Determination of lattice constant in NaCl

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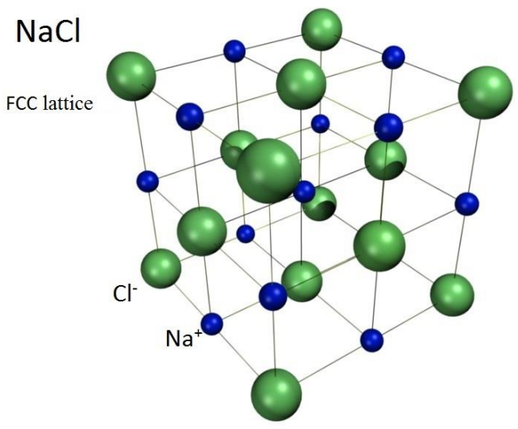
Abstract

Lattice constant of NaCl has been determined by X-ray powder diffractometry. The obtained value of **a** is **5.6413(6) Å**, which is in agreement with the values found in the literature

Basic theory

The NaCl crystal structure:

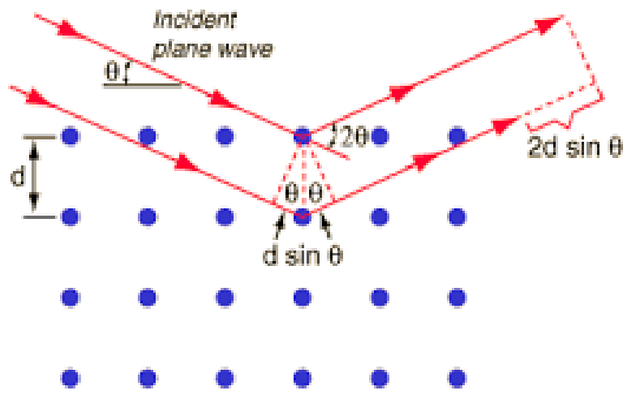


· Crystal is a repetition of an identical group of atoms attached to a mathematical set of points called lattice. The separation between two points in the lattice is the **lattice constant (a)**.

·The structure of NaCl is a face-centered cube, with Cl at (000) position and Na at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ position (It has 2 atoms per lattice point).

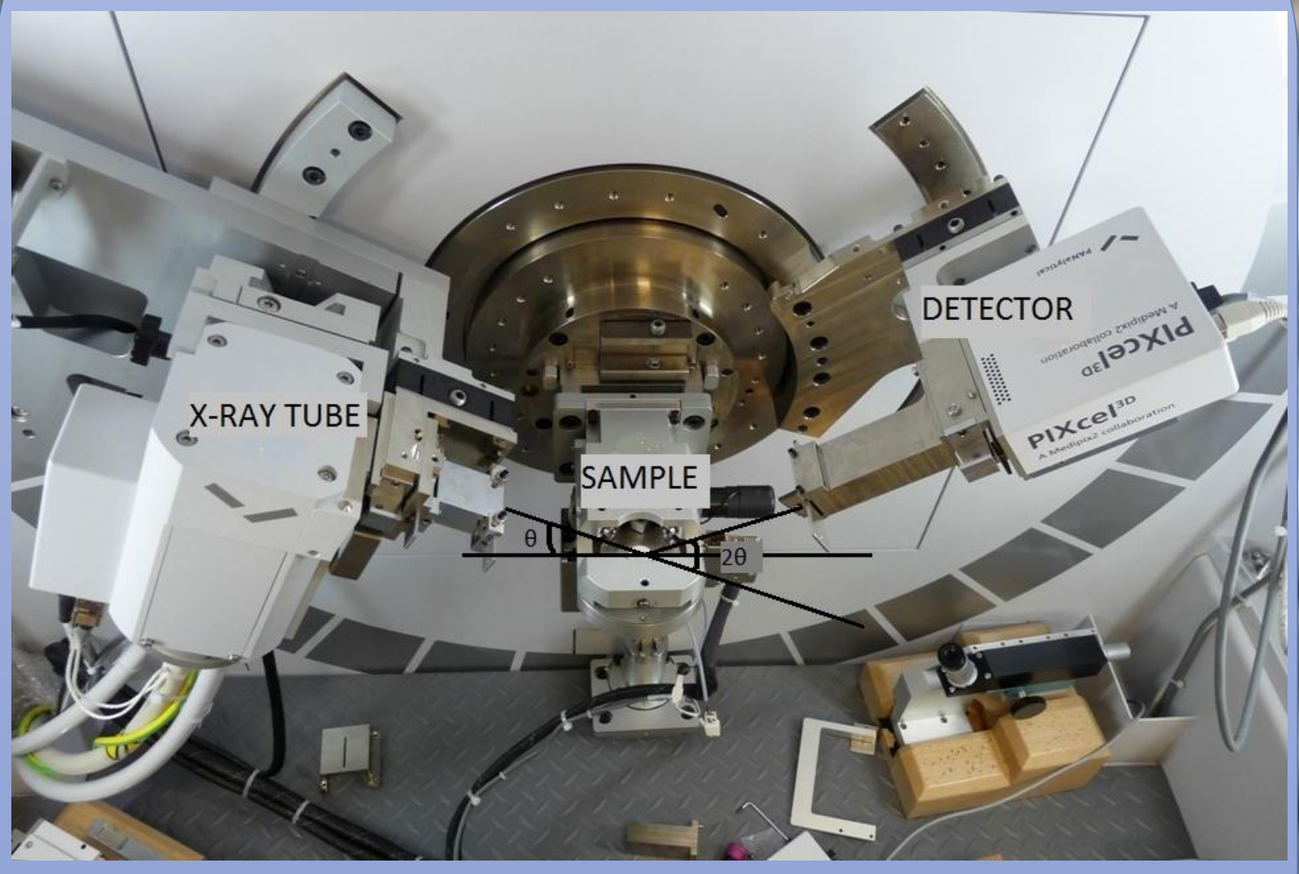
· These points form planes whose orientation is defined by three numbers called **'Miler Index' (hkl)**.

· X-ray beam is reflected by a crystal only in case where rays reflected by adjacent planes make a constructive interference as shown in the figure beside. This leads to, so called, **Bragg's law: 2d(hkl)sinθ=λ.**



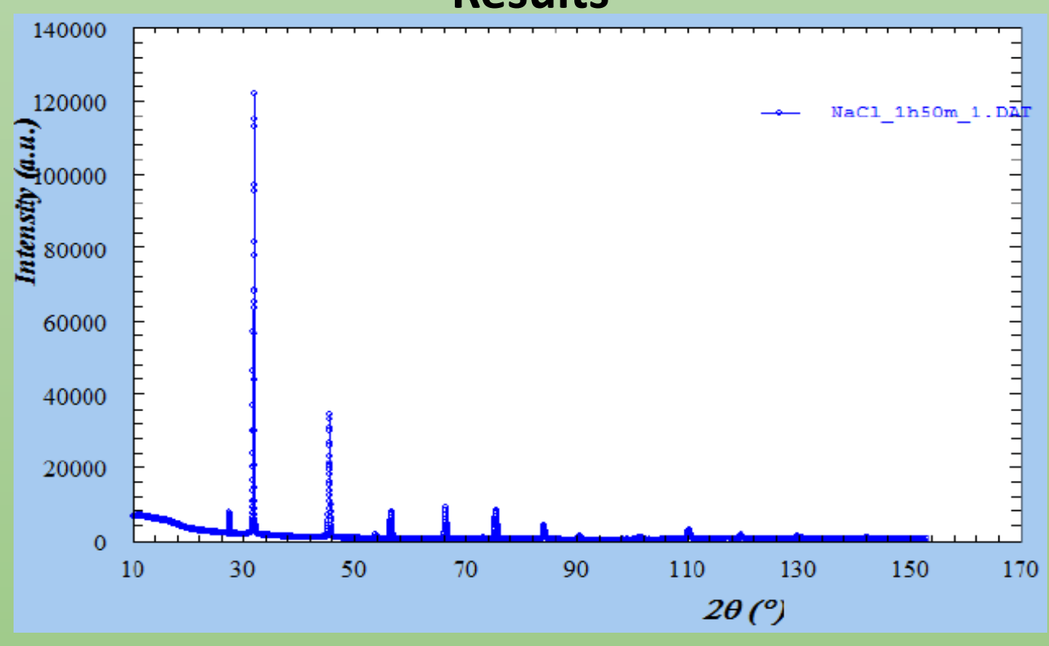
Measurement method

Measurement was done with a powder X-ray diffractometer Empyrean by PANalytical:



The X-ray tube produces X-rays that are emitted in the direction of the sample at an angle θ (see figure above).
The X-rays go through some filters that let pass only a monochromatic wavelength. The detector is orientated at an angle θ.
The sample is powder in order to be characterized by random distribution of crystal orientations. In such a case, when Bragg's law can be satisfied for particular interplanar distance d and angle θ, one will always find a set of appropriate oriented grains.
The computer collects intensity versus angle 2θ.

Results

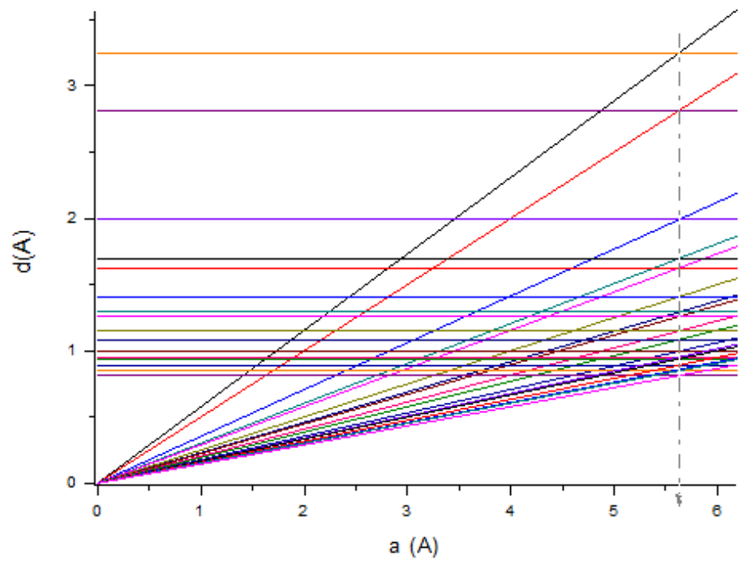


Powder X-ray diffraction pattern collected for NaCl. Using the Bragg's law, d(hkl) is calculated for each of the Bragg's reflections.

Indexing

The graphical technique used is based on equation (valid for regular lattice) :

$$\frac{a^2}{d^2} = h^2 + k^2 + l^2$$



· Tilted lines represent d vs a dependences allowed by selection rules for the fcc lattice.

· in the same graph, experimental values of d are represented as horizontal lines.

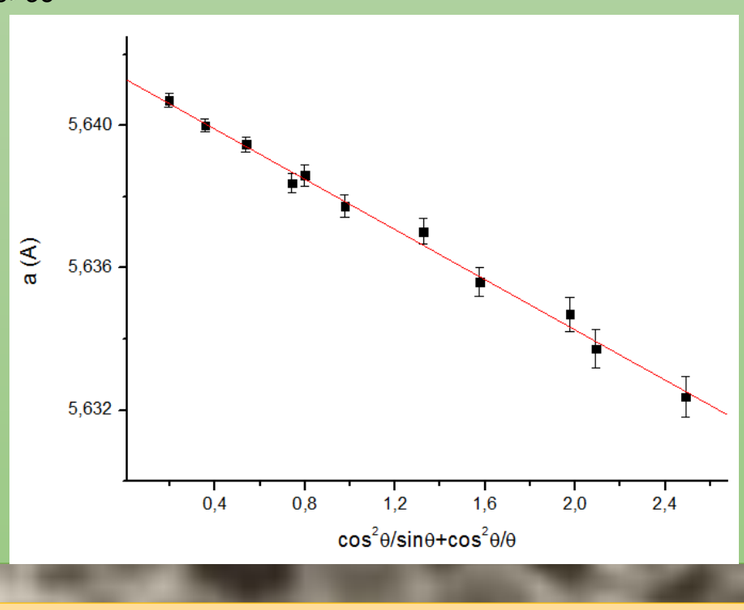
· The value of lattice constant a at which each horizontal line cuts one of tilted lines provides estimation of the real value of lattice constant in the crystal. The index (hkl) of tilted line is the Miller index of the plane characterized by interplanar distance d.

Determination of lattice constant

In order to eliminate systematic errors an extrapolation method is used. It is based on equation:

$$a = a_0 + k\left(\frac{\cos^2\theta}{\sin\theta} + \frac{\cos^2\theta}{\theta}\right)$$

Where a_0 is the estimated value of the lattice constant. The above equation is valid for angles 2θ>60°



Conclusions

The obtained lattice constant of NaCl is **a= 5.6413(6) Å** and it is in agreement with the values found in literature:
·a= 5.640(8) Å [1] ·a= 5.642(2) Å [2] ·a= 5.640(1) Å [3]
While estimating uncertainty of the lattice constant there were taken into account both statistical uncertainties as well as those arising from the angular step of the measurement which was equal to 0.013°.

References

[1] Nickels J E, Fineman M A, Wallace W E; Journal of Physical Chemistry, 53 (1949) 625-628
[2] Urusov V S, Blinov V V, Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, 12 (1970) 278-282
[3] Barrett W T, Wallace W E; Journal of the American Chemical Society, 76 (1954) 366-369
[4] Ch. Kittel, *Introduction to solid state physics*, John Wiley & sons; United States of America; 2005