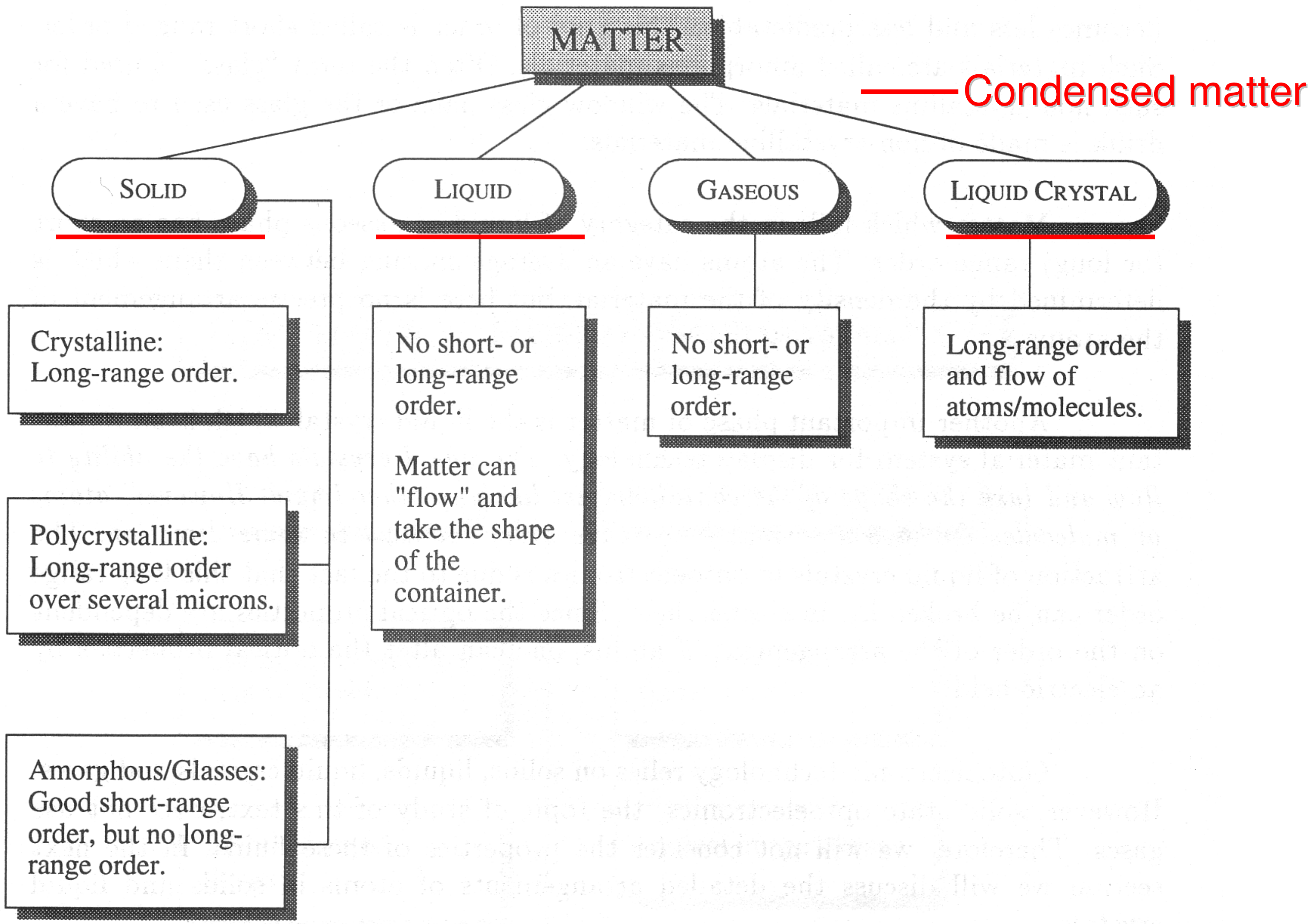
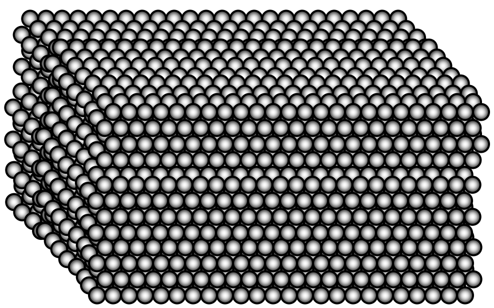
How do atoms condense when they want to minimize energy?

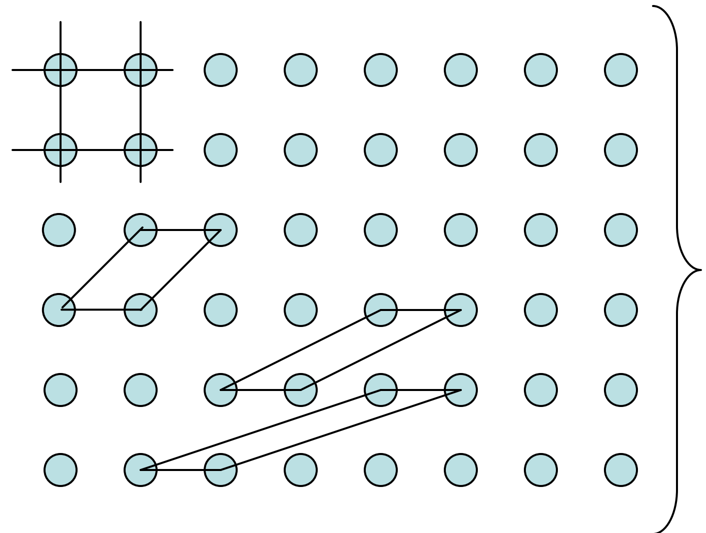
Forms of matter as we know:



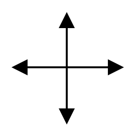
Crystal structures in materials

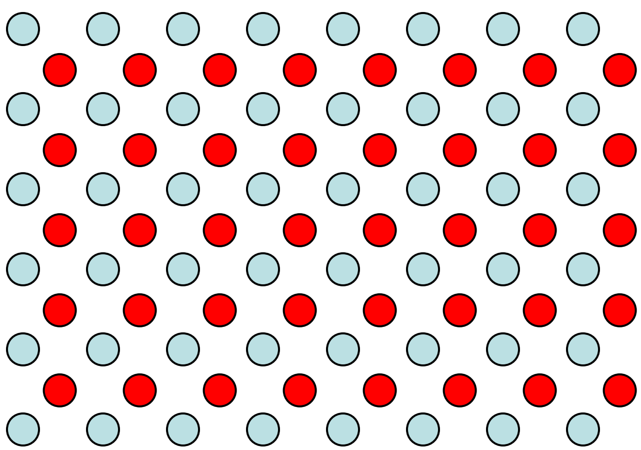
A unique arrangement of atoms that fill space in 3D (Real-life) when repeating (Translational Property)



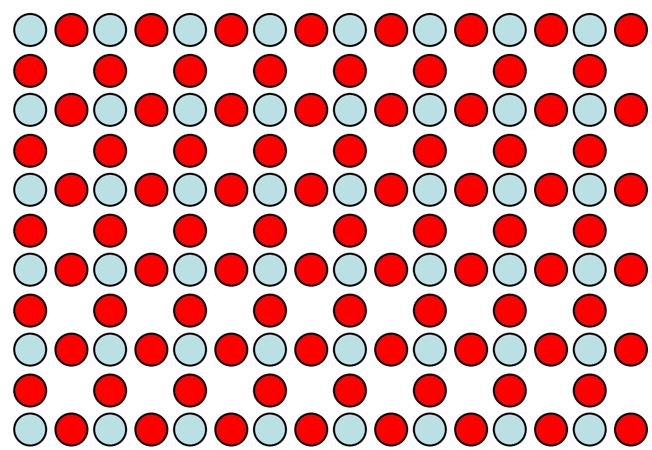


Everytime a unit cell is translated, it must be forming the entire lattice.





2D BCC



2D FCC

Is everything always in a crystalline order?

Abnormal lattice expansion and double periodicity in $La_{0.7}Sr_{0.3}MnO_3$ thin films under electron irradiation

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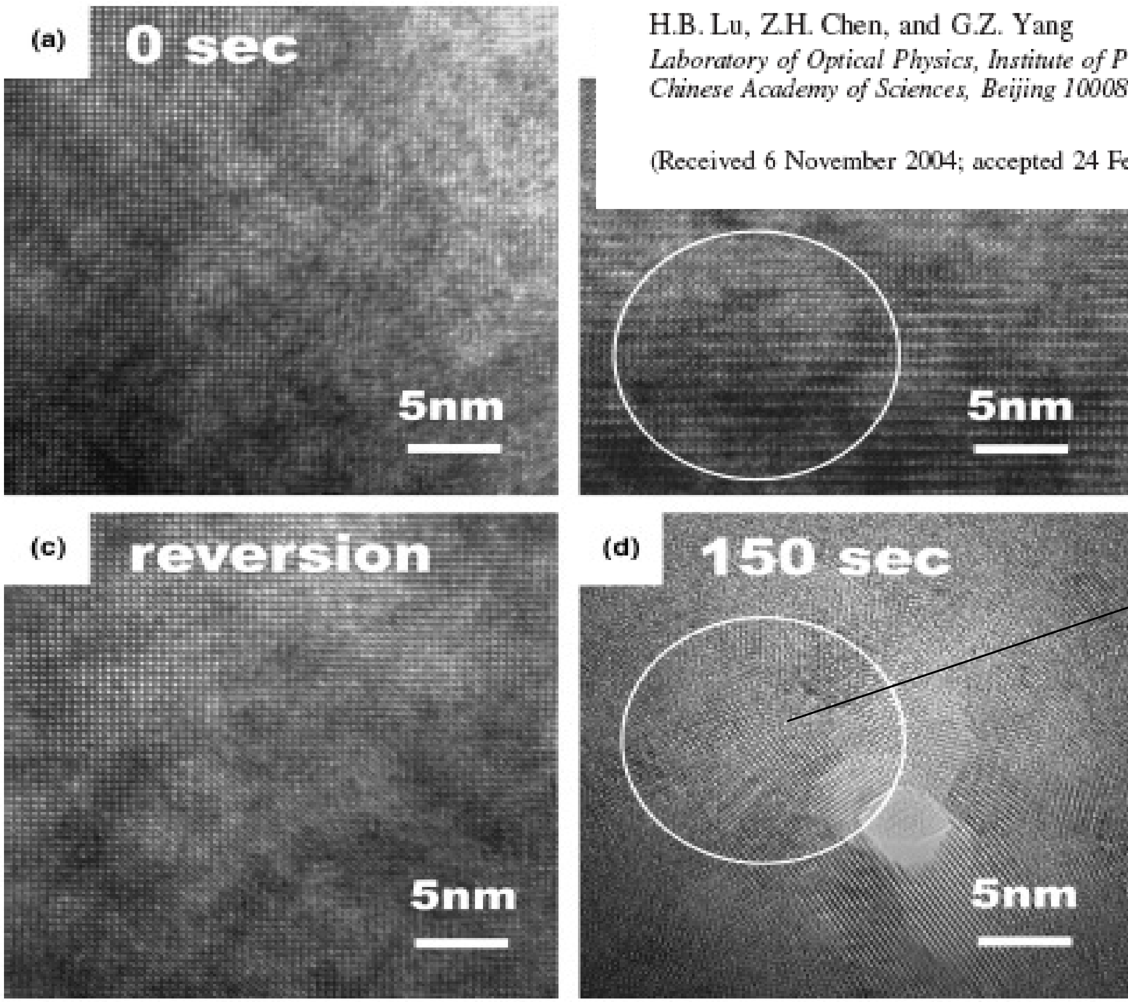
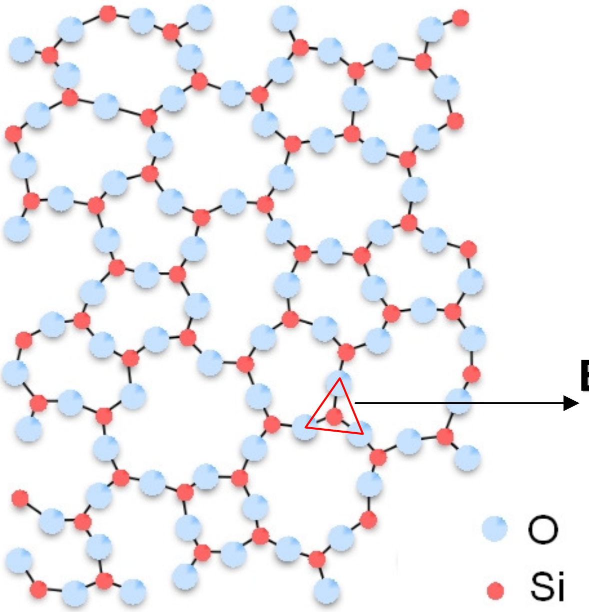


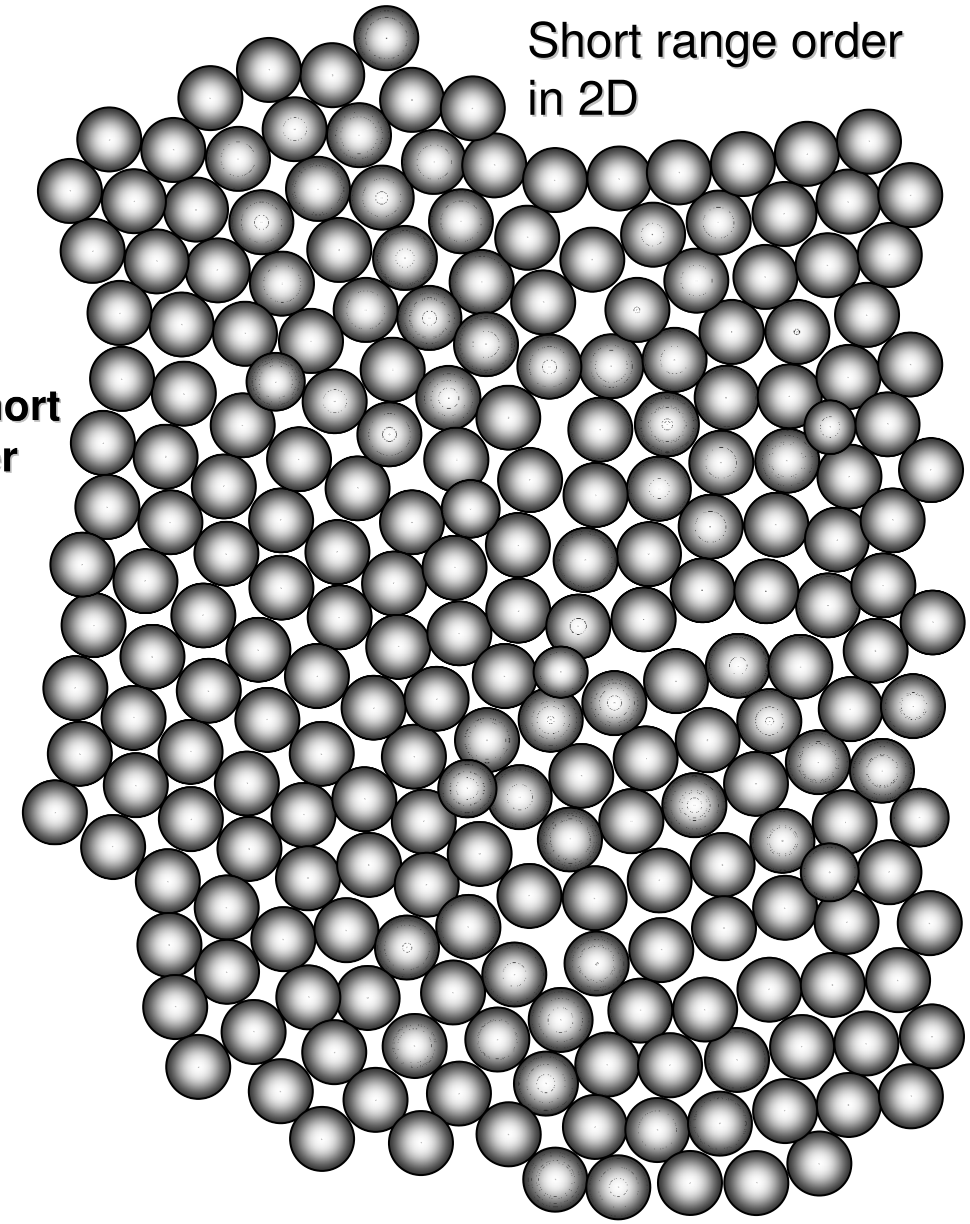
Amorphization under electron bombardment in TEM

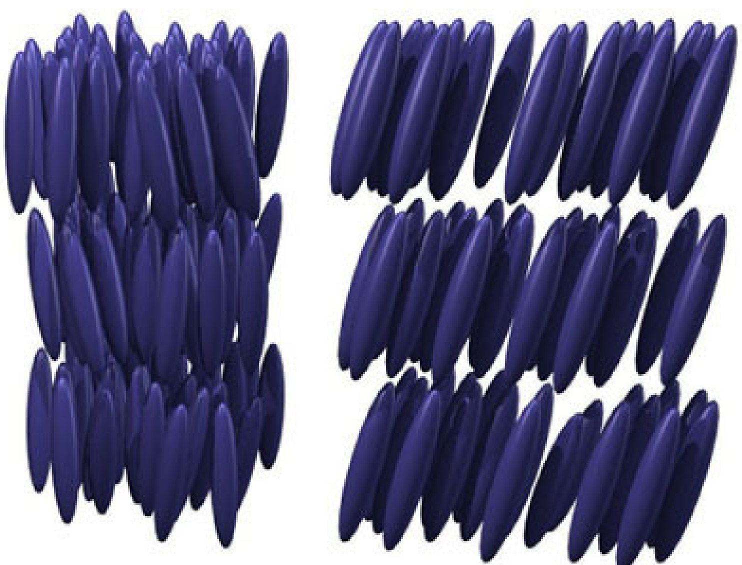


Extremely short range order

Glassy silica (from wikipedia)

Short range order in 2D

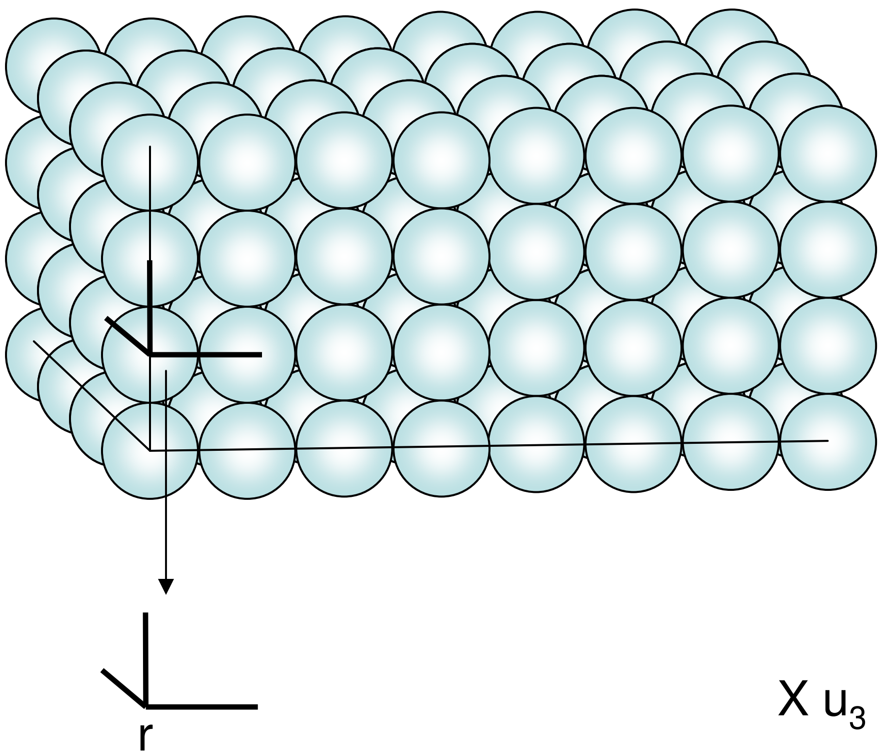




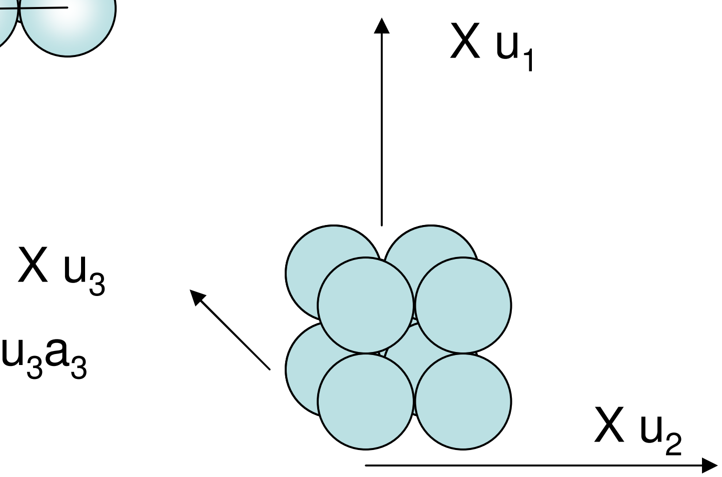
Nematic liquid crystal (orientational long range order)

In 3D, there are seven types of crystal systems that make up 14 Bravais Lattices

Triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic



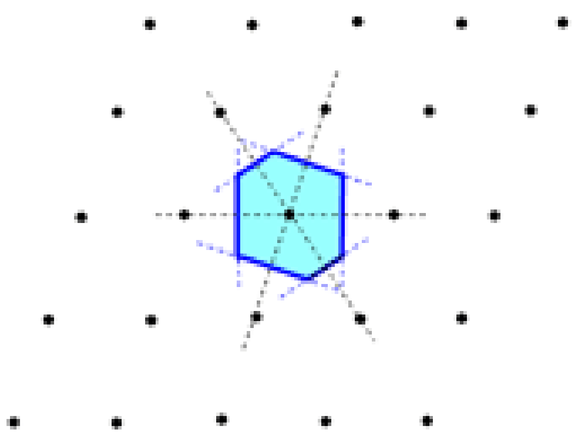
Translation vector = $r^T = r + u_1 a_1 + u_2\, a_2 + u_3 a_3$

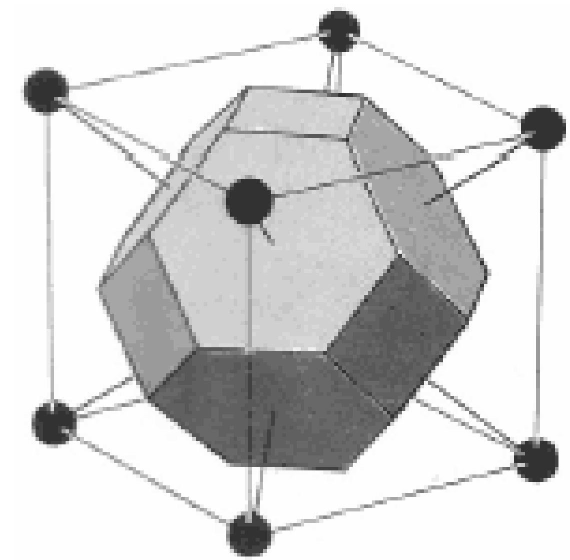


System	Number of lattices	Restrictions on conventional cell axes and singles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^o \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^o$
Tetragonal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

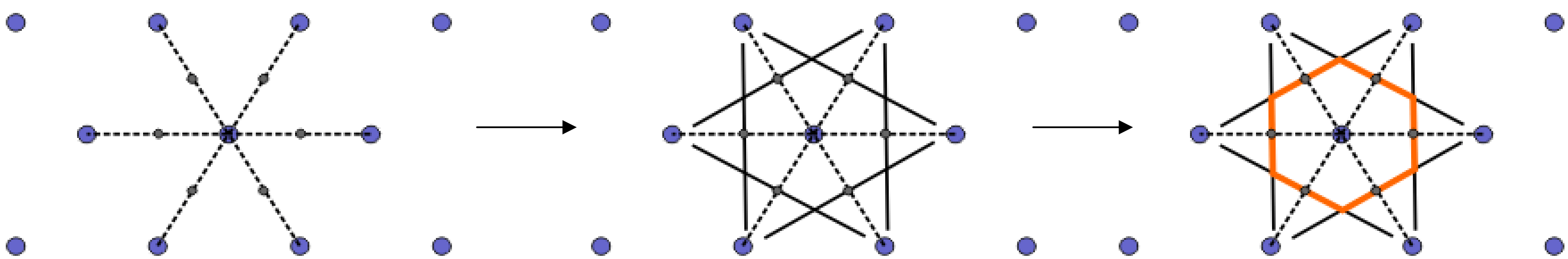
The 14 Bravais lattices and their unit cell characteristics.

The Wigner-Seitz Cell can also be a unit cell





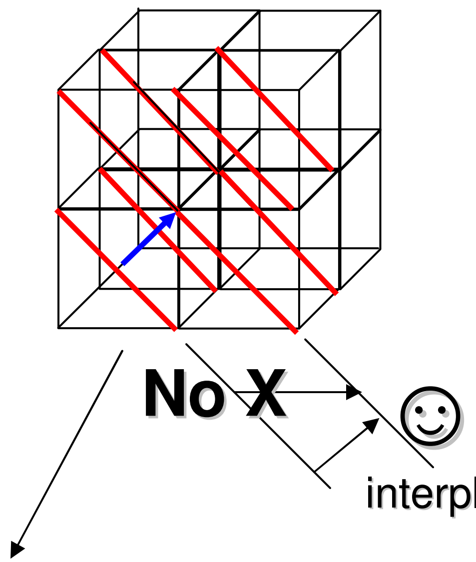
Wigner-Seitz cell for sımple cubic in 3D



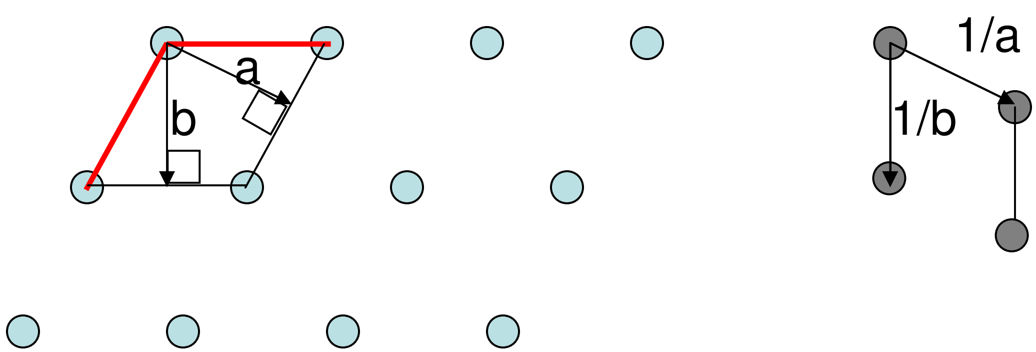
Select a lattice point and draw construction lines to the nearest neighbouring points

Draw lines that perpendicularly bisect the construction lines

The smallest enclosed area represents the Wigner-Seitz cell. Here shown in orange.



We often deal with diffraction data of crystals. A real crystal can be expressed in reciprocal space (space^{-1})



Unit cell in real space

Unit cell in reciprocal space

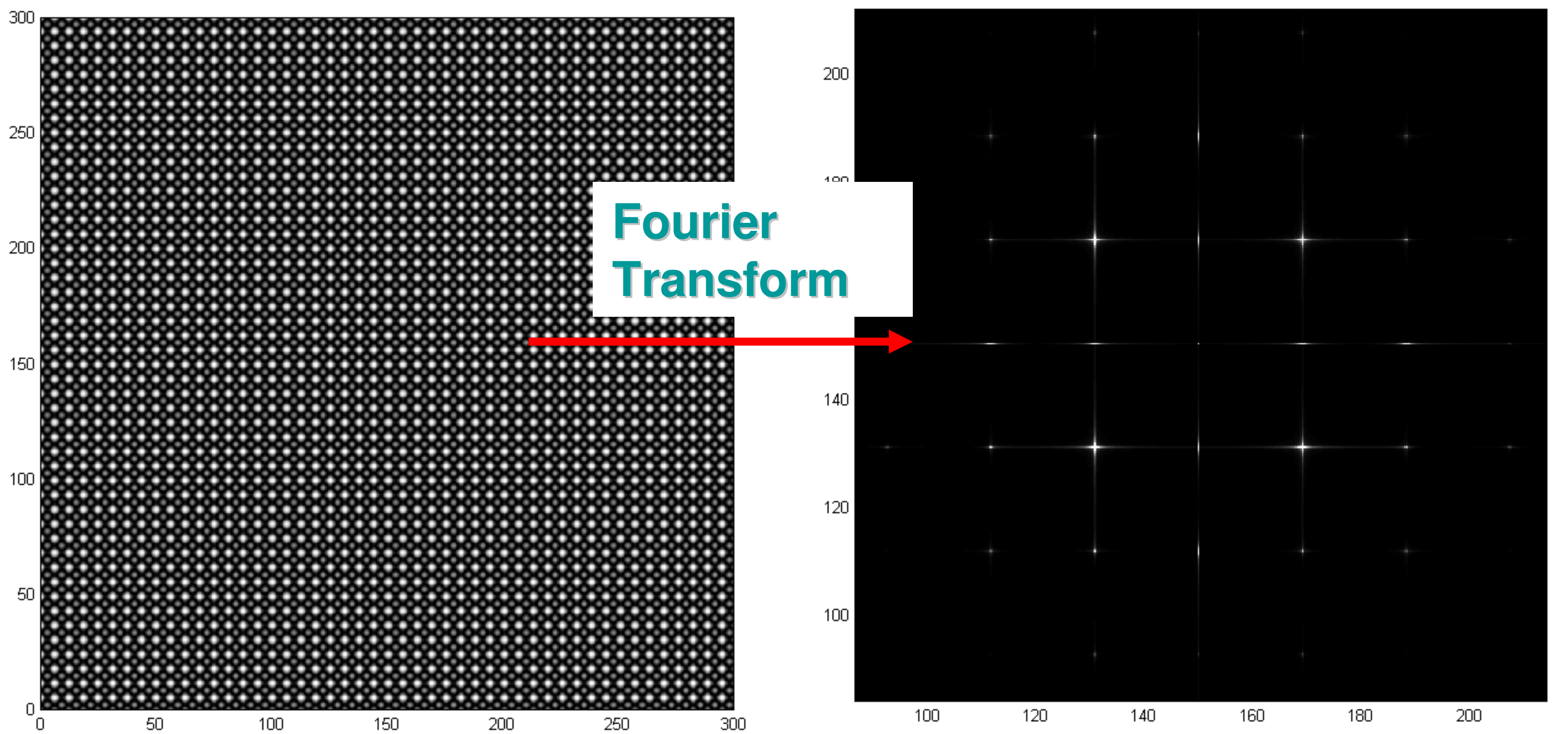
Why deal with the reciprocal lattice?

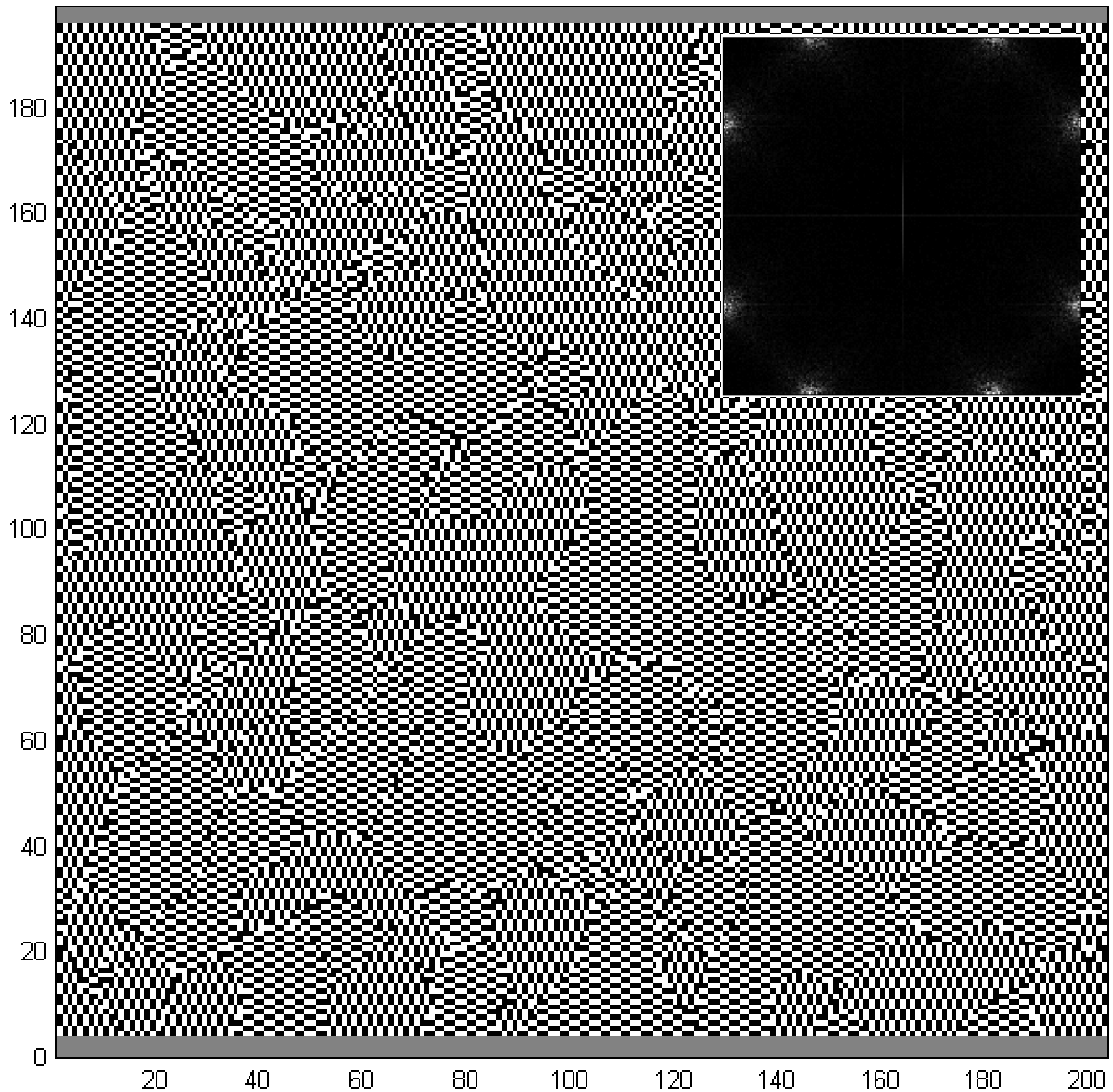
-Easy to deal with points rather than planes.

-Every point represents a set of planes (a period that exists in your crystal).

-Diffraction experiments yield the reciprocal lattice (It is the Fourier transform of a crystal – Believe it or not but nature takes the Fourier transform of your sample when carrying out, for instance, electron diffraction experiments in TEM or XRD).

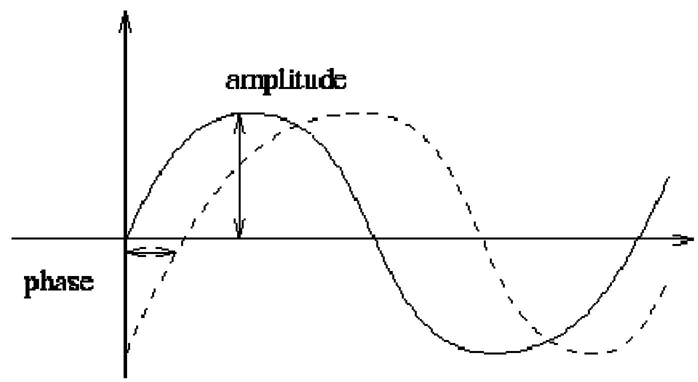
-Very useful when talking about electrons in a crystal (coming soon).





Bragg's equation:

$n\lambda = 2d\sin\theta$



Diffracted waves have to be in phase! (To see a "net reflected" wave)

A crystal can be thought of being a periodic function in a given space.

What is meant by this?

n(r+T) = n(r)

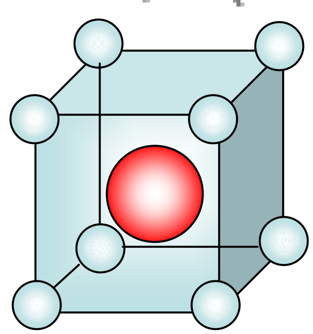
$$\mathbf{b_1} = 2\pi \frac{\mathbf{a_2} \times \mathbf{a_3}}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})}$$

$\mathbf{a_2} \times \mathbf{a_3}$ → Area of parallelogram

$\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})$ Volume of the unit cell

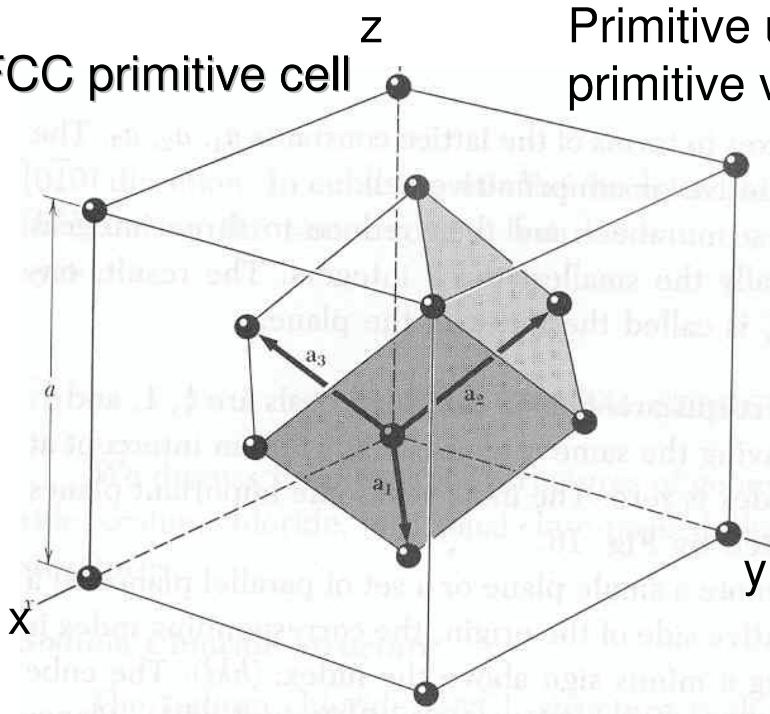
$$\mathbf{b_2} = 2\pi \frac{\mathbf{a_3} \times \mathbf{a_1}}{\mathbf{a_2} \cdot (\mathbf{a_3} \times \mathbf{a_1})}$$

$$\mathbf{b_3} = 2\pi \frac{\mathbf{a_1} \times \mathbf{a_2}}{\mathbf{a_3} \cdot (\mathbf{a_1} \times \mathbf{a_2})}.$$



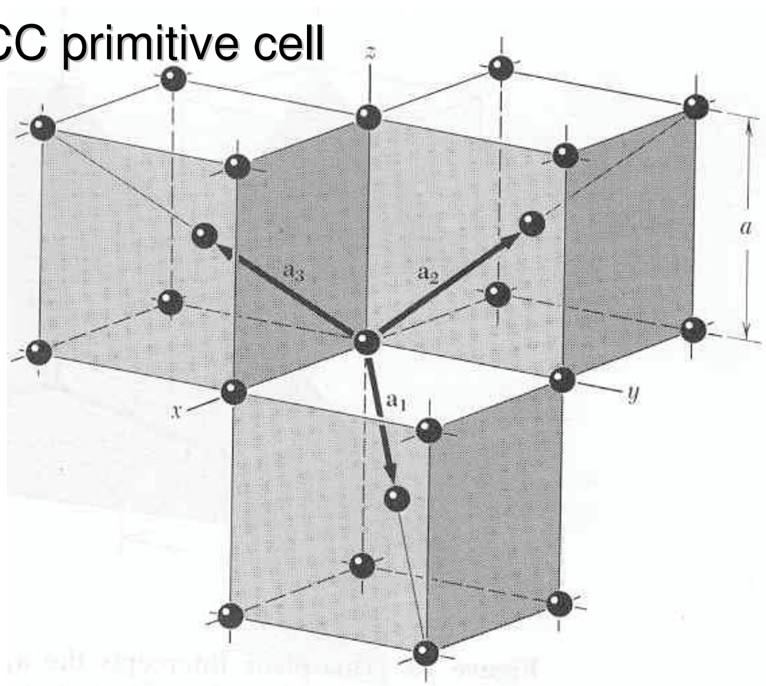
Primitive unit cells needed for the reciprocal primitive vectors

FCC primitive cell



$$\begin{cases} \mathrm{a}_1 = \frac{1}{2}a(\mathrm{x}+\mathrm{y}) \\ \mathrm{a}_2 = \frac{1}{2}a(\mathrm{y}+\mathrm{z}) \\ \mathrm{a}_3 = \frac{1}{2}a(\mathrm{z}+\mathrm{x}) \end{cases}$$

BCC primitive cell



$$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(-\mathbf{x}+\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{x}-\mathbf{y}+\mathbf{z}) \end{cases}$$

From International Union of CRYSTALLOGRAPHY (IUC)

2.1 Definition

Let **a**, **b**, **c** be the basic vectors defining the unit cell of the direct lattice. The basic vectors of the reciprocal lattice are defined by:

$$\mathbf{a}^* = \frac{(\mathbf{b} \wedge \mathbf{c})}{(\mathbf{a}, \mathbf{b}, \mathbf{c})} \quad \mathbf{b}^* = \frac{(\mathbf{c} \wedge \mathbf{a})}{(\mathbf{a}, \mathbf{b}, \mathbf{c})} \quad \mathbf{c}^* = \frac{(\mathbf{a} \wedge \mathbf{b})}{(\mathbf{a}, \mathbf{b}, \mathbf{c})}$$

"The modulus of **a*** is equal to the ratio of the area of the face *OBCG* opposite to **a** to the volume of the cell built on the three vectors **a, b, c**. Referring to Figure below, we may write":

$$\mathbf{a}^* = 1/OA' \quad \mathbf{b}^* = 1/OB' \quad \mathbf{c}^* = 1/OC'$$

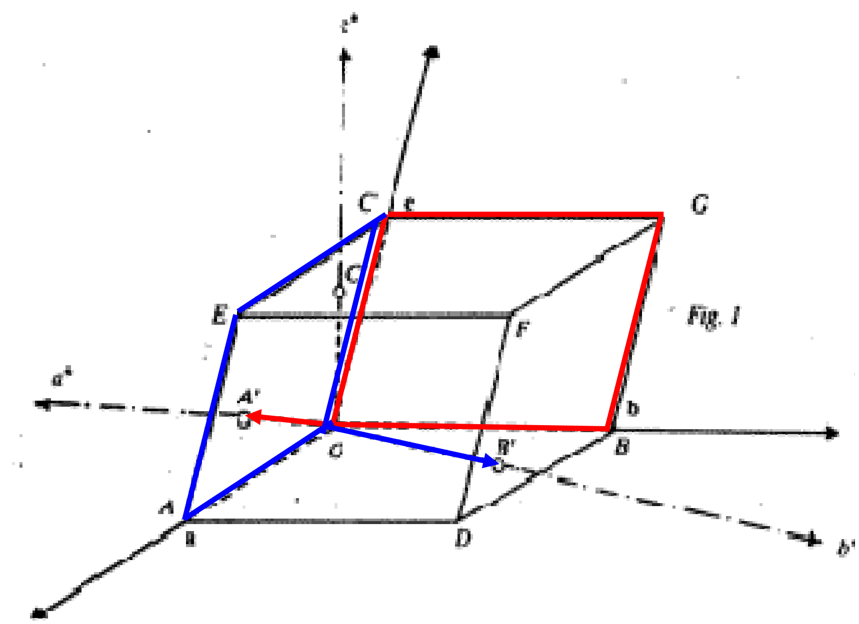
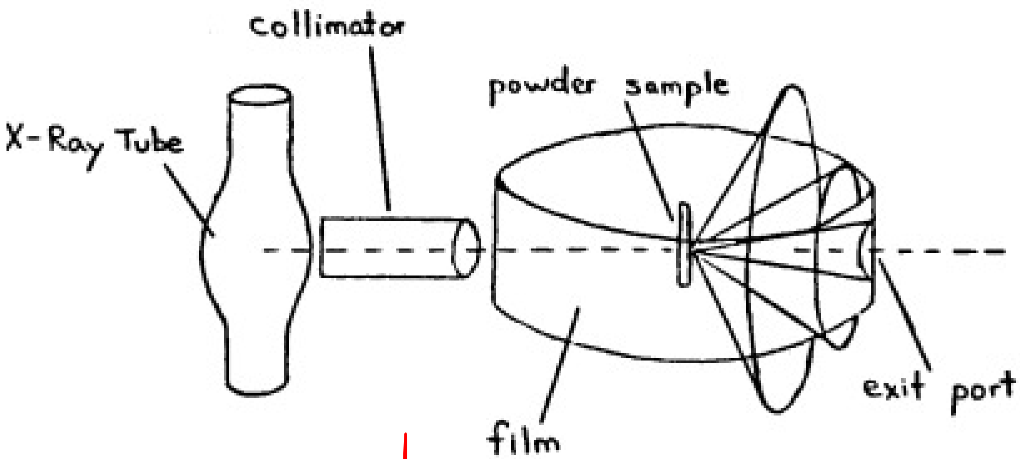
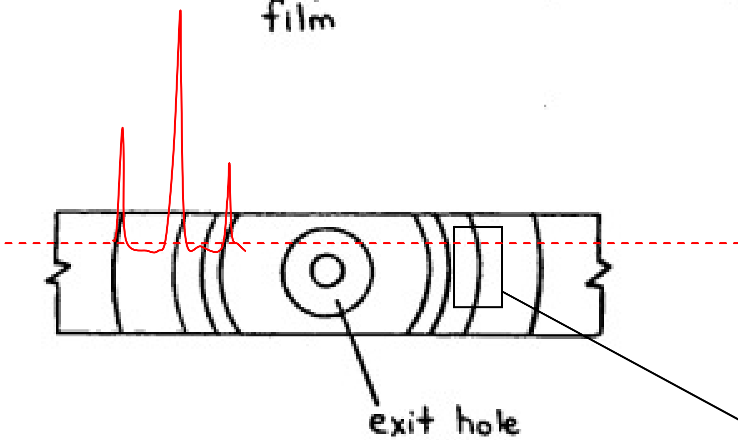


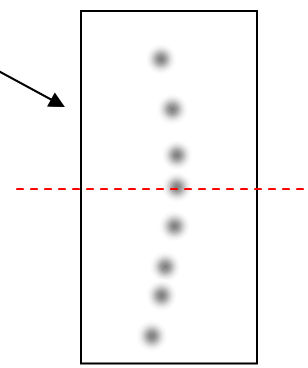
Fig. 1

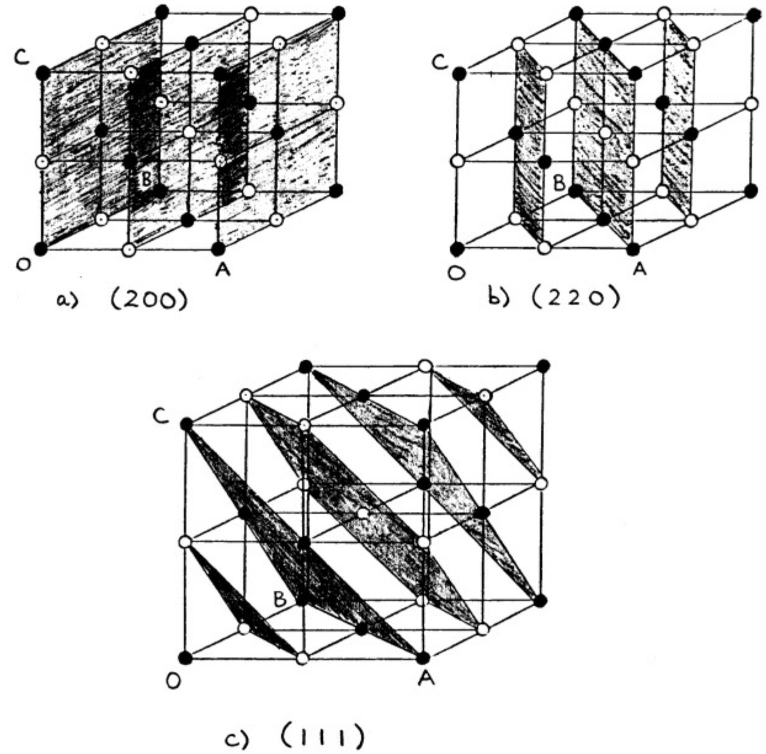
Again, why did we bother with the reciprocal lattice?

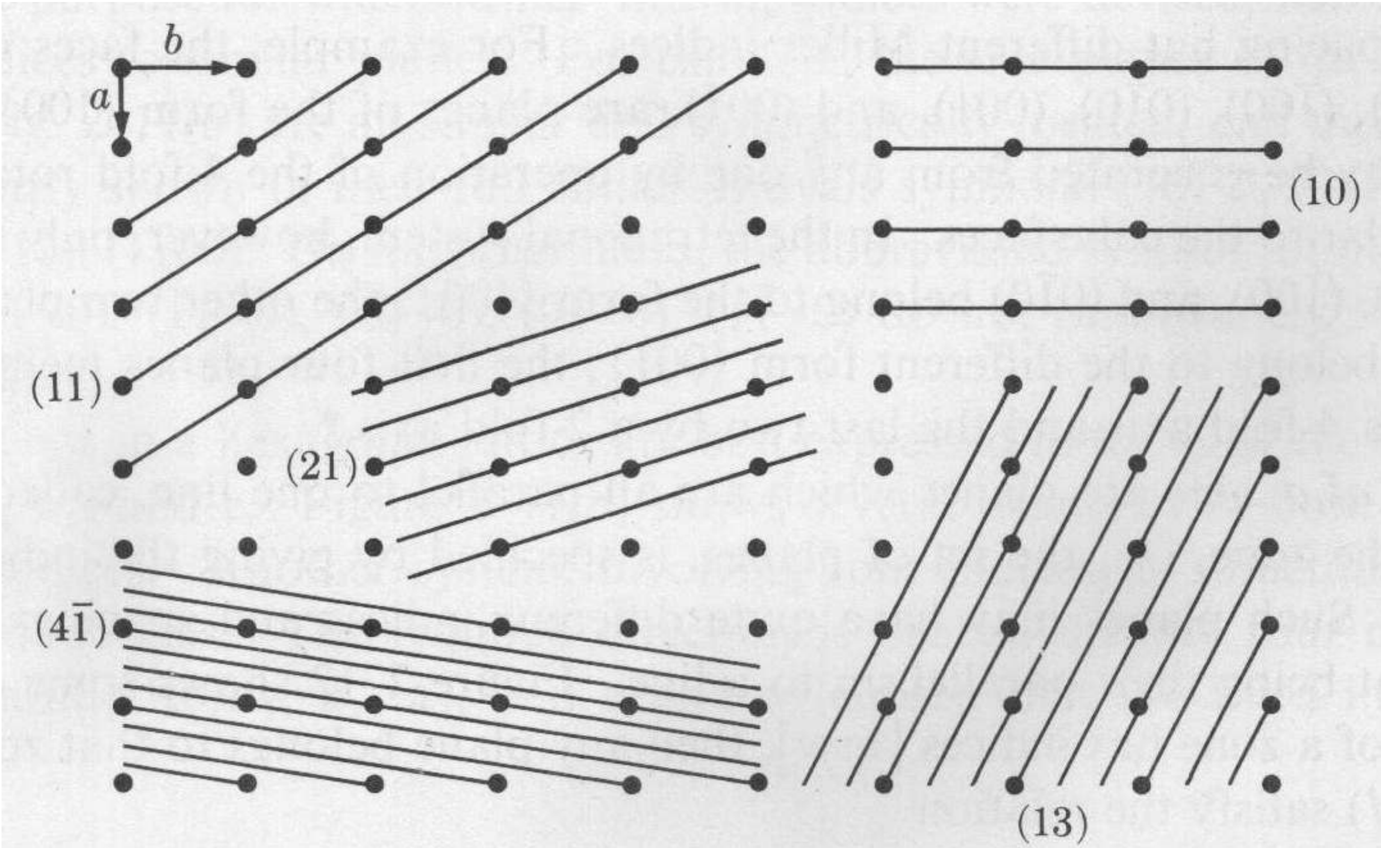




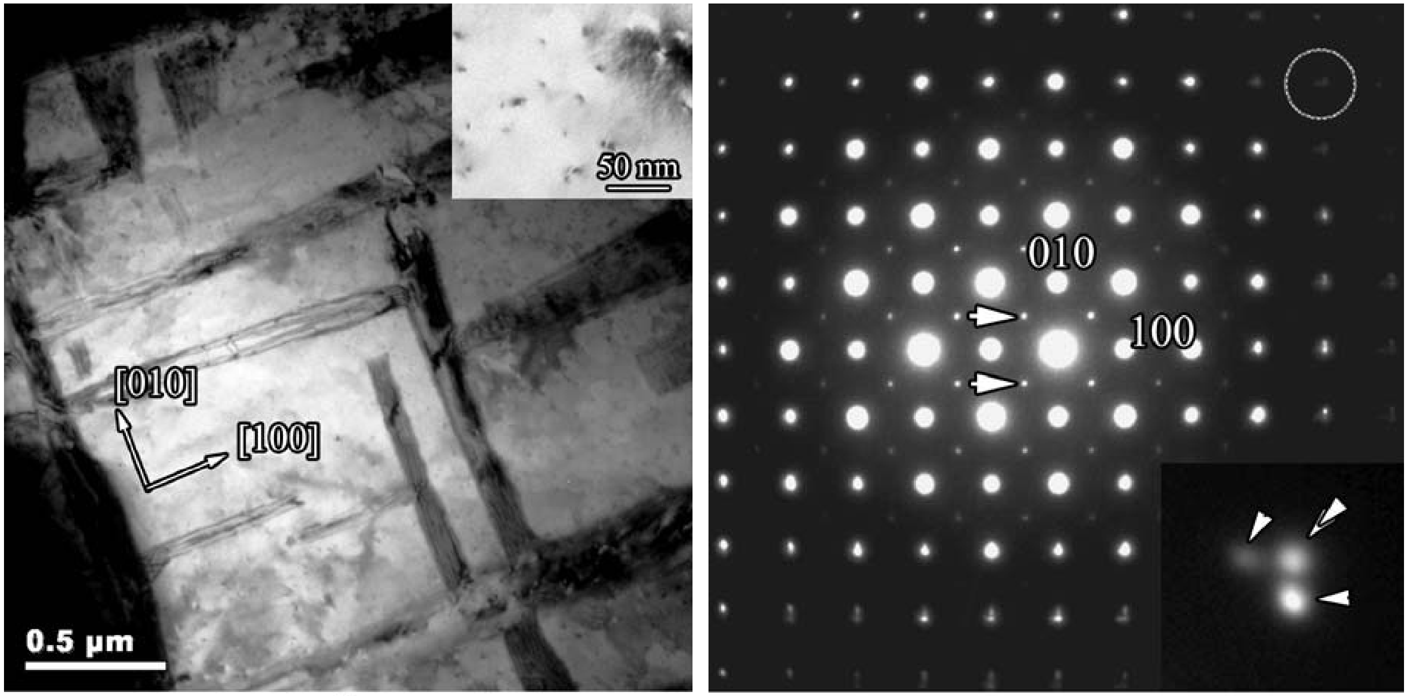
Diffraction Pattern on Film
After Exposure



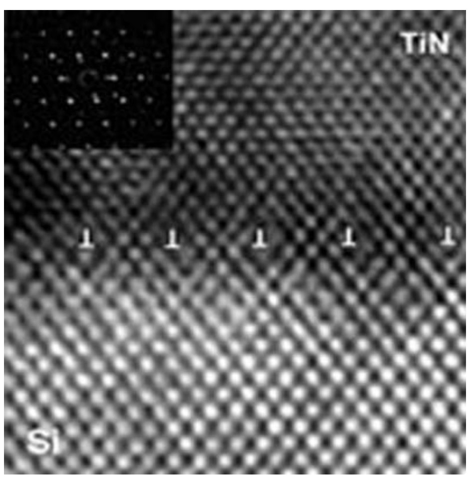




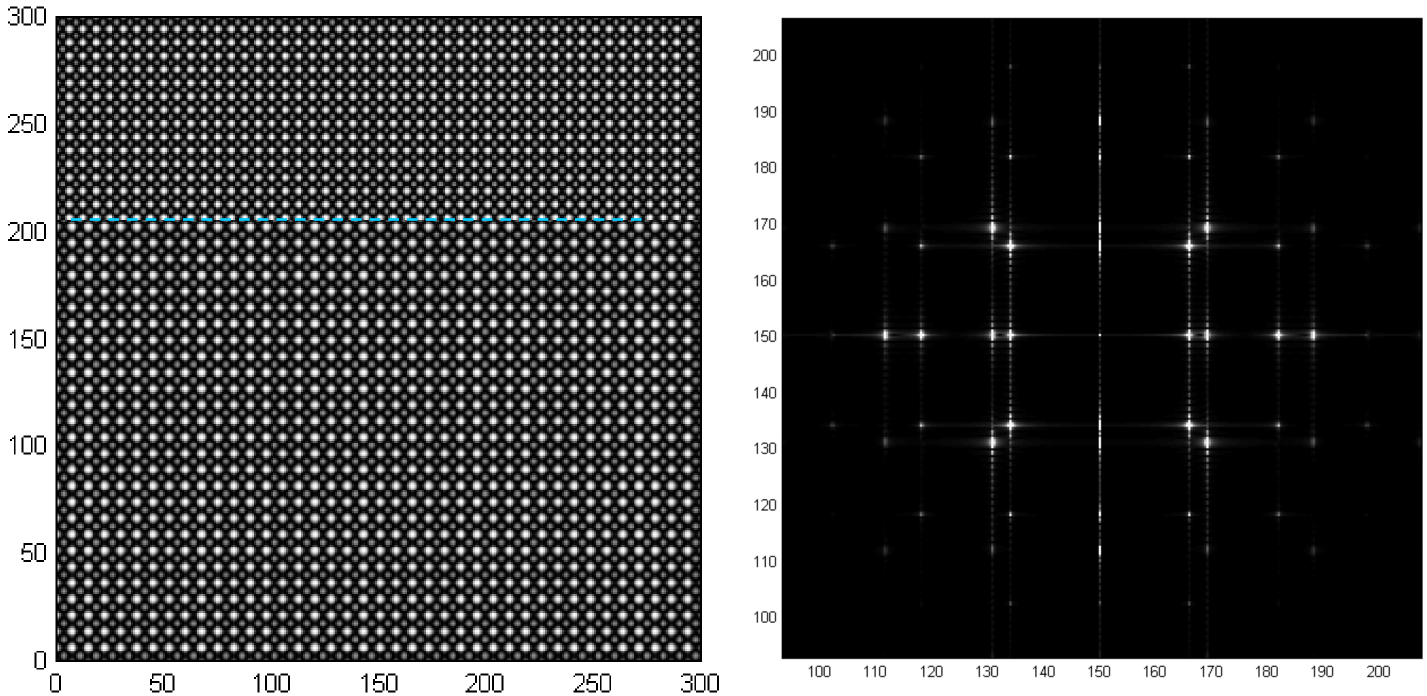
Some examples to sets of planes in a real 2D lattice.



TEM image and electron diffraction pattern from a piezoelectric thin film. How to guess any secondary formations in the structure that might detoriate or enhance your material?

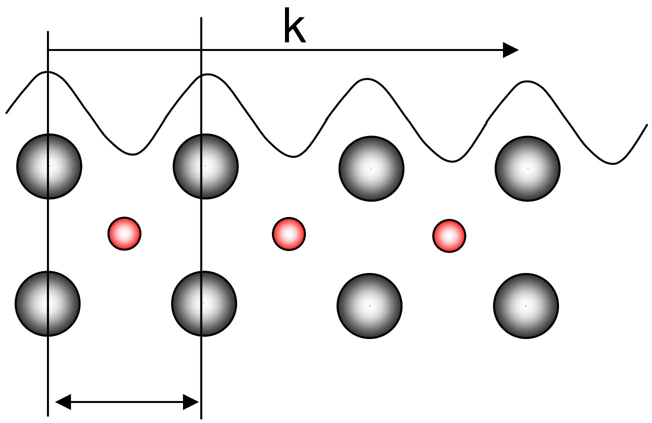


Structural interpretation of a high-k layer grown on Si. Note the dislocations at the interface that form as a result of ‘lattice misfit’.



Matching of epitaxy of semiconductor layers with misfit.

An electron propagating in a crystal with wavelength a ($k = 2\pi/\lambda$)

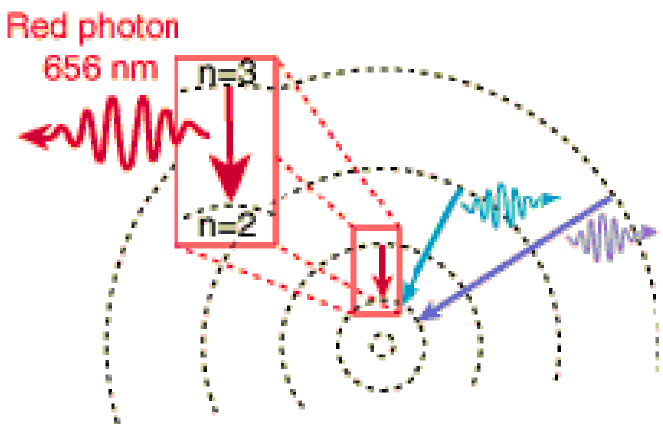


a: lattice constant

$$\boxed{k \equiv \frac{2\pi}{\lambda}} = \frac{2\pi\nu}{v_p} = \frac{\omega}{v_p} = \frac{E}{\hbar c}$$

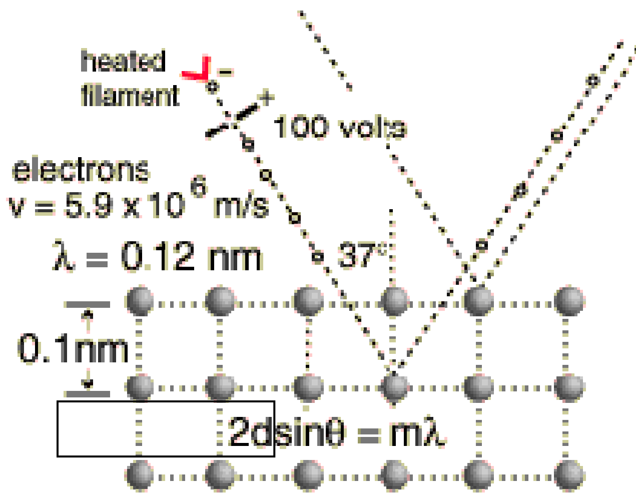
Wave vector: Commonly used in discussing energies of electrons

Larger the k, higher the energy of the electron (inverse of wavelength is quite convenient when representing energies)



$$E_n = \frac{-13.6\ \text{eV}}{n^2}$$

Hydrogen Energy Levels



Electron Diffraction