Day 3: YALE PATHWAYS TO SCIENCE SUMMER WORKSHOP 2021

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Introduction to Materials Science

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

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

Te	empera	ture										+		0° °C		32°°		273≗K
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15 Pnictogens	16 Chalcogens	17 Halogens	18
1	1 H Hydrogen 1.008	Atomic Symbo Name Weight	I [C Soli	olid			Metals		Metallo Po	Nonmeta	als Z						2 He Helium 4.0026
2	3 Li Lithium 6.94	4 Be Beryllium 9.0122	ŀ	ig Liqu H Gas	uid	cali metals	kaline earti etals	Actinoids	ansition me	oids st-transitio	active nmetals	bble gases	5 B Boron 10.81	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
3	11 Na Sodium 22.990	12 Mg Magnesium 24.305	[Rf Unk	known		5,		etals	S .			13 Al Aluminium 26.982	14 Si Silicon 28.085	15 P Phosphorus 30.974	16 S Sulfur 32.06	17 CI Chlorine 35.45	18 Ar ^{Argon} 39.948
4	19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798
5	37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn ^{Tin} 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.60	53 lodine 126.90	54 Xe Xenon 131.29
6	55 Cs Caesium 132.91	56 Ba Barium 137.33	57–71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 TI Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium (226)	89–103	104 Rf Rutherfordium (267)	105 Db Dubnium (268)	106 Sg Seaborgium (269)	107 Bh Bohrium (270)	108 Hs Hassium (277)	109 Mt Meitnerium (278)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (282)	112 Cn Copernicium (285)	113 Nh Nihonium (286)	114 Fl Flerovium (289)	115 Mc Moscovium (290)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.																		
			6	57 La Lanthanum 138.91	58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.05	71 Lu Lutetium 174.97
			7	89 Ac Actinium (227)	90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (266)

PROGRESS OF OUR CIVILIZATION

- 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)

https://www.cpp.edu/~jbputhoff/history.html

Materials Development by Era

Different eras in human history* are named after the <u>materials</u> incorporated in the predominant technologies





Gold Crystal

GOLD

Activity: Type the chemical symbol of Gold



Gold jewellery

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 STRUCTURF

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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

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

For Au, a_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)



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- C) 20.4 Å
- D) 2.04 nm (nanometer, 10⁻⁹ m)
- Nanotechnology is the engineering of materials at nano scale!



Iron

Activity: Type the chemical symbol of Iron





Fe CRYSTAL STRUCTURF

- 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 Å

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





Common Salt





a_NaCl

Cl

Na



- NaCl is a compound made of Na and Cl elements
- This structure is actually known as rocksalt structure
- Lattice parameter (a), a_NaCl = 5.64 Å

NEAREST-NEIGHBORS

- 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-1NN in terms of a?

(Hint: face of a cube is a square)

- A) a/2
- **B)** a/√2
- **C)** a √2

D) a/4



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- A) a/2
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- **C**) a √2
- D) a/4
- Similarly, second nearest-neighbor is d-2NN away, which is ...
- a (lattice constant)





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." Charles Frank

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







DEFECTS IN MATERIALS

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



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- 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!



color due to Ti and Fe



color due to Cr defects





KEY POINTS

- 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

- <u>https://youtu.be/dLPgqobwPGE</u>
- https://steemit.com/life/@zest/the-three-age-system-the-stone-age-the-bronzeage-and-the-iron-age
- <u>https://en.wikipedia.org/wiki/History_of_materials_science</u>
- <u>https://www.doitpoms.ac.uk/tlplib/crystallography3/unit_cell.php</u>
- <u>https://www.nano.gov/timeline</u>
- self-healing material (slightly older video) <u>https://youtu.be/kX_kiECXkvM</u>