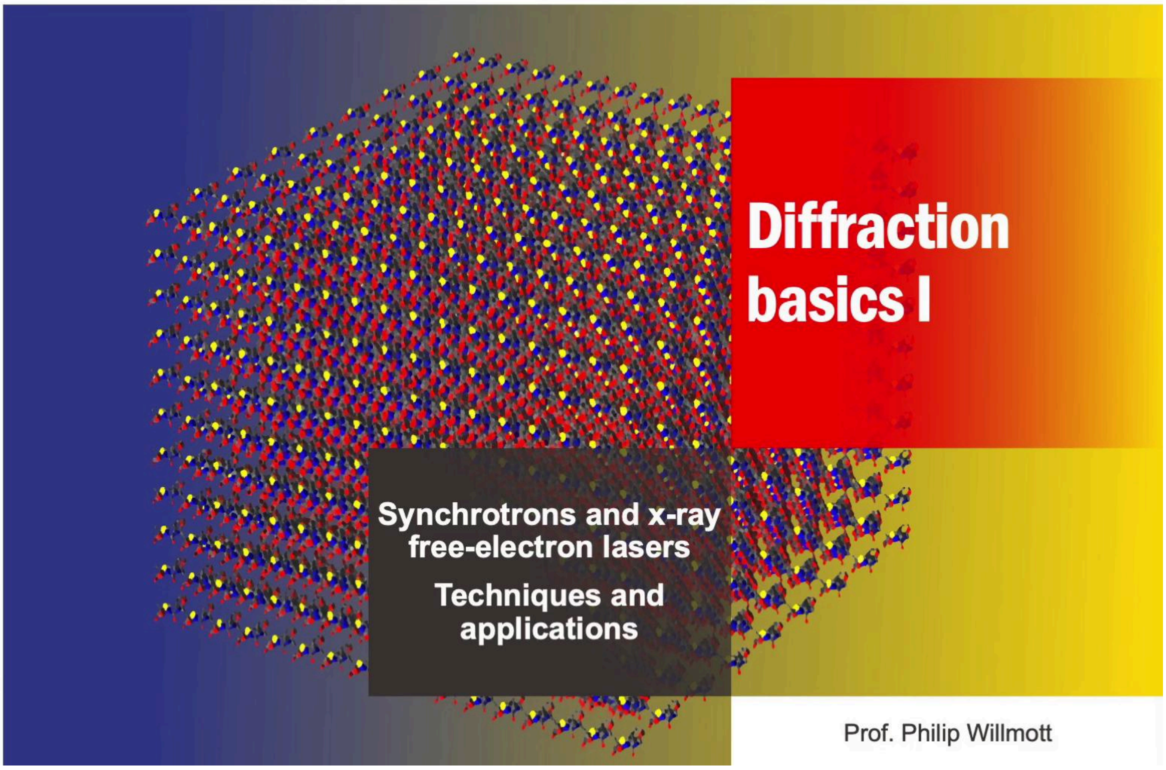
EPFL



École polytechnique fédérale de Lausanne

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Video

EPFL

Contents and objectives of this video

- Description of crystals
- The basis
- Translation vectors
- The unit cell and lattice constants
- Crystal planes and the Miller indices

We begin the first video of the second section of week one with a description of crystals. We concern ourselves here with the classical definition of crystals, invoking translational symmetry, although it should be noted that a new class of materials, quasicrystals, were discovered in the 1980s, which also exhibit sharp diffraction patterns, but which never repeat themselves through translational symmetry. We discuss the so-called basis and Bravais lattice, the unit cell and lattice constants, and the definition of crystal planes via the so-called Miller indices.

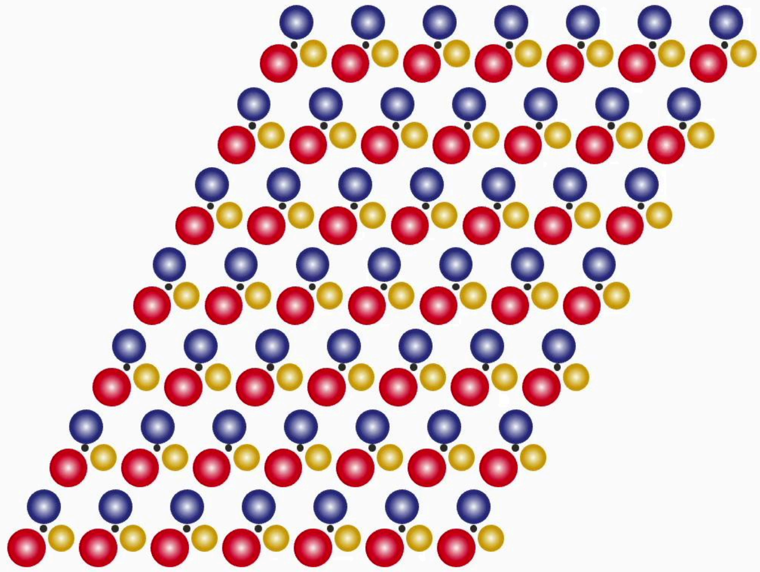
Notes

Summary

0m 05s

What is a crystal?

- Bravais lattice
- ⊗ Basis
- = Crystal



So what is a crystal? A crystal is defined as consisting of a framework of evenly spaced points in space known as the Bravais lattice, plus a so-called basis of atomic positions and types associated with each Bravais lattice point. Mathematically, the convolution of the Bravais lattice with the basis generates a physical crystal.

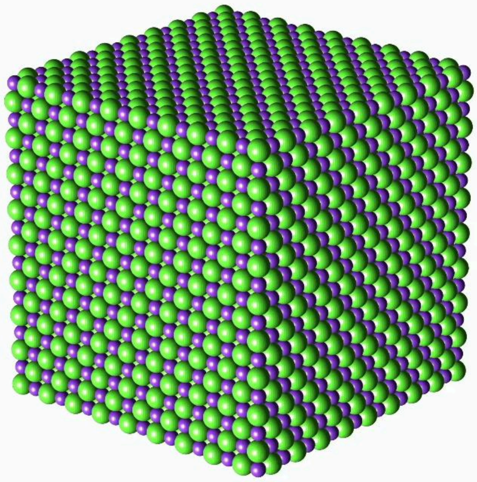
Notes

Summary

0m 45s

What is a crystal?

- Bravais lattice
- ⊗ Basis
- = Crystal



Extension of the 2D schematic shown in the previous slide to three dimensions is trivial, as shown here for the face-centred cubic structure of rock salt.

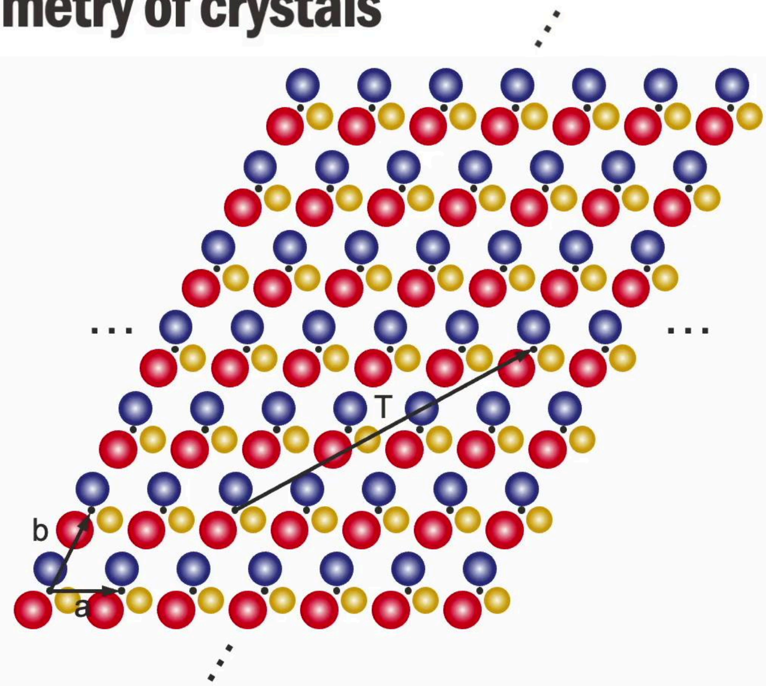
Notes

Summary

1m 14s

Translational symmetry of crystals

- Bravais lattice
- ⊗ Basis
- = Crystal



Translational symmetry T = ma + nb

The separation in three dimensions between adjacent Bravais lattice points is defined by the three lattice vectors a, b, and c, of which a and b are shown here in this two-dimensional representation. The translational symmetry of crystals means that they remain invariant under a translation by a vector t, which is equal to the vector sum of integer multiples of the lattice vectors. In the two-dimensional example shown here, t is equal to 3a plus 2b.

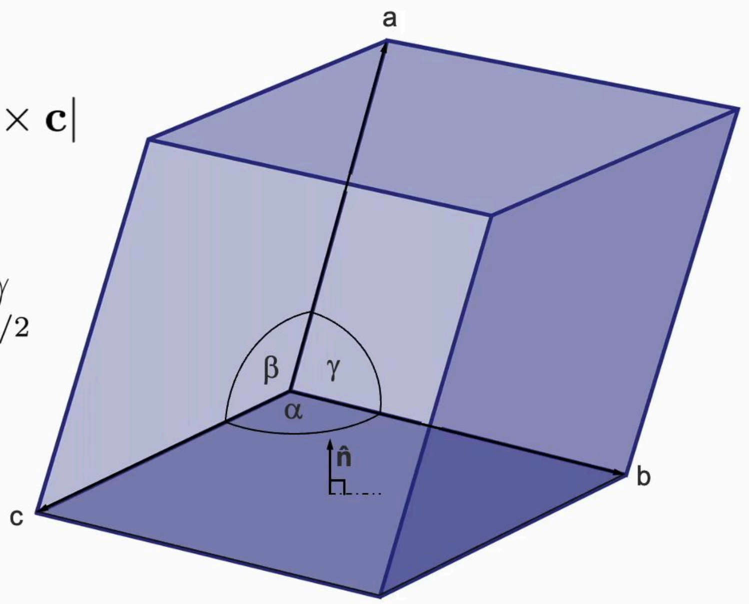
Notes

Summary

1m 28s

Unit cells and lattice constants

- Volume of unit cell $V_c = |\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}|$
- $V_c = abc\left(1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma\right)^{1/2}$



The volume of a unit cell, that is, the repeat unit in three-dimensional space, is the cross product of the area defined by the scalar product of the two vectors b and c, with the vector a to produce the repeat volume. In this vector algebra, the relative angular orientations are implicit. The other three lattice constants are the angles alpha, beta, and gamma, where alpha is the angle opposite a, subtended by b and c, and so forth. Armed with this information, the unit cell volume is given by the expression shown here. Note that in high-symmetry cases such as cubic or orthorhombic crystals, this expression becomes much simpler as all terms involving cosine 90 fall away, 90 degrees, that is.

Notes

Summary

2m 08s

Crystal planes and Miller indices

- Find the intercepts of the crystal plane on the crystal axes in units of their respective lattice constants a, b, and c
- Take the reciprocals of these numbers and then reduce these to the smallest three integers that have the same ratio. The result (hkl) are the Miller indices of that plane

A lattice plane, or more accurately, a family of parallel lattice planes intersects with the Bravais lattice at three non-collinear points that are rational fractions of the lattice vectors that define that Bravais lattice. The integers defining these fractions are the so-called Miller indices. To determine these for a given crystal plane, one needs to find their intercept on the crystal axes, expressed in units of their respective lattice constants a, b, and c. One then takes the inverse of these and then reduce them to the smallest three integers that have the same ratio. These integers, labelled h, k, and l, are the Miller indices.

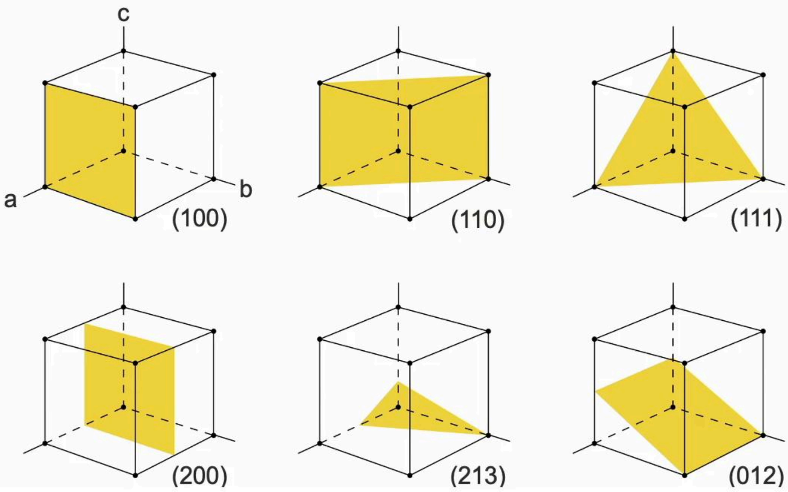
Notes

Summary

3m 10s

Crystal planes and Miller indices

- Find the intercepts of the crystal plane on the crystal axes in units of their respective lattice constants a, b, and c
- Take the reciprocals of these numbers and then reduce these to the smallest three integers that have the same ratio. The result (hkl) are the Miller indices of that plane



In this first example, the 1, 0, 0 plane intersects a at h equals 1, but never intersects b or c. This implies that k and l must equal 0 as b divided by 0 and c divided by 0 equal infinity, the distance required before b and c are intersected by the 1, 0, 0 plane. They never do. Using similar arguments, the top, middle, and top-right examples are clearly the 1, 1, 0 and the 1, 1, 1 planes, respectively. Bottom left shows the 2, 0, 0 because in the a direction, the plane crosses a at a upon 2. In the bottom middle example, the intersection points are 1/2, 1/3, and 1, and hence, this is the 2, 1, 3 plane. The last example is the 0, 1, 2 plane.

Notes

Summary

4m 05s

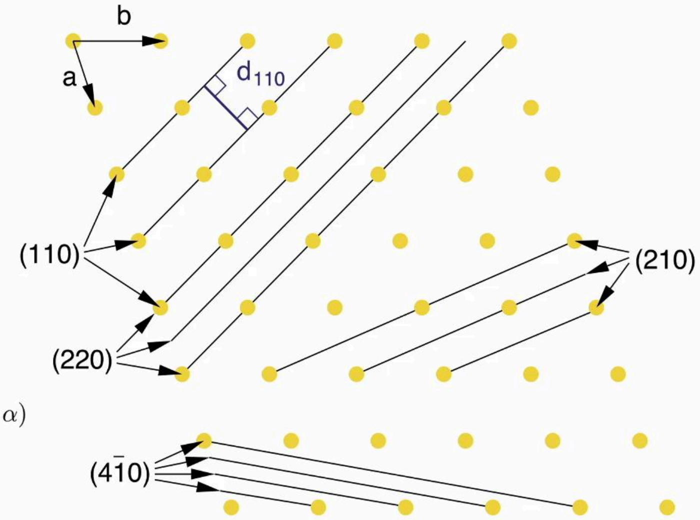
Crystal planes and Miller indices

- Separation between parallel and adjacent (hkl) planes = d_{hkl}

  - $$d_{hkl} = \frac{X}{Y}$$

  - $$X = \left[1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\,\cos\beta\,\cos\gamma\right]^{1/2}$$

  - $$Y = \left[\left(\frac{h}{a}\right)^2 \sin^2\alpha + \left(\frac{k}{b}\right)^2 \sin^2\beta + \left(\frac{l}{c}\right)^2 \sin^2\gamma - \frac{2kl}{bc}(\cos\alpha - \cos\beta\,\cos\gamma) - \frac{2lh}{ca}(\cos\beta - \cos\gamma\,\cos\alpha) - \frac{2hk}{ab}(\cos\gamma - \cos\alpha\,\cos\beta)\right]^{1/2}.$$



The separation between crystallographic planes is given by the lattice constants a, b, c, alpha, beta, and gamma, plus the Miller indices, h, k, l, according to the expressions shown here. Again, although these seem complex for the general case, for a so-called triclinic crystal which exhibits the lowest symmetry, things become much simpler for those cases where one or more angles are right angles and/or two or more of a, b, and c are equal to one another. Examples of families of four different crystal planes in two dimensions are shown on the right-hand side.

Notes

Summary

5m 08s

In the next video...

In the next video, we will consider diffraction basics, beginning with interference between two scattering points in the famous Young's two-slit experiment. This will then lead us to Bragg's law and then general rules associated with it.

Notes

Summary

5m 51s