Introduction to Materials Science

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

Day 3: YALE PATHWAYS TO SCIENCE SUMMER WORKSHOP 2021

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LEARNING GOALS

- What is a material? Why is it important to study Materials Science?
- What is a crystal and its unit-cell?
- What is a defect? Why is it important?
DEFINITION OF A MATERIAL

- Activity: Name an object/material you can see around you? Can you tell what it is made of?

- QUIZ: Which of the following is an element?
  A) Wood
  B) Steel
  C) Salt
  D) Iron

- An element is a pure substance that has atoms with the same number of protons in its nuclei
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### COMMON MATERIALS

- **Periodic table lists all known ‘elements’**
- **Elements form ‘compounds’**
- **Example of Compound: H₂O**
  - We drink water, breathe in O₂, exhale CO₂
- **We use materials for all our daily applications!!**
  - Electric wires: metals
  - Breakfast cereal: ceramic
Human progress has been determined by the development of materials.

The information age is driven by silicon.

Nanomaterials can impact all technology (more on this shortly).
Activity: Type the chemical symbol of Gold

Gold jewellery

Gold Crystal
CRYSTAL STRUCTURE

- Properties of *Crystal*:
  1. three-dimensional (3D) repeating
  2. ordered arrangement

- How do we simplify this large structure?
- **Unit-cell**
  - smallest repeating unit which gives us the crystal structure
Au CRYSTAL STRUCTURE

Properties of Crystal:
1. three-dimensional (3D) repeating
2. ordered arrangement

- How do we simplify this large structure?
- Unit-cell
  - Smallest repeating unit which gives us the crystal structure

For gold, the structure is face-centered cubic (fcc)
- Atoms at corners of the cube
- Atoms at face-centers

We will use VESTA to visualize the structures! (Hands-on)
Lattice parameter (a) is an important characteristic of unit-cell usually in Å units. 1 Å = 10^{-10} m

For Au, \( a_{\text{Au}} = 4.08 \) Å

QUIZ: What is the length of 5 unit-cells of Au?
A) 12.24 Å  
B) 8.16 Å  
C) 20.4 Å  
D) 2.04 nm (nanometer, 10^{-9} m)
LATTICE PARAMETER

- Lattice parameter \((a)\) is an important characteristic of unit-cell usually in Å units. \(1 \text{ Å} = 10^{-10} \text{ m}\)

- For Au, \(a_{\text{Au}} = 4.08 \text{ Å}\)

- QUIZ: What is the length of 5 unit-cells of Au?
  
  A) 12.24 Å
  
  B) 8.16 Å
  
  C) 20.4 Å
  
  D) 2.04 nm (nanometer, \(10^{-9} \text{ m}\))

- Nanotechnology is the engineering of materials at nano scale!
Iron

Activity: Type the chemical symbol of Iron
For iron, the structure is body-centered cubic (bcc)
- Atoms at corners of the cube
- Atoms at center of the cube

Lattice parameter \(a\)
For Fe, \(a_{Fe} = 2.87 \text{ Å}\)

We will use VESTA to visualize the structures! (Hands-on)
Common Salt

Activity: What is the chemical formula of common salt?

- NaCl is a compound made of Na and Cl elements
- This structure is actually known as rocksalt structure
- Lattice parameter (a), $a_{\text{NaCl}} = 5.64\ \text{Å}$
The closest neighbor of an atom is its 'nearest-neighbor'.

Let us consider this one face of a gold (Au) unit-cell.

Quiz: What is the value of $d_{\text{1NN}}$ in terms of $a$?

(Hint: face of a cube is a square)

A) $a/2$
B) $a/\sqrt{2}$
C) $a\sqrt{2}$
D) $a/4$
The closest neighbor of an atom is its ‘nearest-neighbor’

Let us consider this one face of a gold (Au) unit-cell

Quiz: What is the value of $d_{1\text{NN}}$ in terms of $a$?

(Hint: face of a cube is a square)

A) $a/2$
B) $a/\sqrt{2}$
C) $a\sqrt{2}$
D) $a/4$

Similarly, second nearest-neighbor is $d_{2\text{NN}}$ away, which is ...

$a$ (lattice constant)

Volume of unit-cell = $a^3$ (volume of cube)
DEFECTS

- The atoms do not always sit in their usual positions → Defects
- Defects are common in materials and impact the properties

“Crystals are like people: it is the defects in them that make them interesting.”

- Materials Science and Engineering aims to engineer new materials
- Goal is to understand defects and how they impact material properties

Charles Frank

![Diagram showing crystals with and without vacancies](image)
DEFECTS IN MATERIALS

- Types of defects:
  a) vacancies: atom missing from its usual site
  b) interstitials: atom at an *interstitial (void between atoms)* site
DEFECTS IN MATERIALS

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**DEFECTS IN MATERIALS**

- **Types of defects:**
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  c) antisites: different atoms (Na and Cl) swap their usual sites

- Above defects are **intrinsic**, often we introduce defects externally these are called **extrinsic defects**

- Si is **extrinsically doped** to increase the number of charge carriers!

![Sapphire](image1)

- color due to Ti and Fe

![Ruby](image2)

- color due to Cr defects

- pure Al₂O₃ (transparent)
Materials are everywhere around us, their development is linked to our progress.

We represent a crystal structure using its unit-cell with a lattice parameter.

Defects in materials can be of intrinsic as well as extrinsic type.

Defects can play a key role to tune the desired properties of materials.

Materials Science and Engineering aims to understand materials at a fundamental level and try to design new ones by engineering defects in the material.
RESOURCES

- https://youtu.be/dLPqgobwPGE
- https://www.doitpoms.ac.uk/tlplib/crystallography3/unit_cell.php
- https://www.nano.gov/timeline
- self-healing material (slightly older video) https://youtu.be/kX_kiECXkvM