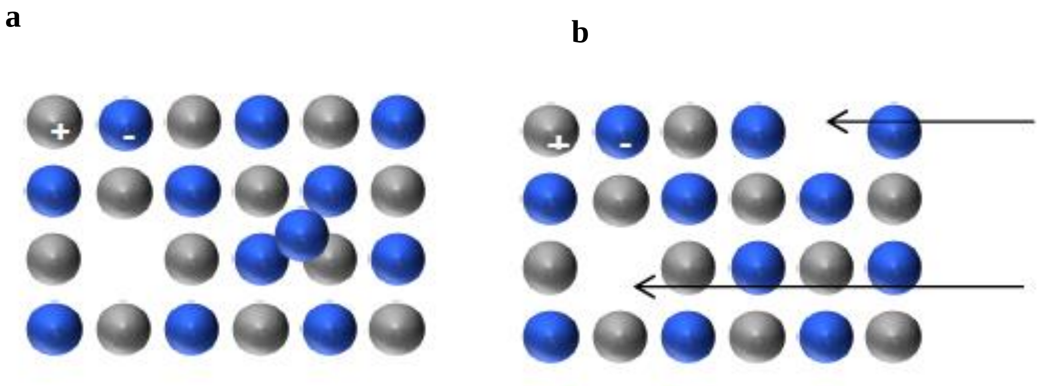
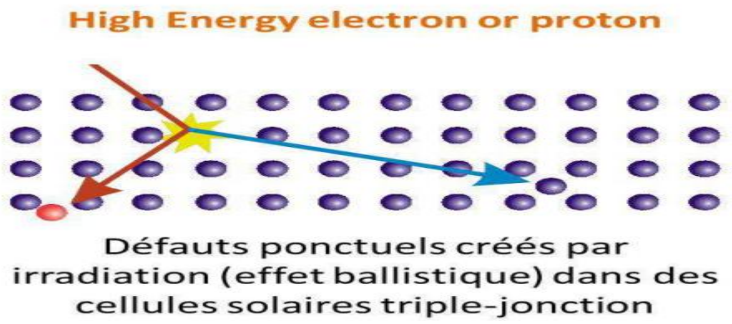


Figure 4.(a) Frenkel Defect, (b) Schotky Defect

III. Creating holes

In some cases, the concentration of a crystal is higher than the equilibrium concentration. Thus, rapid cooling (quenching) from a high temperature allows to keep, at low temperature, a relatively high concentration in gaps One also obtains a higher concentration in gaps by irradiating the material with ionizing radiation (γ (rays γ for example). The presence of a high concentration of gaps significantly changes the behaviour of metallic materials, especially during phase transformations



IV. How many vacancies are there?

The Boltzmann distribution can be used to estimate the number of vacancies Nv, which is predicted by statistical thermodynamics to have a substantial dependency on temperature T.

$$N_V = N\exp(\frac{-Q_V}{K_B T})$$

Where

N :is the total number of regular lattice sites , (total number of atomic sites).

Q_V : is the energy required to form a vacant lattice site in a perfect crystal.

K_B :is the Boltzmann's constant , = $1.38 * 10^{-23}$ J/ atom .K

T : is the temperature in Kelvin (K).

V. colored center in ionic crystals

Heated in an atmosphere containing sodium vapours, a NaCl crystal turns yellow (KCI heated in potassium vapor turns purplish red).

Chapter 3

Linear defects

In materials science, linear defects observed in crystals are called dislocations. A dislocation corresponds to a discontinuity in the organization of the crystalline structure. A dislocation can be seen simply as a "quantum" of elemental deformation within a crystal possessing a long-range stress field.

I. Definition

Mutability (the amplitude of a material to be deformed) and ductility (the amplitude of a material able to be stretched into threads) which can facilitate the plastic deformation of metals and their alloys for example comes from the presence of a type of crystalline defects of linear shape called dislocations.

It is characterized by:

- The direction of its line;
- A vector called "Burgers' vector" whose standard represents the amplitude of the deformation it generates.

Dislocations are of crucial importance for the physical properties of crystalline materials:

- They are the ones that propagate plastic deformation as they move. Thus, they allow metal parts to be shaped.
- The distortions of the crystal lattice that they induce facilitate the diffusion of atoms. They can trap defects around them (Cottrell cloud).
- They influence the electronic properties of semiconductors

Dislocations are obtained by sliding b of a part of the crystal along a plane. The dislocation line itself is the line of the glide plane separating the part of the crystal that has slipped from the one that has remained motionless. The slide vector b is called the dislocation **Burgers vector**.

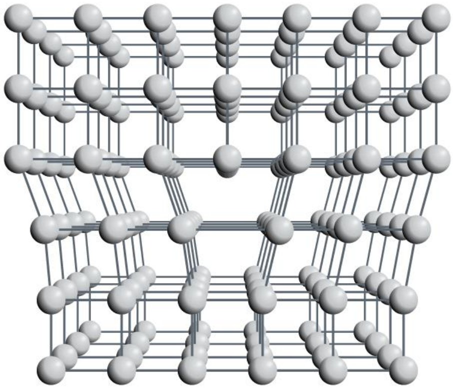
II. Geometric description

There are two types of straight dislocations: coin dislocations and dislocations vis. In practice, dislocations often show, in a given proportion, the coin character and the screw character: we then speak of mixed dislocations. These dislocations are curved (or left) and at each point, we can decompose them into a corner component and a screw component.

II.1. Corner dislocations

Geometrically, a corner dislocation can be understood as resulting from the introduction of an atomic half-plane inside a perfect crystal. The location of the dislocation is defined as the boundary of this additional half plane in the otherwise perfect crystal (see Fig.).

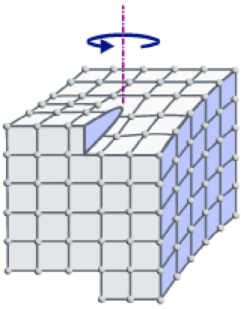
The deformation is identical to that created by introducing an additional plane of atoms to the upper part of the crystal. The atoms of the upper half-crystal are compressed, the others are dilated.

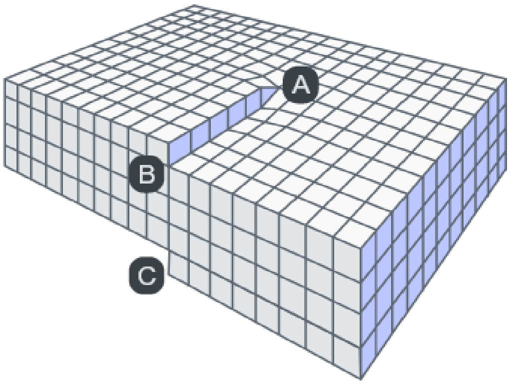


II.3. Dislocations vis

We can imagine a screw dislocation by imagining that a notch is made in the crystal and that one of the edges of this notch is slid relative to the other by an interatomic distance.

A screw dislocation transforms the successive atomic planes into a helical surface, hence its name (see Fig.).





III. Vector of Burgers

A dislocation is entirely defined by its position in the crystal and by a vector called Burgers vector. The **Burgers vector** noted as b, is defined as the closing fault of a circuit or circuit of Burgers connecting neighbouring atoms and encircling the dislocation line, characterizing the amplitude, direction and direction of displacement of the atoms of dislocation. This method consists of taking a circuit on a reticular plane perpendicular to the dislocation line. The circuit passes around dislocation figure 1. the direction of the circuit is by convention that of the hands of a clock. The start of the circuit, which has an identical number of steps in all directions, is made from any atom of the plane and taken as a starting point. In a perfect crystal figure1.a, the point of arrival of the circuit coincides with that of departure and consequently, the vector of Burgers, $b = 0$.

In the case of a corner dislocation (figure 2) screw dislocation (figure 3), the point of arrival does not coincide with that of departure. The circuit closing fault shown on the diagram represents the vector of Burgers b.

- It is noted that the vector of Burgers and the dislocation line are always perpendicular in the case of a corner dislocation. They are parallel in the case of a dislocation vis.
- A dislocation never ends inside the crystal. It extends from a mixed surface, the vector of Burgers makes an angle with the dislocation line.

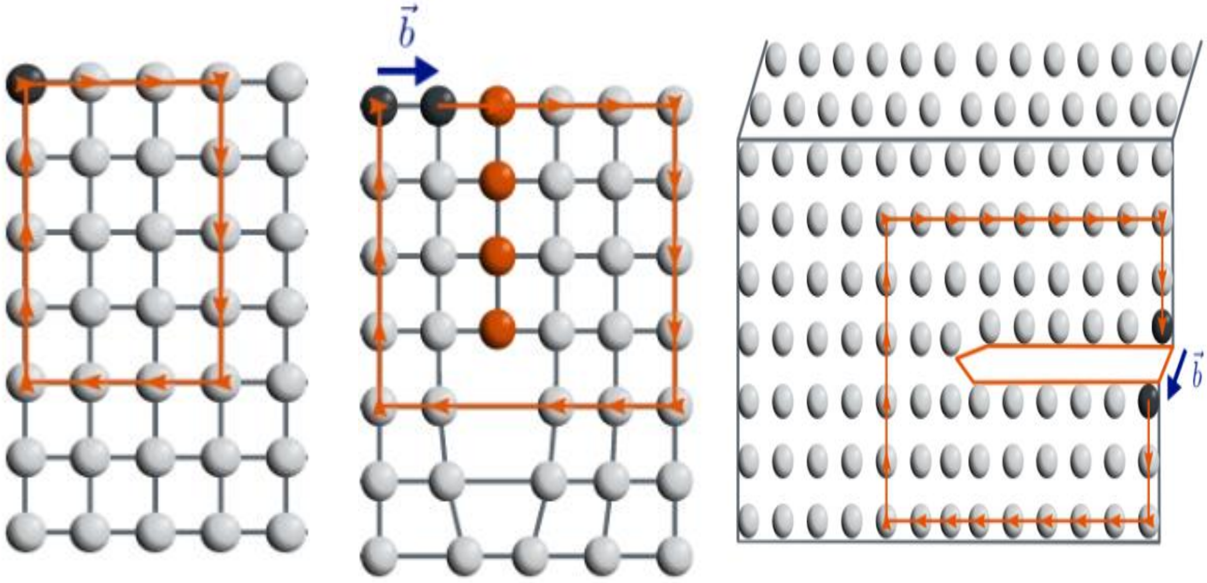
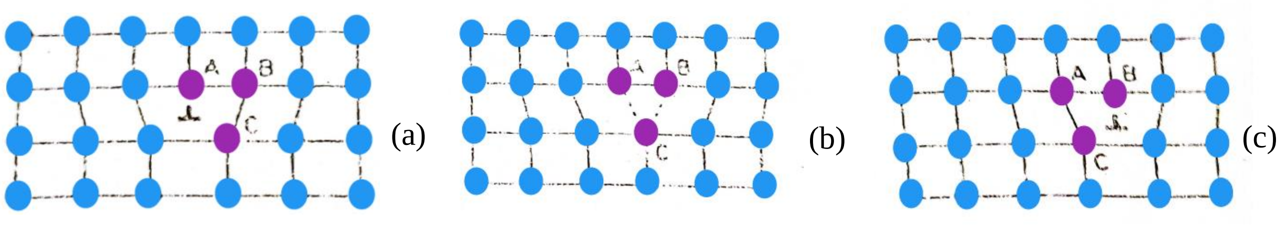


Figure - Burgeurs circuit. (a) Circuit in a perfect crystal (b) circuit around a dislocation corner (figure 2) circuit around a dislocation screw.

IV. Motion of dislocations

In a crystal, dislocations can move in their sliding planes. Their presence facilitates movement and the constraints applied for such a displacement are relatively low. This dislocation displacement process is the basis of the low temperature plastic deformation mechanism (T<0.4Tf) in most crystalline materials and particularly metals and their alloys, resulting in a



Permanent change of shape

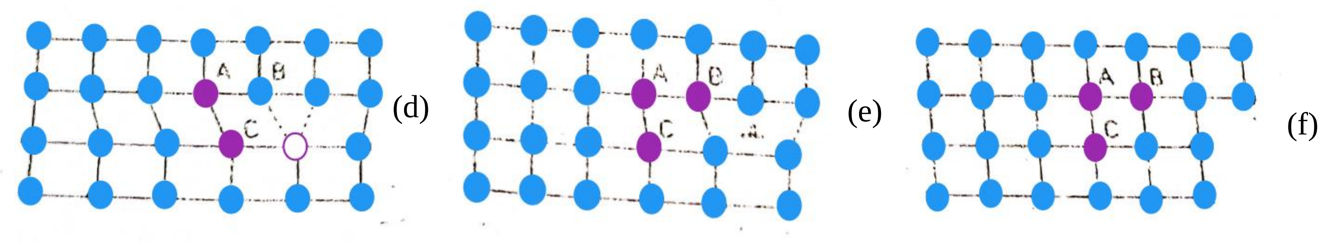
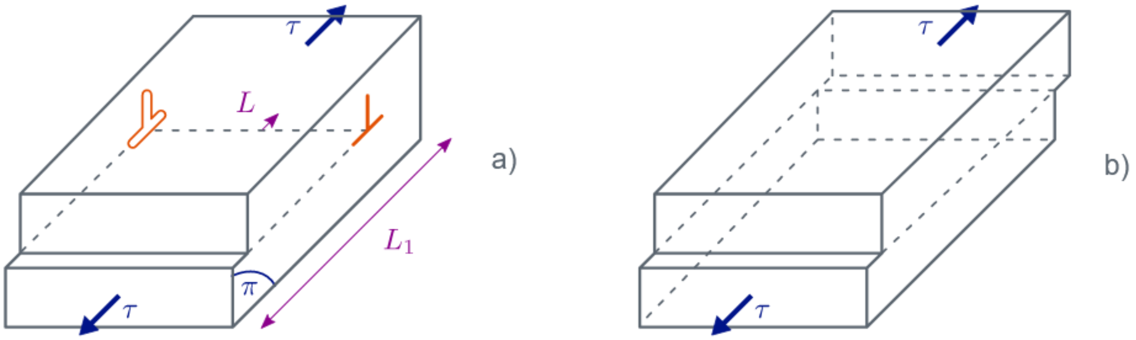


Figure 9. Movement of atoms involved in the displacement of a dislocation -coin under the effect of the stress τ

Figures 9 show the movement of a coin dislocation through a crystal subjected to stresses indicated by τ. Note the limited number of atoms involved as well as bonds to be broken at the same time. The dislocations move easily and without any difficulty causing at the end, a deformation of the crystal. The motion of a dislocation is always in a direction perpendicular to the dislocation line.

The presence of steps on the surface of a crystal does not give any indication as to the type of dislocation that contributed to the formation of these steps. The displacement of a corner dislocation is parallel to the direction of the applied stress. In this case, the dislocation line is parallel to the step left on the crystal surface by the emergence of the dislocation, as shown in Figure 10.



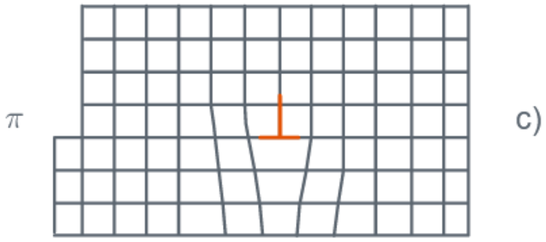


Figure 10. Direction of displacement and deformation produced by a corner dislocation

A corner dislocation can also move perpendicular to its sliding plane. This is called the dislocation rise. Unlike sliding, which is a conservative movement occurring without transport of matter, the rise in dislocations is assisted by atomic scattering phenomena. Figure 11 describes two ascending processes assisted by diffusion of interstitial atoms and gaps.

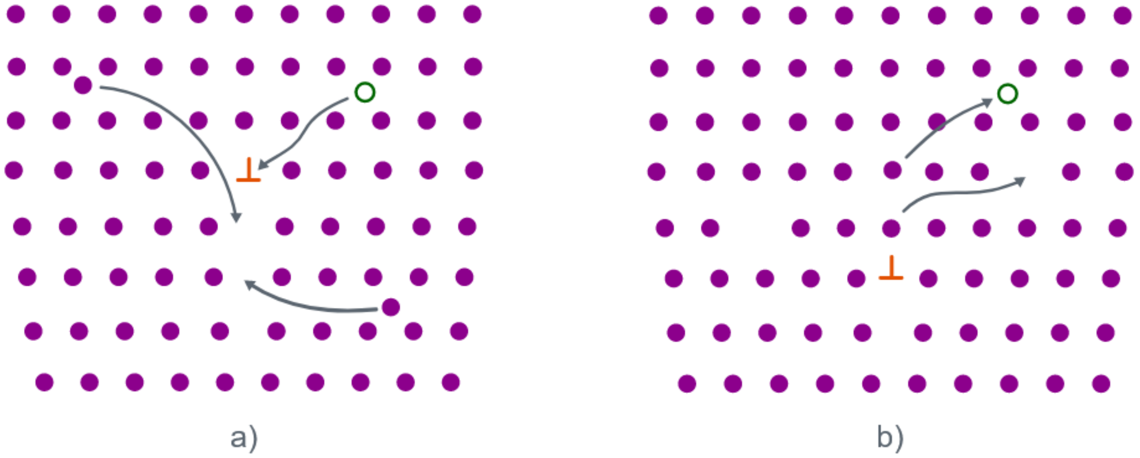


Figure 11. Rise of a dislocation by (a) addition of atom to the additional half-plane and (b) removal of atom from the additional half-plane

The transport phenomena of point defects occur more easily at high temperature than at low temperature. The rise of dislocations, unlikely at low temperature, can therefore be thermally activated. It makes it possible, in particular, to interpret the phenomena of creep under high stress. It is noted that the final deformation is the same as in the case of the corner deformation, but the dislocation line is here perpendicular to the step left on the surface (see Figure 12). Note that the dislocations vis are not subject to upward movement. Under certain conditions, to avoid obstacles, the dislocations vis can change their sliding plane. This is called deflected sliding, which is also a thermally activated phenomenon (Figure 13).

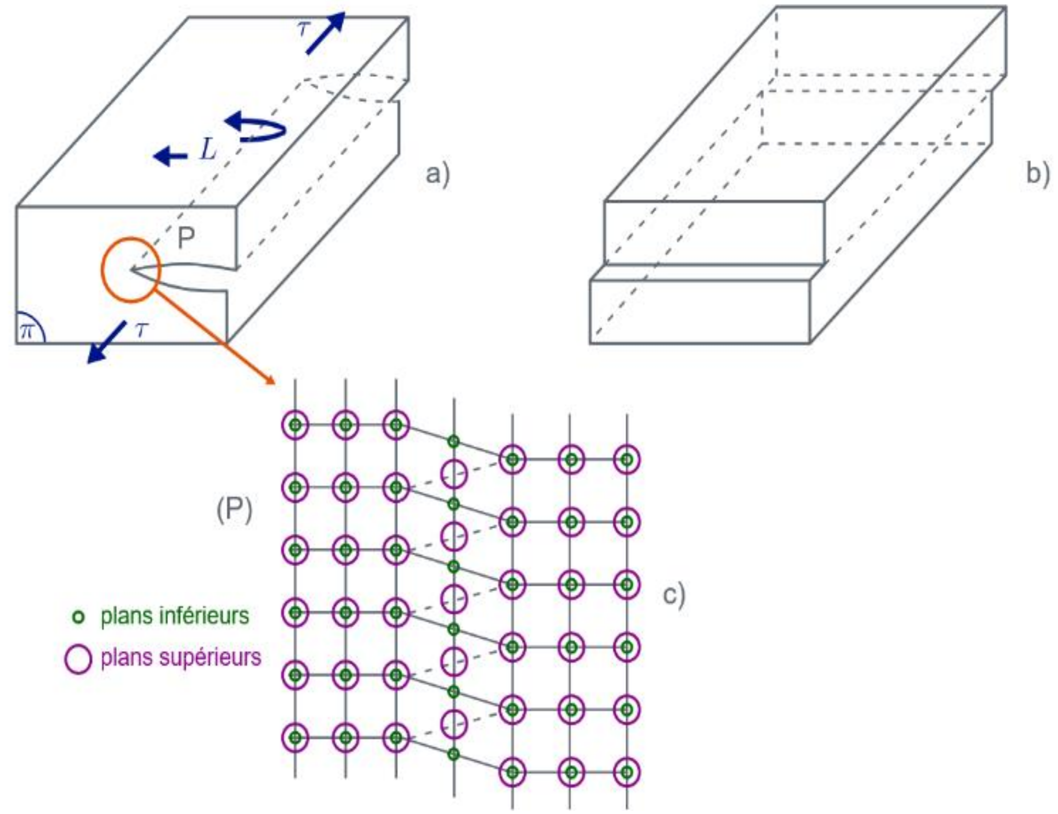


Figure 12. Direction of displacement and deformation caused by a screw dislocation

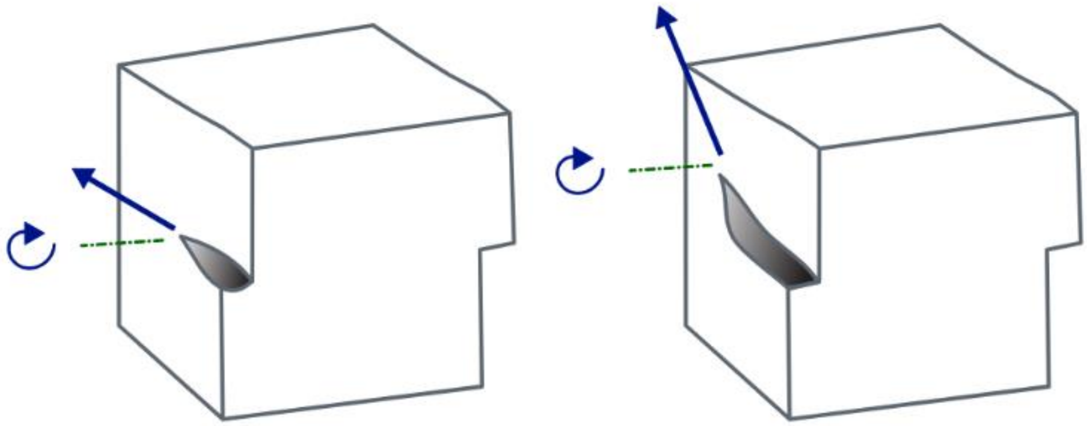


Figure 13. Deflected slide from a screw dislocation

V. Elastic properties of dislocations

When a stress is applied to a crystal, it deforms. If the crystal takes its shape when the stress is relaxed, the deformation is called elastic and is governed by Hooke's law which establishes the proportionality between stress and deformation. The coefficient of proportionality is the elastic modulus which is expressed in unit of stress since the deformation is a dimensionless quantity.

V.1. Tensile load

The stress is applied and the resultant deformation ε is the relative elongation (see Fig. ci-a On a:EE where E is the Young's module (E=200GPa) for steels,100 GPa for Cu , 10 Gpa for Pb). The elongation is accompanied by a lateral contraction rr0 where is the coefficient of Poisson.près).

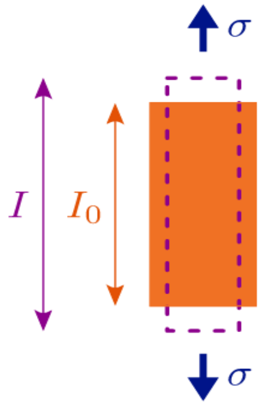


Figure. Tensile loads

V.2.Shear loading

In this case, the stress applied, called cission, is not normal but tangential parallel) to the faces on which it is exerted (see Fig.). The deformation γ is expressed in relative value by the displacement per unit of thickness, that is to say by the angle shown γ on the figure. Hooke's law is written: τ=μγ oùγ is the module of Coulomb or shear module [μ=E2(1+θ)].

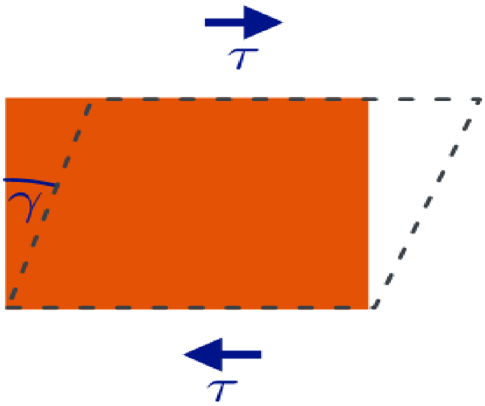


Figure 15: Shear loads

VI. The interaction between dislocations

is an important concept in materials science, particularly in the field of plastic deformation of crystalline materials. Dislocations are linear crystallographic defects that play a crucial role in the mechanical behaviour of materials.

When a material is subjected to external stress, dislocations can move and interact with each other. This interaction can occur in different ways:

- **Dislocation attraction/repulsion:** Two dislocations of the same polarity (i.e., with vectors of Burgers in the same direction) can attract or repel each other depending on their mutual distance and relative orientation of their sliding planes. It also depends on the characteristics of dislocations, such as type, density and orientation.
- **Annihilation:** When two dislocations of opposite polarities (a line dislocation and an antidislocation) meet, they can cancel each other's effects. This usually occurs when the dislocations are close enough that their stress fields overlap and cancel.
- **Formation of dislocation loops:** When a dislocation loops on itself, it can form a dislocation loop. These loops can be of a varied nature, such as coiled loops, screw loops, etc. Dislocation loops can interact with each other, move along the glide planes or be absorbed by other dislocations.
- **Snapping and pinning:** The dislocations can be stopped or slowed down by various obstacles in the crystal structure, such as grain joints, precipitates, surface defects, etc. This phenomenon is called snagging or pinning of dislocations. The interaction between dislocations and these obstacles can significantly influence material strength and ductility.

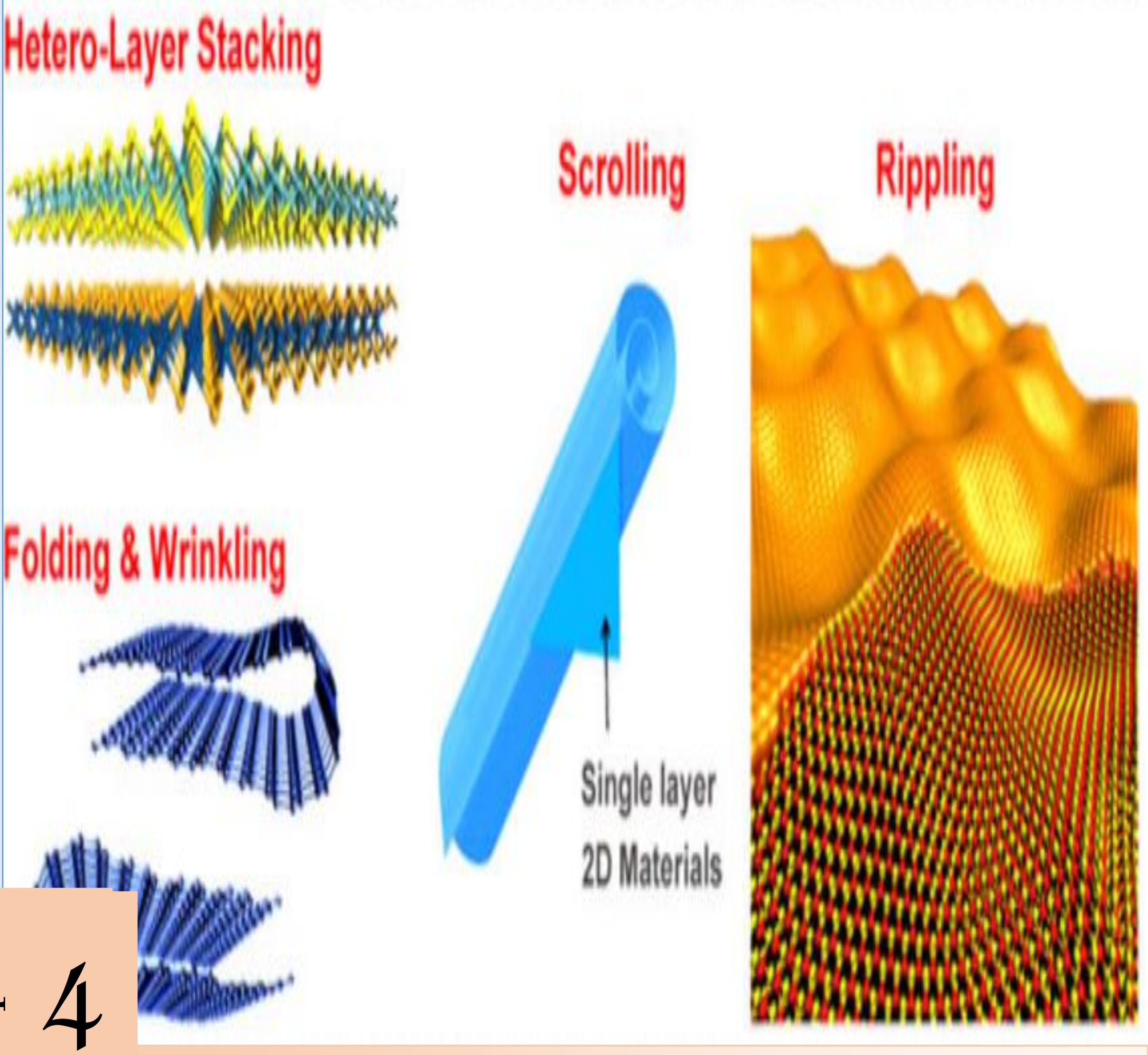
VII. Methods for observation of dislocations

Observation of dislocations is essential to understanding the structure and properties of crystalline materials. Some of the main methods for dislocation observation are:

1. **Transmission electron microscopy (TEM):** TEM is one of the most powerful techniques for observing dislocations. It uses an electron beam transmitted through a thin sample to form a high-resolution image of the crystal structure. Dislocations appear as dark lines or contrasting lines due to their interaction with the electron beam.
2. **High-resolution transmittance electron microscopy (MET-HR):** The MET-HR is a variant of the MET that allows for even higher resolution, allowing dislocations to be

observed with great precision. This technique is particularly useful for studying low-density dislocations and the details of their structure.

3. **Scanning electron microscopy (SEM)**: The SEM is used to observe the topography of a sample surface. Although dislocations are not directly visible in SEM, they can often be detected by associated surface defects such as dislocation stairs or crystal growth stages.
4. **Atomic force microscopy (AFM):** AFM is a surface microscopy technique that uses an extremely fine tip to scan the surface of the sample. Although AFM is not as commonly used as TEM or SEM for the observation of dislocations, it can be useful in studying surface defects associated with dislocations.
5. **X-ray diffraction:** X-ray diffraction is a powerful method for determining the crystal structure of a material. Dislocations can be detected by deformations in the diffraction peaks, called Debye-Scherrer peaks, which are associated with local deformations of the crystal structure.
6. **Polarized light microscopy:** Polarized light microscopy can be used to observe dislocations in transparent or translucent materials. Dislocations appear as dark lines or contrasting lines under a polarized microscope because of their effect on the polarization of light.



Chapter 4

Bidimensional Defects

Bidimensional defects, also known as planar defects, are imperfections in a crystal structure that extend over a two-dimensional plane within the material. These defects disrupt the regular arrangement of atoms along a surface or boundary, affecting the material's mechanical, electrical, and optical properties.

Types of Bidimensional Defects

1. Grain Boundaries

In general, solid matter consists of an assembly of microcrystals. At the junction of these microcrystals, small cavities form, where impurities typically accumulate. The contact surface between microcrystals constitutes the "grain boundaries." Thus, a grain boundary is the surface that separates two crystals with different orientations, as illustrated in the figure below.

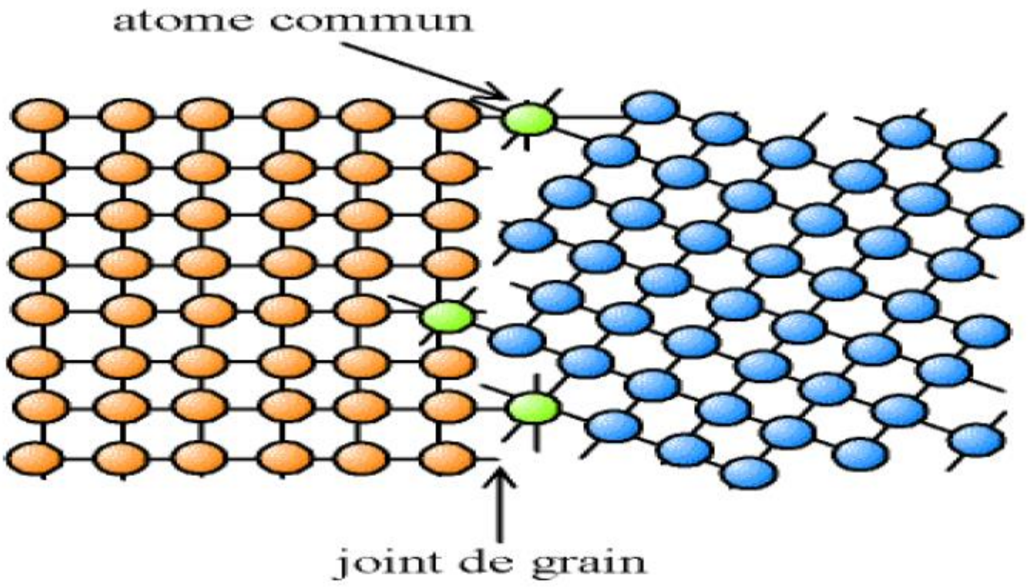


Figure: *Grain Boundaries*

2. Stacking Faults and Twins

The crystalline structure can be regarded as a regular stacking of planes following a specific pattern that repeats indefinitely. This can be characterized by a stacking sequence.

For example, in the face-centered cubic (FCC) structure, the stacking sequence of the [111] planes follows the pattern […ABCABCABC…], as illustrated in the diagram below.

A stacking fault refers to an alteration in the stacking sequence. These defects can be classified as follows:

- **Intrinsic** (see figure below): This occurs when a plane is missing, resulting in a stacking sequence of the type […ABCACABC…].

Intrinsic defects can also occur if the "upper" part of the crystal is displaced relative to the "lower" part by a/6[111], thereby shifting the B plane into position C.

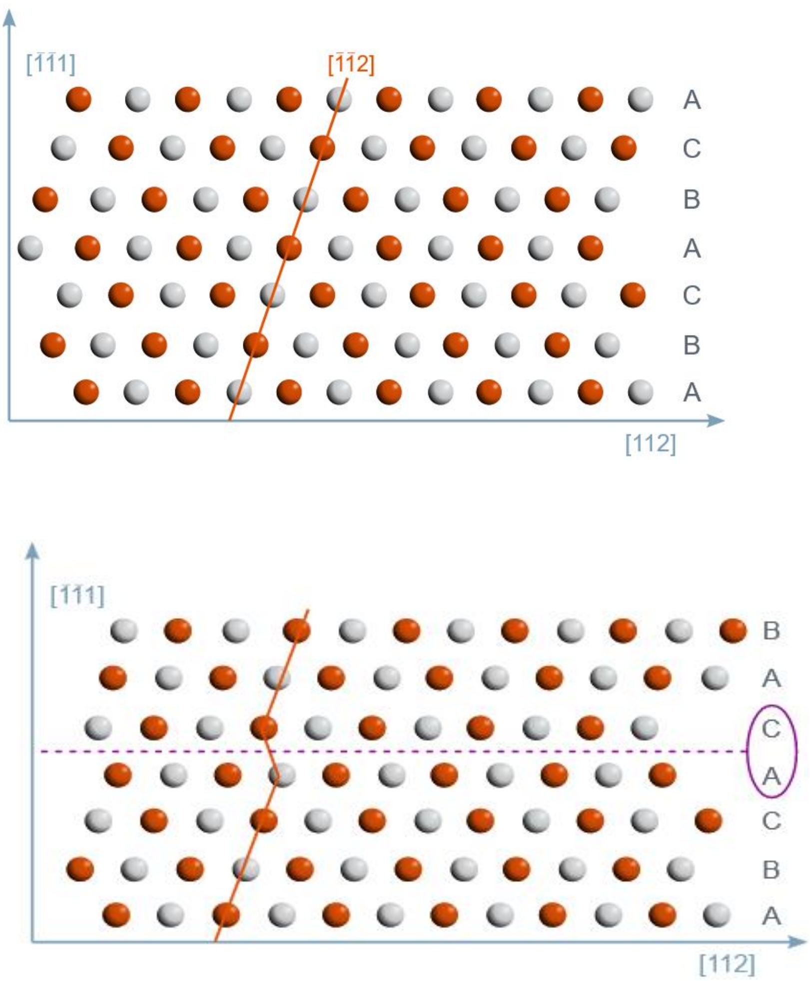


Figure: *Intrinsic Stacking Fault in the Structure FCC*

Extrinsic: This occurs when an additional plane is introduced, resulting in a stacking sequence of the type […ABCACBABC…].

Extrinsic defects can also occur if the "upper" part of the crystal is displaced relative to the "lower" part by a/6[111], shifting the C plane into position A, and if the "lower" part is displaced relative to the "upper" part by a/6[111], moving the A plane into position C.

The defect of stacking does not cross the whole crystal, it is then bordered by one (or two) dislocation(s) whose Burgers vector is not a translation of the network but is of type a/(6[111]) . Such partial dislocation is called Shockley dislocation (see Fig. below).

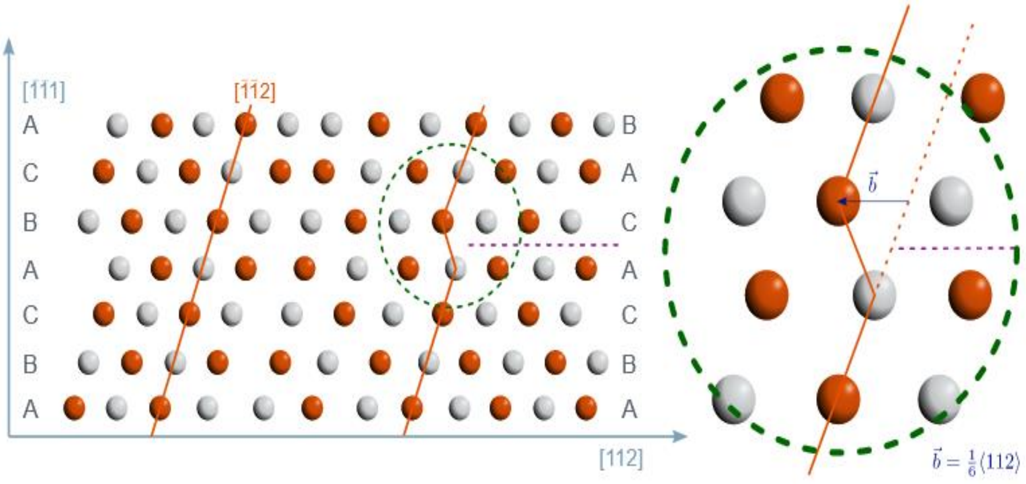


Figure: *Shockley Dislocation*

The stacking sequence may also locally transform into a symmetric structure, such as […CBACBACBA…], during processes like solidification or recrystallization. The resulting sequence is […ABCABCACBACBA…]. The stacking fault caused by this sequence alteration is known as a twin, and the corresponding plane is called a twinning plane (see figure).

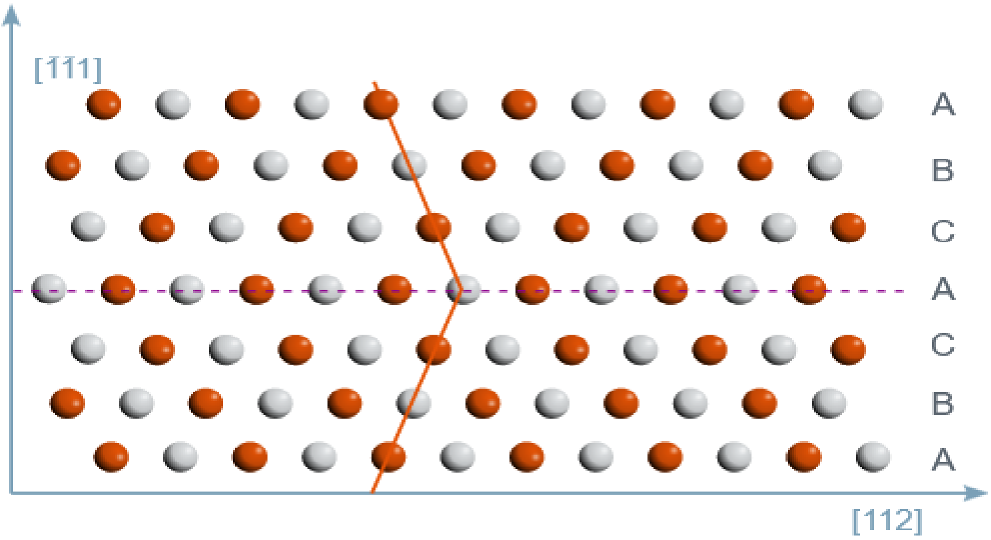
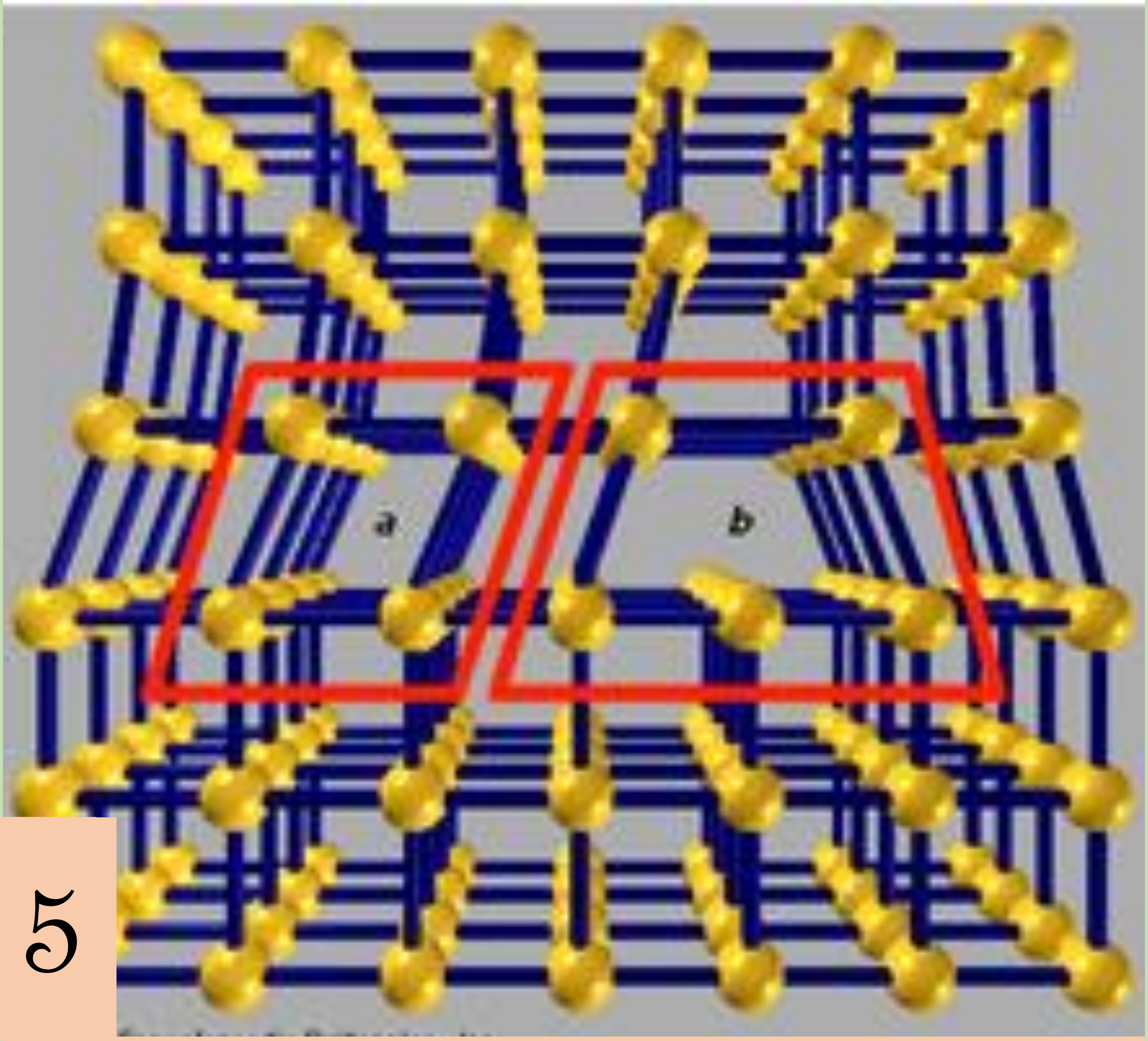


Figure: Schematic Representation of a Twin in the FCC Lattice



Chapter 5

Three-Dimensional Defects

Three-dimensional (3D) defects, also known as volumetric defects, are imperfections in a crystal structure that extend in all three spatial dimensions. These defects disrupt the periodic arrangement of atoms within a material and can significantly impact its mechanical, electrical, and optical properties.

Classification of Three-Dimensional Defects in Materials

Three-dimensional (3D) defects in materials significantly impact their mechanical, electrical, and thermal properties. These defects include **precipitates, voids and pores, inclusions, and grain boundaries.** Below is an explanation of each type with relevant figures.

e. Precipitates (Coherent and Incoherent)

Precipitates, also known as volumetric defects, are second-phase particles formed by the combination of metal atoms with alloying element atoms.

Inclusions are impurities that typically originate during the solidification process of the sample from its liquid state. They are generally composed of sulfides, oxides, or silicates.

The diagram below schematically illustrates two categories of precipitates. Coherent precipitates maintain crystallographic continuity with the matrix—the crystal lattices of the matrix and the precipitate are similar, although their lattice parameters may differ, causing elastic distortion in the matrix. Incoherent precipitates, on the other hand, have no crystallographic relationship with the matrix. Inclusions are always incoherent. Lastly, semi-coherent precipitates exhibit coherence with the matrix only along certain planes.

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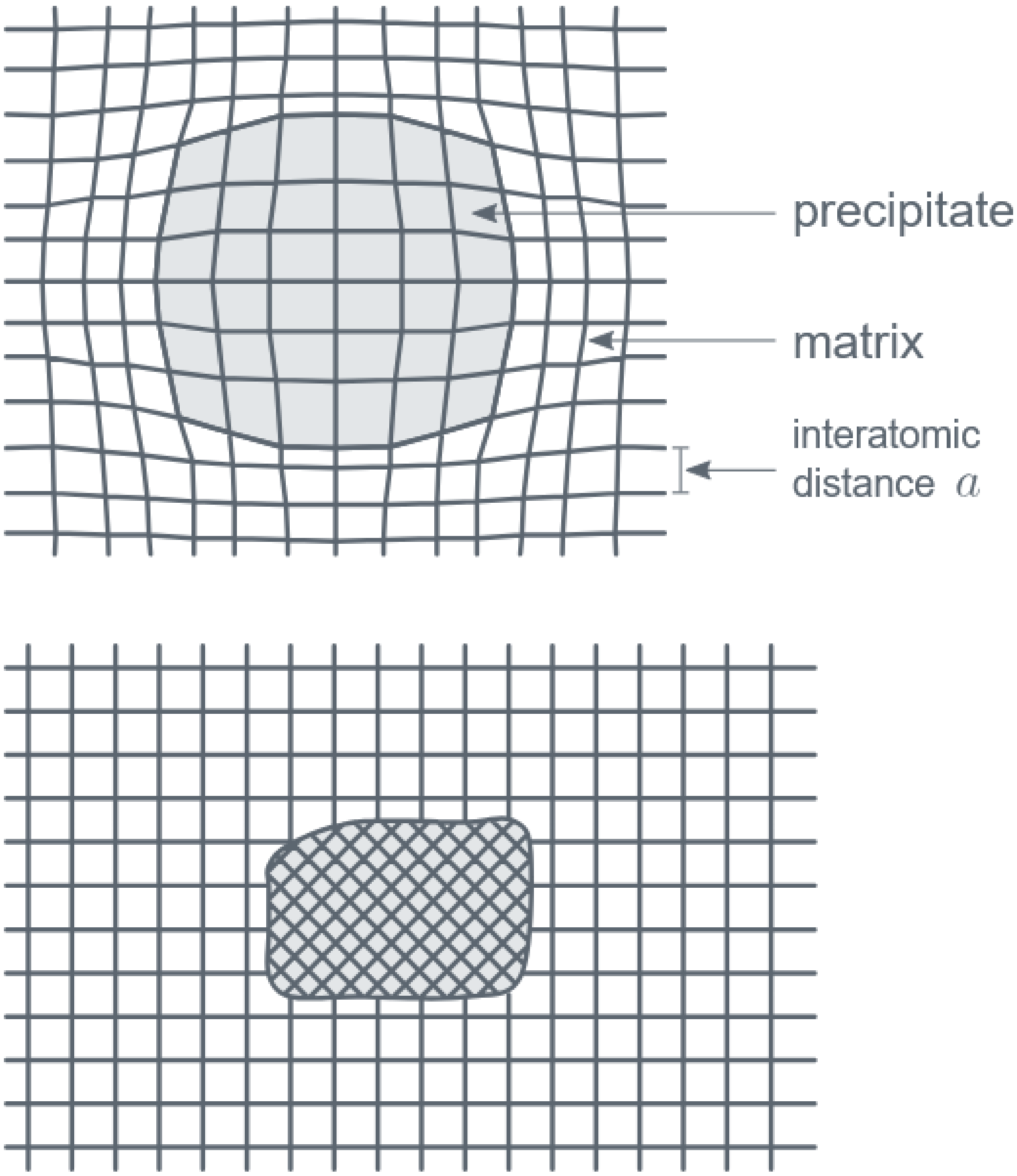


Figure. Different types of precipitates: coherent and incoherent

f. Voids and Pores

Voids and pores are empty spaces in a material, either due to **manufacturing defects, gas entrapment, or radiation damage**

3. Inclusions

Inclusions are **foreign particles** (oxides, sulfides, or carbides) trapped inside a material during manufacturing.

4. Grain Boundaries

Grain boundaries are **interfaces between individual crystallites (grains)** in a polycrystalline material.

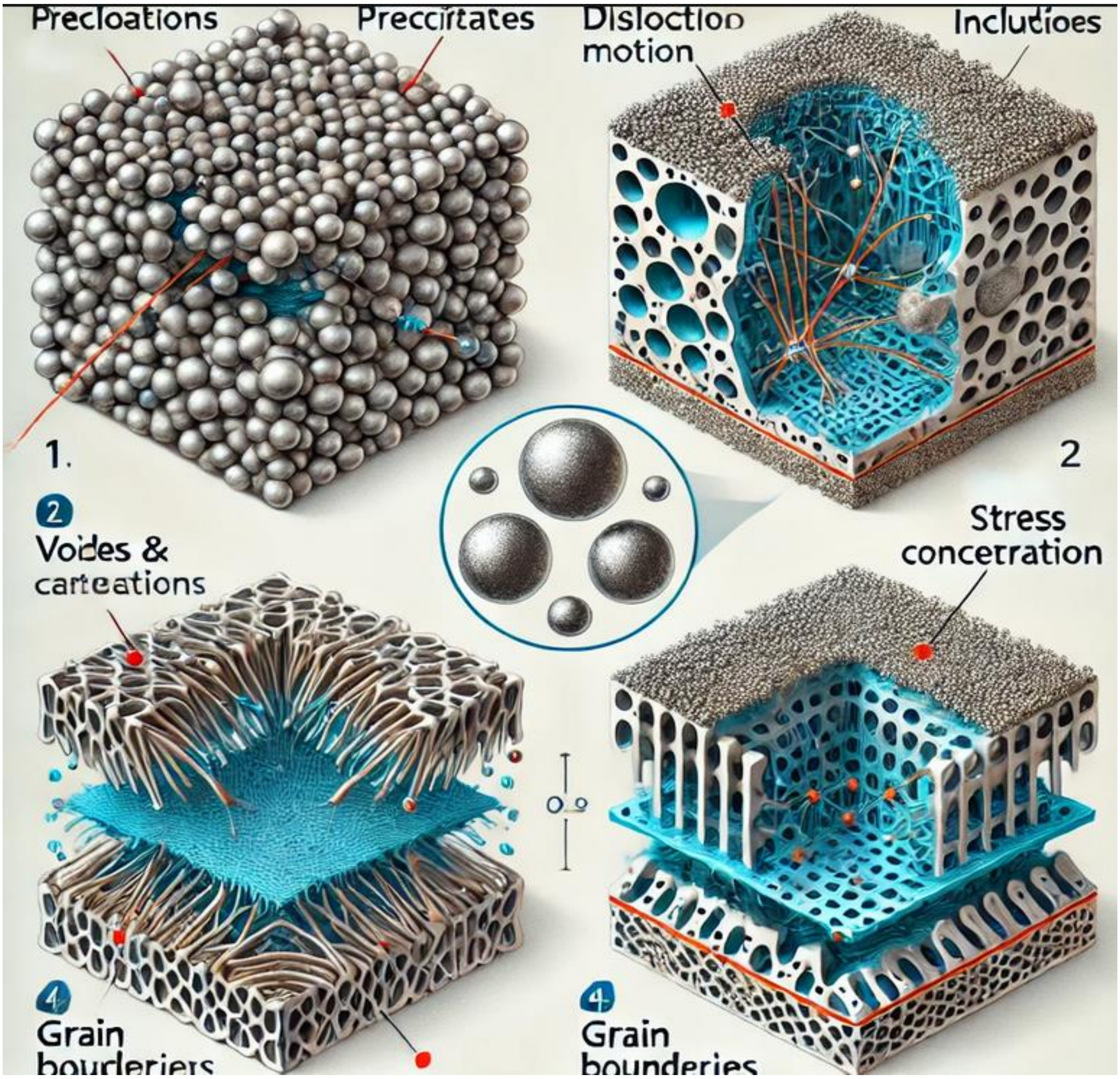
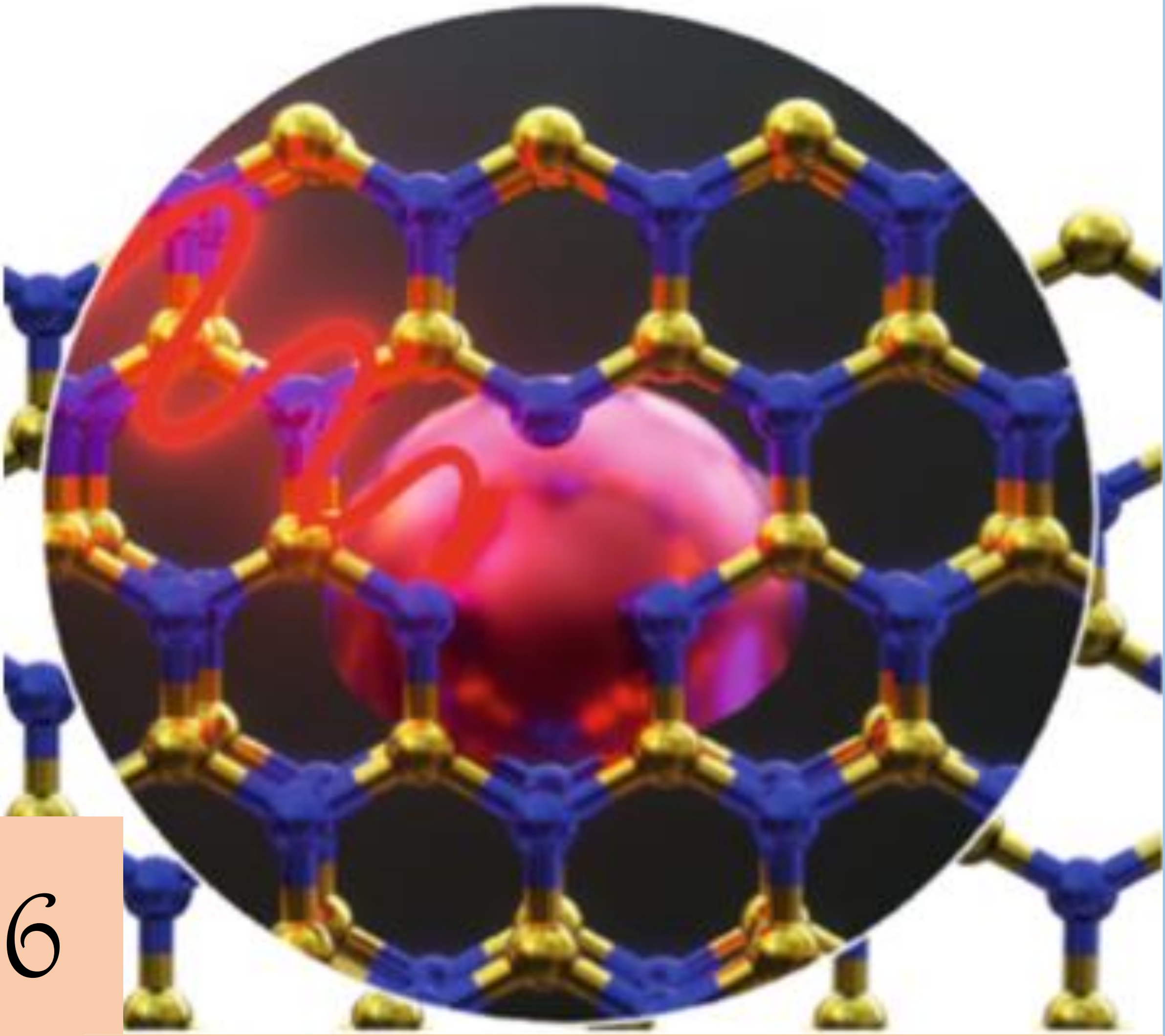


Figure 5.2. scientific diagram illustrating the four types of three-dimensional material defects: **Precipitates, Voids and Pores, Inclusions, and Grain Boundaries.**



Chapter 6

Factors Influencing the Electrical Conductivity and Hardness of a Material

V. Electrical Conductivity

Electrical conductivity is an essential property of materials that determines how well they can conduct electricity. The ability to conduct electricity depends on several factors, including the nature of the material, temperature, and the presence of impurities. Understanding these factors is critical for designing and optimizing electrical systems and devices. In this section, we will discuss the factors that affect electrical conductivity and how they influence the flow of current through a material

VI. Law of Electrical Conductivity:

The Nernst-Einstein equation provides an accurate calculation of the electrical conductivity of a material, whether in liquid or solid form. The formula for electrical conductivity is given by:

$$\sigma = \frac{Dz^2e^2}{kT}$$

To estimate electrical conductivity, it is necessary to gather information on:

- D : The diffusion coefficient of the material

- z : The number of charges carried by the material

- e : The elementary charge

- c : The concentration of the material

- k : The Boltzmann constant (approximately 1.3806×10^{-23} $J \cdot K^{-1}$)

- T : The absolute temperature

VII. Factors Affecting Electrical Conductivity

Several factors influence the electrical conductivity of a material. These include in this figure:

1. **Nature of the Material**

The electrical conductivity of a material depends on its atomic structure and the number of free electrons it has. Metals, for example, are excellent conductors of electricity because they have a high number of free electrons that can move freely through the lattice structure. Non-metals, on the other hand, have a lower number of free electrons and are poor conductors of electricity.

2. **Temperature**

The conductivity of a material changes with temperature. In general, the conductivity of metals decreases with temperature, while that of semiconductors and insulators increases. This is because the increase in temperature causes the atoms to vibrate more, which disturbs the movement of electrons, reducing their ability to move freely.

3. **Presence of Impurities**

The presence of impurities in a material can significantly affect its conductivity. Impurities can create localized regions with high or low electron density, which can either enhance or hinder the flow of current. For example, adding impurities like boron or phosphorus to silicon can create regions with excess or fewer electrons, respectively, making it an excellent material for making electronic devices like transistors and diodes.

4. **Crystal Structure**

The crystal structure of a material can also influence its conductivity. Materials with highly ordered crystal structures, like diamonds, are poor conductors of electricity because they lack free electrons. In contrast, materials with disordered crystal structures, like amorphous silicon, can be good conductors of electricity because they have a high number of free electrons.

Electrical conductivity is a complex property that depends on several factors. Understanding these factors is essential for designing and optimizing electrical systems and devices. By controlling these factors, we can develop materials with unique electrical properties suitable for specific applications.

VIII. Factors Influencing the Conductivity of a Material

1. The nature of the material: Some materials are better conductors than others, with metals being a prime example.
2. The temperature of the material: As the temperature decreases, the conductivity increases.

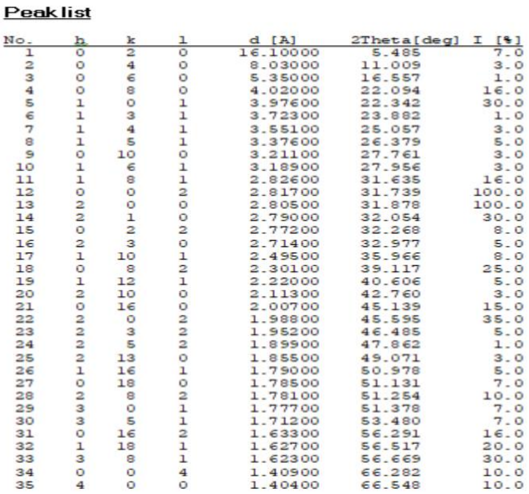
   Explanation: The hotter the wire or component, the more energy its molecules have, allowing them to resist the flow of current more effectively. This increased resistance leads to a decrease in conductivity..
3. The diameter of the material: A wire with a larger diameter has better conductivity than a wire with a smaller diameter. However, it is important not to confuse this with wire gauge, as a higher gauge number corresponds to a smaller wire diameter.
4. The length of the material: Electrons travel more easily through a shorter component. Therefore, as the length increases, the conductivity of the component decreases

Summary Table

3D Defect	Cause	Effect on Properties
Precipitates	Phase separation, supersaturation	Strengthening, but possible brittleness
Voids & Pores	Casting, radiation, fatigue	Reduced density, stress concentration
Inclusions	Impurities from manufacturing	Crack initiation, brittle failure
Grain Boundaries	Crystallographic misalignment	Affects strength, conductivity, and creep resistance

Applications

Exercise n°1: Determine based on the following results



Peak list

```
No.    h    k    l       d [A]      2Theta[deg]  I [%]
  1    0    2    0    16.10000        5.485       7.0
  2    0    4    0     8.03000       11.009       3.0
  3    0    6    0     5.35000       16.557       1.0
  4    0    8    0     4.02000       22.094      16.0
  5    1    0    1     3.97600       22.342      30.0
  6    1    3    1     3.72300       23.882       1.0
  7    1    4    1     3.55100       25.057       3.0
  8    1    5    1     3.37600       26.379       5.0
  9    0   10    0     3.21100       27.761       3.0
 10    1    6    1     3.18900       27.956       3.0
 11    1    8    1     2.82600       31.635      16.0
 12    0    0    2     2.81700       31.739     100.0
 13    2    0    0     2.80500       31.878     100.0
 14    2    1    0     2.79000       32.054      30.0
 15    0    2    2     2.77200       32.268       8.0
 16    2    3    0     2.71400       32.977       5.0
 17    1   10    1     2.49500       35.966       8.0
 18    0    8    2     2.30100       39.117      25.0
 19    1   12    1     2.22000       40.606       5.0
 20    2   10    0     2.11300       42.760       3.0
 21    0   16    0     2.00700       45.139      15.0
 22    2    0    2     1.98800       45.595      35.0
 23    2    3    2     1.95200       46.485       5.0
 24    2    5    2     1.89900       47.862       1.0
 25    2   13    0     1.85500       49.071       3.0
 26    1   16    1     1.79000       50.978       5.0
 27    0   18    0     1.78500       51.131       7.0
 28    2    8    2     1.78100       51.254      10.0
 29    3    0    1     1.77700       51.378       7.0
 30    3    5    1     1.71200       53.480       7.0
 31    0   16    2     1.63300       56.291      16.0
 32    1   18    1     1.62700       56.517      20.0
 33    3    8    1     1.62300       56.669      30.0
 34    0    0    4     1.40900       66.282      10.0
 35    4    0    0     1.40400       66.548      10.0
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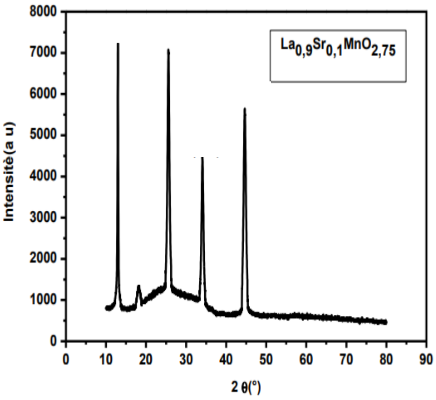
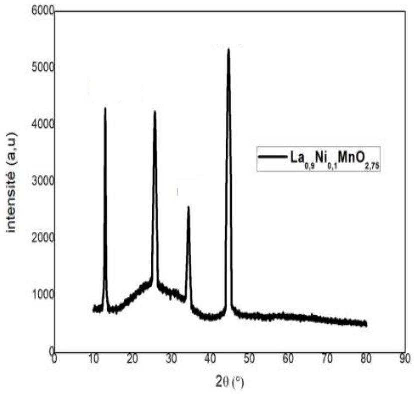
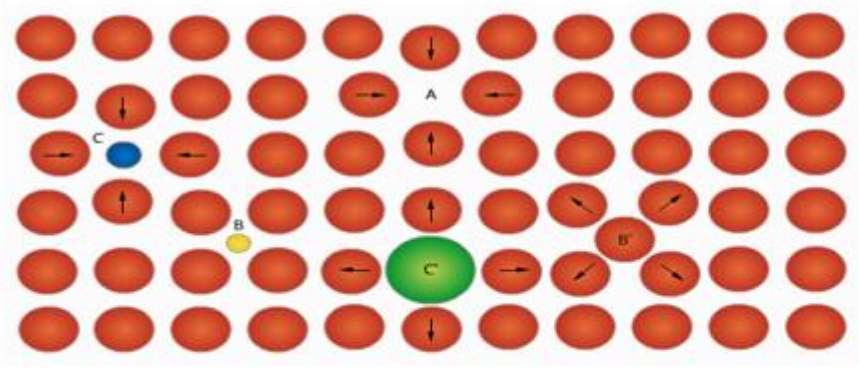
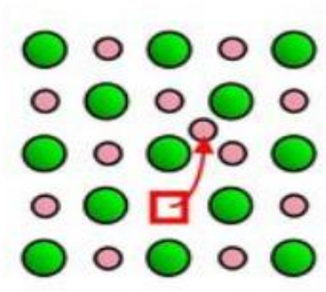


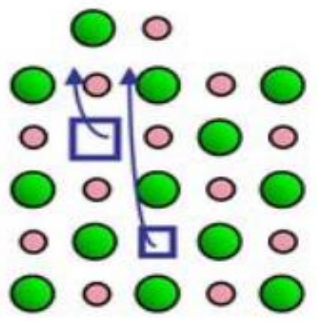


1. La distance inter-réticulaire d_{hkl} sachant que la structure est orthorhombique
2. Les paramètres des mailles a, b et c.
3. La taille des grains
4. Le coefficient de Texture
5. Le coefficient de stress
6. La densité de dislocation.

Exercise n°2 : Identify the types of defects present in the following slices of a metal crystal:







Exercise n°2 :

Find the number of gaps in $1m^3$ of Cu at 100°C.

Exercise n°3 :

During the crystallization of NaCl, there is formation of a cubic structure. Taking the molecular weight of NaCl equal to 58.46 and the density equal to $2.167 g/cm^3$, calculate the interatomic distance (distance between two neighbouring atoms).

Exercise n°4 :

An ionic crystal with the chemical formula AB_2 is considered. This crystal contains gap defects. The A^+ and B^{2-} ions have ion radiations of 100 pm and 200 pm respectively.

- Calculate the gap density if the ion concentration B^{2-} is 4.0×10^{20} $ions/cm^3$ and the temperature is 1000 K.
- What is the energy of forming a gap?
- Calculate the fraction of A sites occupied by gaps if the gap concentration is $5.0 \times 10^{16}/cm^3$.

Exercise n°5 :

A germanium crystal is doped with phosphorus to produce a carrier concentration $n = 10^{16}$ cm^{-3}. Knowing that the atomic density of germanium is 4.42×10^{22} cm^{-3} and the atomic mass of germanium is 72.6 g/mol, calculate the fraction of sites of germanium occupied by phosphorus atoms.

Exercise n°6 :

A sodium chloride crystal contains a Schottky defect concentration of 1.2 x 10^{19} cm^{-3} at 500 K. Since the formation energy of each Schottky defect is 2.5 eV, calculate the density of Schottky defects in the crystal.

Exercise n°7 :

A silver crystal contains a Frenkel defect concentration of 1.5 x 10^{18} cm^{-3} at 500 K. Since the formation energy of each Frenkel defect is 0.7 eV, calculate the density of Frenkel defects in the crystal.

Exercise n°8 :

A sodium chloride crystal contains a Schottky defect concentration of 1.2 x 10^{19} cm^{-3} and a Frenkel defect concentration of 2.5 x 10^{18} cm^{-3} at 500 K. Knowing that the formation energy of each Schottky defect is 2,5 eV and that the formation energy of each Frenkel defect is 0.7 eV, calculate the total density of defects in the crystal.

Exam of defect properties -May 2024-

Course question: (15pts)

1/ What is the important role of gaps in the behaviour of materials at high temperatures?

A. Stabilize crystal structure
B. Decrease thermal conductivity of materials
C. Increase strength of materials
D. Facilitate the movement of crystal atoms (diffusion)

A. 2/ What kind of point defect is a gap in a crystalline structure?

A. An atom surrounded by close neighbors located in different positions
B. A substitution of atoms
C. A void left in the structure at a site normally occupied by an atom
D. An interstitial atom

3/ In ionic crystals, how are point defects created to preserve the electrical neutrality of the material?

A. By creating only anionic gaps
B. By clustering multiple defects
C. Independent of each other
D. In pairs of opposite signs

4/What type of point defect consists of an anionic gap and a cationic gap in an ionic crystal?

A. Frenkel defects

B. Interstitial ions

C. Schottky defects

5/What is the mechanism for the incomplete migration of atoms in a crystalline network?

A. Rearrangement of the crystal lattice

B. Formation of new chemical bonds

C. Change of position between atoms and gaps

D. Increase in atomic density

6/In what cases can the crystal's concentration in gaps be higher than the equilibrium concentration?

A. Addition of metallic impurities

B. Low temperature gradual heating

C. Exposure to ionizing radiation

D. Fast cooling from high temperature

7/What disturbance of the crystalline order do point defects cause?

A. On dimensions limited to a crystallographic mesh

B. In a specific crystal plane

C. On the entire crystal structure

D. At the interface of crystalline grains

8/ What are the three types of linear dislocations?

A. Straight dislocations, curved dislocations, twisted dislocations

B. Primary dislocations, secondary dislocations, tertiary dislocations

C. Single dislocations, complex dislocations, multiple dislocations

D. Corner dislocations, dislocations vis, mixed dislocations

9/ What is the coefficient of proportionality between stress and deformation in an elastic material according to Hooke's law?

A. Coefficient of Poisson

B. Elastic module

C. Young's module

D. Coulomb Module

10/ How is the vector of Burgers defined in the context of crystalline dislocations?

A. The vector of Burgers is defined as the failure to close a circuit connecting neighbouring atoms and encircling the dislocation line.

B. The vector of Burgers is defined as the force needed to move a dislocation in a crystal.

C. The Burgers vector is defined as the density of dislocations in a crystalline material.

D. The vector of Burgers is defined as the distance between two parallel crystalline planes.

11/ In which case are the vector of Burgers and the dislocation line always perpendicular?

A. Linear dislocation

B. Mixed dislocation

C. Dislocation coin
D. Dislocation vis

12/ How important are dislocations for the physical properties of crystalline materials?

A. They influence the electronic properties of semiconductors.
B. They facilitate the diffusion of atoms and trap defects around them.
C. They are obtained by sliding a part of the crystal along a plane.
D. They propagate plastic deformation and allow the metal parts to beshaped.

13/ How do dislocations affect the plastic deformation of materials?

A. They strengthen the crystal structure, making the material more rigid.
B. They cause fractures in the material when subjected to stress.
C. They facilitate the sliding of crystalline planes, thus allowing deformation without rupture.
D. They reduce material ductility by limiting its ability to deform.

14/ What method of dislocation observation uses an electron beam transmitted through a thin sample to form a high-resolution image of the crystal structure?

A. Polarized optical microscopy
B. Transmission Electron Microscopy (TEM)
C. Scanning Electron Microscopy (SEM)
D. X-ray diffraction

15/ What method is used to observe the topography of a sample surface and can be useful for studying surface defects associated with dislocations?

A. X-ray diffraction
B. Atomic force microscopy (AFM)
C. Scanning Electron Microscopy (SEM)
D. Polarized Optical Microscopy

Exercise : (5pts)

A sodium chloride crystal contains a Schottky defect concentration of 1.2 x 10^{19} cm^{-3} and a Frenkel defect concentration of 2.5 x 10^{18} cm^{-3} at 500 K. Knowing that the Schottky defect density volume is 2,27 10^{18} cm^{-3} and the Frenkel defect density is 1.38 10^{15} cm^{-3}

1. Define and illustrate the Schottky and Frenkel defect
2. Rename this defect.
3. Calculate the formation energy of each defect.

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