Modulated structures and subsolidus phase relations of Labradorite Feldspars

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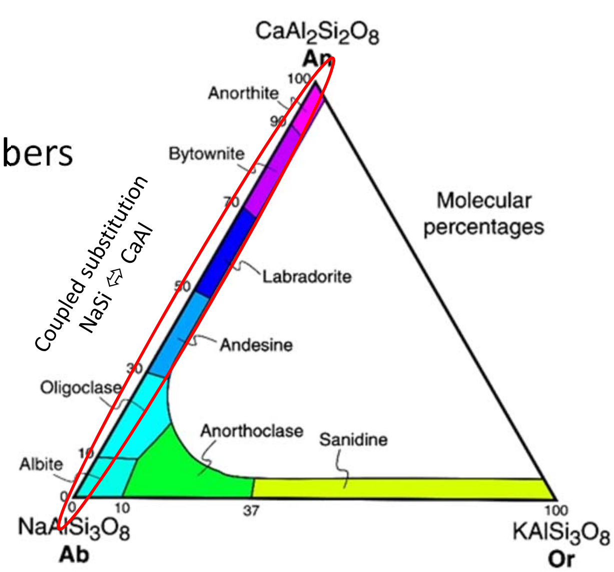
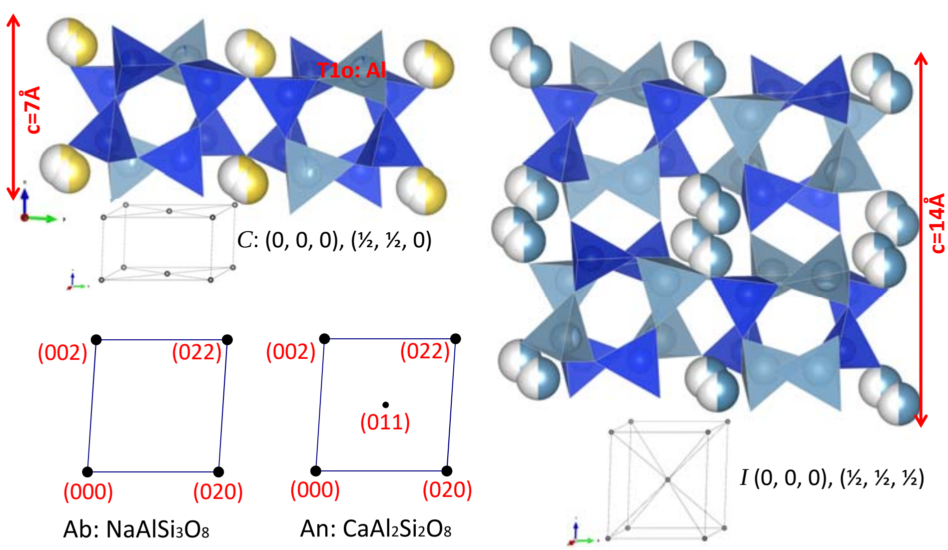
Wisc Nano-Geoscience

Feldspar Minerals

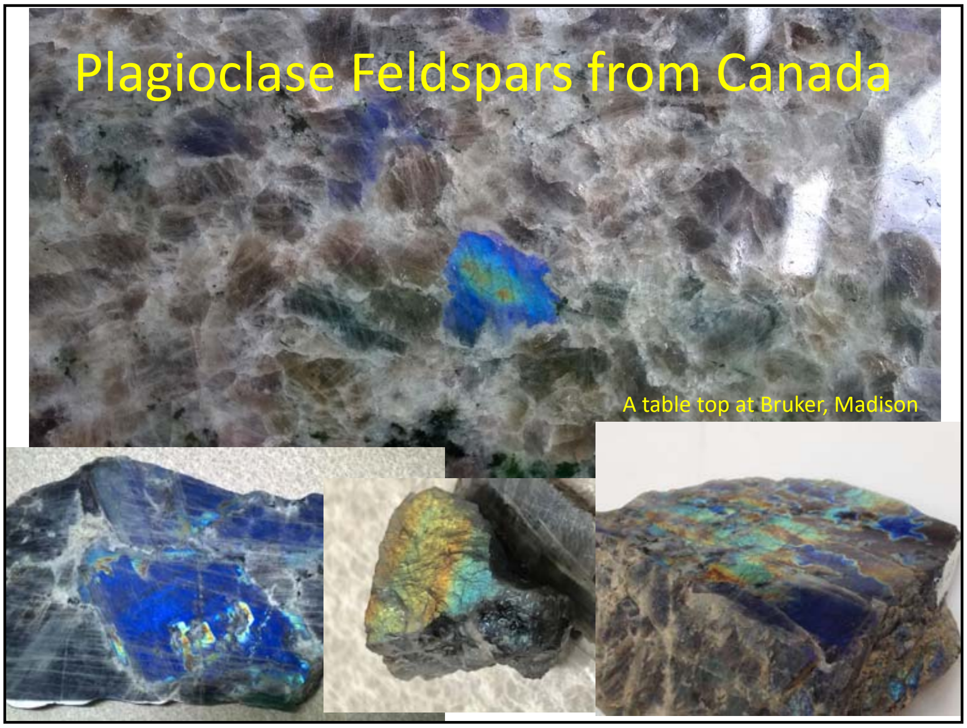
- Most abundant
- Tectosilicate
- Three end members (Or, Ab, An)
- Two series
- Plagioclase
- Alkali feldspar



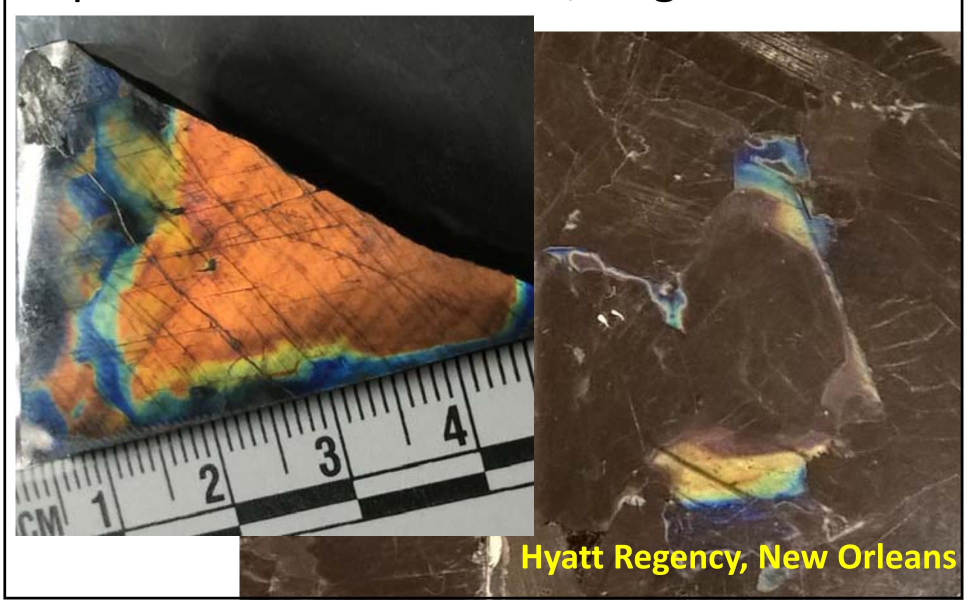
Albite ($C\bar{1}$) vs Anorthite ($I\bar{1}$)



Plagioclase Feldspars from Canada

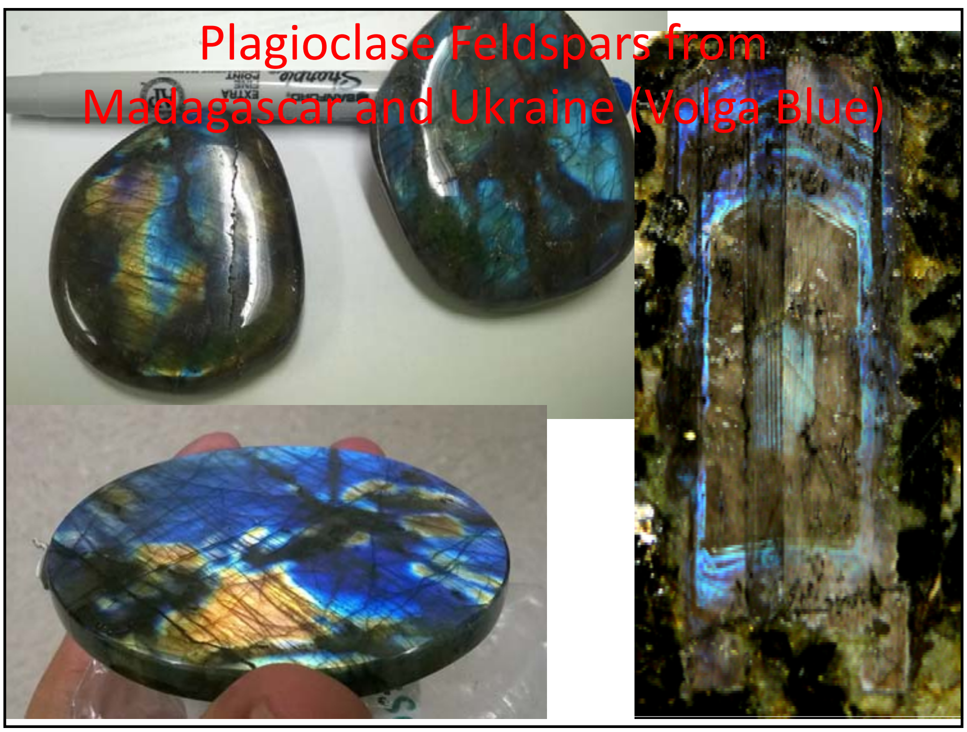


Plagioclase Feldspars:
Spectrolite from Finland; Angola Brown



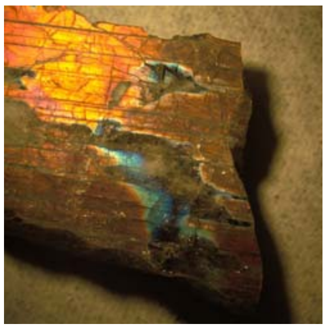
Sunstones from Oregon and Norway

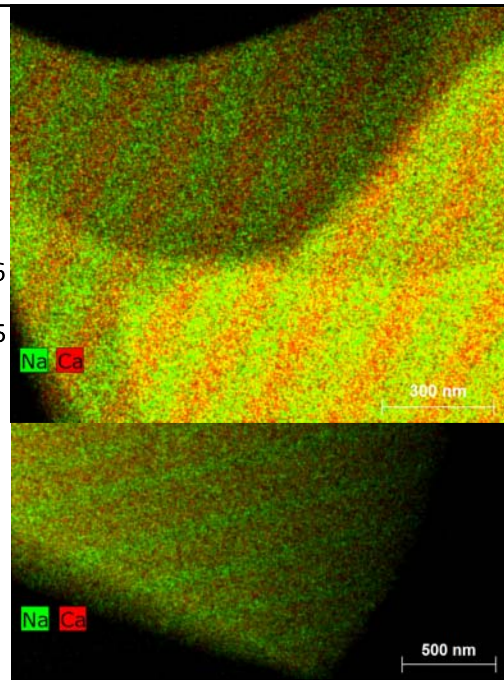
Plagioclase Feldspars from Madagascar and Ukraine (Volga Blue)



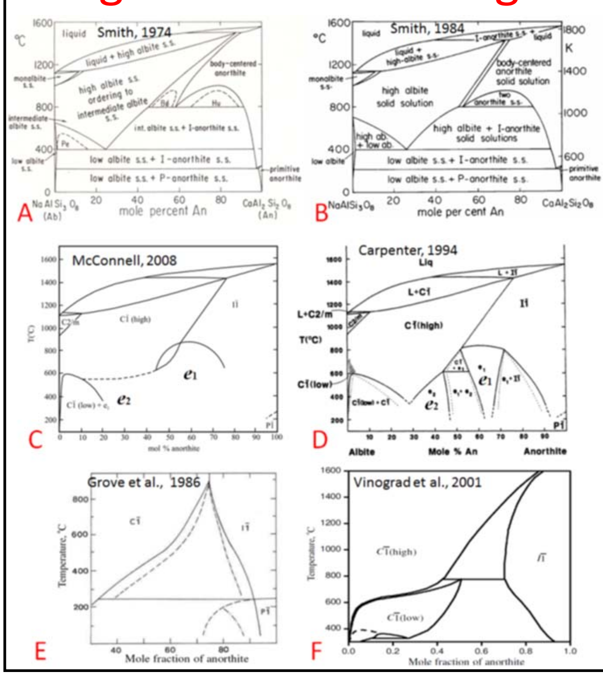
Sweden

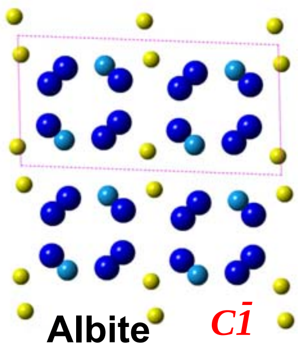
- Sweden
- Red: $An_{52}=An_{56}+An_{46}$
- Blue: $An_{50}=An_{55}+An_{45}$

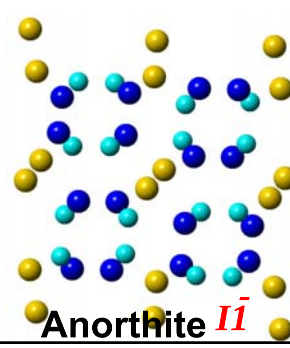




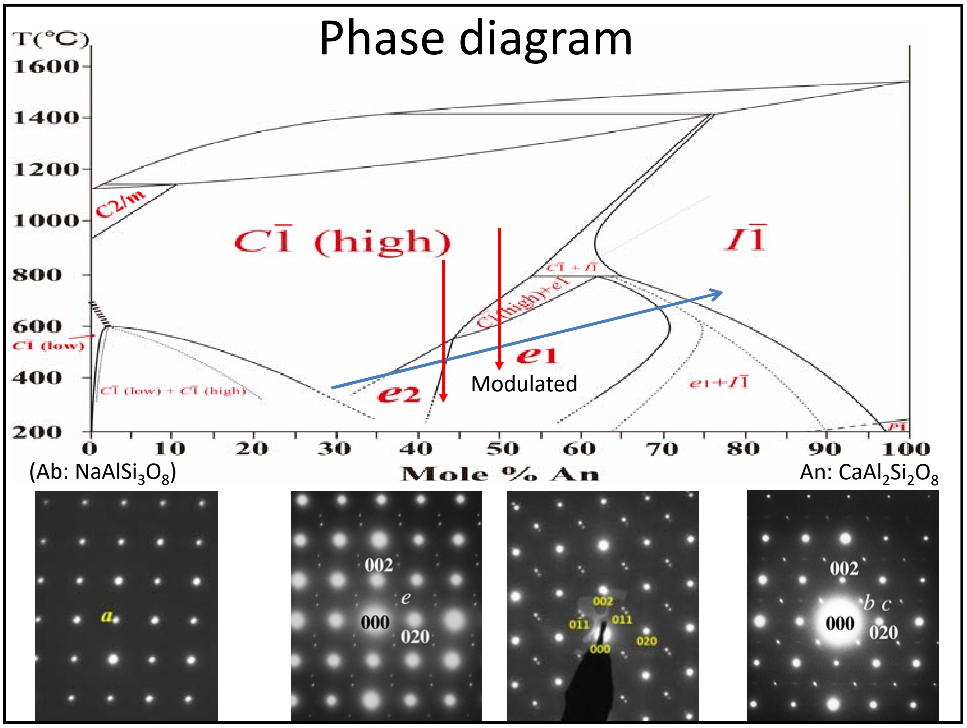
Plagioclase Phase Diagram





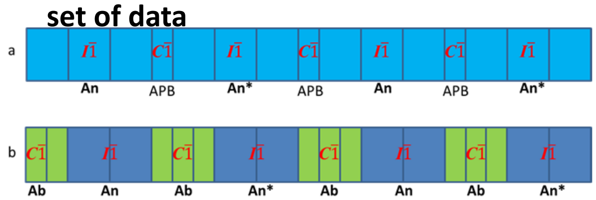


Phase diagram



Structure Models for *e*-plagioclase

- First discovered in 1940 by Chao and Taylor
- All reported models are lamellar models:
- $I\bar{1}$ (An) domains + APBs
- $I\bar{1}$ (An) + $C\bar{1}$ (Ab) + $I\bar{1}$* (An) + $C\bar{1}$ (Ab)
- **Very different models (Jogodzinski group, 1981; Yamomoto and Morimoto group, 1984) were proposed based on exact same set of data**



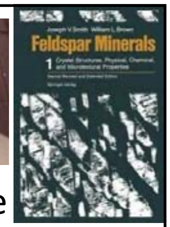
(Ab: $NaAlSi_3O_8$) An: $CaAl_2Si_2O_8$

Megaw, McConnell,
Bailey's group,
Wenk's group,
Jogodzinski's group,

Smith & Ribbe,
Morimoto's group,
Grove,
Toman & Frueh,

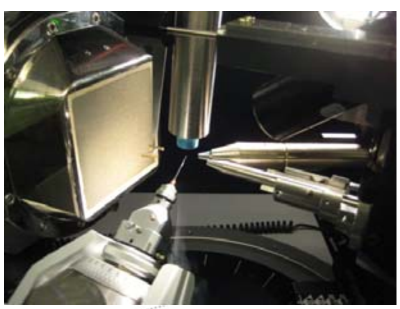
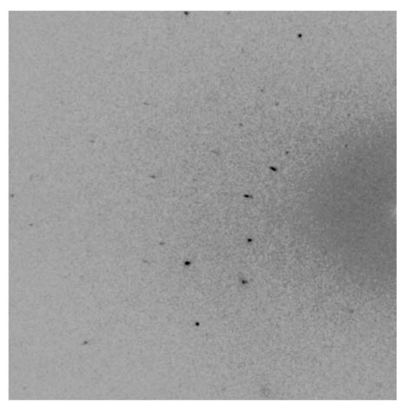
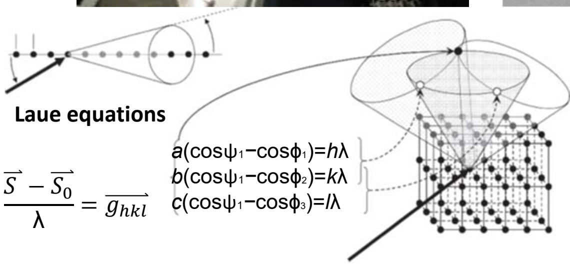
e-plagioclase problem





Smith & Brown (1988) (page 113) described the problem quite well: "*It must be stated that quite frankly, although each group of scientists has produced an impressive set of data and conclusions, there has been no comprehensive attempt to make comparative tests in the true spirit of scientific inquiry. All models appear to contain considerable truth, but it is not clear how much of the 'elephant' has been described! The hunters must set up a joint safari, and collect new data at low temperature on specimens which span the entire composition range* of *e*-plagioclase."

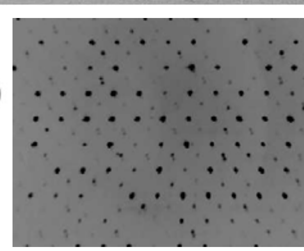
Single-crystal XRD

Laue equations

$$\frac{\vec{S} - \vec{S_0}}{\lambda} = \overrightarrow{g_{hkl}}$$

$a(\cos\psi_1 - \cos\phi_1) = h\lambda$
$b(\cos\psi_1 - \cos\phi_2) = k\lambda$
$c(\cos\psi_1 - \cos\phi_3) = l\lambda$



Neutron Time-of-Flight Laue

Combine de Broglie's equation with Bragg's law

$$\lambda = \frac{h}{mv} = \frac{ht}{m(L_1 + l_2)}$$

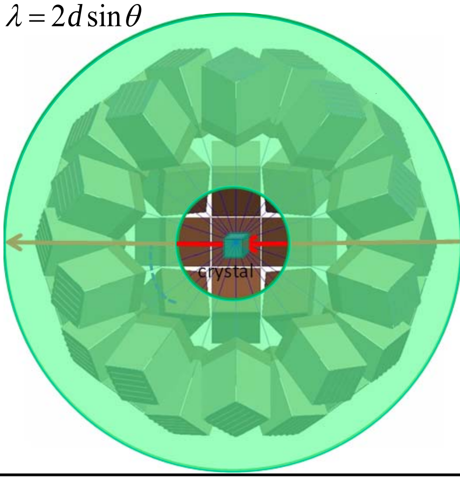
$$\lambda = 2d\sin\theta$$

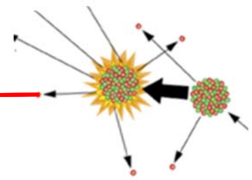
$$t = \frac{m}{h}(L_1 + l_2) \times 2d\sin\theta$$

Neutron Time-of-flight Laue

(**Wavelength-resolved Laue**)

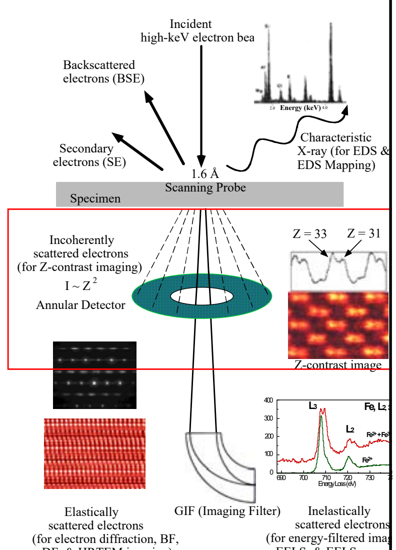
3-*D* Reciprocal Space Mapping



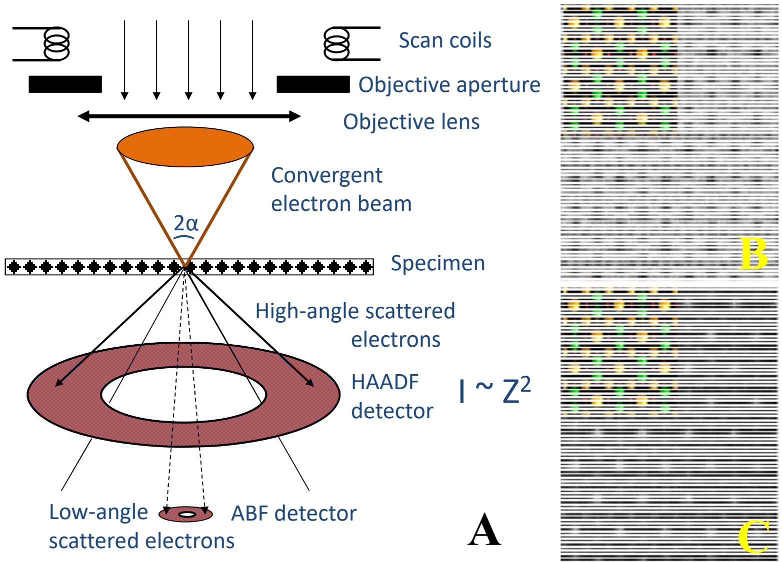


TEM/STEM: a nano-lab, not just a lens

NSF-MRI: DMR-0619368



STEM (scanning transmission electron microscope):
HAAD (high-angle annular dark-filed) imaging, or
Z-contrast imaging because of **I ~ Z²**



Xu et al., 2014a

All early models are wrong!

$I\bar{1}$

No APBs,

$I1$-like

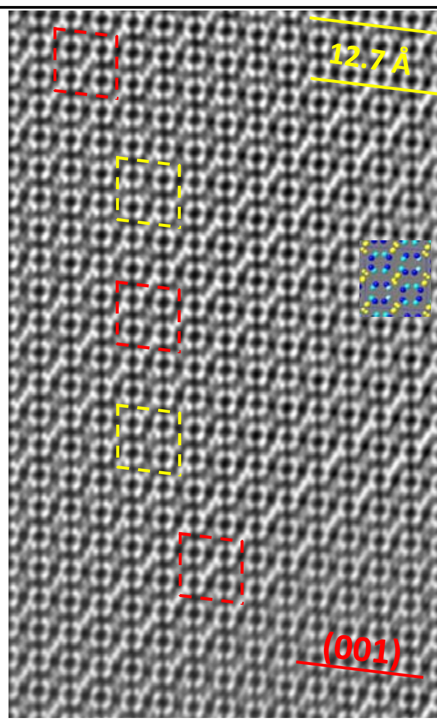
but Inversion twins

$I\bar{1}$

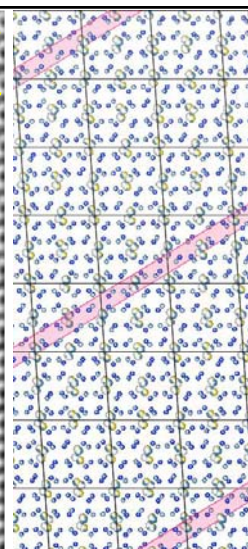
$I1$-like

Z-contrast image

Xu, 2016



$X\bar{1}$



Structure from XRD

An_{70}

American Mineralogist, Volume 102, pages 21–32, 2017

Solved: The enigma of labradorite feldspar with incommensurately modulated structure

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ABSTRACT

Intermediate plagioclase feldspars are the most abundant minerals in the Earth's crust. Their incommensurately modulated structure has puzzled geologists and crystallographers for decades since the phenomenon in a labradorite was reported in 1940. Solving the structure is a necessary step toward mapping the complex subsolidus phase relations of plagioclase solid solution. The structure of a homogeneous labradorite (An_{51}) single crystal from a metamorphic rock is solved and refined from single-crystal X-ray diffraction. The result structure can be simplified as alternating *I*1-like lamellae domains related by inversion twins. The inversion boundary shows an anorthite-like structure with $I\bar{1}$ symmetry and is richer in Ca than the neighboring domains with opposite polarity. No albite-like subunits appear in the

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Incommensurate density modulation in a Na-rich plagioclase feldspar: *Z*-contrast imaging and single-crystal X-ray diffraction study

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e-plagioclase: $X\bar{1}$

- Intermediate composition
- ~An25 - ~An75

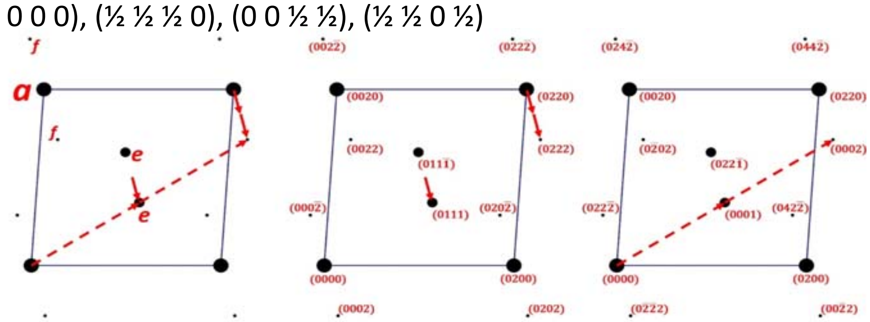
$X\bar{1}$(αβγ)0

$X\bar{1}$($\delta h\ \delta k\ \delta l$)0

3+1D space group:
$X\bar{1}$(αβγ)0 superspace group setting, with c~14Å subcell and a centering condition of (0 0 0 0), (½ ½ ½ 0), (0 0 ½ ½), (½ ½ 0 ½)

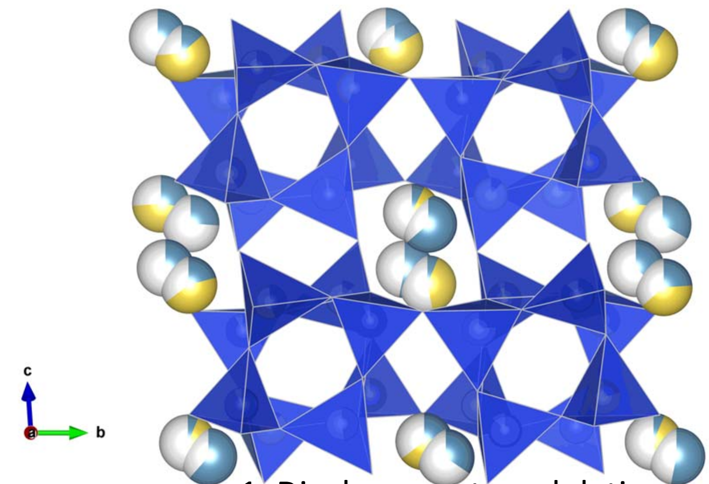
Wave vector

$\mathbf{q} = \delta h + \delta k - \delta l$



A *Miller index: (hkml)* **B** Xu, Jin, & Noll, 2016 **C**

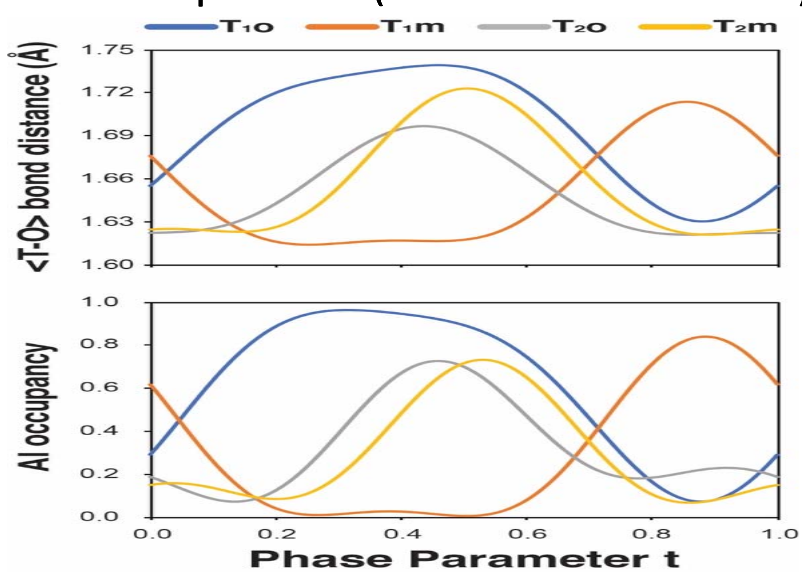
Structure of a plagioclase (An51): $X\bar{1}$
Movie: [100]-zone axis



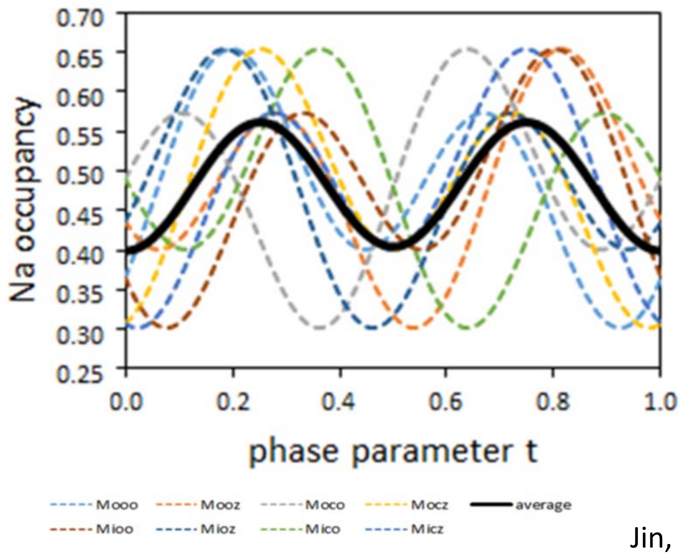
Jin, & Xu, 2017a

1. Displacement modulation

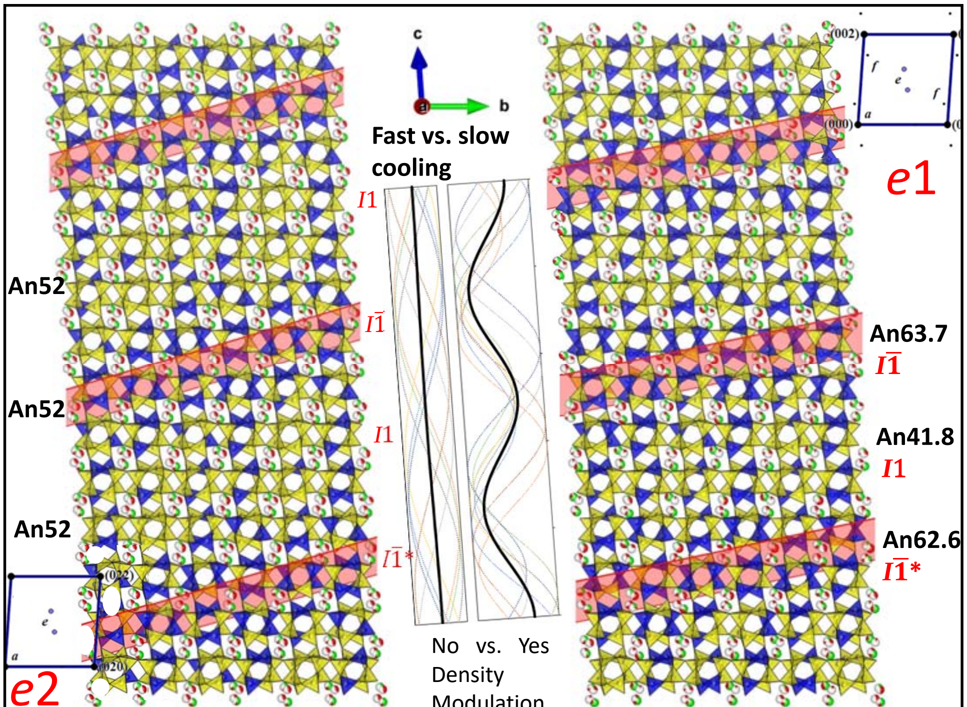
2. Occupational modulation:
Al-Si occupancies (neutron diffraction)



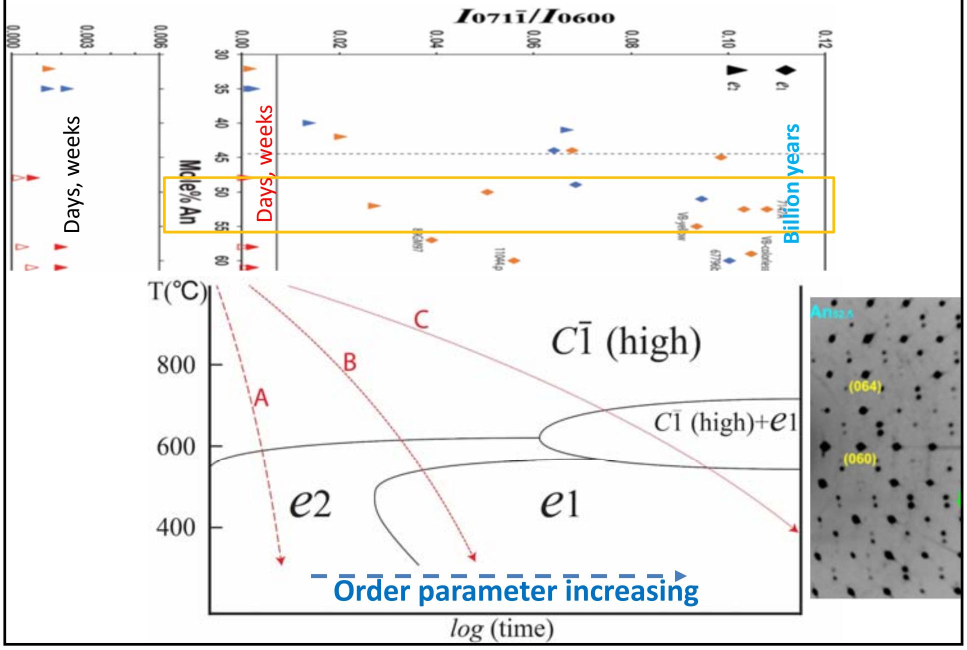
3. Density modulation (first observation)
8 M (Ca+Na) sites within one unit cell



Jin, & Xu, 2017a



Schematic T-T-t diagram: An52



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