5 Concepts

An ideal crystal is an infinite repetition of a group of atoms. It can be constructed via two elements:

– The basis, which is the group of atoms.

– The lattice, which is the set of points to which the basis is attached. Or equivalent:

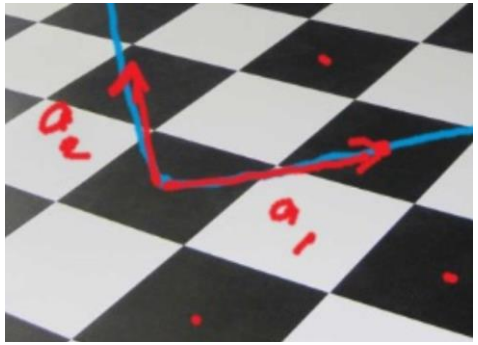
A lattice is the set of points, which can be reached by the lattice translation vector $\vec{T} = \sum_{i=1}^{N} u_i \cdot \vec{a}_i \ \ \forall u_i \in \mathbb{Z}$ where the translation vectors $\vec{a}_i$ must be such, that given an arbitrary point $\vec{r}$, the atomic structure at $\vec{r} + \vec{a}_i$ is identical with the one, seen from $\vec{r}$.

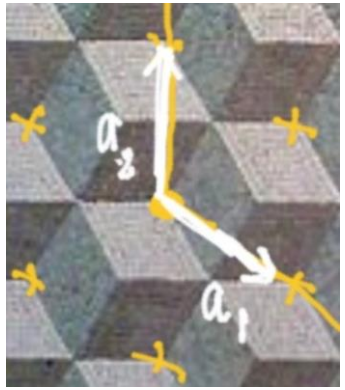
The translation vectors are said to be primitive if for any two points $\vec{r}$, $\vec{r'}$ from which the atomic structure looks the same, there exists a translation vector $\vec{T}$, such that $\vec{r'} = \vec{r} + \vec{T}$.

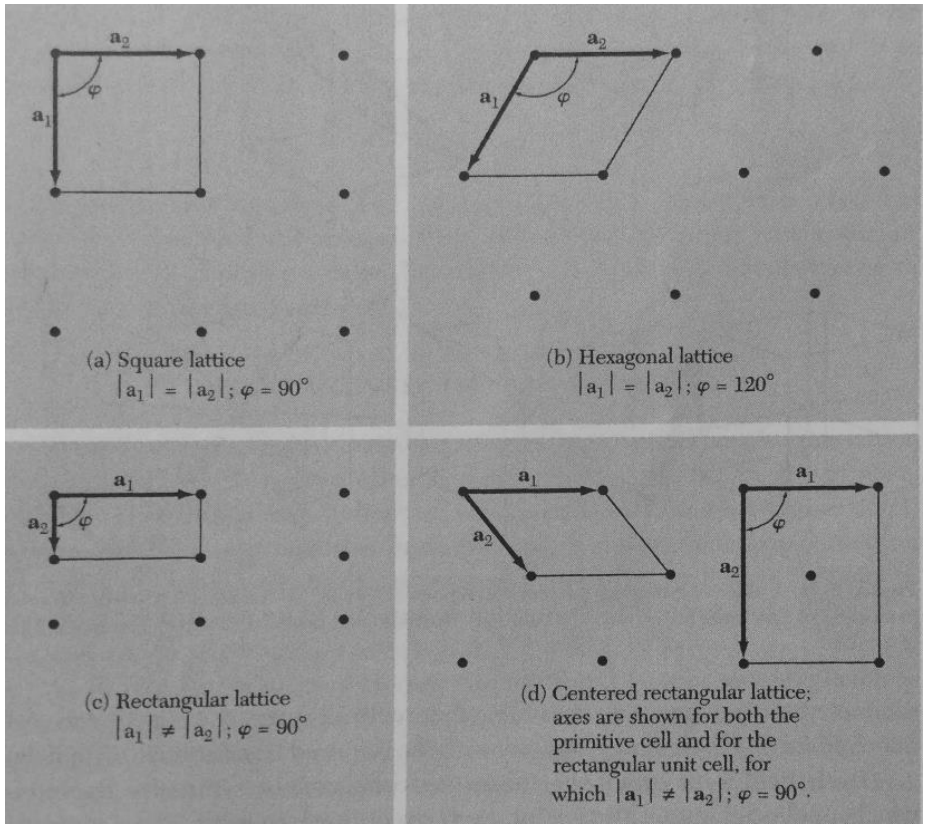
A lattice type is a lattice with special symmetry properties.

Bravais Lattices (2D)

Lattice Type	Restrictions
Square	$a_1 = a_2,\ \phi = 90^\circ$
Hexagonal	$a_1 = a_2,\ \phi = 120^\circ$
Rectangular	$a_1 \neq a_2,\ \phi = 90^\circ$
Centered rectangular	$a_1 \neq a_2,\ \phi = 90^\circ$
	(for the rectangular unit cell)

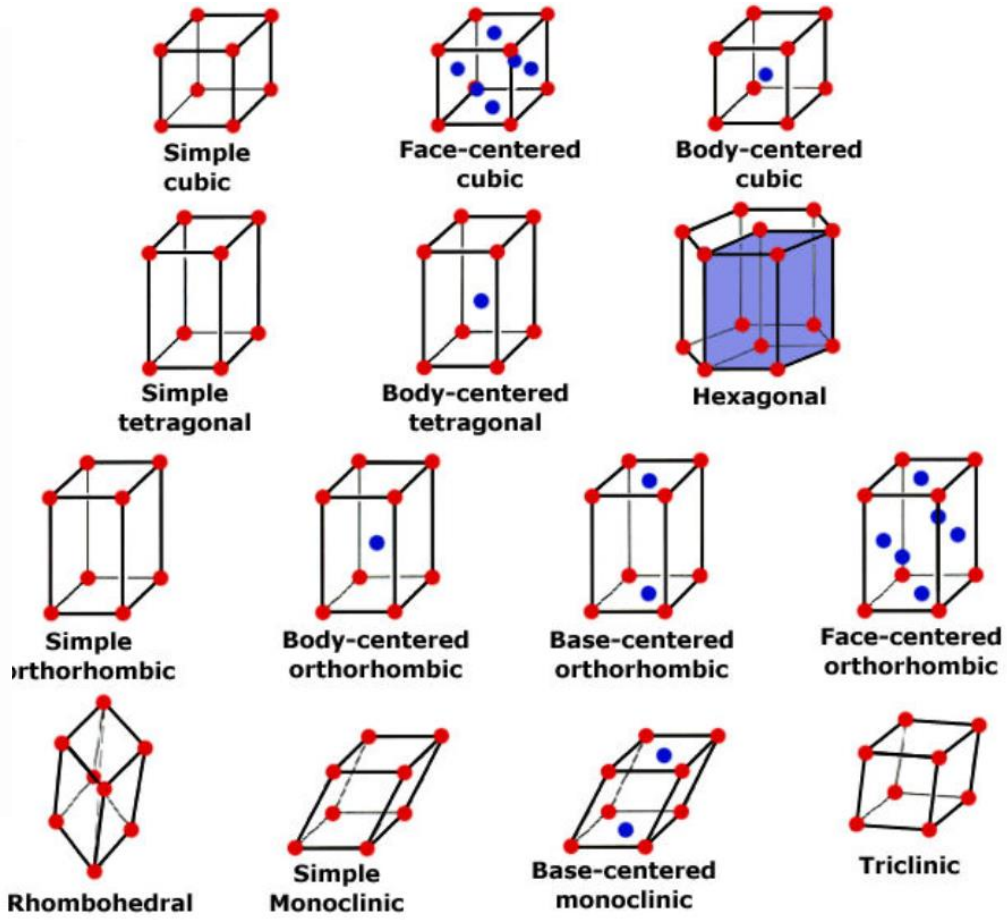




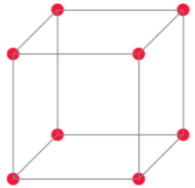
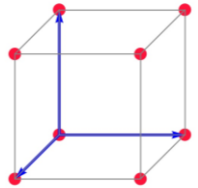
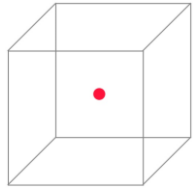
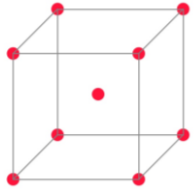
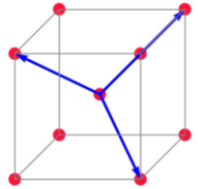
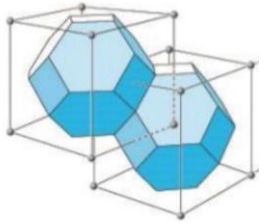
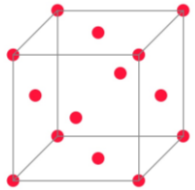
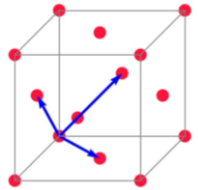
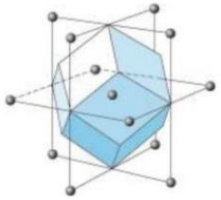


Bravais Lattices (3D)

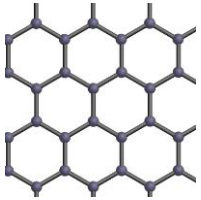
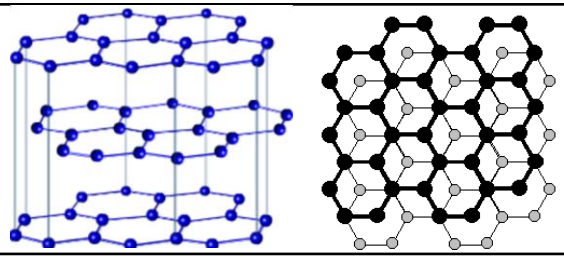
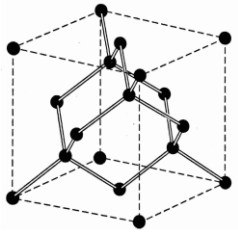
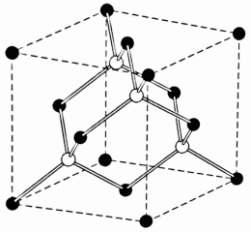
System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90° \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90°$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90°$ $\gamma = 120°$



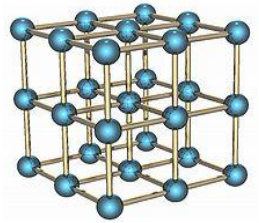
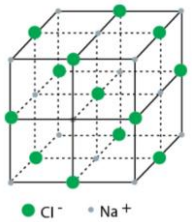
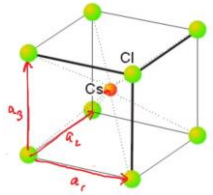
Bravais Lattices (3D): Cubic

	Conventional Cell	Primitive Translation Vectors	Wigner-Seitz Cell
sc			
bcc			
fcc			

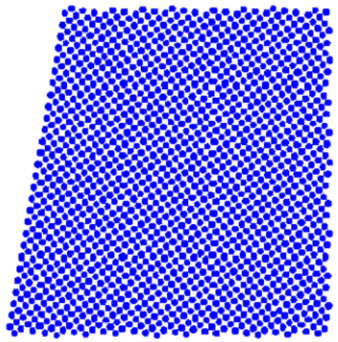
Examples

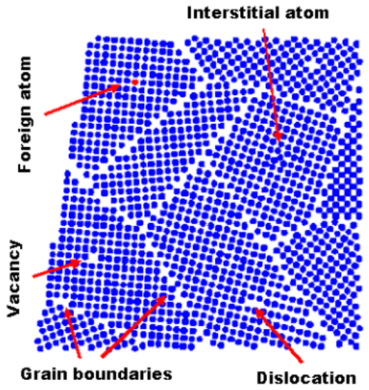
Graphene		Hexagonal Primitive Basis: 2 C atoms
Graphite		Hexagonal Primitive Basis: 4 C atoms
Diamond Structure		Fcc Primitive Basis: 2 C atoms
Cubic Zinc Sulfide Structure		Fcc Primitive Basis: 1 Zn, 1 S atom

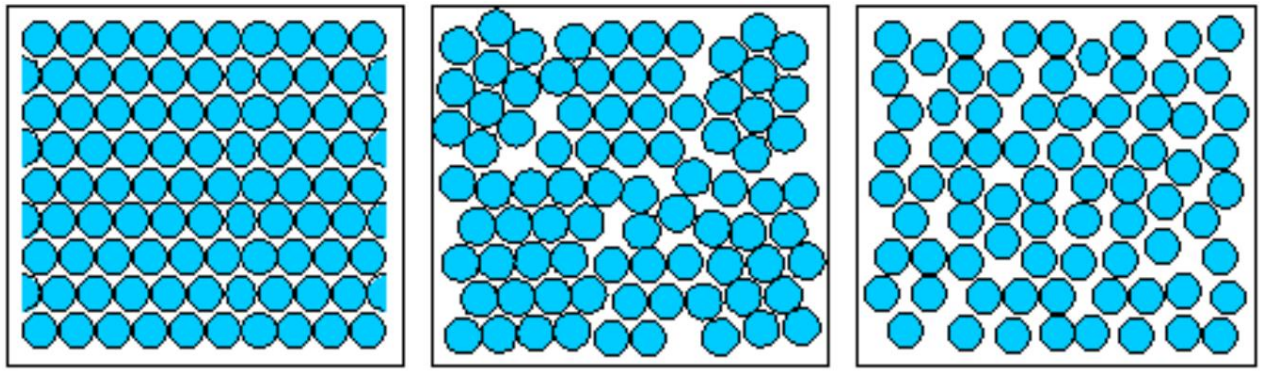
Examples

Alpha-Polonium		Sc Primitive Basis: 1 Po atom
Sodium Chloride Structure		Fcc Primitive Basis: 1 Cl-, 1 Na+ atom
Caesium Chloride Structure		Sc Primitive Basis: 1 Cl, 1 Cs atom

Single Crystal / Polycrystal / Amorphous solid







Single crystal

Periodic across the whole volume.

Polycrystal

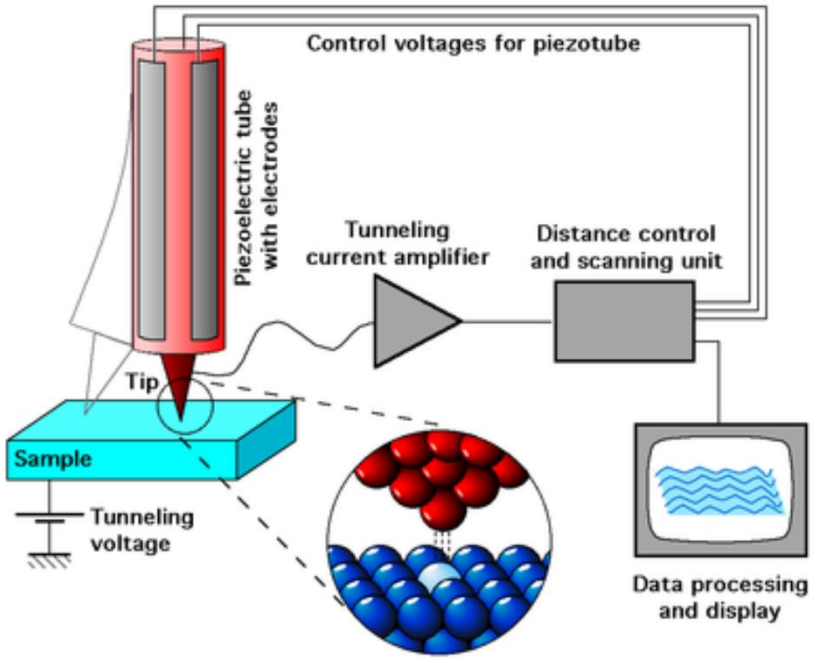
Periodic across each grain.

Amorphous solid

Not periodic.

Measuring Crystal Structures

STM
(Scanning tunneling microscope)



HRTEM
(High-resolution transmission electron microscope)