X-ray studies of phase transitions of (Ca,Sr)-åkermanite solid solutions

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Contents

- Melilites and Åkermanites
- Modulations and Superstructures
- Phase transitions and modulations in solid solutions

Åkermanites are a member of the melilite family

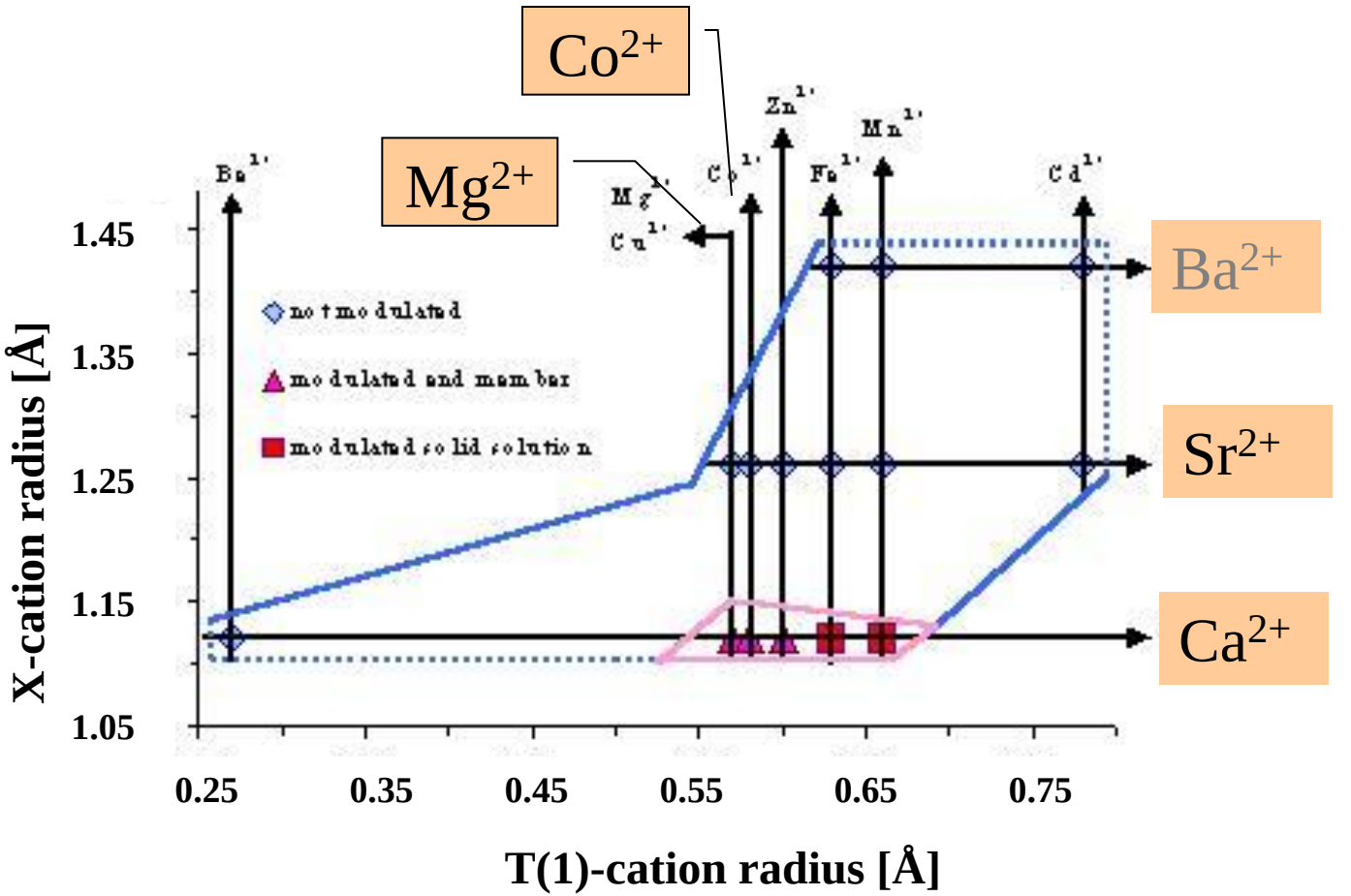
$$X_2T(1)T(2)_2O_7$$

Melilites	
X	Ca, Na, Sr, Pb, Ba, rare earth-El.
T(1)	Be, Mg, Cu, Co, Zn, Fe, Mn, Cd, Al, Ga
T(2)	Si, Ge, Al, Fe
Anion	O, F, S

T(2) = Si

Anion = O $\Rightarrow$ Åkermanites

Åkermanites and modulated structures



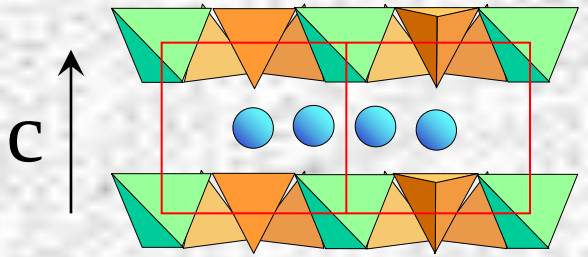
(Röthlisberger et al.,1990)

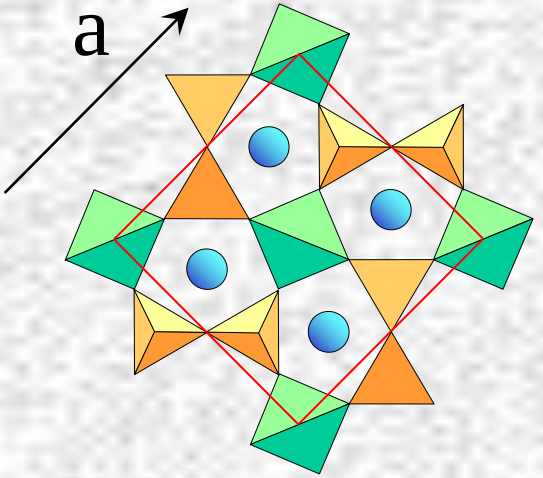
The basic structure

= CoO_4

= Si_2O_7

= Ca,Sr





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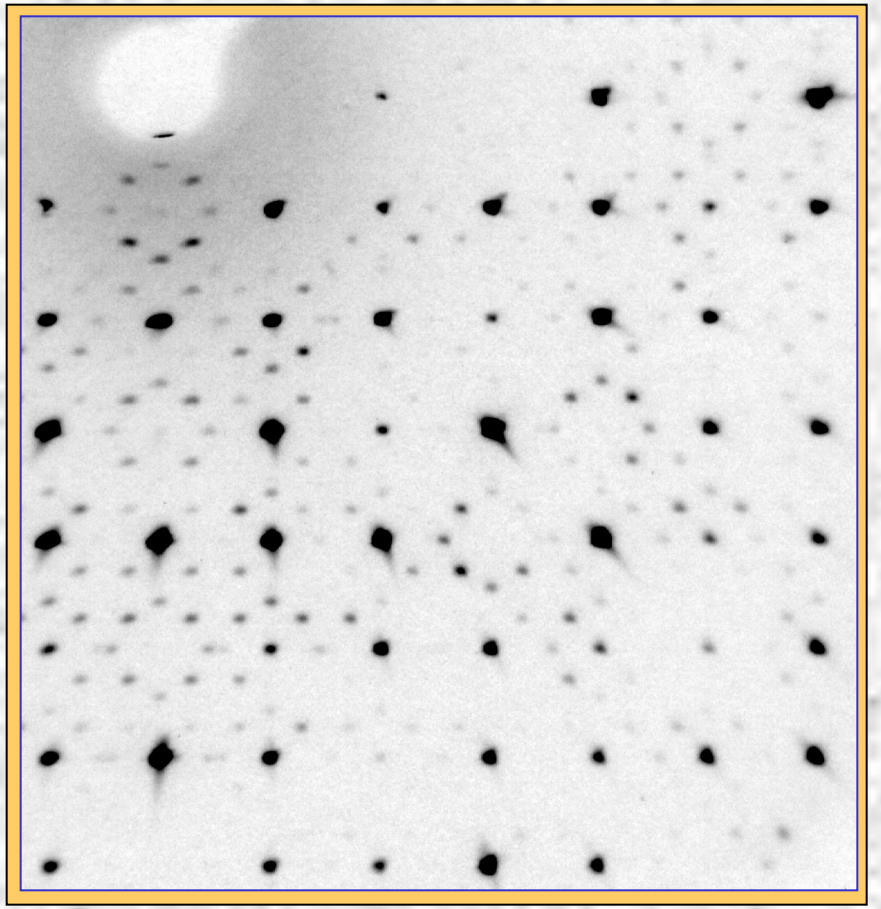
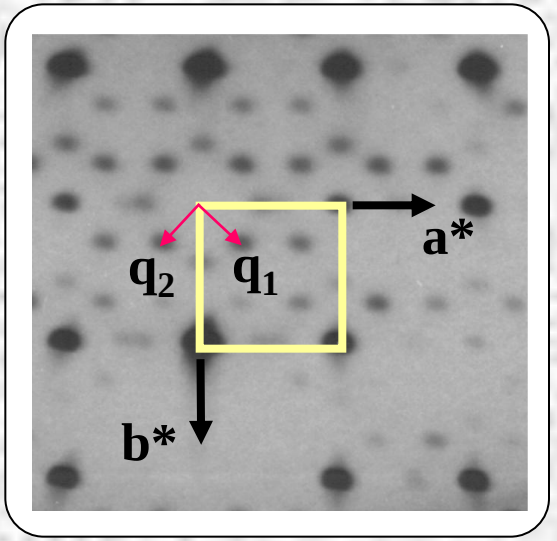
Modulations in $Ca_2CoSi_2O_7$

A diffraction pattern

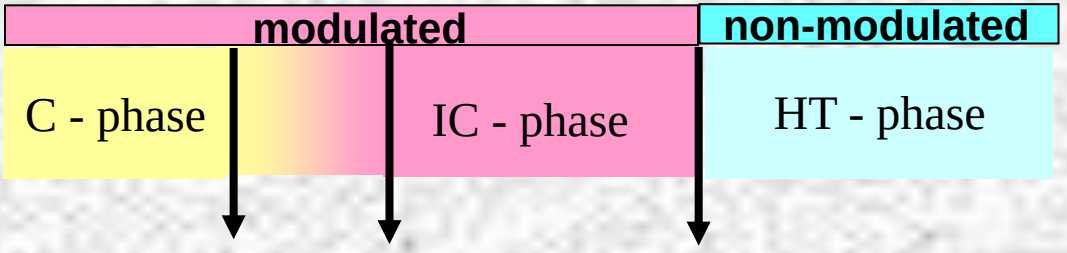




Precession Photograph
(h k 0)- layer of the reciprocal lattice at T=300K .

$q_1 = \alpha(a^*+b^*)$,
$q_2 = \alpha(-a^*+b^*)$
$\alpha = 0.291$

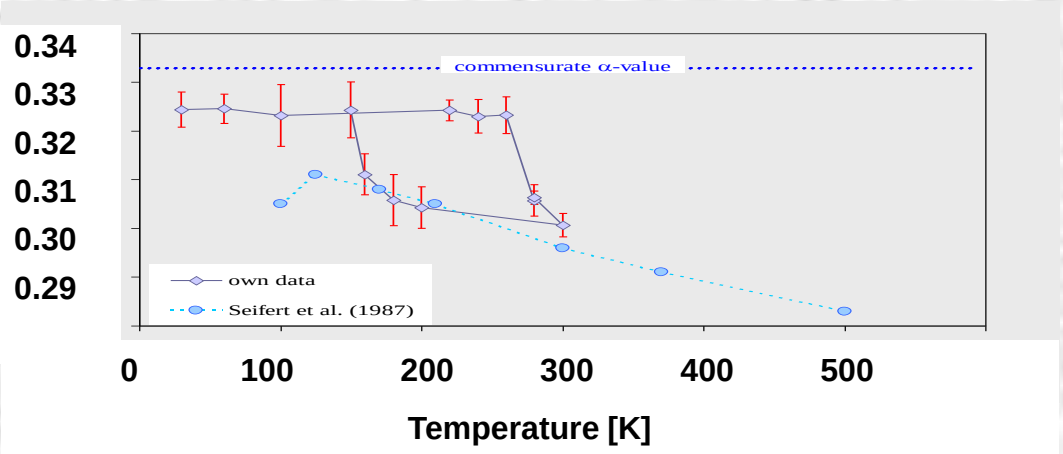
Sequence of phases



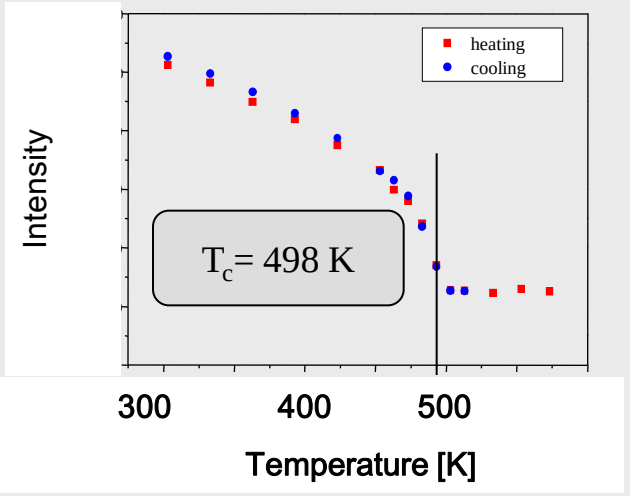
T_c = 155 K - 270 K

T_c = 498(1) K

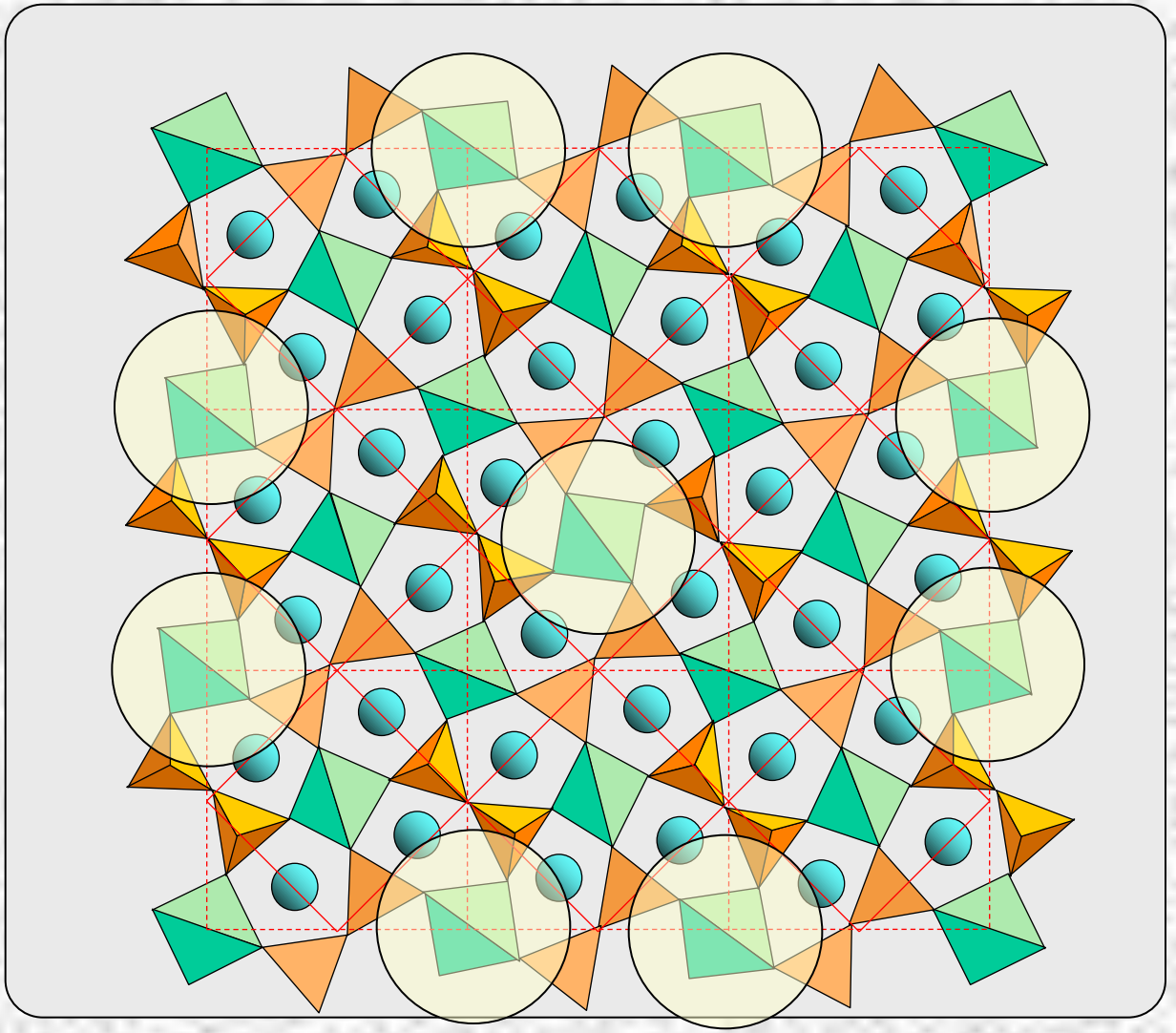
Variation of the q-vector

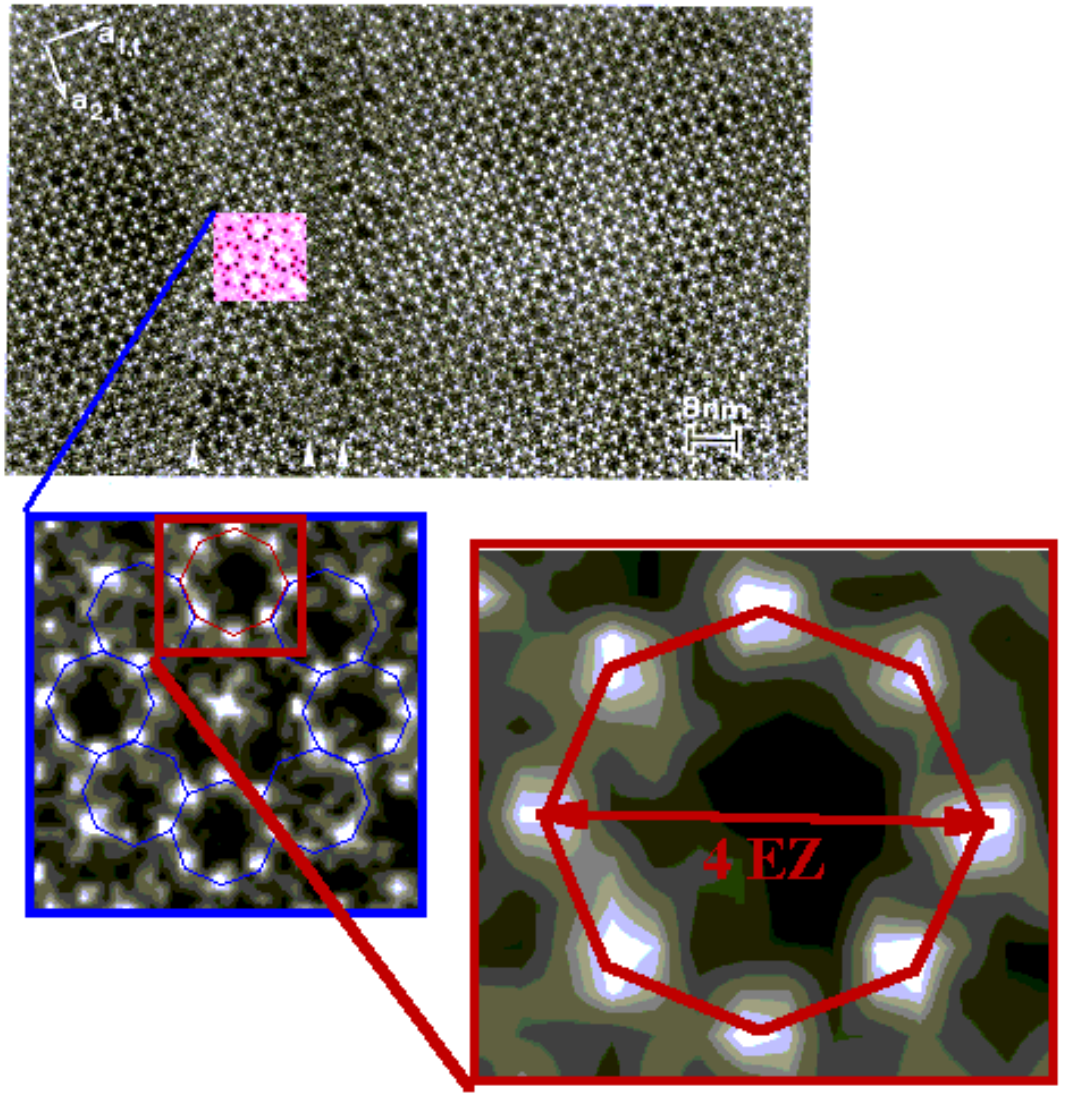


Satellite intensity



Commensurate superstructure

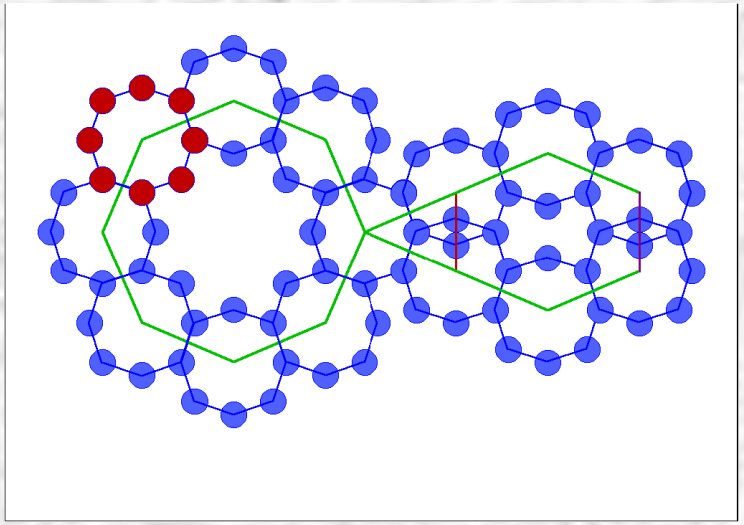




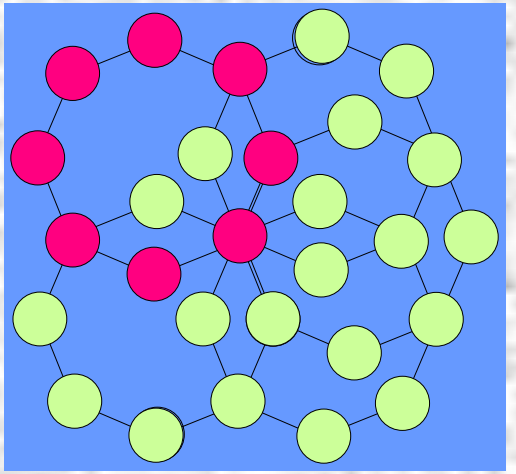
TEM image of the incommensutate RT phase.

After Van Heurk et al., 1992

Hypothesis: The incommensurate and the commensurate structure are condensations of **octagonal rings** consisting of 6-fold coordinated Calcium with a different degree of order.



Incommensurate structure



Commensurate structure

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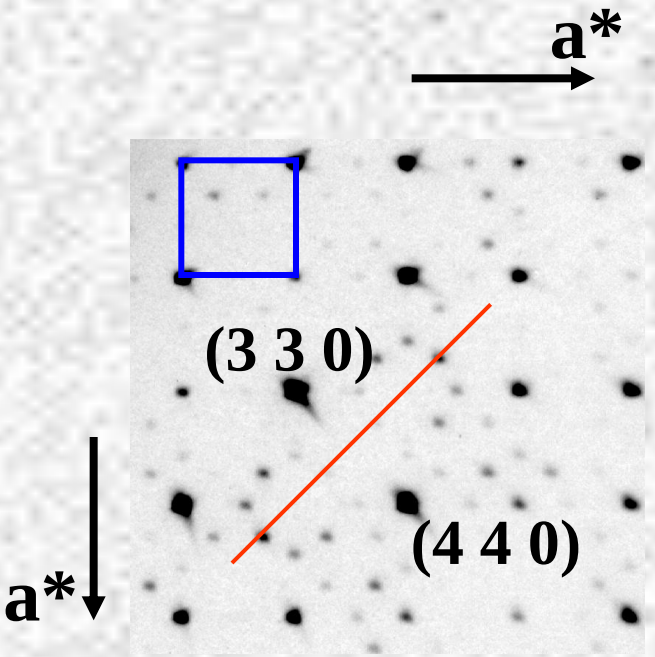
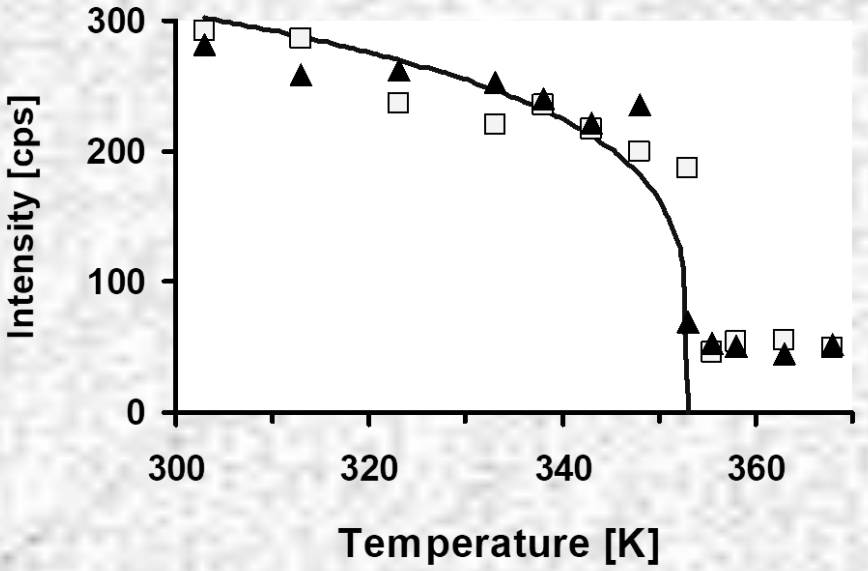
Modulations in **solid solutions**

$Ca_{1-x}Sr_xMgSi_2O_7$; ***x = 0***

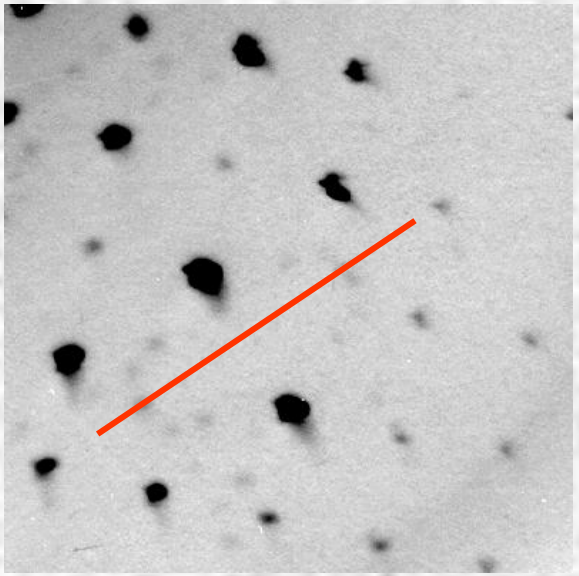


T = 300 K

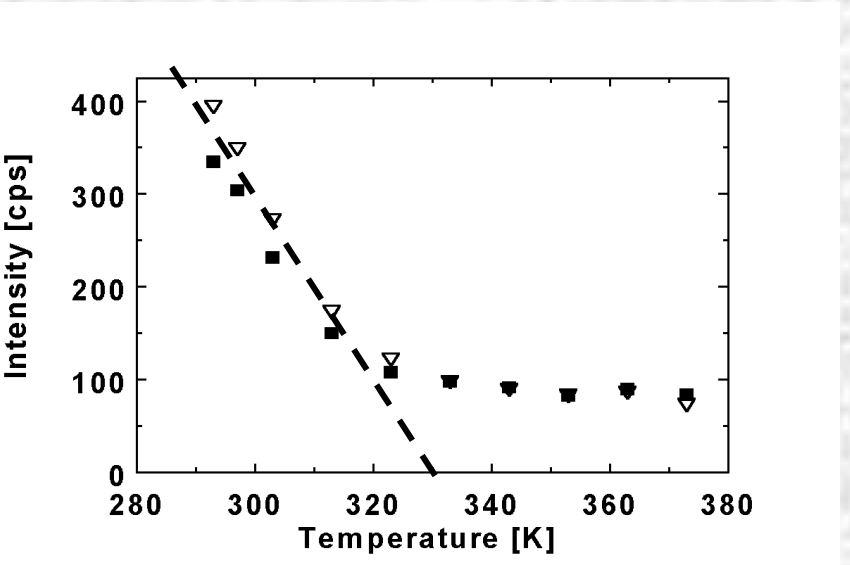


Tc = 354 K

$Ca_{1-x}Sr_xMgSi_2O_7$; *x = 0.08*

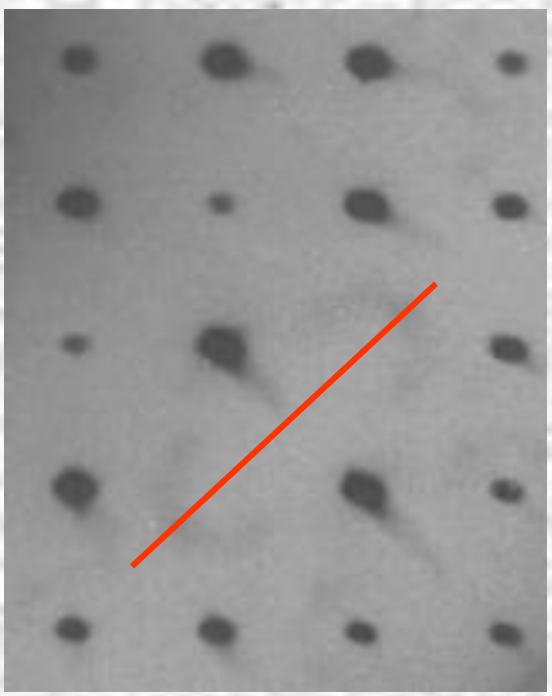


T = 300 K

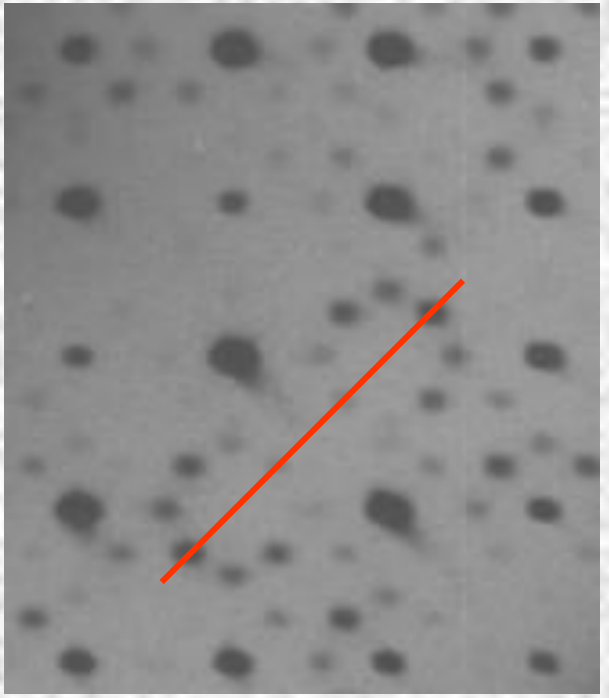


Tc = 330 K

$Ca_{1-x}Sr_xMgSi_2O_7$; *x = 0.16*

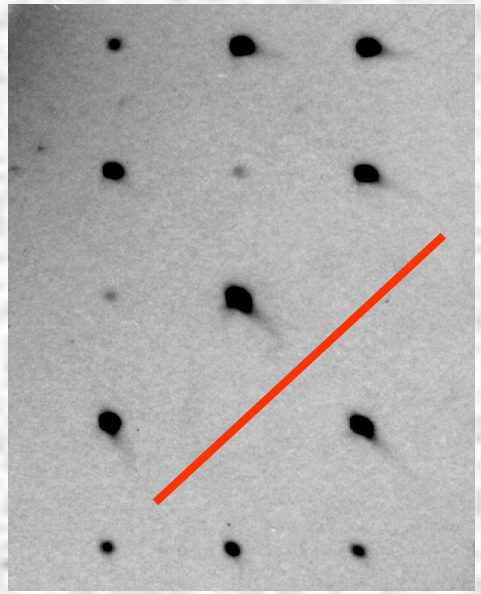


T = 300 K

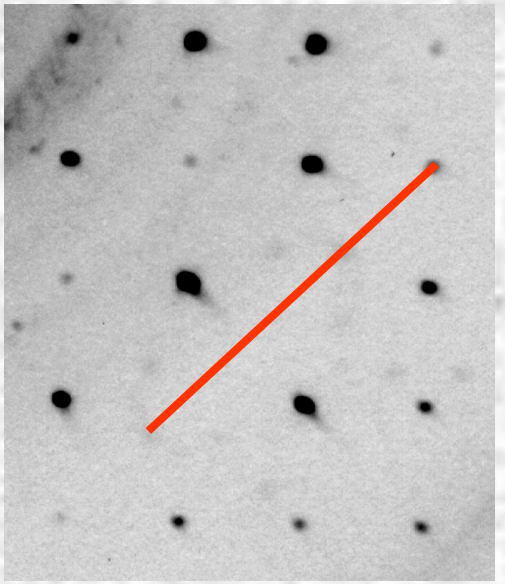


T = 130 K

$Ca_{1-x}Sr_xMgSi_2O_7$; *x = 0.32*



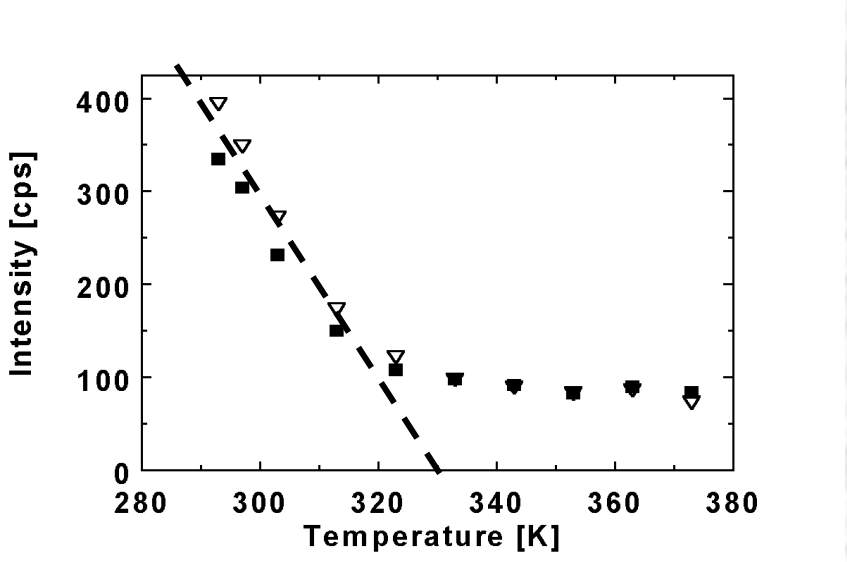
T = 300 K

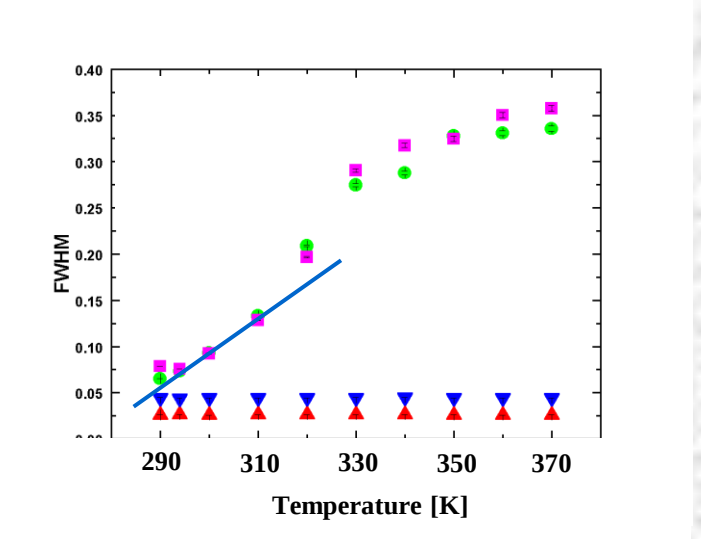


T = 130 K

Transformation temperature

$Ca_{1-x}Sr_xMgSi_2O_7$; *x = 0.08*

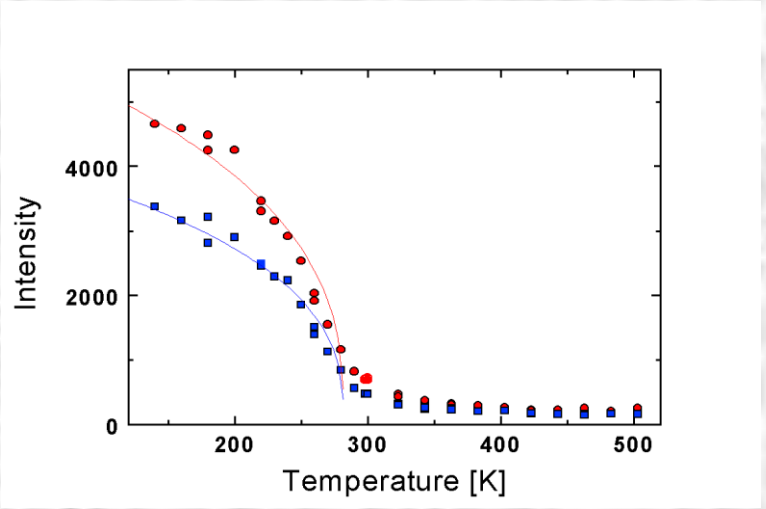


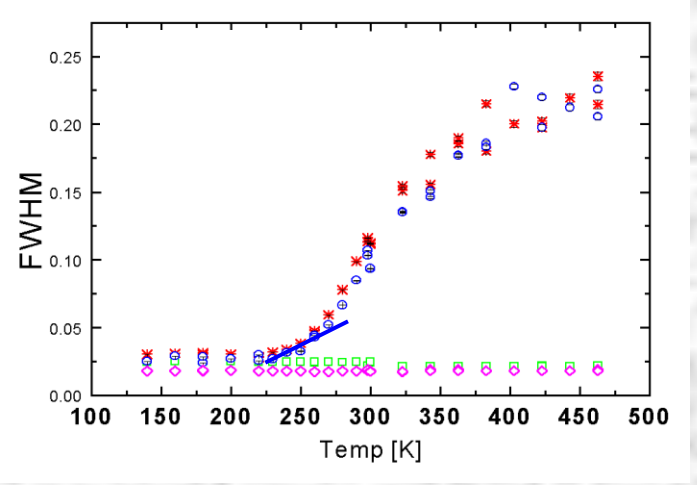


Tc = 330 K

Tc = 280 K

$Ca_{1-x}Sr_xMgSi_2O_7$; $x = 0.16$

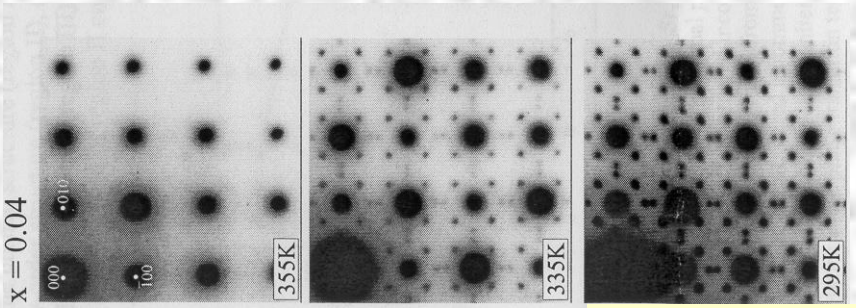




Tc = 277 K ? ⇔ ? Tc = 250 K

Transformation temperature

TEM diffraction of the incommensutate phase.
x=0.04



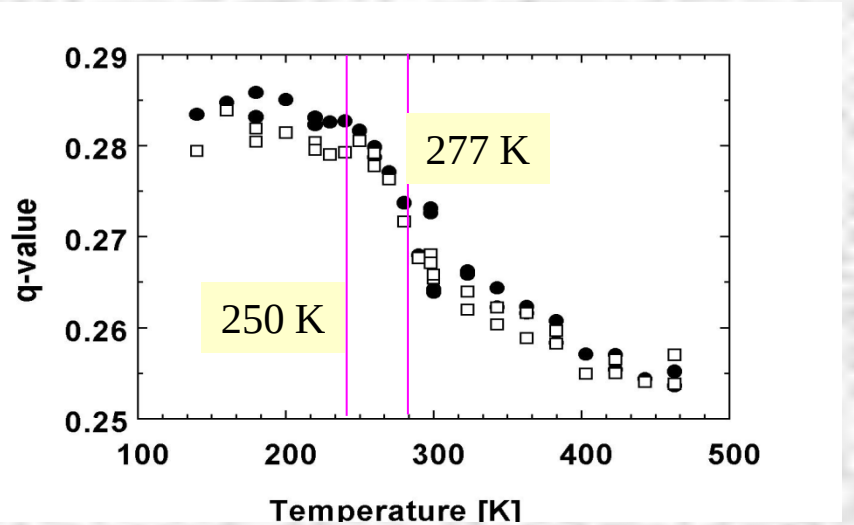
T = 355 K
No satellites

T = 335 K
1. order satellites

T = 295 K
1.and 2. order satellites

After M. Schosnig et al., 2000

Variation of the q-value for *x=0.16*



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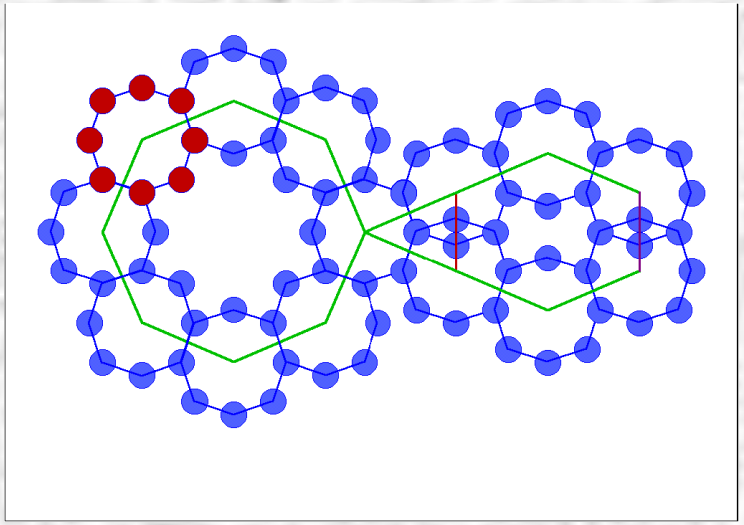
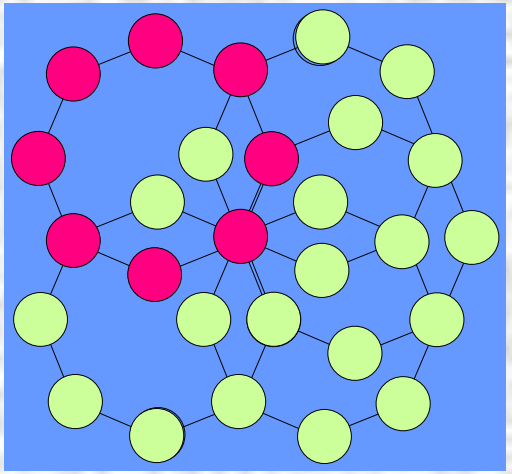


Incommensurate structure



Commensurate structure