

Today's program

Concepts

- Crystal structures
- Lattice + Basics
- Primitive translation vectors

- Unit cells
- Conventional cells
- Wigner-Seitz cells

- Packing factor
- Nearest neighbours

Examples

2-dimensions (Square & hexagonal)

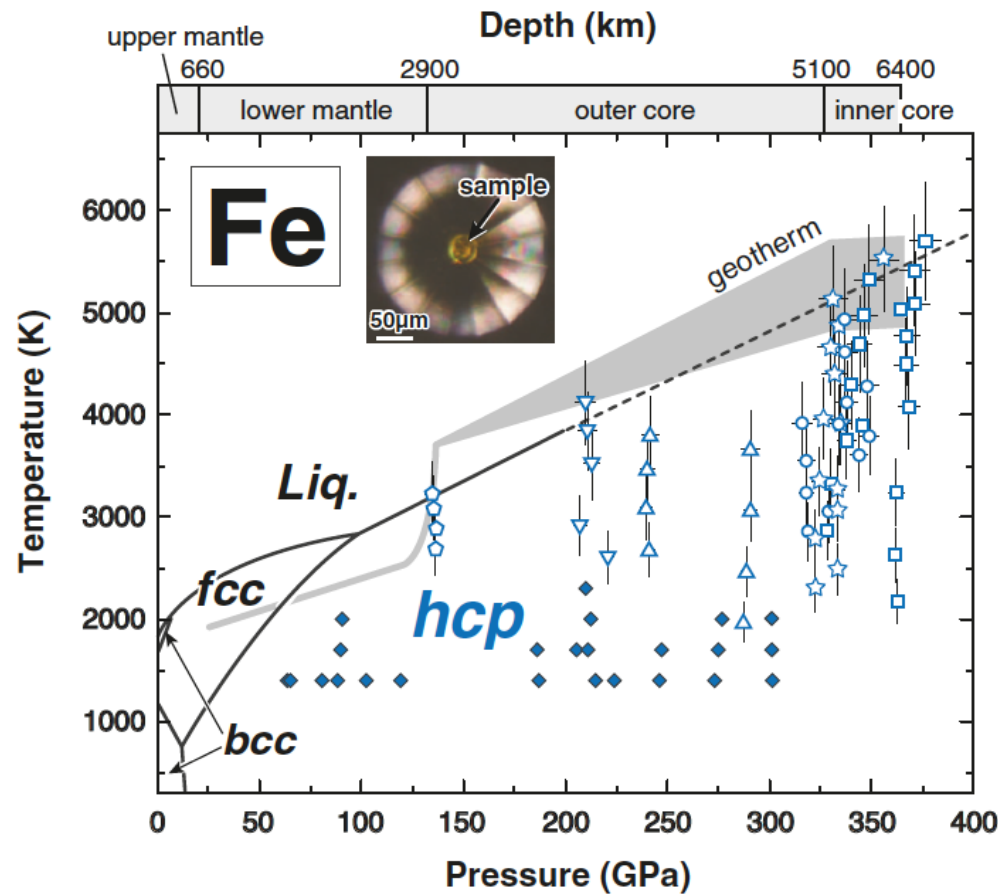
- Concept / vocabulary
- Graphene (Nobel prize 2010)

3-dimensions structures

- Cubic crystal structures
- Quiz
- Discuss diamond & table salt

Tasks for next week:

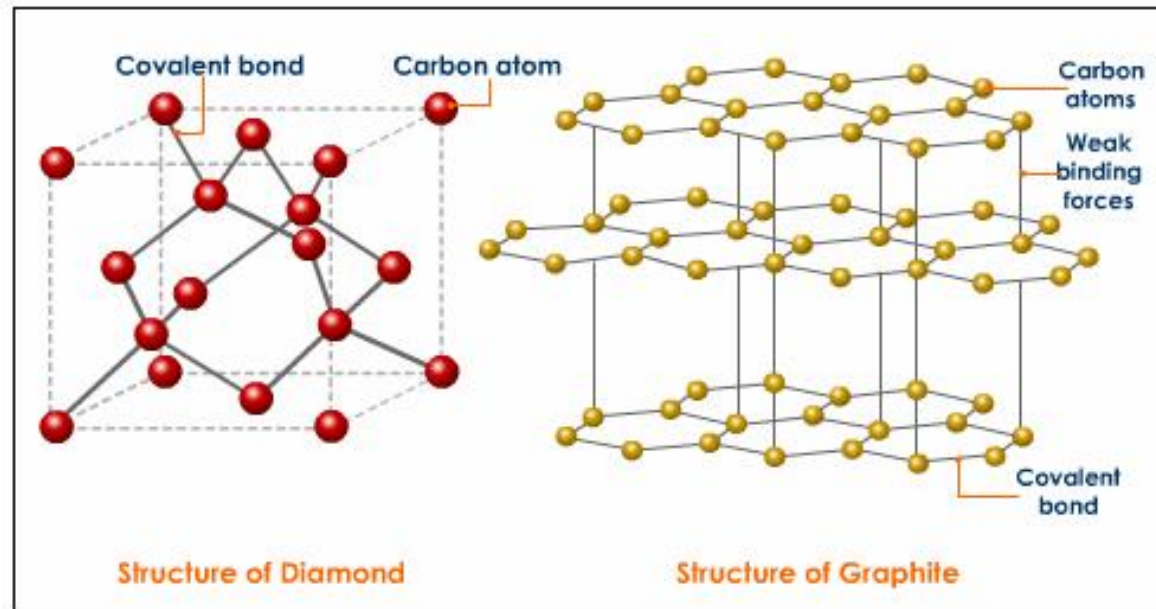
Structure of Iron in the Earth's Inner Core



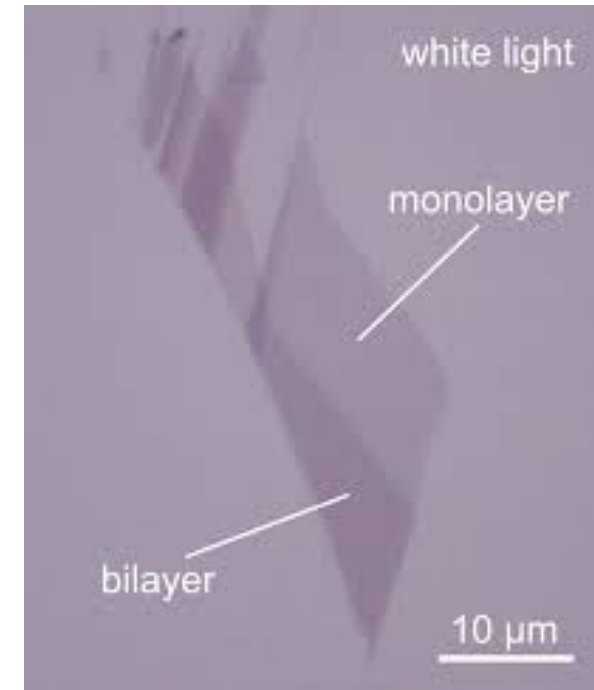
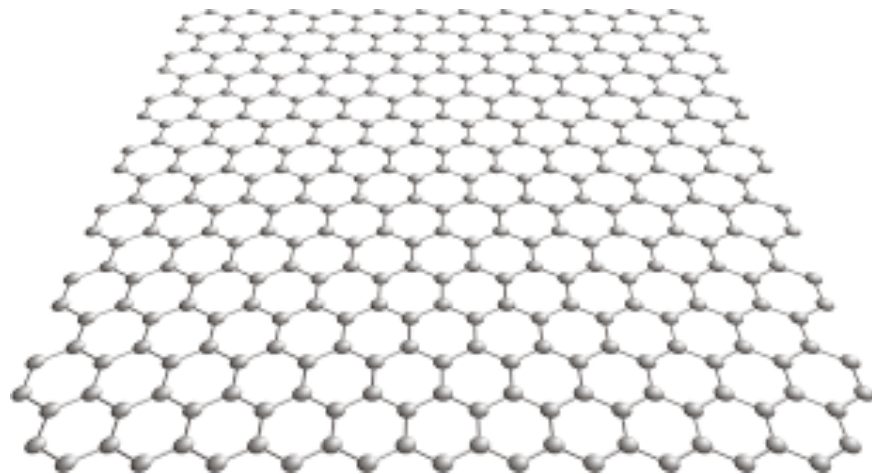
**Temperature-Pressure:
Phase diagram**

Science **330**, 359 (2010)

Same Material – Different crystal structures



Graphene – monolayer of graphite



Nobel Prize 2010
Andre Geim & Konstantin Novoselov

Red - thread

(1) Description of crystal structures (Today)

Concepts & Vocabulary

Examples

Quizzes

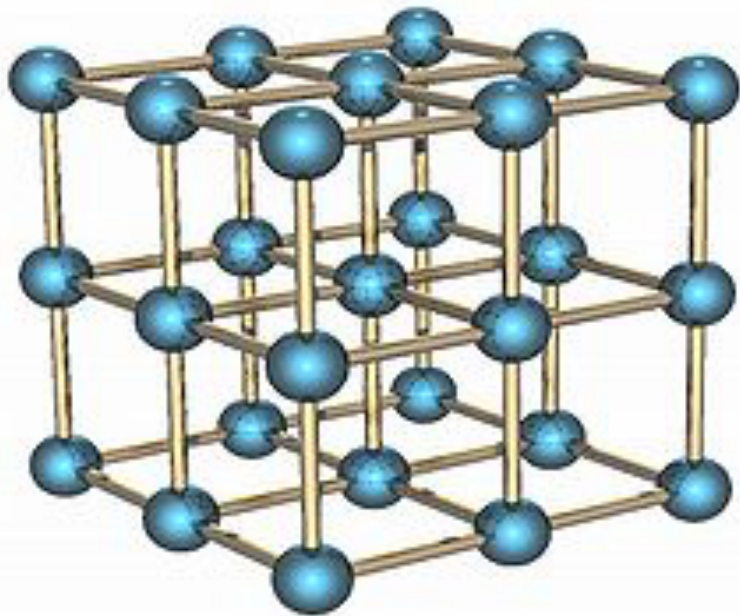
(2) How to measure crystal structure (next Wednesdays)

Deriving the crystal structure of new superconductor

Reciprocal space

Scattering theory

Polonium: Rare example of elementary simple cubic structure.



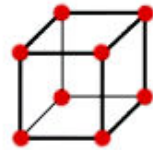
The alpha form of solid polonium.



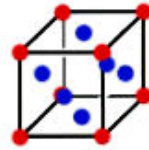
Alexander Litvinenko

first confirmed victim of lethal [polonium-210](#)-induced [acute radiation syndrome](#)

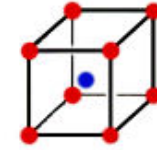
3D Lattices



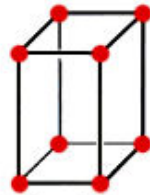
Simple cubic



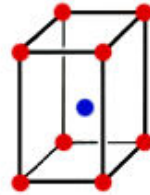
Face-centered cubic



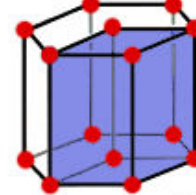
Body-centered cubic



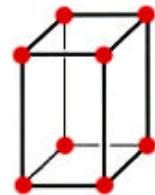
Simple tetragonal



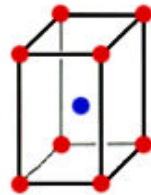
Body-centered tetragonal



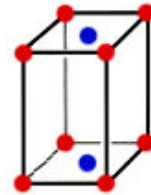
Hexagonal



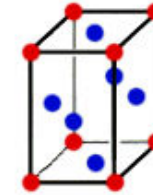
Simple orthorhombic



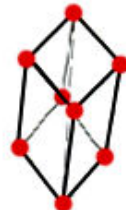
Body-centered orthorhombic



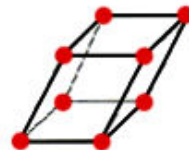
Base-centered orthorhombic



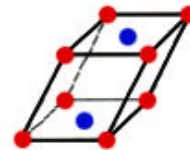
Face-centered orthorhombic



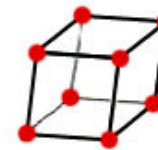
Rhombohedral



Simple Monoclinic

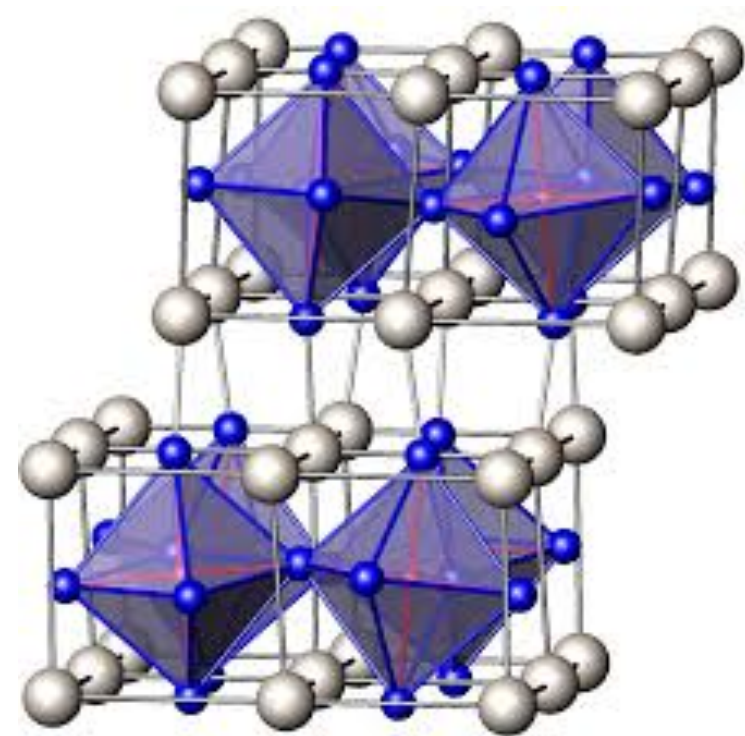
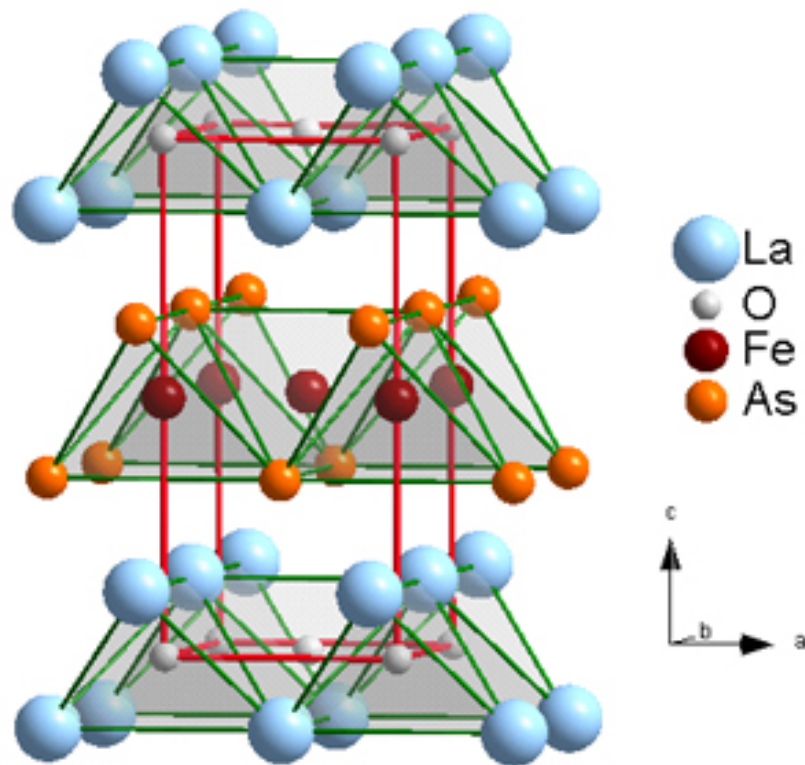


Base-centered monoclinic



Triclinic

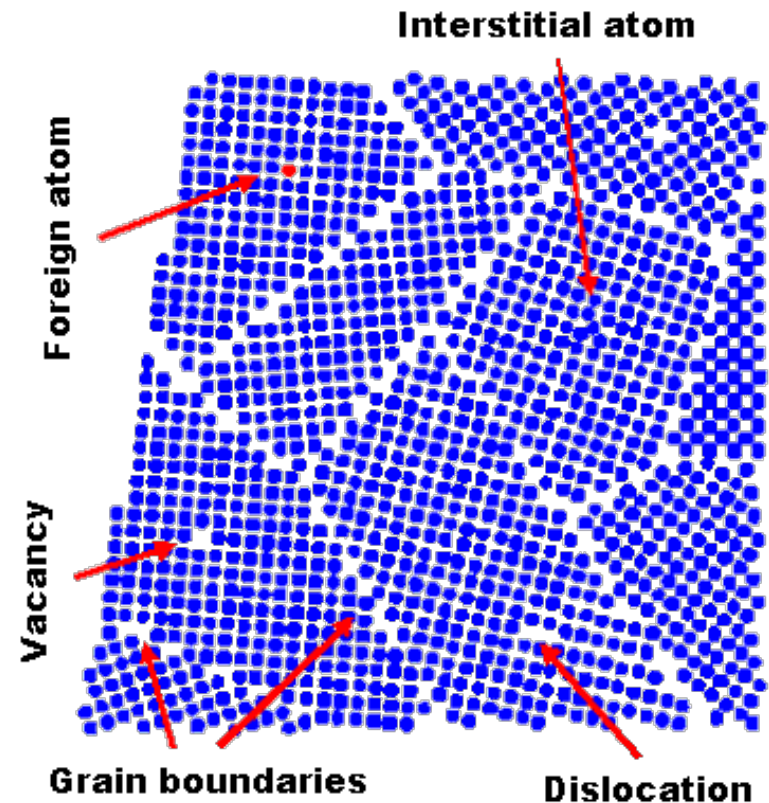
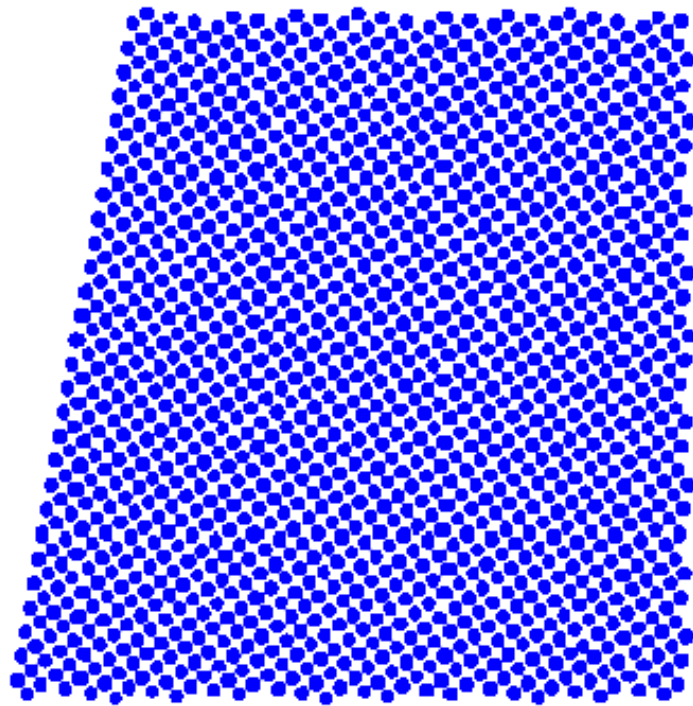
Complicated Crystal Structures



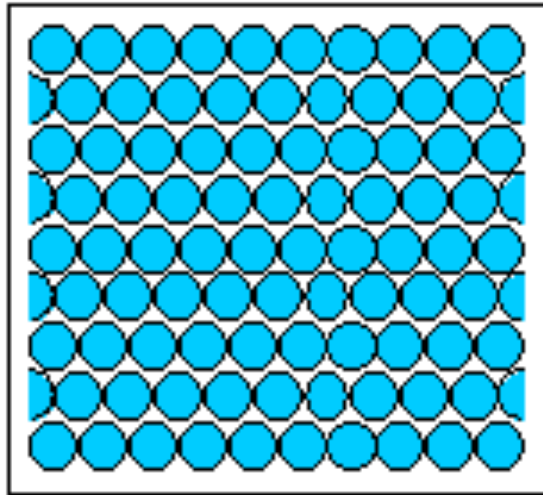
<http://www.wou.edu/~rmiller09/superconductivity/>

Phys. Rev. Lett. 104, 226401 (2010)

Single crystal versus Polycrystal

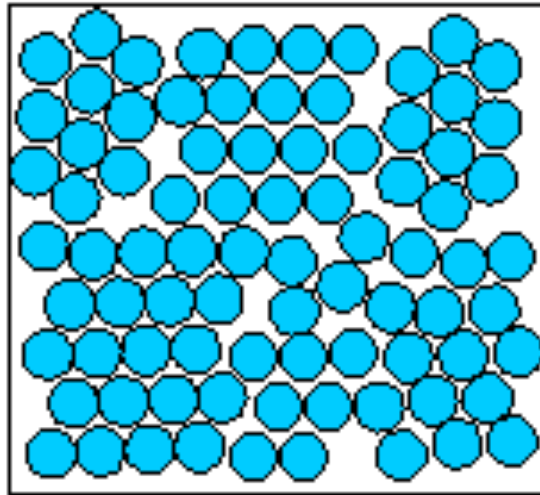


Amorphous solid



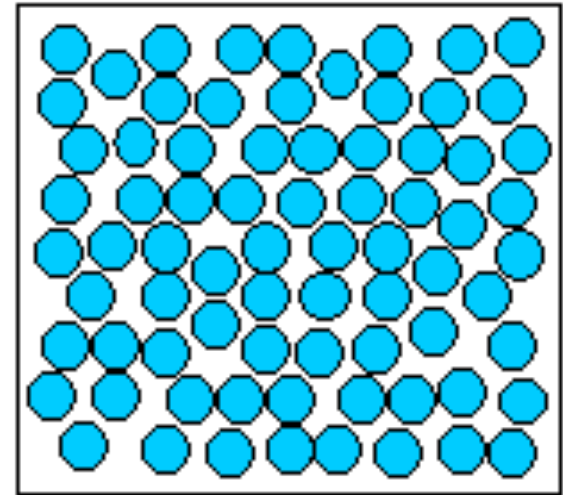
Single crystal

Periodic across the
whole volume.



Polycrystal

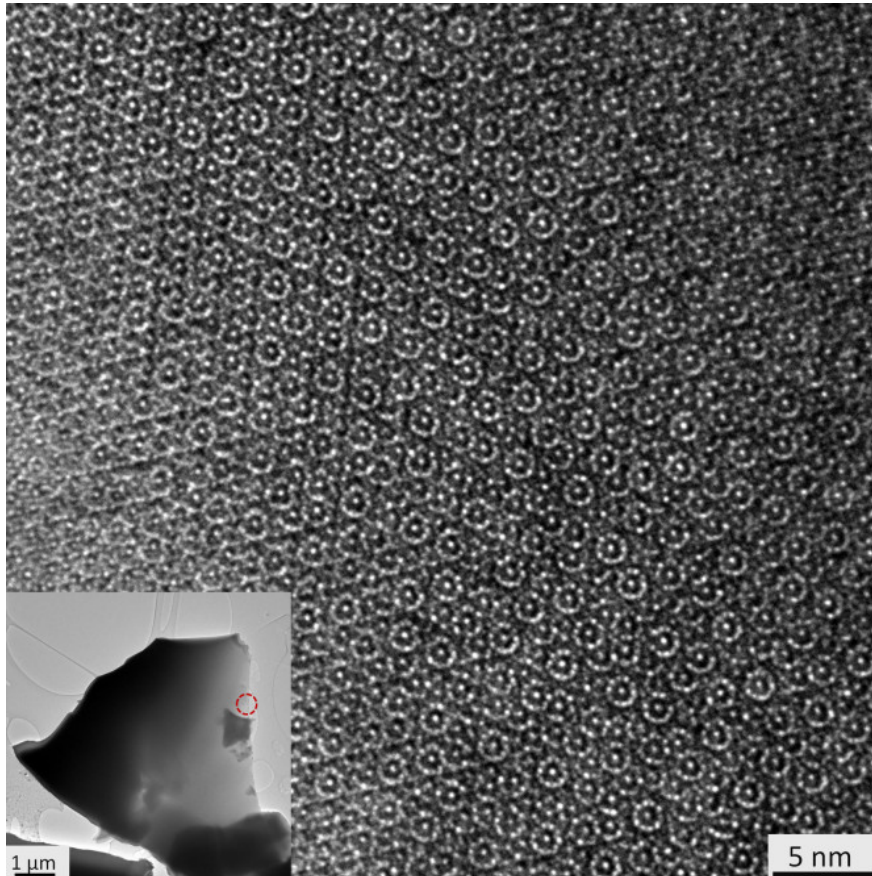
Periodic across
each grain.



Amorphous solid

Not periodic.

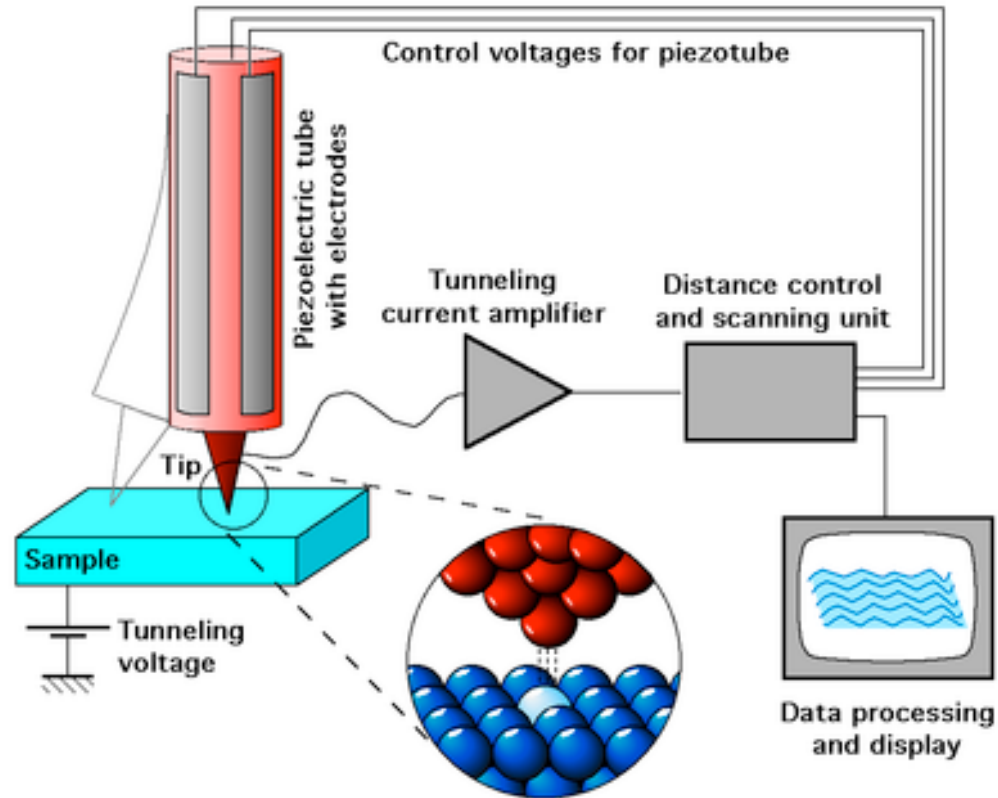
Quasi-crystals



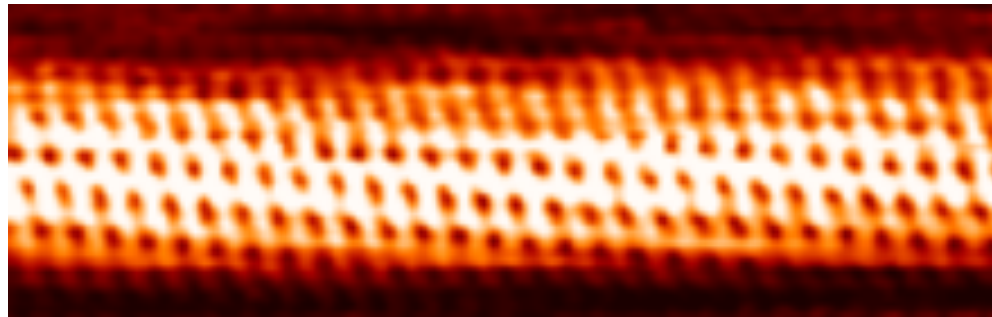
High-resolution transmission electron microscopy (HRTEM) image showing that the real space structure consists of a homogeneous, quasiperiodic and ten-fold symmetric pattern.

Sci Rep. 2015; 5: 9111

Scanning tunneling microscope (STM)

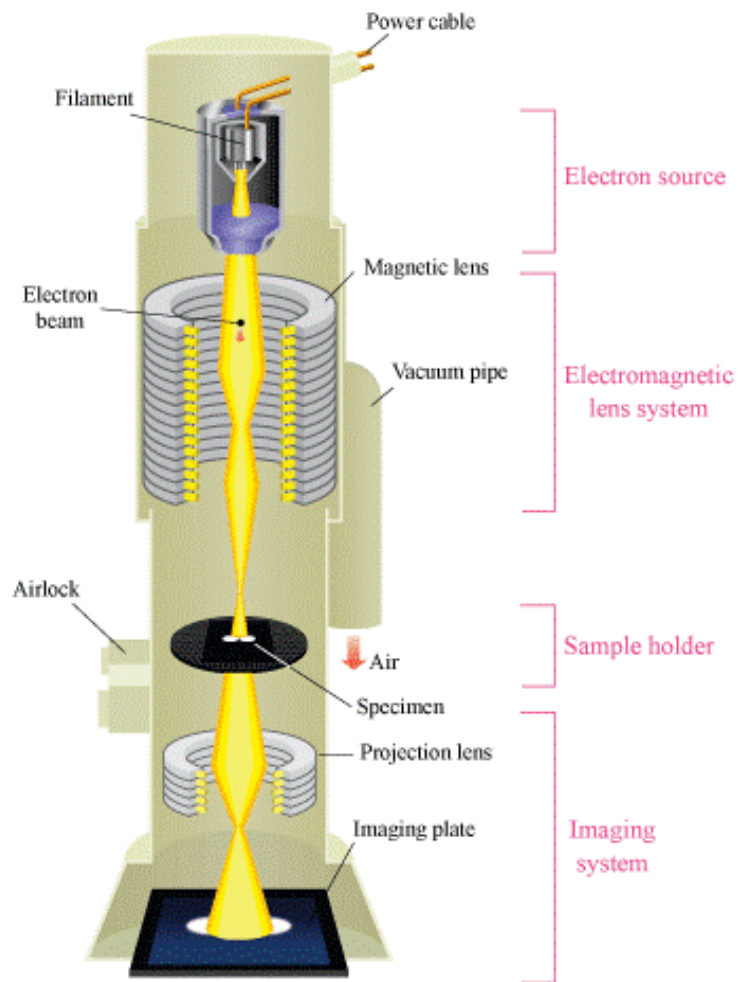


PRINCIPLES OF STM



Carbon Nano-tube

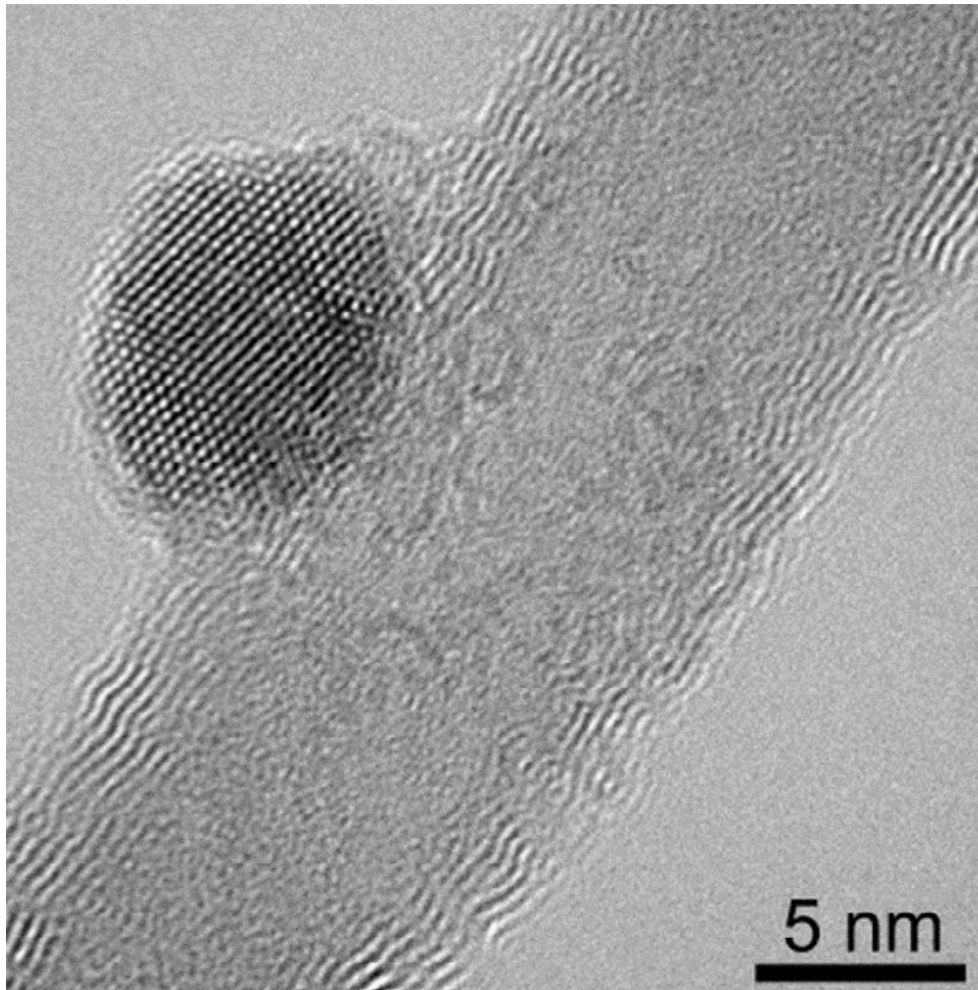
High-Resolution Transmission Electron Microscope (HRTEM)



http://www.hk-phy.org/atomic_world/tem/tem02_e.html

<http://www.dstuns.iitm.ac.in/microscopy-instruments.php>

High-Resolution Transmission Electron Microscope (HRTEM)



HRTEM image and focal series reconstruction of the MWCNTs with Fe₃O₄ nanoparticles attached.

<https://www.int.kit.edu/1745.php>

Tasks for next week

(1) Read chapter 2 :

Braggs Law

Scattering wave amplitude (read fast, don't spend time on the derivation)

Reciprocal Lattice vectors

Diffraction conditions

Laue Equations

Brillouin Zones

Reciprocal lattice (bcc, fcc)

Fourier Analysis of Basis (read fast, don't spend time on the derivation)

Structure factor (bcc, fcc)

(2) Read about: Fermi Golden rule & Fourier transforms

(3) Solve exercise sheet 1

Exercise 1 *Crystal lattice*

Why is there no tetragonal base-centred crystal lattice? (Draw a figure!)

Exercise 2 *Cubic lattice system*

For simple cubic, bcc, and fcc lattices with lattice constant a , calculate the following quantities expressed in units of a :

- Volume of the conventional unit cell
- Number of primitive lattice points per unit cell
- Volume of the primitive cell
- Number of nearest neighbours (coordination number)
- Distance between nearest neighbours
- Packing density for spherical and touching atoms

Exercise 3 *Lattice constant of silver*

Silver has a cubic fcc lattice and a density of 10.49 g/cm^3 . Calculate the lattice constant, the distance between nearest neighbours, and the radius of a silver atom if they were touching spheres.

Exercise 4 *Wigner-Seitz cell*

Construct the Wigner-Seitz cell of the orthorhombic base-centred lattice for $a_1 : a_2 : a_3 = 4 : 2 : 3$.

Exercise 5 *Sphere packings*

Calculate the ratio c/a of an ideal hexagonal dense sphere packing (hcp) and its packing density. Compare the packing density to that of an fcc lattice and explain your findings.