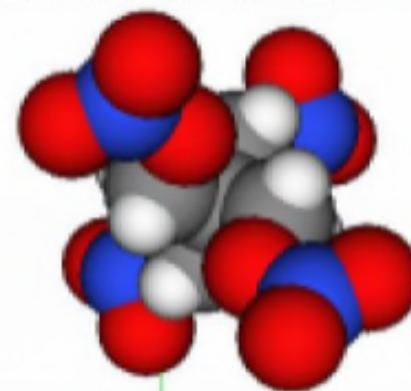


STACKING FAULT MODELING OF CLAYS IN GSAS-II

GSAS-2



ROBERT B. VON DREELE
Advanced Photon Source,
Argonne National Laboratory,
Lenomt, IL 60439 USA
vondreele@anl.gov

June 6, 2017
Edmonton, Alberta, Canada

INTRODUCTION: GSAS-II MODERN GUI – 3 FRAME LAYOUT + CONSOLE

The screenshot displays the GSAS-II software interface. The main window is divided into three frames. The left frame shows a 3D ball-and-stick model of a crystal structure. The right frame is split into two panes: the top pane shows a hierarchical data tree, and the bottom pane shows a table of phase data for Quinuclidine SO3. Red arrows point to various UI elements: the main menu, data tree, submenu, data tabs, data window, drawing tabs, and graphics window.

GSAS-II Plots

Powder Patterns Quinuclidine SO3

GSAS-II data tree

File Data Calculate Import Help

Loaded Data: D:\pygsasii\testing\calcite.bck0

Notebook

Controls

Phase

calcite

H3OSbF6

Quinuclidine SO3

PETN-II data

Phase Data for Quinuclidine SO3

General Data Atoms Draw Options Draw Atoms

	Name	Type	x	y		Sym Op	Style	Label	Color
1	S1	S	0.63369	0.25000	0.31848	1	ellipsoids		Yellow
2	O2	O	0.63521	0.25000	0.55230	1	ellipsoids		Red
3	O3	O	0.68718	0.38684	0.22311	1	ellipsoids		Blue
4	O4	O	0.68718	0.11316	0.22311	1	ellipsoids		Blue
5	N5	N	0.40625	0.25000	0.22311	1	ellipsoids		Blue
6	C6	C	0.37782	0.25000	-0.01774	1	ellipsoids		Blue
7	C7	C	0.32553	0.38769	0.31349	1	ellipsoids		Blue
8	C8	C	0.32553	0.11231	0.31349	1	ellipsoids		Blue

save as: m Phase data v New rotation: -10.50, -12.00, 4.00

11:33 AM 5/2/2011

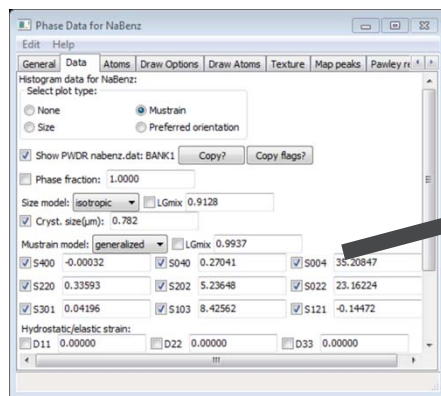
Graphics window

Drawing tabs

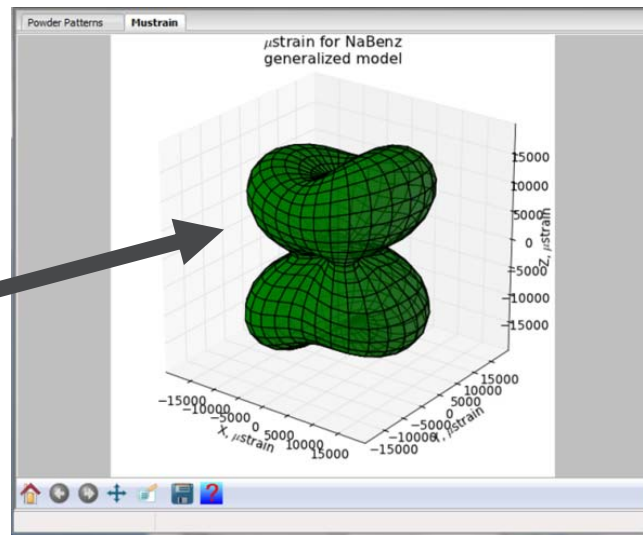
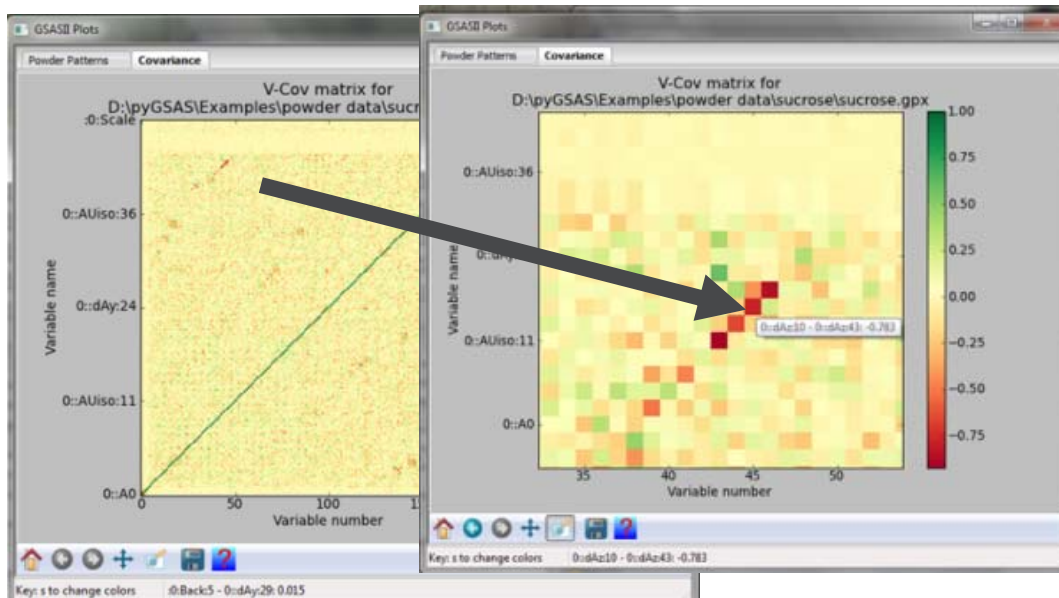
NB: Dialog box windows will appear wanting a response

ADVANCED VISUALIZATION IN GSAS-II: NUMBERS AS PICTURES

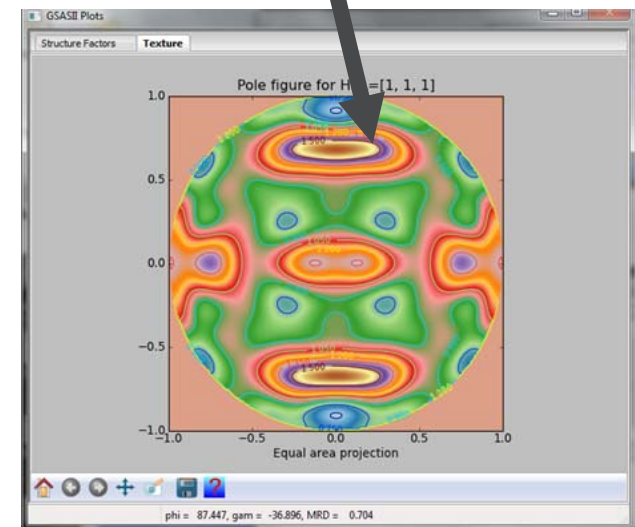
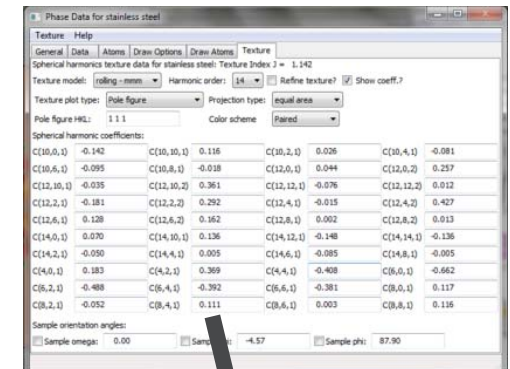
μ strain surface



v-cov matrix



Texture – sph. harmonics



GSAS-II CAPABILITIES & EXAMPLES

Powder data

- 2D Images:
 - calibration & integration → 1D patterns
 - Direct strain fitting → 3 strain tensor elements
- 1D patterns
 - Peak picking & fitting
 - Indexing & space group selection → make new phase
- Multidata X-ray/neutron, CW/TOF → all combinations possible
- Structure solution
 - Stochastic – Monte Carlo/Simulated Annealing
 - Deterministic – Charge Flipping (3D & 4D)
- Structure Refinement – Rietveld Method
 - Modified Levenberg-Marquardt SVD LS
 - Pawley/LeBail refinement (needed for Structure Solution)
 - (3+1) Incommensurate structures
 - Constraints & restraints
 - Rigid bodies (2 kinds)
 - Texture Analysis → spherical harmonics
- **Stacking Faults → DIFFaX simulations (NB: no refinement)**
- Pair Distribution Function → data transformation (e.g. make PDF)
 - PDF peak fitting

DIFFaX – STACKING FAULT SIMULATION

Treacy, Newsam & Deem, *Proc.Roy. Soc.Lond.* A433, 499–520(1991).

- Classic crystallographic Fortran program
 - Deck of cards input: (for e.g. diamond/lonsdaleite simulation)

```
INSTRUMENTAL          {Header for instrumental section}
X-RAY                  {Simulate X-ray diffraction}
1.5418                 {X-ray wavelength}
{gaussian 0.1 trim}    {Instrumental broadening (much faster)}
PSEUDO-VOIGT 0.1 -0.036 0.009 0.6 TRIM {Instrumental broadening (much slower)}
STRUCTURAL             {Header for structural section}
2.52 2.52 2.06 120.0   {unit cell coordinates, a, b, c, gamma}
6/MMM                 {hexagonal, c = cubic [111]}
2                     {111 sheet, plus its mirror}
infinite               {Layers are very wide in the a-b plane}
LAYER 1
CENTROSYMMETRIC
C 1 -.333333 -.166667 -.125 1.0 1.0
{C 2 .333333 .166667 .125 1.0 1.0, related to 1 by -1}
LAYER 2
CENTROSYMMETRIC
C 1 .333333 .166667 -.125 1.0 1.0
{C 2 -.333333 -.166667 .125 1.0 1.0, related to 1 by -1}
STACKING               {Header for stacking description}
recursive              {Statistical ensemble}
infinite               {Infinite number of layers}
TRANSITIONS            {Header for stacking transition data}
{Transitions from layer 1}
0.7 0.666667 0.333333 1.0 {layer 1 to layer 1}
0.3 0.0 0.0 1.0 {layer 1 to layer 2}

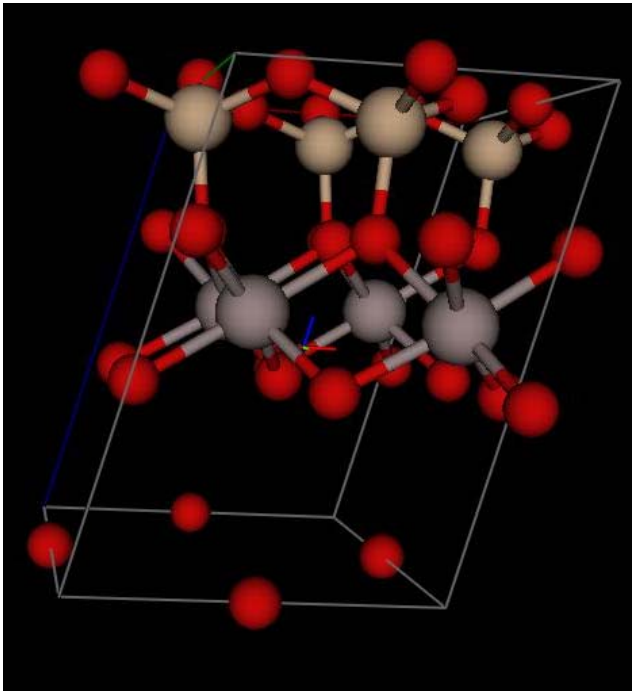
{Transitions from layer 2}
0.3 0.0 0.0 1.0 {layer 2 to layer 1}
0.7 -0.666667 -0.333333 1.0 {layer 2 to layer 2}
```

- Must construct this by hand following manual
- Need a separate plotting pgm to view result
- Trials: edit input, rerun & replot....

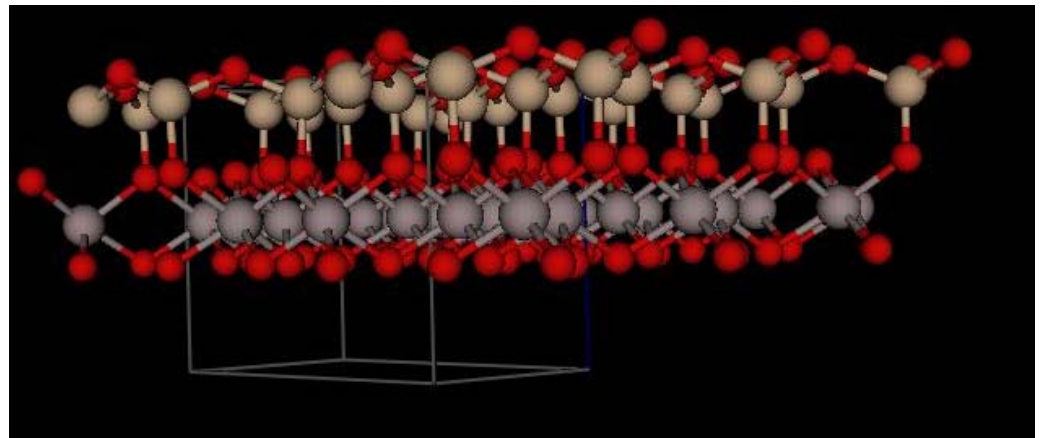
GSAS-II & DIFFaX

GUI interface & structure plotting

- Model development
 - Layers
 - hand input; ok if very simple (e.g. diamond)
 - transform from known structure (e.g. kaolinite)



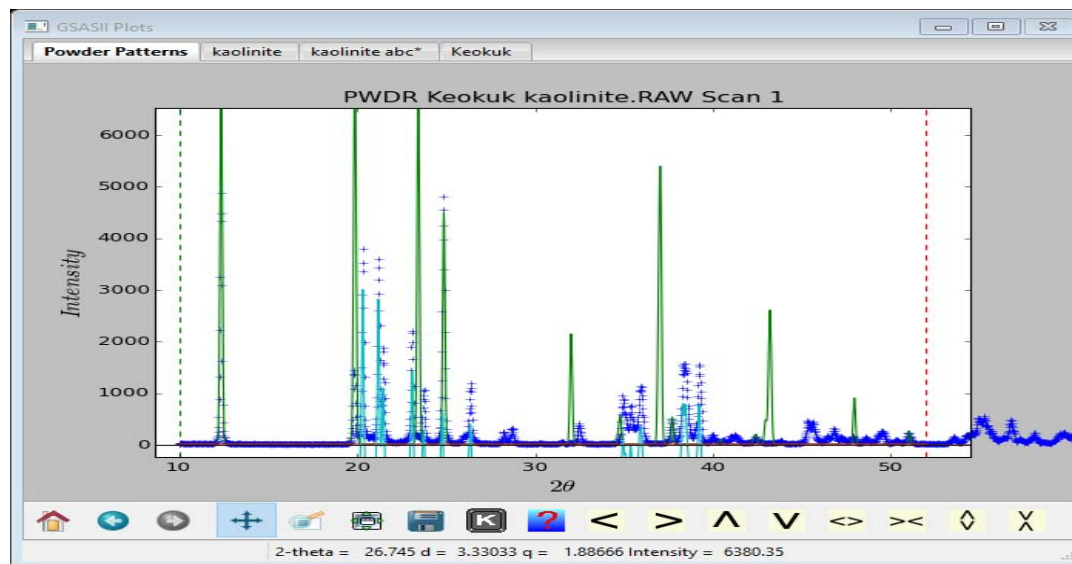
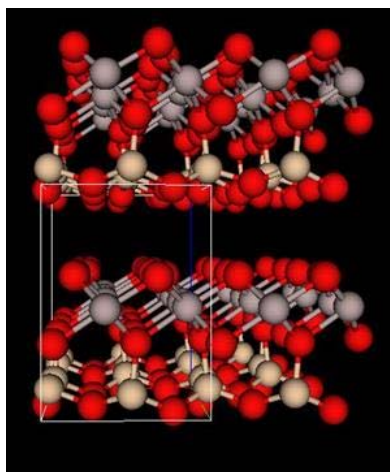
Kaolinite - triclinic



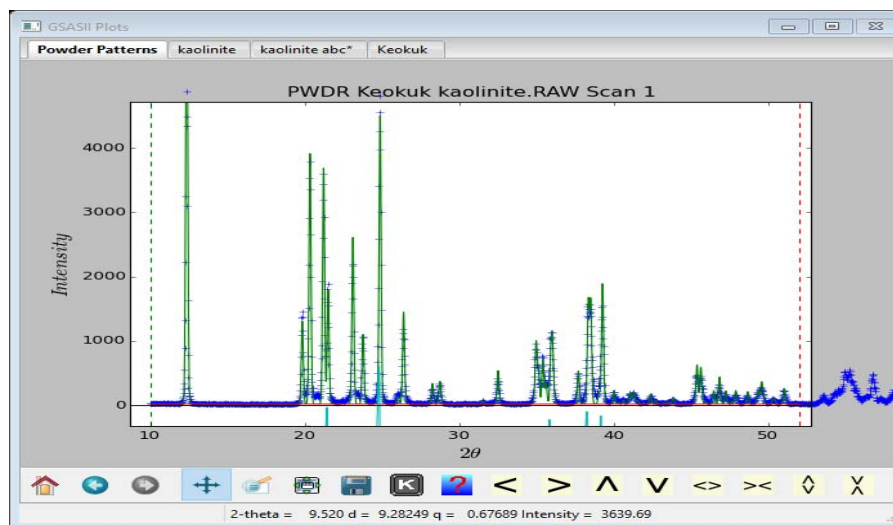
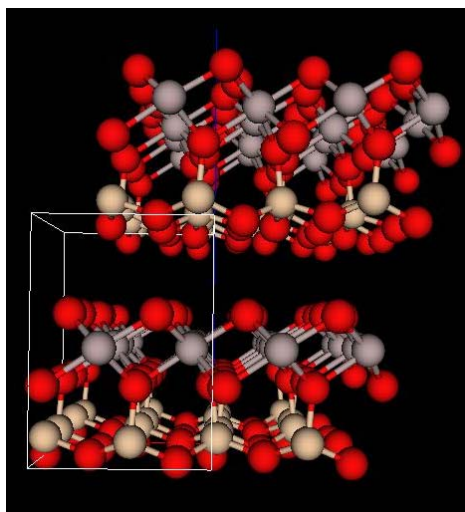
Transform: $abc \rightarrow abc^*$
Can be stacked

GSAS-II & DIFFaX – KEOKUK KAOLINITE

- Model development
 - Stacking model



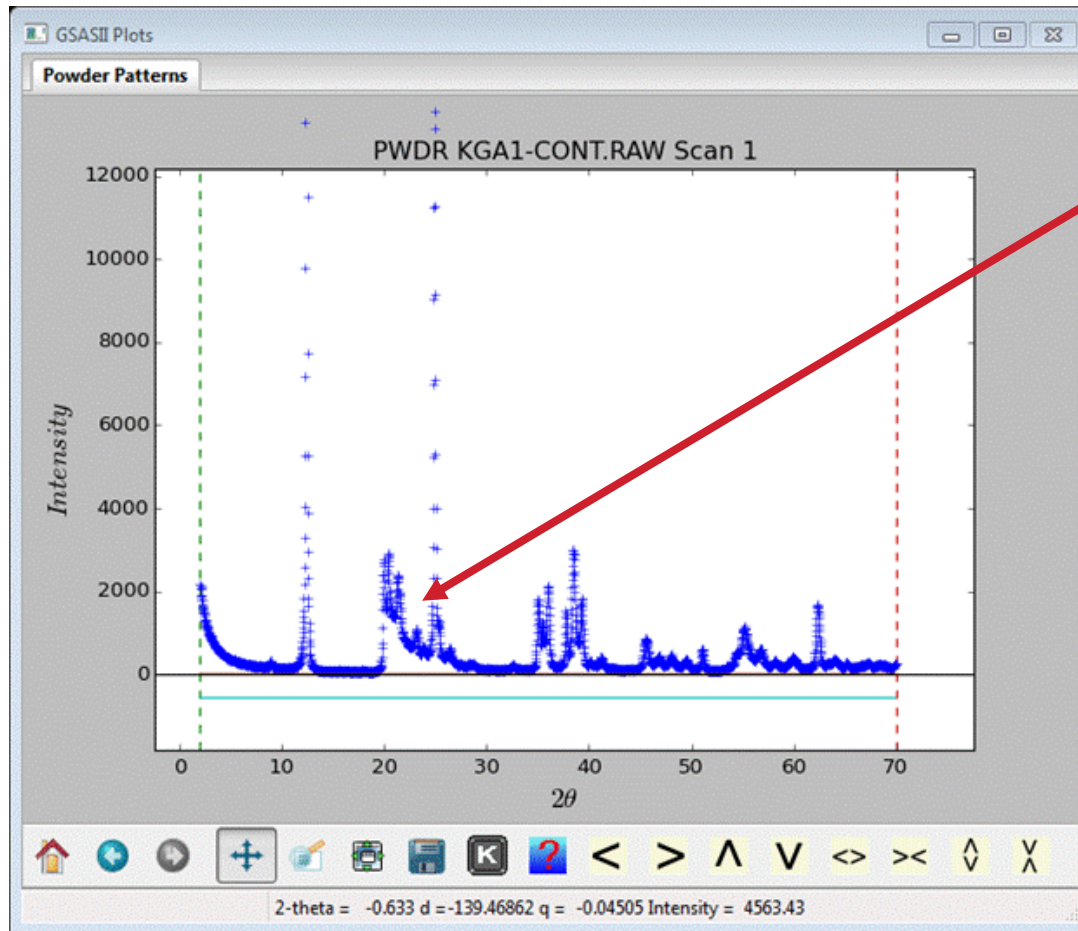
No offset on x,y – crummy simulation



Kaolinite x,y offset – much better (no ⁷surprise)

GEORGIA KAOLINITE – CMS KGa-1b

Faulted kaolinite



Obvious stacking faults

Modeling?

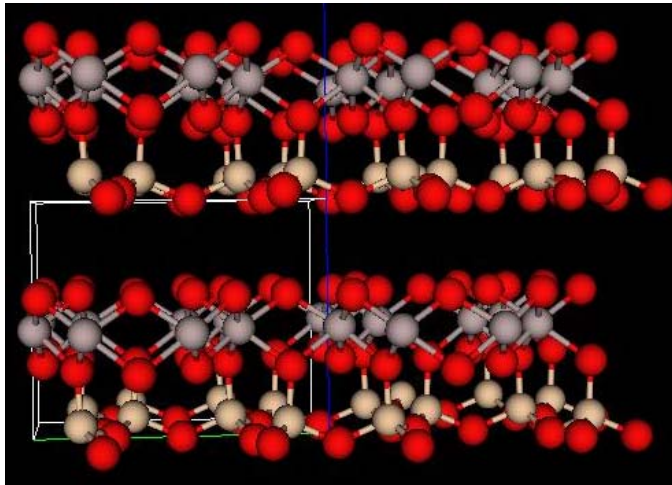
Need at least 2 layers for faulting to have A-A, A-B, B-A & B-B stacking

Both kaolinite with different offsets

NB: pattern has a bit of anatase (TiO_2)

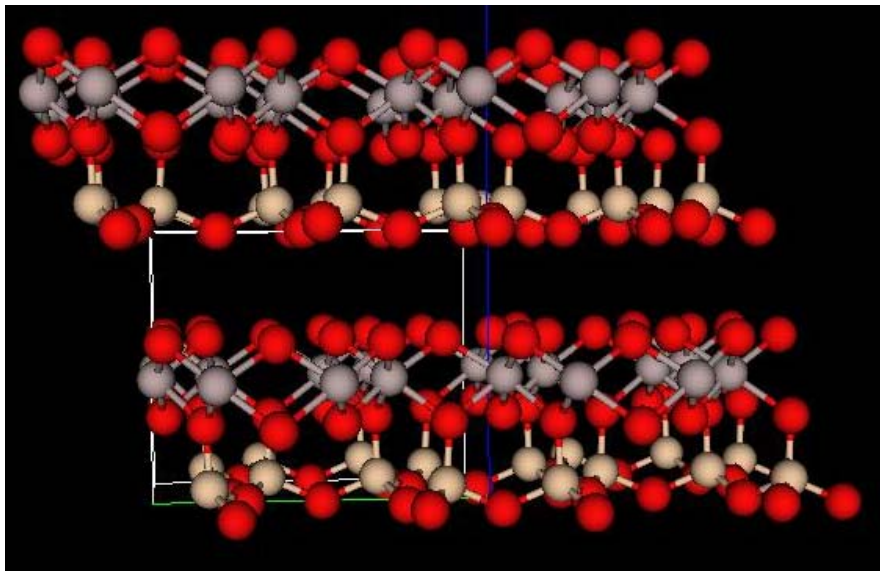
GEORGIA KAOLINITE

2 different offsets:



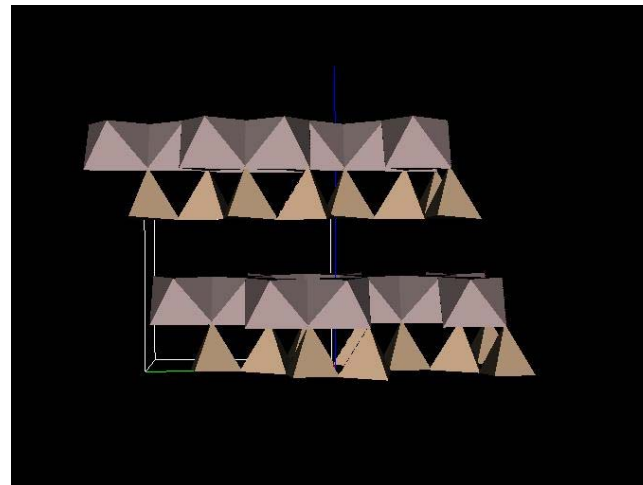
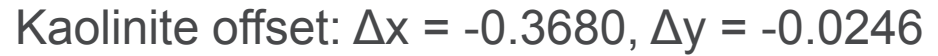
Kaolinite offset: $\Delta x = -0.3680$, $\Delta y = -0.0246$

$\Delta y \rightarrow$



Fault offset: $\Delta x = -0.3680$, $\Delta y = -0.0246 + 1/3$
NB: not dickite stacking

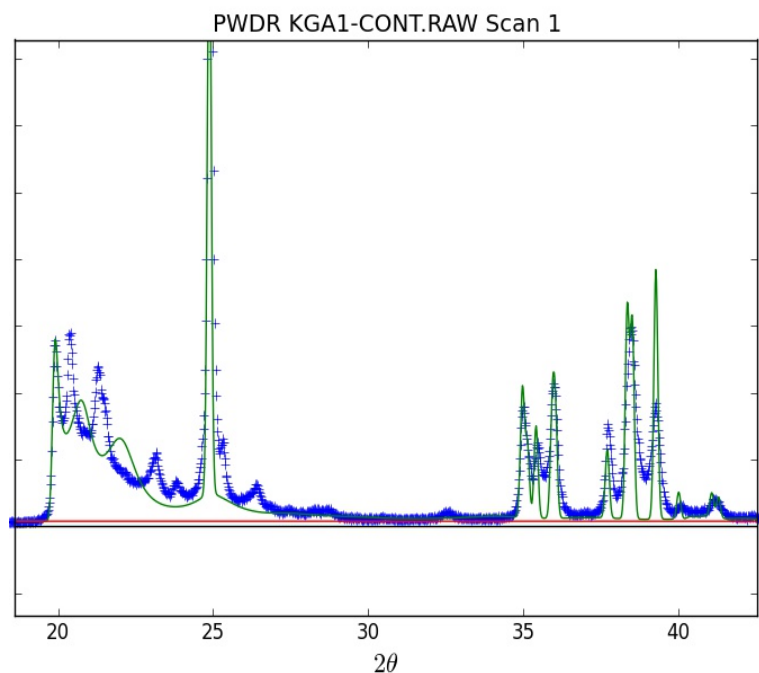
Top view



GEORGIA KAOLINITE

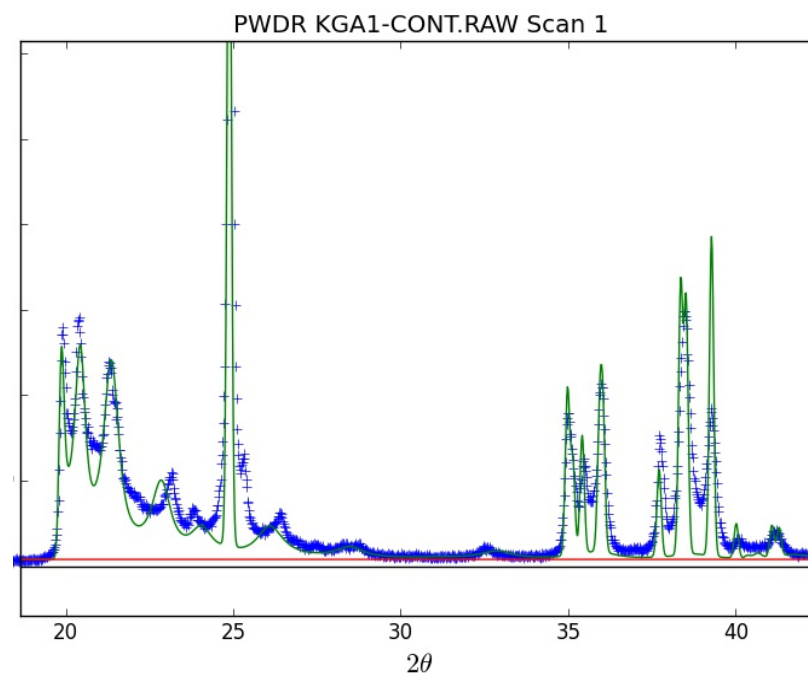
Stacking probabilities – A-A/A-B?

- 50-50%



- Not so great
- Model may need more elaborate stacking to fully model data
- Another offset direction? – add a layer C with new C-A & C-B offsets & probabilities

- or 80/20%



much better but not perfect

**GSAS-II –
EASY VISUALIZATION OF STACKING MODELS
INTERFACE TO DIFFaX**

THANK YOU