Simulation of Classical and Quantum mechanics

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- The Universe consists of three main components: dark energy, dark matter, and ordinary matter. (The Europian Space Agence, 2013)

Figure 1: The Hubble Ultra-Deep Field image shows some of the most remote galaxies visible to present technology (diagonal is 1/10 apparent Moon

Categories of solid-states materials based on their chemical, physical, and structural characteristics

1. **Metals**: Metals compose of one or more metallic elements. Example are, Iron (Fe) and Brass.

Figure 2: : Familiar objects made of metals and metal alloys (from left to right): silverware, scissors, coins, a gear, a wedding ring, and a nut and bolt

Categories of solid-states materials based on their chemical, physical, and structural characteristics

2. Ceramics: Ceramics are compounds with properties between metallic and nonmetallic elements. Examples, Magnesium Oxide,

Figure 3: Common objects made of ceramic materials: scissors, a china teacup, a building brick, a floor tile, and a glass vase.

Categories of solid-states materials based on their chemical, physical, and structural characteristics

3. **Polymers**: Polymers include the familiar plastic and rubber materials. Examples are polyethylene and pvc.

Figure 4: Several common objects made of polymeric materials: plastic tableware, billiard balls, a bicycle helmet, two dice, a lawn mower wheel, and a plastic milk carton.

Categories of solid-states materials based on their chemical, physical, and structural characteristics

4. **Composites**: The resultant product of two or more groups of the solid materials.

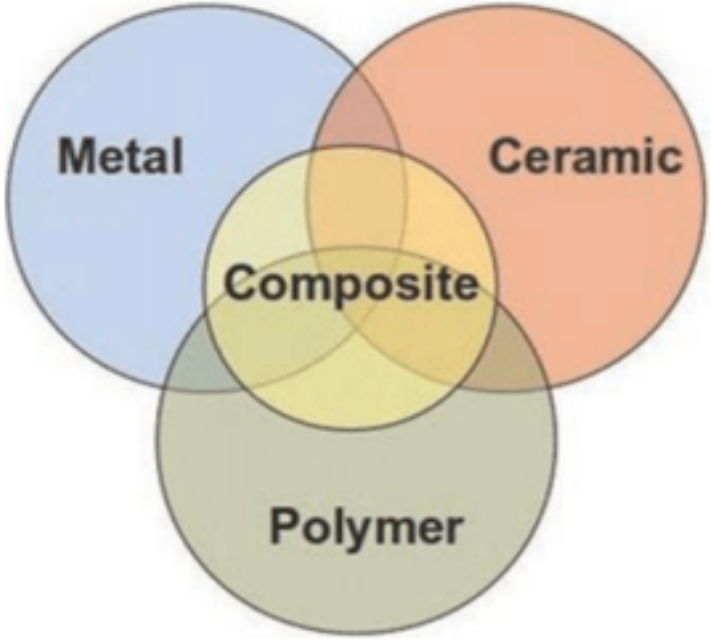


Figure 5: schematic diagram of the composition of composites

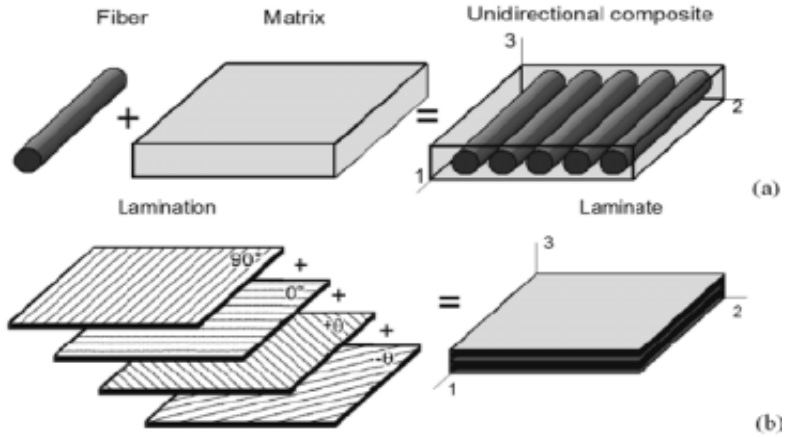


Figure 6: Diagrams a and b represent fibre reinforced matrix composite and laminated composite. Bicycle frames and plywoods respectively

Advanced Materials

- Advanced materials represent another material group.
- They are products of traditional materials whose properties have been enhanced.
- They include biomaterials, semiconductors, nanomaterials, and smart materials.

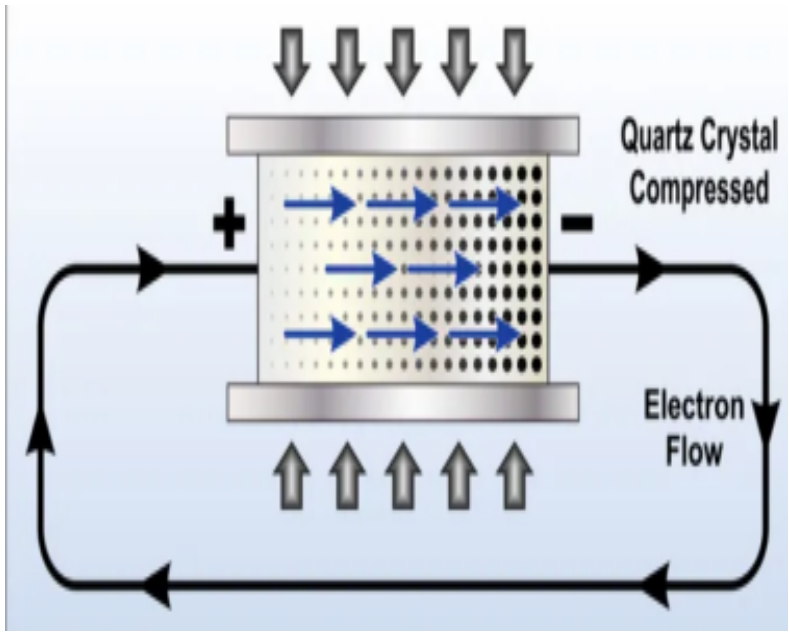


Figure 7: Piezoelectric Effect

Crystalline and Armorphous Solid Materials

- This category of materials is classified based on the order of their constituent particles.

CRYSTALLINE SOLIDS

- Atoms are arranged in regular 3 dimension
- Sharp melting point
- Anisotropic
- True solid
- Symmetrical
- More rigid
- Long range order

AMORPHOUS SOLIDS

- They do not have regular arrangement
- No particular melting point
- Isotropic
- Pseudo solid
- Unsymmetrical
- Less rigid
- Short range order

Crystalline and Armorphous Solid Materials

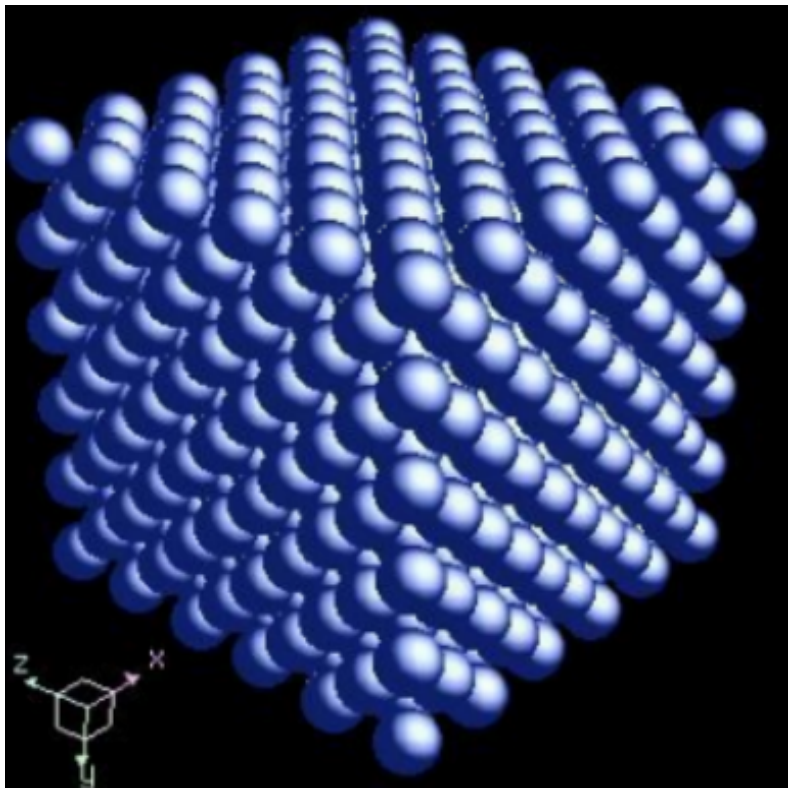


Figure 8: : Crystal structure of a Cu structure exhibiting a repeated order of atoms.

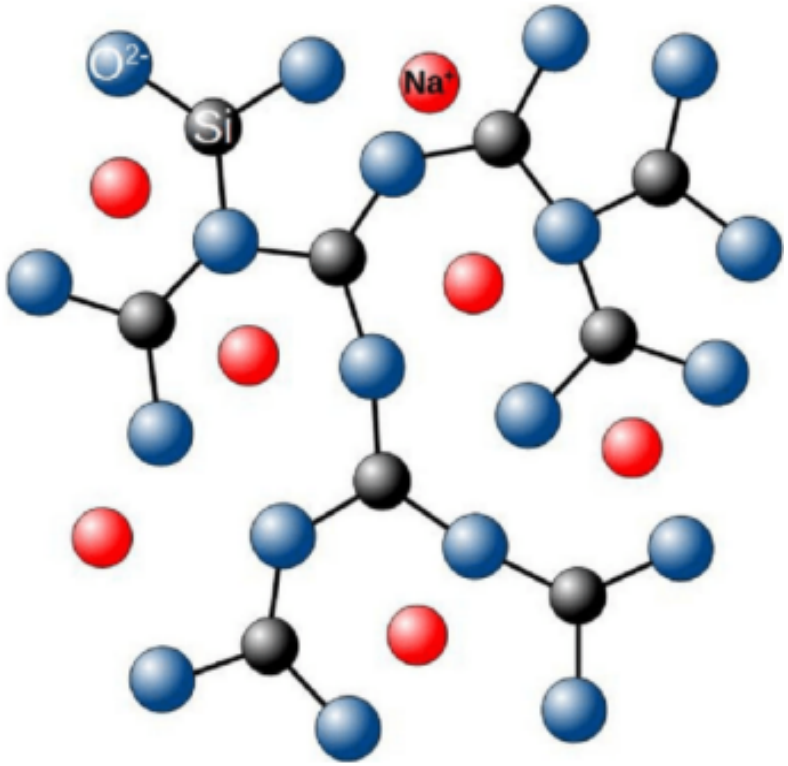


Figure 9: Amorphous structure of a Soda glass with no definite repeating order of atoms.

CRYSTAL LATTICE

- **Lattice**: An array of points in two or three dimensional space.

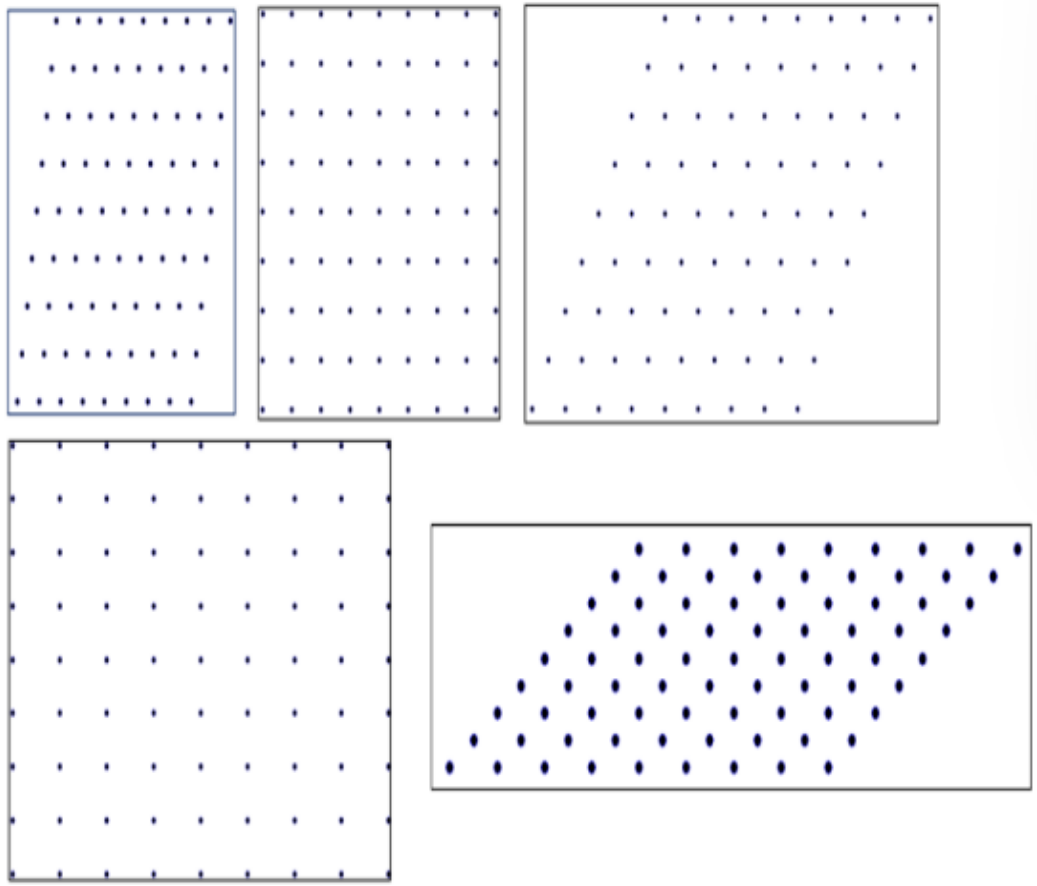


Figure 10: Different sets of lattices according to different symmetries

- **Group**: Refers to a mathematical concept related to the symmetry operations that can be applied to a crystal lattice. These operations include rotations, reflections, and translations that leave the crystal structure unchanged.

- The geometrical entity (such as a point, line, or plane) about which symmetry operations can be performed to generate equivalent arrangements is known as symmetry element.

1. ROTATIONAL SYMMETRY

- Rotational symmetry involves rotating the crystal lattice by a certain angle about an axis passing through a lattice point.
- The axis of rotation is a an imaginary line, passing through a fixed point around which the crystal may be rotated such that it present the same appearance more than once during a complete revolution of 2π.
- Lattices can be found such that one-, two-, three-, four-, and sixfold rotation axes carry the lattice into itself, corresponding to rotations by 2π, $2\pi/2$, $2\pi/3$, $2\pi/4$, and $2\pi/6$ radians and by integral multiples of these rotations.

- For example, a 90-degree ($2\pi/4$) rotation around a fourfold (C4) axis leaves the crystal structure unchanged. This symmetry is known as a tetragonal symmetry.

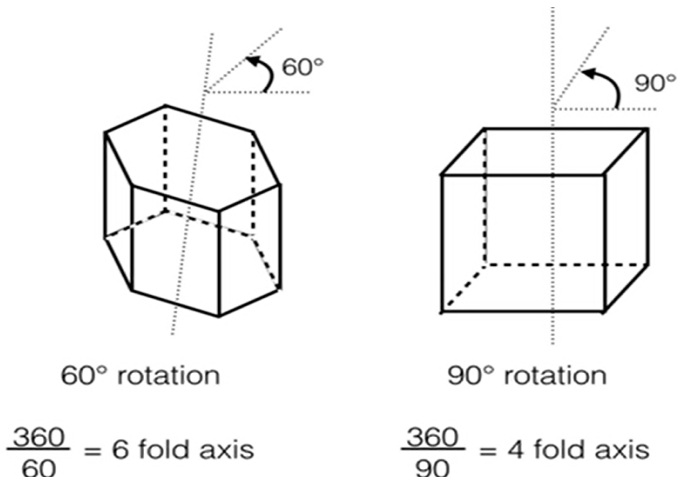


Figure 11: 6 and 4 fold axis of a hexagonal and cubic lattice

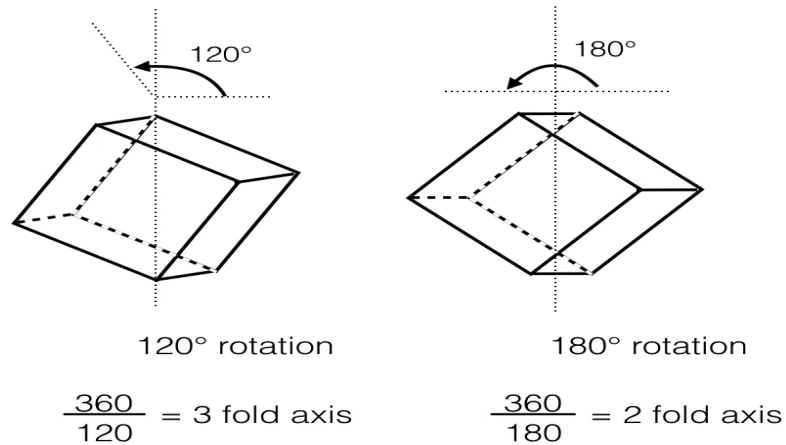


Figure 12: Other forms or axis of symmetries in a cubic lattice

2. TRANSLATION SYMMETRY

- The Crystal lattice in two or three dimensional space may be defined by primitive translation vectors a_i. They are the smallest set of linearly independent vectors that define the lattice translation.

- Any point in the lattice can be represented as a linear combination of these primitive translation vectors with integer coefficients.

- Any lattice point R, can be expressed as
  $R = u_1 a_1 + u_2 a_2 + u_3 a_3$ in 3D and
  $R = u_1 a_1 + u_2 a_2$ in 2D where u_1, u_2, u_3 are integers.

- The volume of the primitive cell is given by the triple product of the primitive vectors.

$$V = |a_1 \cdot (a_2 \times a_3)|$$

- The primitive translation vectors are often used to create the crystal axis of the primitive parallelepiped

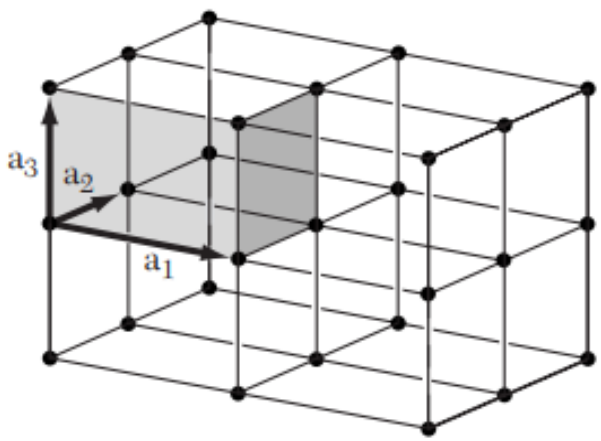


Figure 13: 3D array of a crystal lattice

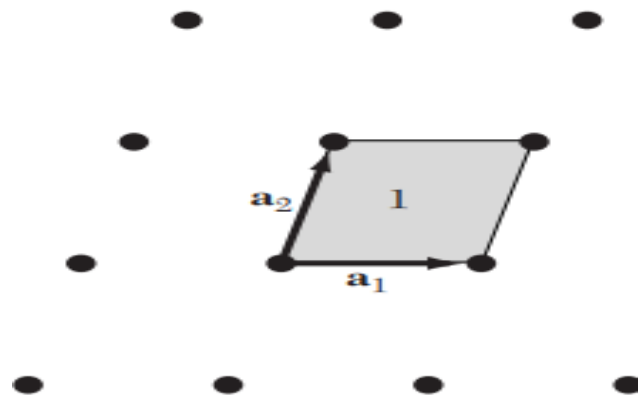


Figure 14: A 2D array of a crystal lattice

3. REFLECTION / MIRROR SYMMETRY

- Reflection symmetry, also called mirror symmetry or inversion symmetry, means a crystal's atomic arrangement looks identical when reflected across a flat surface (plane) or a single point.
- The operation involves reflecting each point across the reflection plane so that the position of each point on one side of the plane is mirrored on the other side.

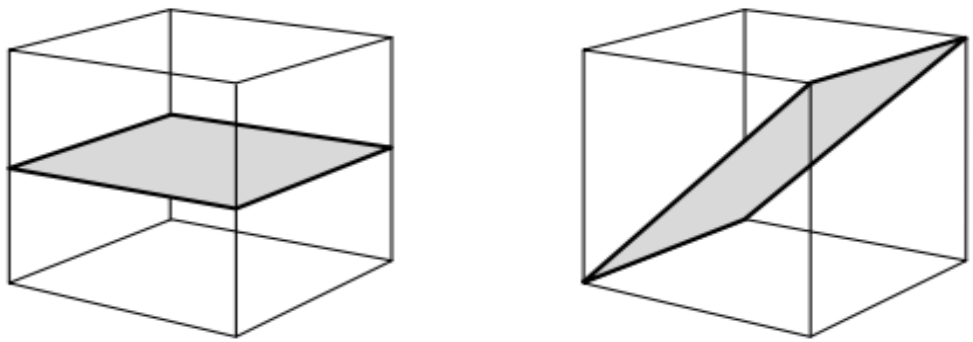


Figure 15: (a) A plane of symmetry parallel to the faces of a cube. (b) A diagonal plane of symmetry in a cube.

- If r represent the position vector of an atom relative to the reflection plane, then it's reflection is r′ can be given by

$$\mathrm{r}' = -\mathrm{r}$$

  This means that each coordinate of the atom is multiplied by -1, effectively mirroring it across a plane.
- The planes of reflections are often governed by miller indices (hkl), which are integers representing the intercept of the plane with the three crystallographic axis (a_1, a_2, a_3).

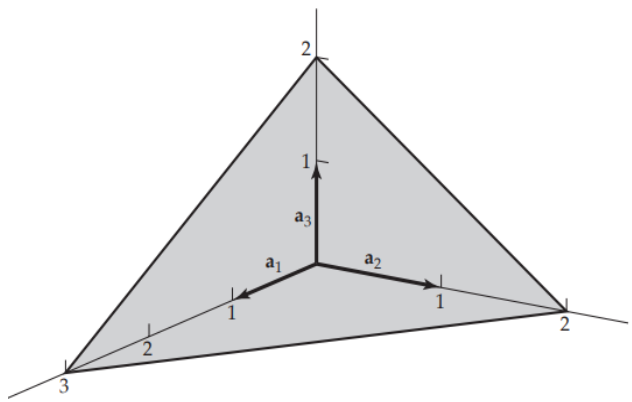


Figure 16: This plane intercepts the a_1, a_2, a_3 axes at $3a_1, 2a_2, 2a_3$. and thus the indices of the plane are (233).

2D BRAVAISE LATTICES

- There are four main different symmetries of 2D lattice (oblique, square, hexagonal and rectangular). The symmetry of a lattice is referred to as CRYSTAL SYSTEM.

- Rectangular CRYSTAL SYSTEM (2 fold axis and 2 mirror planes) is accepted by two different type of lattices.

- Each CRYSTAL SYSTEM has the conventional choice of two lattice basis vectors, a and b, where the orientation of these vectors are specified by the orientation of symmetry elements

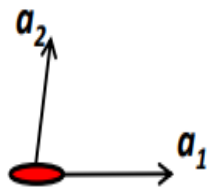
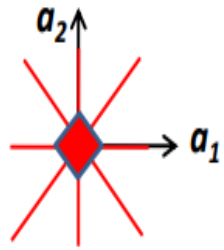
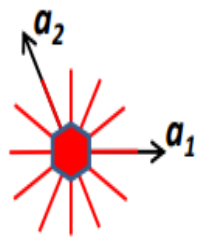
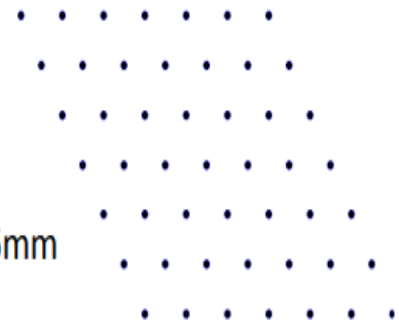
Crystal system	Basis vectors / Symmetry elements	Lattice constants	Lattice type
1. Oblique		a ≠ b, α ≠ 90 deg	p2 
2. Square		a = b, α = 90 deg	p4mm 
3. Hexagonal		a = b, α = 120 deg	p6mm 

Figure 17: 2D Lattices I

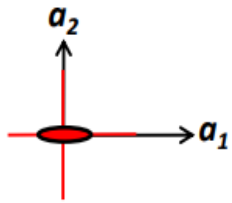
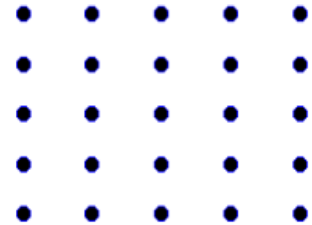
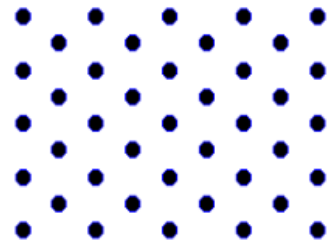
Crystal system	Basis vectors / Symmetry elements	Lattice constants	Lattice type
4. Rectangular		**a ≠ b, α = 90 deg**	pmm2 
			cmm2 

Figure 18: 2D Lattices 2

3D BRAVAISE LATTICES

- For the case of 3 D lattice there are 7 different symmetries (crystal systems).
- The lattice vectors a, b and c chosen according to the conventional rules form the NON-PRIMITIVE UNIT CELL, which has additional lattice points inside. This correspond to the CENTERING OF A UNIT CELL.
- For three dimensions all distinct lattices may be described by a few types of centering. It gives 14 3D Bravais lattice.

MODELLING WITH VESTA AND ASE

Introduction to VESTA

VESTA stands for Visualization for Electronic and Structural Analysis. It's a powerful tool for visualizing crystal structures, molecules, and other materials.

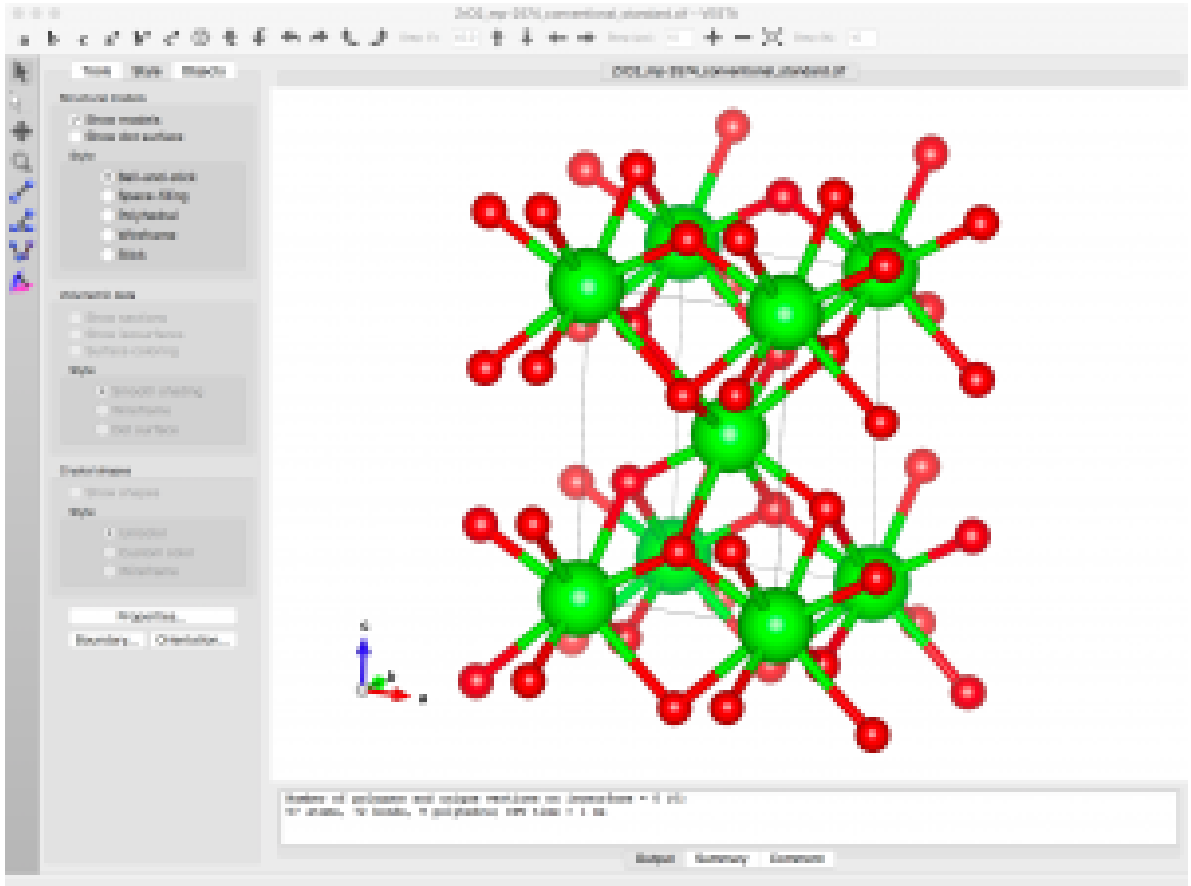


Figure 19: VESTA INTERFACE

What You Can Do In Vesta

- Crystal Structure Visualization: VESTA allows users to visualize crystal structures in three dimensions. It supports various crystallographic file formats, including CIF (Crystallographic Information File), POSCAR/CONTCAR (used in VASP), and others.

- Molecular Visualization: In addition to crystal structures, VESTA can also visualize molecular structures. This includes organic molecules, inorganic molecules, and biomolecules. Users can load molecular structure files in formats such as XYZ, PDB, and others.

- Customization and Analysis Tools: VESTA provides a range of customization options for visualizing and analyzing structures. Users can adjust atom sizes, colors, and styles, as well as bond lengths and angles. V

What You Can Do In Vesta

- Symmetry Analysis: One of the key features of VESTA is its ability to analyze the symmetry of crystal structures. Users can identify symmetry elements and operations within a crystal structure.
- Export and Sharing: VESTA allows users to export visualizations in various formats. This includes static images, as well as interactive 3D models.

Space Groups

- Space groups are mathematical descriptions of symmetries exhibited by the arrangement of atoms or molecules in a crystal lattice. It describe the ways in which this lattice can be translated, rotated, or reflected in three-dimensional space while still maintaining its overall symmetry.

- There are a total of 230 space groups in three-dimensional space. Each space group has its own unique set of symmetry elements, such as rotations, reflections, and translations, which define its particular symmetry properties

Lattice Parameters

- Lattice parameters are the values that define the size and shape of a unit cell in a crystal lattice. In three dimensions, a crystal lattice can be described by three edge lengths (a, b, c) and three interaxial angles (α, β, γ) between these edges.

- These parameters define the dimensions and orientation of the unit cell.
  The edge lengths (a, b, c) represent the lengths of the edges of the unit cell.
  The interaxial angles (α, β, γ) represent the angles between these edges.

Structure Parameters

Structural parameters refer to the specific characteristics or properties that describe the arrangement of atoms, ions, or molecules within a material's crystal lattice. These parameters provide detailed information about the spatial arrangement of the constituents within the crystal structure

- Atomic positions: The coordinates of each atom or ion within the unit cell, typically described in terms of **Fractional** or **Cartesian** coordinates.

Modelling in VESTA

- Get and install VESTA: Go to the official Vesta link and download the VESTA zip file compatible with your operating system (OS), extract it and launch the .exe file
- Create a New Structure: Go to "File" then "New Structure" to create a new crystal structure.
- Set your Space Group and Lattice Parameters for your crystal structure by specifying the lengths of the unit cell edges (a, b, c). The angles (α, β, γ) are automatically defined base on the crystal system selected.
- Add Atoms: Once the lattice parameters are set, you can start adding atoms to the unit cell. Go to "Edit" then "Add Atom" or use the shortcut (Ctrl + Shift + A) to add atoms to the unit cell.

Modelling in VESTA contd.

- Adjust Display Settings: Customize the display of the crystal structure by adjusting parameters such as atom size, bond radius, and color scheme. Use the "Edit" then "Data/Display Style" menu to access display settings.

- Analyze: Once your crystal structure is built, you can analyze it using various tools available in VESTA. Use tools such as symmetry analysis, bond length analysis, and coordination polyhedra analysis to study the structure.

- Save Your Work: Once you are satisfied with your crystal structure, save your work by going to "File" then "Save" or "Save As...". You can also export to an appropriate file format (eg. xyz, CIF, .vasp, etc).

Examples

- Fe body centered cubic structure
- Fe face cetered cubic structure
- Fe2O3 body centered cubic structure
- NaCl cubic structure

Introduction to Materials Project

- The Materials Project is indeed an extensive online database containing information about materials, molecules, and related properties.
- It provides a wide range of data on various materials such as Crystal structure information.
- You can create an account and access materials project here.

Materials Project - Composition

The composition of a material refers to the specific elements and the proportions that make up the material.

- Chemical Elements: The database includes data on the chemical elements present in each material. This information identifies the types of atoms that comprise the material, such as carbon, oxygen, silicon, etc.
- Elemental Proportions: In addition to listing the chemical elements, the database also provides information about the relative proportions of each element within the material. This helps characterize the material's chemical composition more precisely.
- Structural Formulas: For complex materials with multiple chemical components, the database may include structural formulas or chemical formulas that depict the arrangement of atoms and the ratios of the elements.

Materials Project - Crystal Structure Information

Crystal structure information is crucial for understanding the arrangement of atoms within a material, which greatly influences its properties and behavior.

- For example, one well-known crystal structure is that of diamond. In diamond, carbon atoms are arranged in a face-centered cubic (FCC) lattice, with each carbon atom bonded to four neighboring carbon atoms in a tetrahedral geometry. The space group for diamond is Fd-3m, and its lattice parameter a is approximately 3.567 Å. These details provide insights into the symmetry and spatial arrangement of atoms within the diamond crystal lattice.

What is ASE and why ASE

The atomic simulation environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. The code and documentation is freely available here.

- **Python**: Ensure you have Python installed on your system. ASE is compatible with both Python 2 and Python 3, but Python 3 is recommended.
- **Requirements**: Ensure these packages are installed, Numpy, SciPy and Matplotlib (optional)
- **ASE itself**: You can install ASE using the "pip" package manager. Type "pip install ase" in your terminal or command prompt.

Modelling in ASE

To start, you have to import "atoms" with this command; **from ase import Atoms**.
It is a Python statement that imports the **Atoms** class from the **ase** package.

- **from ase**: This specifies that we're importing something from the **ase** package.
- **import Atoms**: This specifies that we're specifically importing the **Atoms** class from the **ase** package.