

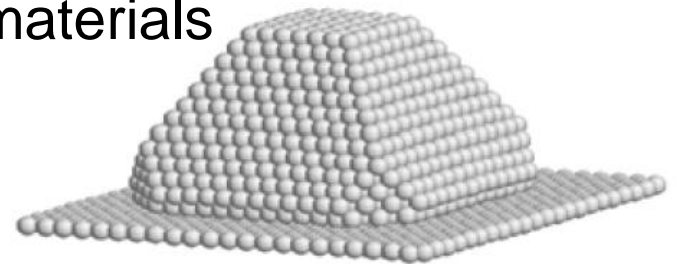


# NTNU

Norwegian University of  
Science and Technology

## **TMT4320 Nanomaterials** **August 24<sup>th</sup>, 2016**

- Unique properties of Nanomaterials



# Unique properties-Learning objectives

- Defects in nanocrystalline materials (day 2)
- Effect of grain size on physical properties (melting point, elastic constants, diffusivity, magnetic, electrical, optical and thermal properties)-(day 3)
- Effect of grain size on mechanical properties (hardness, yield strength, ductility, toughness and creep) – (day 4)
- Grain growth behaviour in nanomaterials- (day 5)

# Microstructure and defects

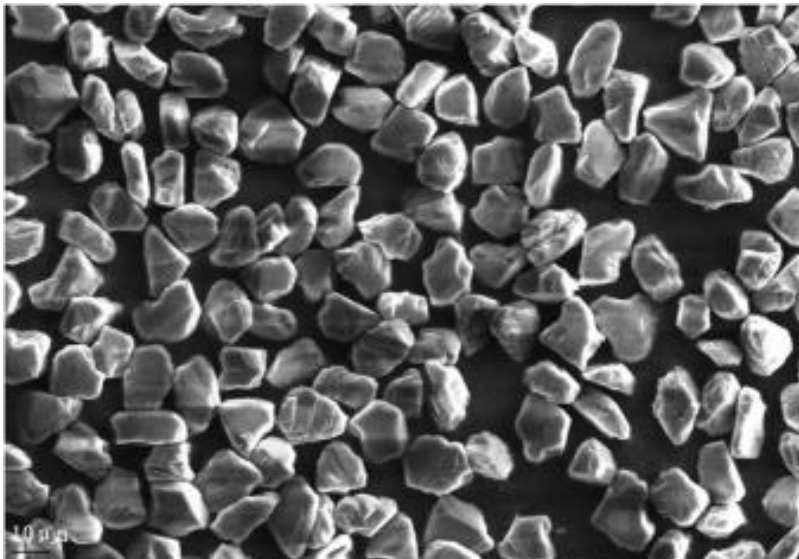
## Introduction

If we are able to arrange atoms in graphite we could make diamonds!

# Microstructure and defects

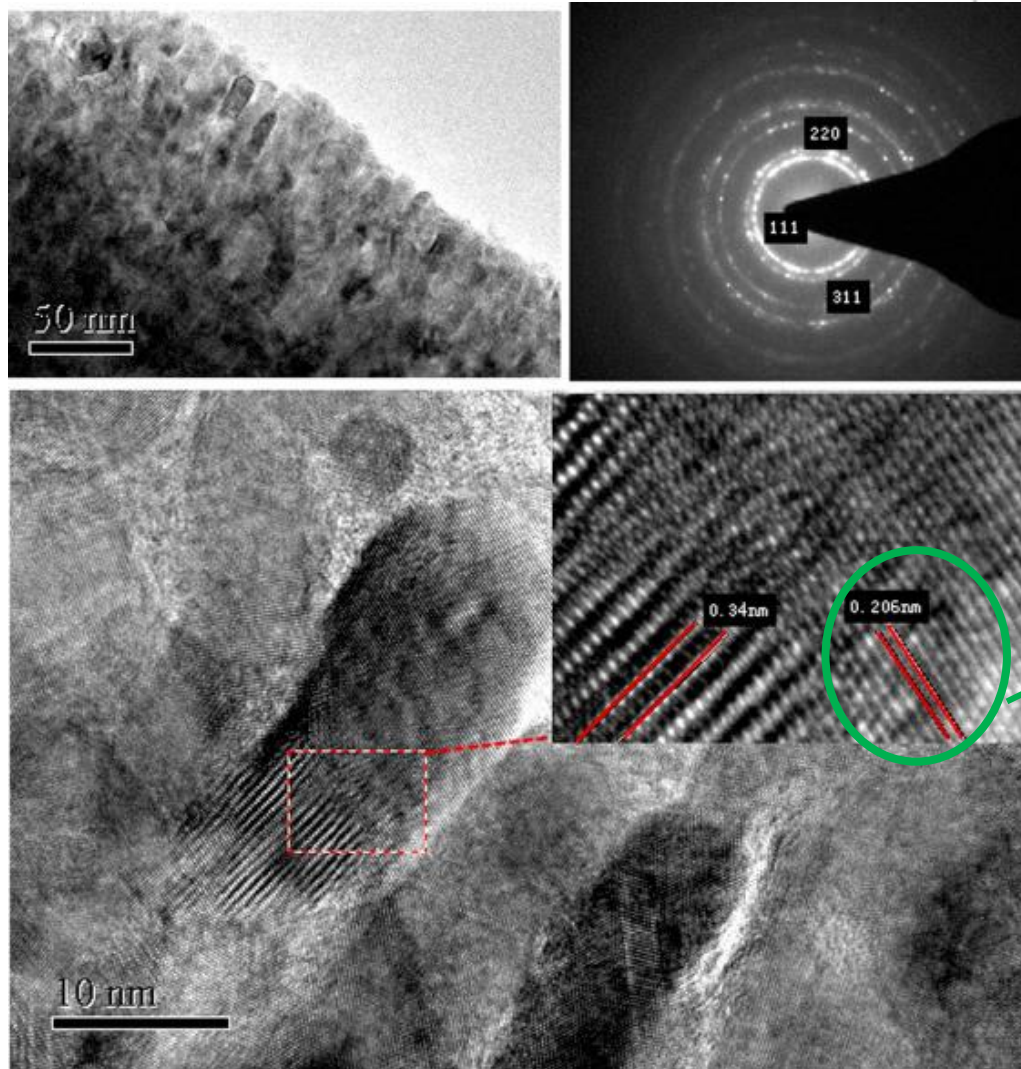
## Introduction

If we are able to arrange atoms in graphite we could make diamonds!



SEM (left) photograph of synthetic fine diamond particles.

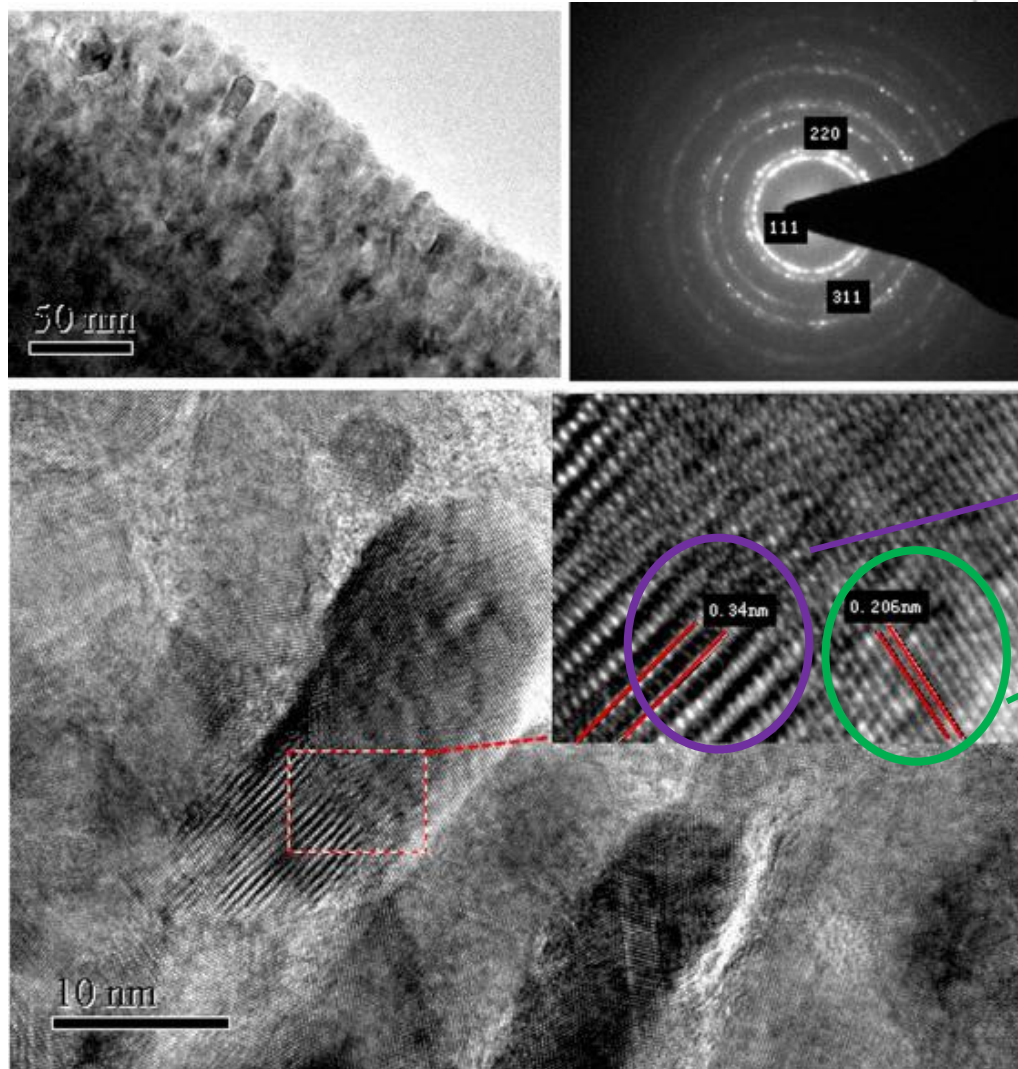
# Microstructure and defects



(111) plane of diamond.

HRTEM image of synthetic fine diamond particles.

# Microstructure and defects



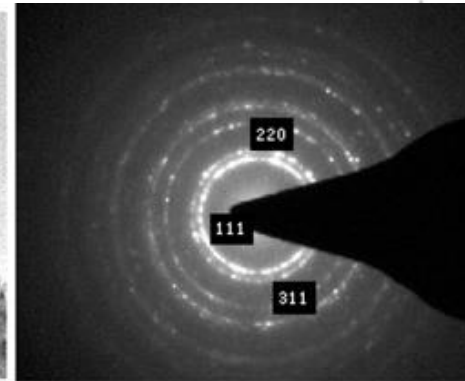
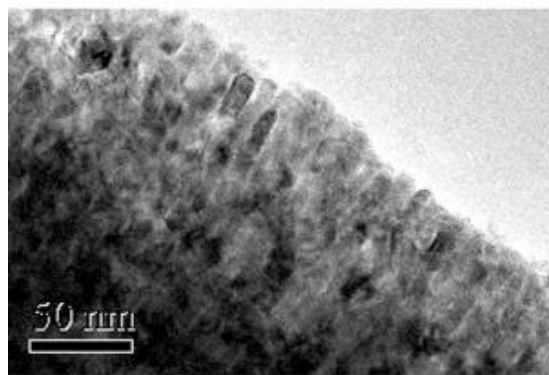
(002) planes  
of graphite.

(111) plane  
of diamond.

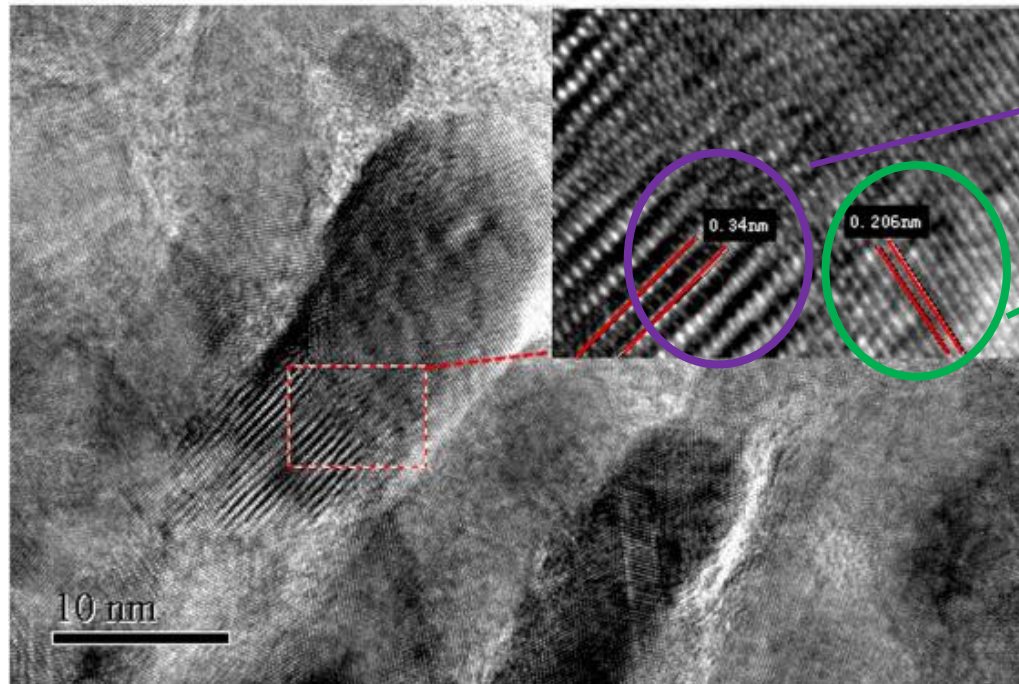
HRTEM image of synthetic fine diamond particles.



# Microstructure and defects



SAED  
image



(002) planes  
of graphite.

(111) plane  
of diamond.

HRTEM image of synthetic fine diamond particles.

# Microstructure and defects

## Introduction

Important to understand relationship between structure and properties.

Microstructural features in nanomaterials include:

- Grain size, distribution and morphology.
- The nature of grain boundaries and interphase interfaces.
- Nature of intragrain defects
- Composition profiles across grains and interfaces
- Residual impurities from processing.



# Microstructure and defects

## Defects in Crystalline materials

What is a crystal?

What is a defect?

How are defects classified?

# Microstructure and defects

## Defects in Crystalline materials

What is a crystal?

- Crystals are three-dimensional, periodic arrangements of atoms/molecules in space

What is a defect?

- Defects are any imperfection that lead to a disruption of this periodicity.

How are defects classified?

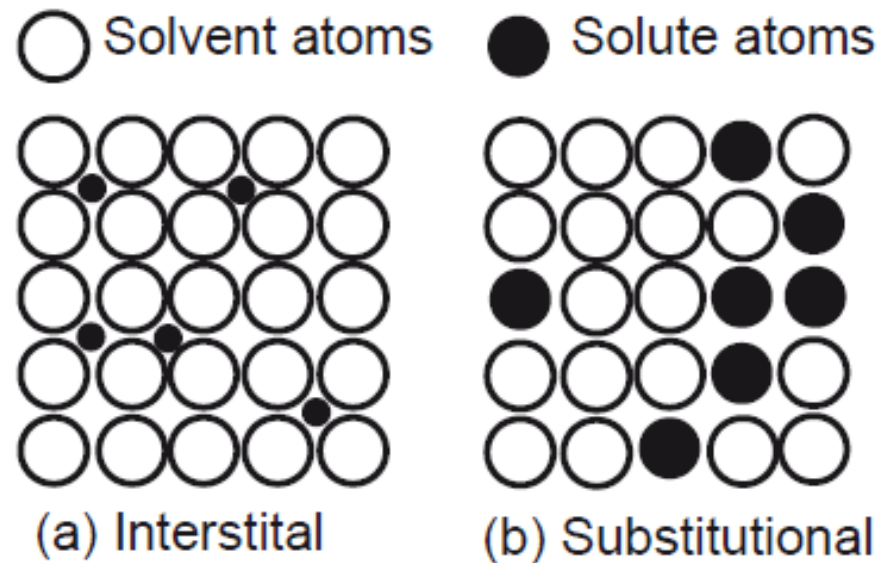
- Point defects (0D)
- Line defects (1D)
- Surface defects (2D)
- Volume defects (3D)

# Microstructure and defects

## Defects in Crystalline materials

How are defects classified?

- Point defects (0D)
  - Metal and alloys → Vacancies, substitutional and interstitial



Common point defects

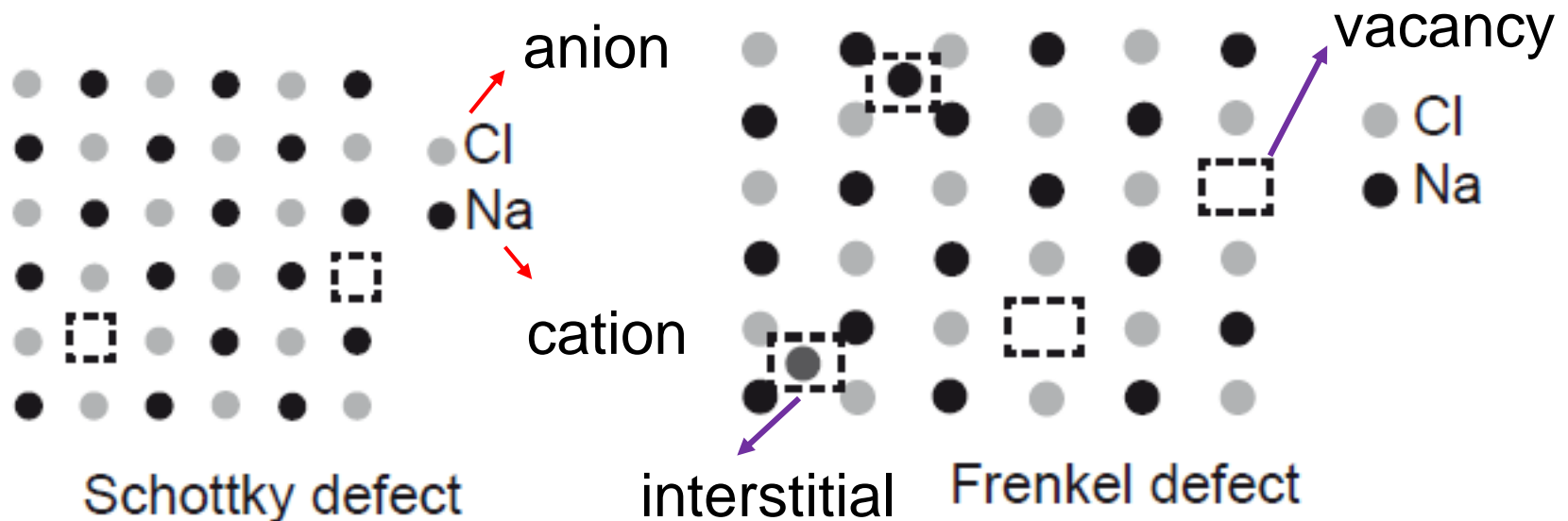
# Microstructure and defects

## Defects in Crystalline materials

How are defects classified?

– Point defects (0D)

- Metal and alloys → Vacancies, substitutional and interstitial
- Ionic solids → **Schottky** (anion-cation vacancy pairs) and **Frenkel** (vacancy-interstitial pairs) defects

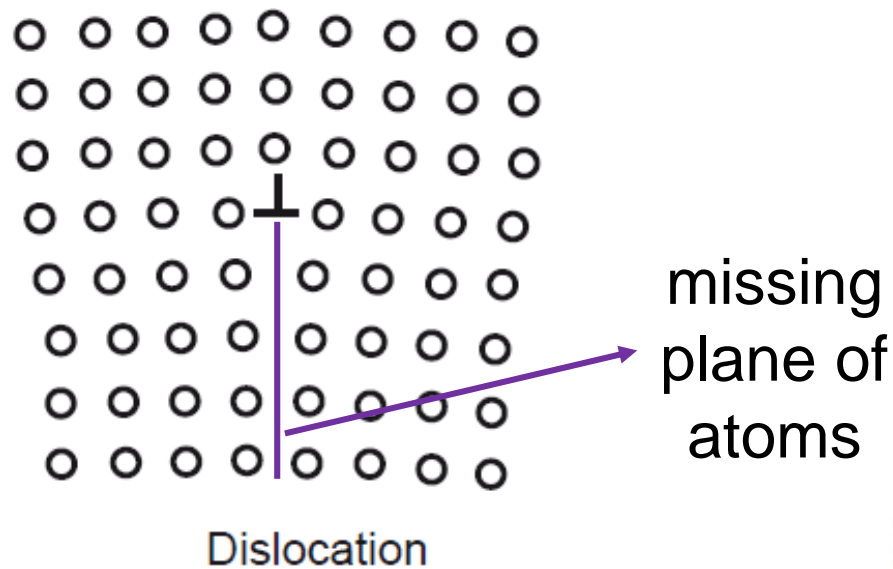


# Microstructure and defects

## Defects in Crystalline materials

How are defects classified?

- Point defects (0D)
- Line defects (1D)
  - Dislocations: missing plane of atoms



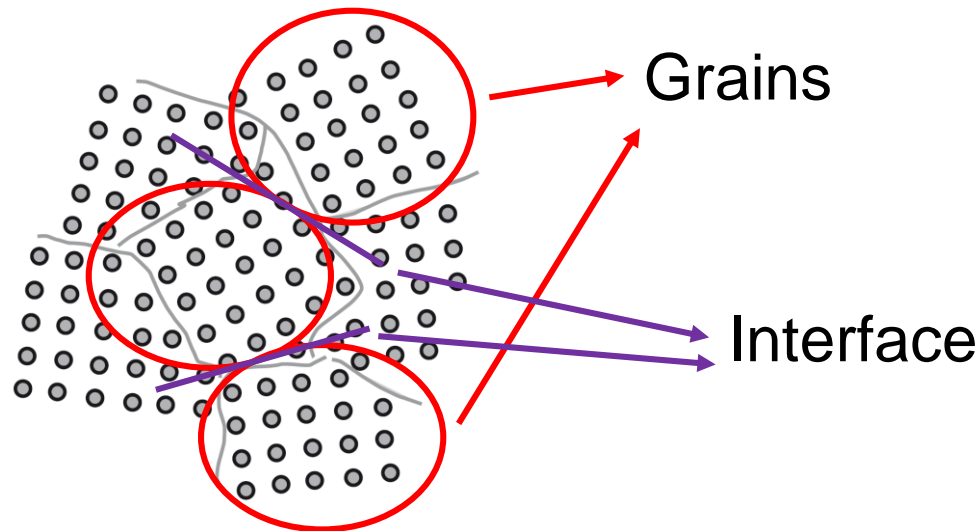


# Microstructure and defects

## Defects in Crystalline materials

How are defects classified?

- Point defects (0D)
- Line defects (1D)
- Surface defects (2D)
  - Grain boundaries, twins and stacking faults



Grain boundaries

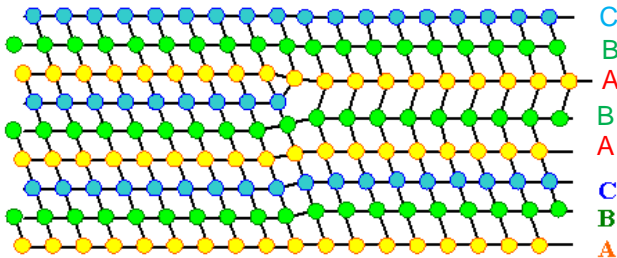
**Grain boundary**  
**(GB)**: the interface  
between two grains,  
or crystallites, in a  
polycrystalline  
material

# Microstructure and defects

## Defects in Crystalline materials

How are defects classified?

- Point defects (0D)
- Line defects (1D)
- Surface defects (2D)
  - Grain boundaries, twins and stacking faults



Stacking faults

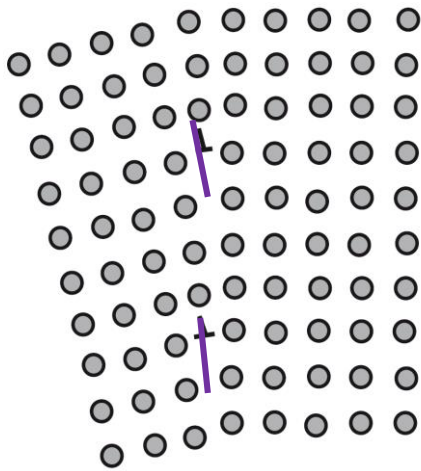
**Stacking fault:**  
Incorrect stacking  
of crystal planes  
associated with  
the presence of  
partial dislocations

# Microstructure and defects

## Defects in Crystalline materials

### How are defects classified?

- Point defects (0D)
- Line defects (1D)
- Surface defects (2D)
  - Grain boundaries, twins and stacking faults



Twin boundary

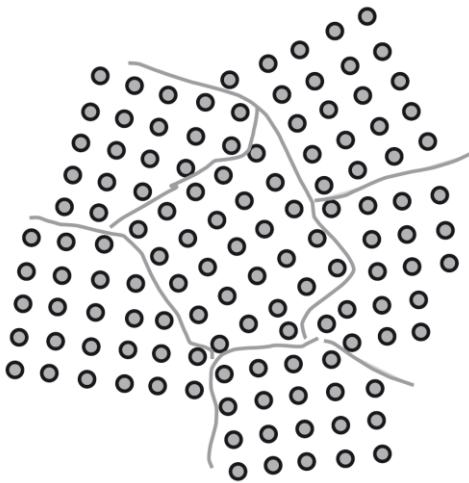
**Twin boundary:** A  
slight  
misorientation that  
exists between  
two crystals

# Microstructure and defects

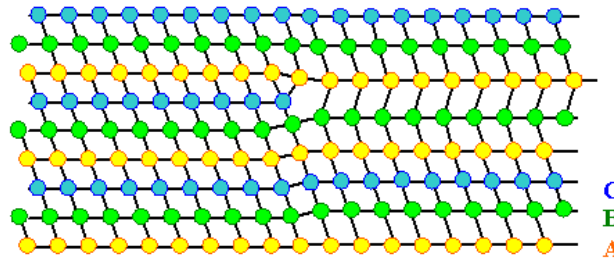
## Defects in Crystalline materials

### How are defects classified?

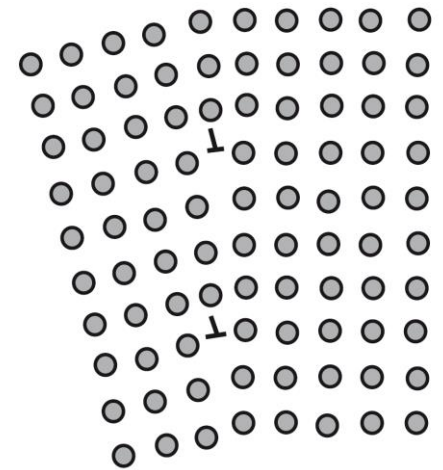
- Point defects (0D)
- Line defects (1D)
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  - Grain boundaries, twins and stacking faults



Grain boundaries



Stacking faults



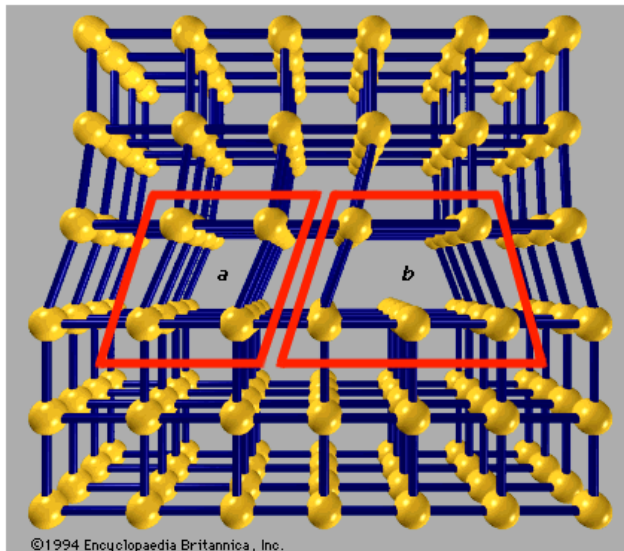
Twin boundary

# Microstructure and defects

## Defects in Crystalline materials

### How are defects classified?

- Point defects (0D)
- Line defects (1D)
- Surface defects (2D)
- Volume defects (3D)
  - Voids and microcracks.



**Void**: The absence of a number of atoms to form internal surfaces in the crystal

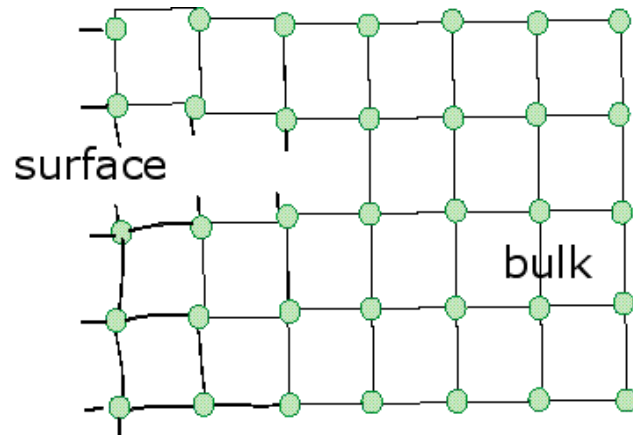


# Microstructure and defects

## Defects in Crystalline materials

### How are defects classified?

- Point defects (0D)
- Line defects (1D)
- Surface defects (2D)
- Volume defects (3D)
  - Voids and microcracks.



A **Microcrack** occurs where internal broken bonds create new surfaces.

# Microstructure and defects

## Defects in Crystalline materials

How are defects classified?

- Point defects (0D)
  - Metal and alloys → Vacancies, substitutional and interstitial
  - Ionic solids → Schottky (anion-cation vacancy pairs) and Frenkel (vacancy-interstitial pairs) defects
- Line defects (1D)
  - Dislocations: missing plane of atoms
- Surface defects (2D)
  - Grain boundaries, twins, stacking faults and free surfaces.
- Volume defects (3D)
  - Voids and microcracks.

# Summary

- Introduction to Nanomaterials
  - Definition of Nanomaterials
  - Introduction to properties, applications, challenges and concerns
  - Problem A
- Unique properties of Nanomaterials
  - Basic definitions
  - Classification: 0D, 1D, 2D, 3D

# Next lecture

- Defects
  - Examples
  - Problem B
- Physical properties: size effects
  - Lattice constant
  - Melting point