

Katowice

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β -Eucryptite, a phase with many open questions

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Introduction

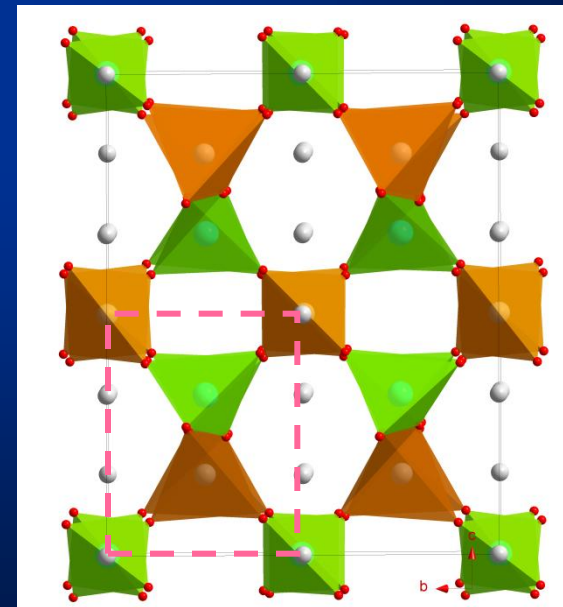
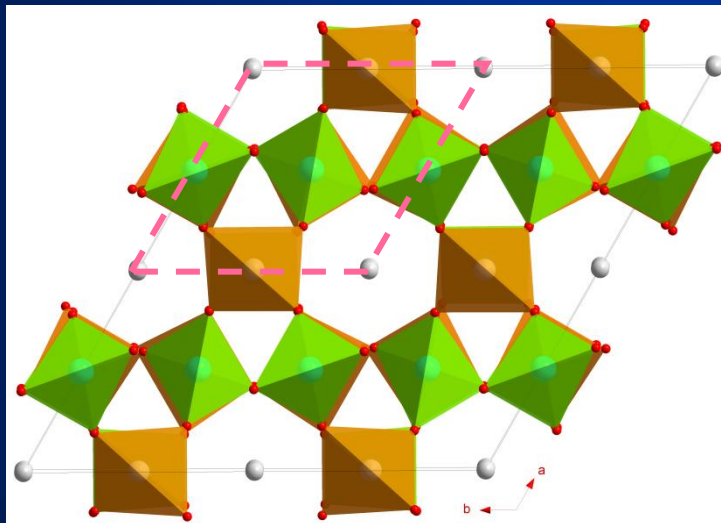
β -Eucryptite, LiAlSiO_4

What is basic knowledge on the structure ?

It is a derivative of the β (high)-quartz structure.

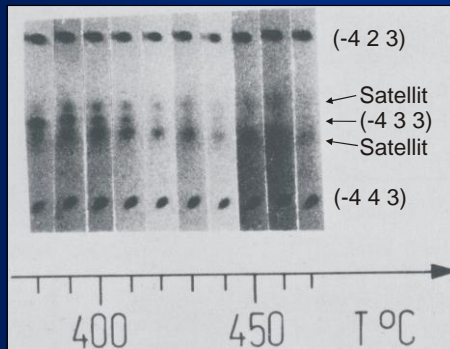
SG: $P6_422$, Isostructural replacement of Si by Al.

2x2x2 superstructure as compared to quartz

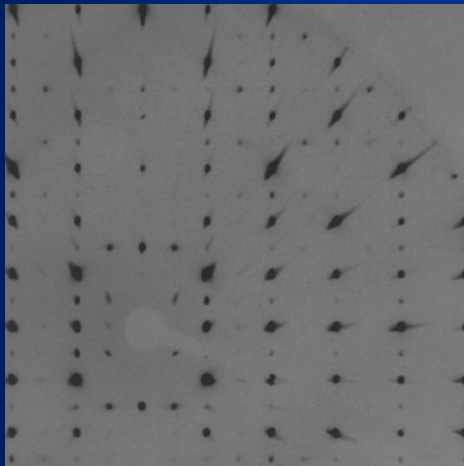


Sequence of phases

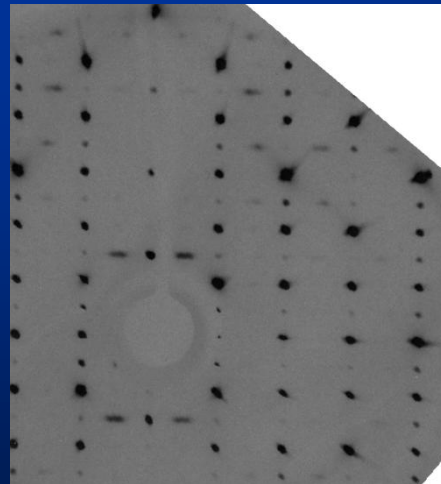
β -Eucryptite exhibits a modulated structure at higher temperatures



The historically first picture showing the appearance of satellite reflections

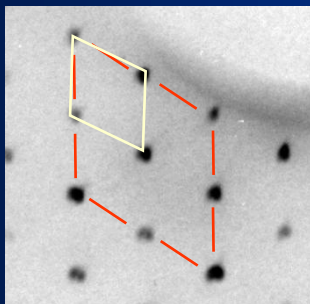
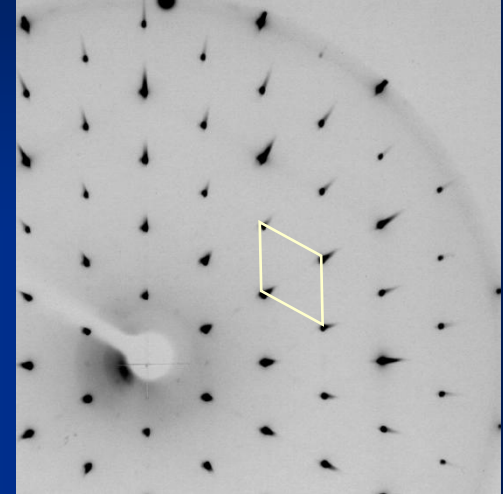
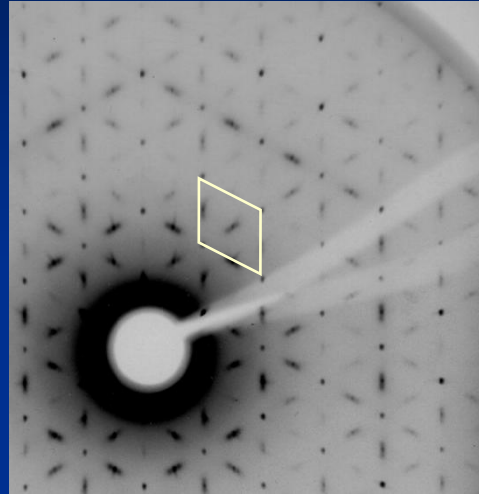
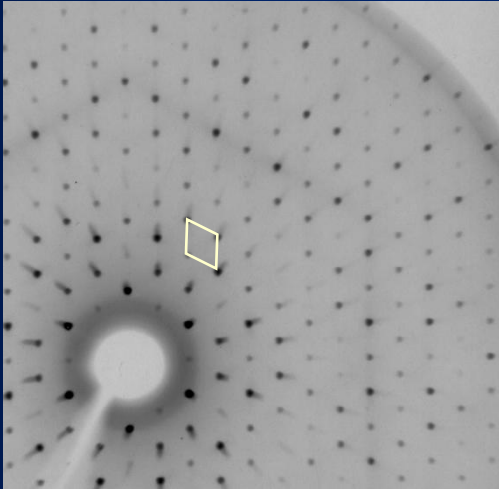


At 25 °C

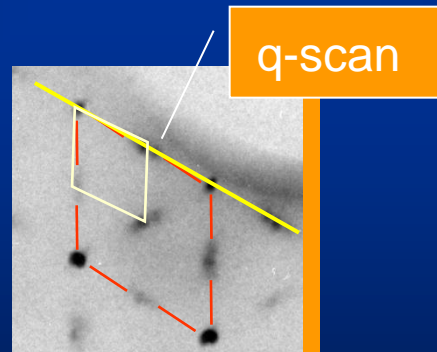


At 380 °C

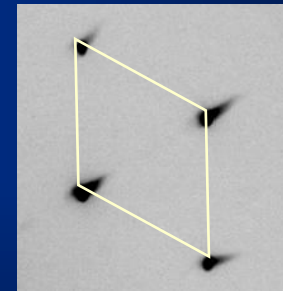
Sequence of phases



$T = 25\text{ °C}$



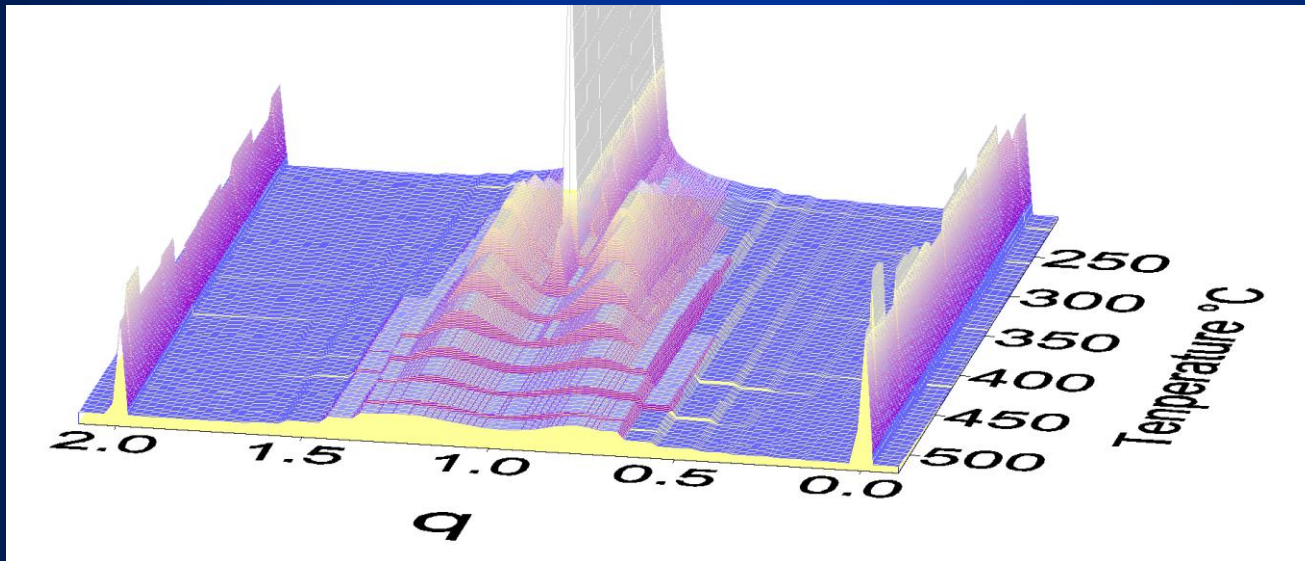
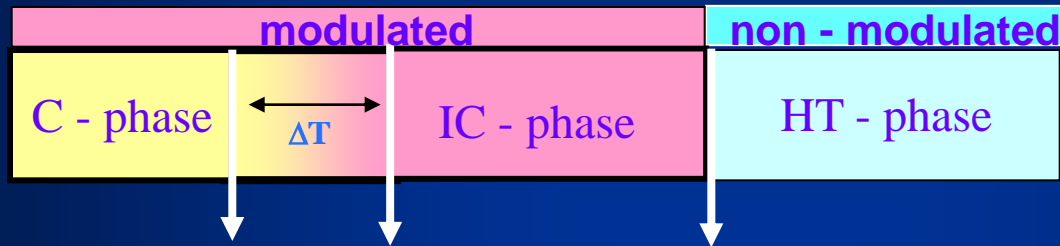
$T = 380\text{ °C}$



$T = 460\text{ °C}$

Sequence of phases

Typical sequence of phases for modulated structures:



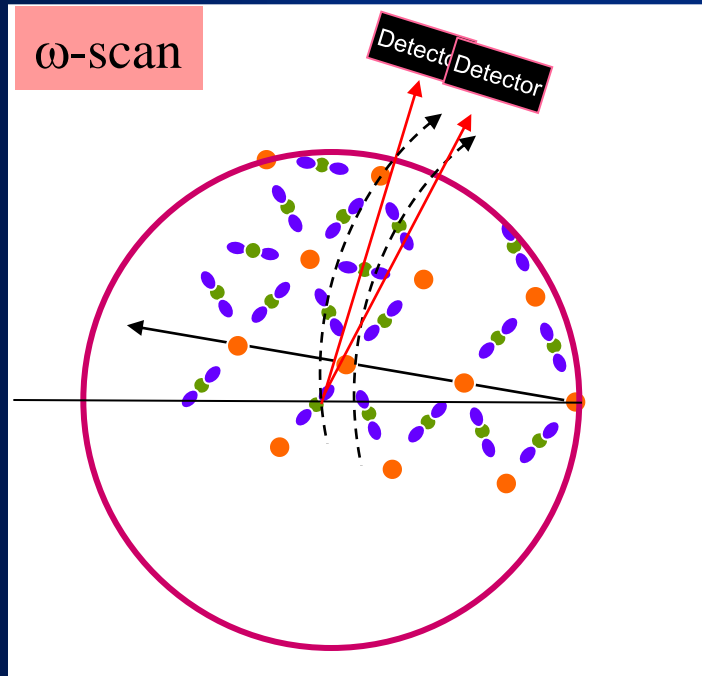
Structure determination.

Problems for the structure determination

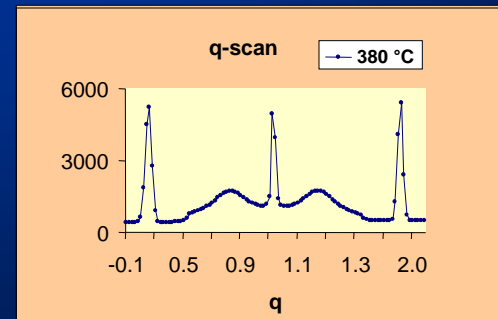
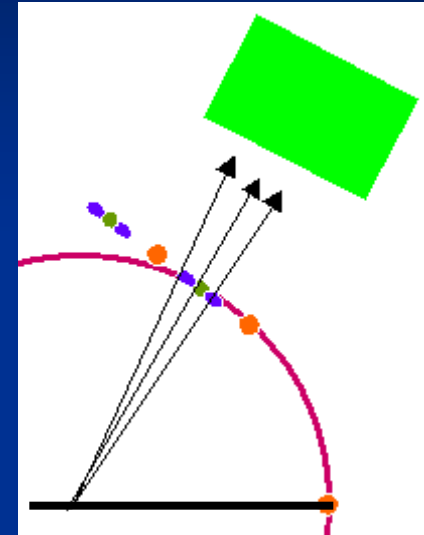
- ◆ The satellite reflections are diffuse
- ◆ The satellite reflections are not well resolved
- ◆ The satellite reflections are overlapping the adjacent a-reflections

Data collection

ω -scan is not possible
for the satellites

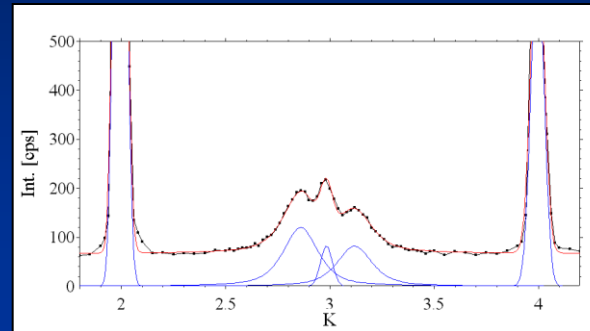
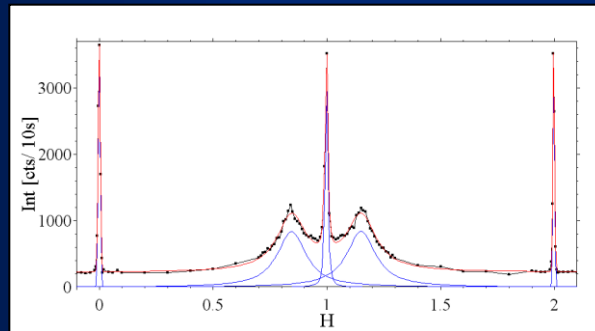


q-scan is the solution



T = 380 °C

Data collection



Profile fitting for overlapping intensities
by least squares methods

- ◆ The area under the profile function determines the intensity.
- ◆ The FWHM of the profile function is related to the number number of periods which contribute to coherent scattering

Structural concepts

- ◆ The modulation period is about 12×12 lattice constants of the high quartz structure.
- ◆ The modulated phase (diffuse reflections) and the superstructure (sharp reflections) have different areas of coherent scattering
 - \Rightarrow 11-16 periods for the modulated structure
 - \Rightarrow 100 periods for the superstructure
- ◆ The range of coherence is limited by anti-phase boundaries.
- ◆ Only tilts of the tetrahedra are responsible for the structural modulation.