Lecture 3: Crystal Imperfections and Solidification of Metals and Alloys

1. Introduction

In materials science, the **atomic structure of solids** strongly influences their **mechanical, electrical, magnetic, and thermal properties**.

Perfect crystals are idealized concepts; in reality, **all crystals contain defects**, which are deviations from the perfect periodic arrangement of atoms.

Why defects matter:

- Determine **strength, hardness, and ductility**
- Affect **electrical conductivity and magnetic behavior**
- Influence **diffusion, corrosion, and fracture mechanisms**
- Crucial for **designing alloys and engineering materials**

Studying defects allows engineers to **control material behavior** for specific applications.

2. Classification of Crystal Defects (Dimensional View)

Defects are classified by **dimensionality**:

Defect Type	Dimension	Examples
Point Defects	0D	Vacancy, Interstitial, Substitutional, Frenkel, Schottky
Linear Defects	1D	Edge Dislocation, Screw Dislocation
Interfacial Defects	2D	Grain Boundaries, Twin Boundaries
Bulk Defects	3D	Pores, Cracks, Inclusions

3. Point Defects (0D)

Definition: Localized defects involving one or a few atoms.

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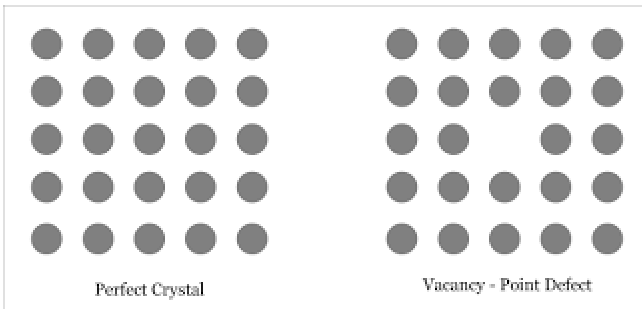
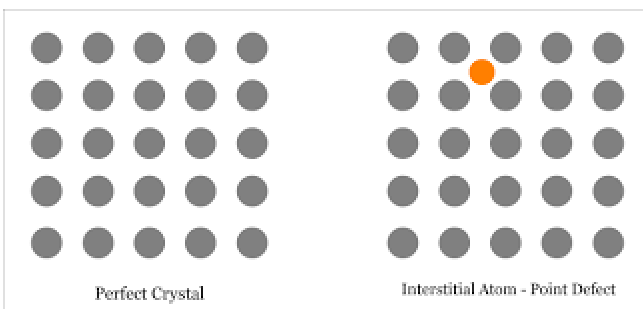
Types and Examples:

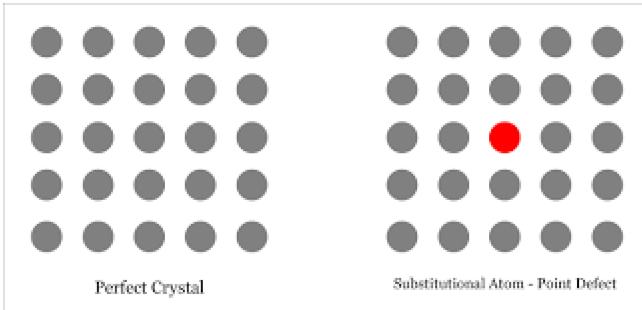
1. **Vacancy Defect**
    - Atom missing from its lattice site
    - Increases with temperature
    - *Effect:* Enhances atomic diffusion
    - *Example:* Missing copper atom in FCC copper



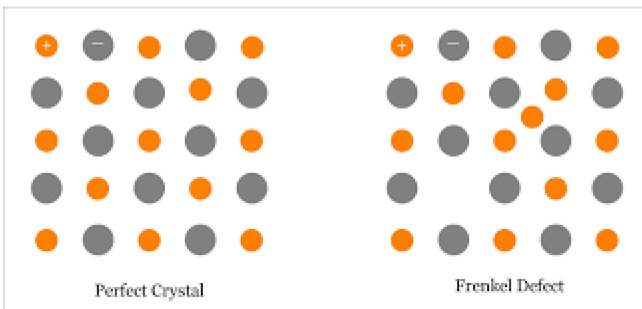
2. **Interstitial Defect**
    - Extra atom in the space between lattice atoms
    - *Effect:* Lattice distortion, increased hardness
    - *Example:* Carbon in interstitial site of iron (steel)



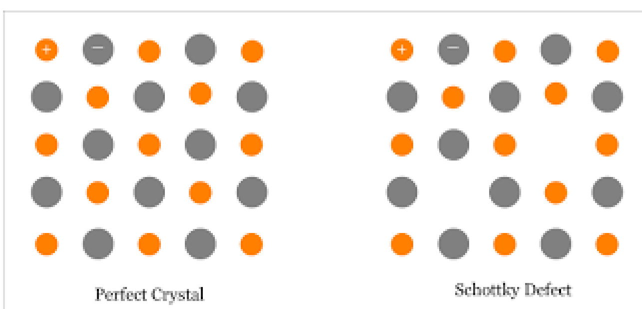
3. **Substitutional Defect**
    - Atom replaced by a different atom of similar size
    - *Effect:* Alters electrical, thermal, and mechanical properties
    - *Example:* Zinc replacing copper in brass alloy



4. **Frenkel Defect**
    - Atom moves from lattice site to interstitial position
    - *Effect:* Vacancy-interstitial pair affects ionic conductivity
    - *Example:* Silver ion in AgCl



5. **Schottky Defect**
    - Equal number of cation and anion vacancies to maintain charge neutrality
    - *Effect:* Reduces density of ionic crystals
    - *Example:* NaCl with missing Na+ and Cl− ions



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4. Linear Defects (1D) – Dislocations

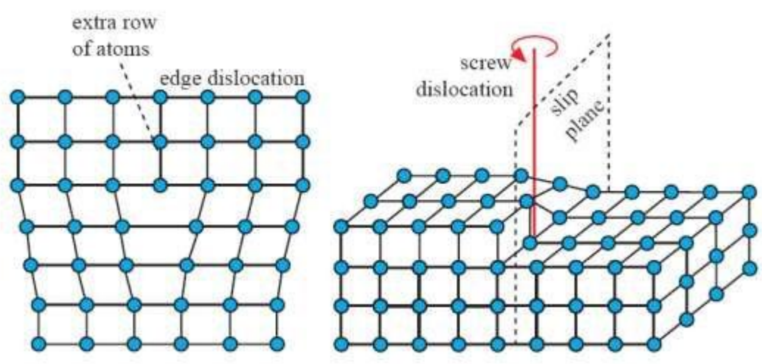
Definition: Line defects enabling **plastic deformation**.

Types:

1. **Edge Dislocation**
   - Extra half-plane of atoms inserted
   - Distorts surrounding lattice
   - *Effect:* Material deforms under stress
2. **Screw Dislocation**
   - Atoms displaced in a spiral around the dislocation line
   - *Effect:* Enables shear deformation

Importance:

- Dislocations are responsible for **plasticity** in metals
- High dislocation density → stronger but less ductile

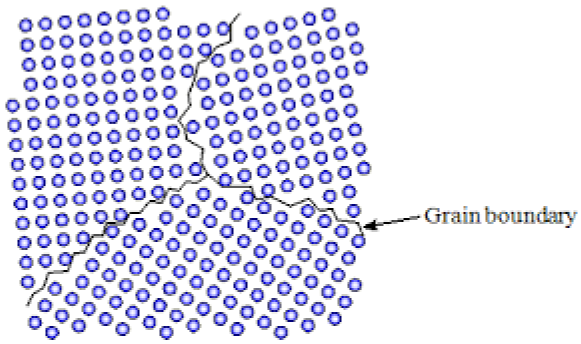


5. Interfacial Defects (2D)

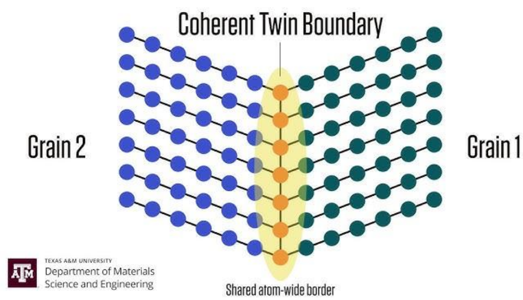
Definition: Defects along a plane separating regions.

Examples:

1. **Grain Boundaries**
   - Boundary between differently oriented grains
   - *Effect:* Blocks dislocation motion → increases strength (Hall-Petch effect)
   - *Observation:* Smaller grains → stronger material



2. **Twin Boundaries**
   - Mirror symmetry across a plane
   - *Effect:* Can strengthen material or allow plastic deformation



6. Bulk Defects (3D)

Definition: Large-volume defects that affect material integrity.

Examples:

- **Pores:** Empty regions; reduce density and strength
- **Cracks:** Stress concentrators; initiate failure
- **Inclusions:** Foreign particles; reduce toughness

7. Solidification of Metals

Definition: Transformation of **liquid metal to solid** during cooling.

Stages:

1. **Nucleation**
   - Formation of small solid particles (nuclei)
   - Homogeneous: in pure liquid
   - Heterogeneous: on impurities or mold walls
2. **Growth**
   - Atoms attach to nuclei → grains form

Result: Polycrystalline structure with distinct grains separated by grain boundaries

8. Solidification of Alloys

Alloys contain two or more elements → more complex solidification.

Types:

1. **Solid Solution Formation:** Uniform mixing of atoms
2. **Eutectic Reaction:** Liquid → two solid phases ($L \rightarrow \alpha + \beta$)
3. **Dendritic Growth:** Tree-like crystals in alloys

Cooling Rate Effects:

Cooling Rate	Grain Size	Effect
Fast	Small	Harder and stronger
Slow	Large	Softer and more ductile

9. Questions for Students

1. Define vacancy and interstitial defects with examples.
2. How do edge and screw dislocations differ?
3. How do grain boundaries affect material strength?
4. Explain nucleation and growth during solidification.
5. How does cooling rate influence alloy properties?

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10. References

1. Callister, W. D., & Rethwisch, D. G. (2018). *Materials Science and Engineering: An Introduction*, 8th Edition. Wiley.
2. Shackelford, J. F. (2015). *Introduction to Materials Science for Engineers*, 8th Edition. Pearson.
3. Smith, W. F., Hashemi, J. (2011). *Foundations of Materials Science and Engineering*, 5th Edition. McGraw-Hill.
4. Van Vlack, L. H. (1985). *Elements of Materials Science and Engineering*, 6th Edition. Addison-Wesley.