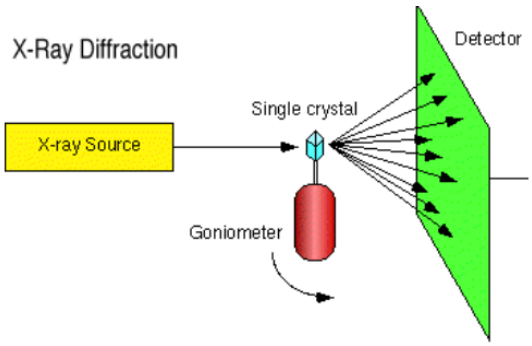
- **<u>The key-feature of X-ray diffraction is the interaction between the crystal and the incoming X-ray radiation</u>**

  X-rays in the crystal are scattered by electrons - Thomson scattering: the electron oscillates in the electric field of the incoming X-ray beam and an oscillating electric charge radiates electromagnetic waves. This is elastic coherent scattering: frequencies and wavelengths of the incoming X-rays and scattered/diffracted X-rays are the same/unchanged. This scattering is becoming very discrete in terms of directions, some scattered waves are reinforced, some weakened as we are dealing here with the diffraction reflections, which is amplified by millions of copies of the same atoms (electrons) in the same position in the crystal space due to crystal periodic, repetitive unique character.
  We cannot measure (yet) the X-ray scattering produced by a single chemical entity (organic molecule) is it is too weak, but we can use crystals as 3-D amplifier of scattering produced by single crystal motif.
  X-ray diffraction is well welcomed "side-effect" of this process due to amplifying or cancelling effect of scattering radiation emitted by electrons. There are also other types of interactions of X-rays with electrons, e.g. excitations. This type of high-energy phenomenon would damage the single molecule almost immediately. In the crystal there are thousands of molecules - some of them survive long enough to give a measurable radiation.
- **<u>Most serious problem with X-ray diffraction:</u>**

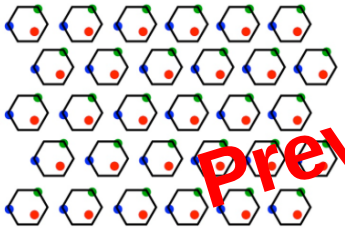


In X-ray diffraction we do not have lenses, which could focus, diffracted rays back to the crystal structure, refractive index for X-rays in all media: **n=1** **$I \approx F^2$** **$\sqrt{I} = \sqrt{F^2} = |F|$**
Information directly available from an X-ray single crystal diffraction experiment:

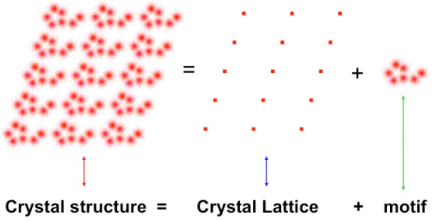
1) Intensities, I, of diffracted X-rays therefore only |F| amplitudes of diffractive X-rays.
2) Directions of the diffracted X-rays

The phase α must be reconstructed in rather complex, difficult experimental and computing methods:
Phase problem = phase solution methods

- **<u>Lattices, crystal planes, hkl indices</u>**



The 3-D periodicity of the crystal can be simplified and represented by an abstract crystal lattice.



Crystal lattice is described by 3 translations: a, b, c and the angles between them. They cannot be just any translations, they to reproduce all crystal motives (lattice points) if applied to any single lattice point (or motif's atoms).
The a, b, c lattice translations determine the unit cell it:

- Has to be a lattice 'building block', which edges correspond to a, b, c
- Should give the whole crystal lattice if moved by a, b, c
- Has to be of the right handed system
- Has to have the smallest possible volume
- Possesses the highest possible symmetry characteristic for the lattice (this is why some unit cells are not primitive)

Unit cells are defined in terms of lengths of the three vectors and the three angles between them.
To get the structure of the motive we have to first get the information about the unit cell size and it's arrangement.