Refinement of modulated structures with Jana examples

Michal Dušek
Institute of Physics, Prague, Czech Republic

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Outline

- Structure factor formula for simple harmonic modulation
- Diffraction pattern induced by modulation function
- What can be modulated? Which parameters are refined?
- Program Jana2006
- Two ways how to solve modulated structure
- Example: sodium carbonate by classical method
- Verification of results from Fourier maps
- Distances and t-plots
- Plotting of modulated structures
- Example: Chromium diphosphate solved by charge flipping
- Discontinuous functions
- Commensurate refinement
- Composite structures [skipped]
- Magnetic structures
- Where to get more information?

Structure factor and diffraction pattern

$\mathbf{r}_\nu = \mathbf{r}_{\nu,0} + \mathbf{u}_\nu(\tau)$,

where τ is x_4 of undisplaced position.

The displaced position has $x_4 = \tau + \mathbf{q}\mathbf{u}_\nu$

Contribution of an interval $d\tau$ to the Fourier coefficient h_1, h_2, h_3, m:

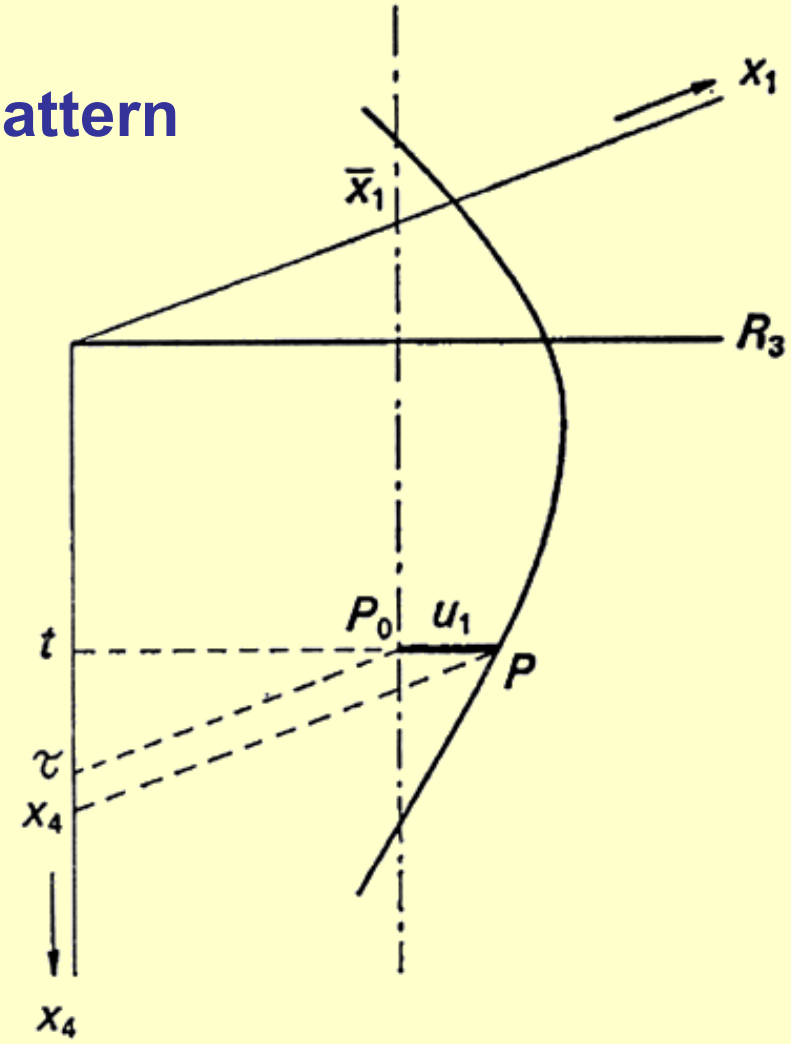
$$f_\nu d\tau \exp\left[2\pi i\left(h_1x_1 + h_2x_2 + h_3x_3 + mx_4\right)\right] =$$

$$f_\nu d\tau \exp\left[2\pi i\left(\mathbf{H}\mathbf{r}_\nu + mx_4\right)\right] =$$

$$f_\nu d\tau \exp\left[2\pi i\left(\mathbf{H}\mathbf{r}_{\nu,0} + \mathbf{H}\mathbf{u}_\nu + m\mathbf{q}\mathbf{u}_\nu + m\tau\right)\right]$$

$$F\left(h_1,h_2,h_3,m\right) = \sum_\nu f_\nu \exp\left(2\pi i\mathbf{H}\mathbf{r}_{\nu,0}\right)$$

$$\times \int_0^1 d\tau \exp\left[2\pi i\left(\mathbf{H} + m\mathbf{q}\right)\mathbf{u}_\nu + m\tau\right]$$



(de Wolff, Acta Cryst. A30,777)

The integral can be calculated by Gaussian method.

An older way uses analytical method with Bessel functions. The analytical calculation shows clearly relationship between modulation waves and diffraction pattern.

Positional modulation with a simple harmonic wave

$$\mathbf{r}_\nu(\mathbf{n}) = \mathbf{r}_{\nu,0} + \mathbf{U}_{\nu s1}\sin\left[2\pi\mathbf{q}\left(\mathbf{r}_{\nu,0}+\mathbf{n}\right)\right]$$

Contribution from atom at $\mathbf{r}_\nu + \mathbf{n}$: (form factors corrected for temperature movement)

$$F_{\nu,\mathbf{n}}(\mathbf{Q}) = f_\nu^T(\mathbf{Q})\exp\left[2\pi i\mathbf{Q}\cdot\left(\mathbf{r}_\nu+\mathbf{n}\right)\right] = f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_\nu\right)\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{n}\right)$$

$$F_{\nu,\mathbf{n}}(\mathbf{Q}) = f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0}\right)\exp\left\{2\pi i\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\sin\left[2\pi\mathbf{q}\left(\mathbf{r}_{\nu,0}+\mathbf{n}\right)\right]\right\}\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{n}\right)$$

Jacobi - Anger expansion :

$$\exp\left(iz\sin\alpha\right) = \sum_{l=-\infty}^{\infty} J_l(z)\exp\left(il\alpha\right)$$

In our case $z = 2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}$

$$F_{\nu,\mathbf{n}}(\mathbf{Q}) = f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0}\right)\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{n}\right)\sum_{l=-\infty}^{\infty} J_l\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)\exp\left[2\pi il\mathbf{q}\left(\mathbf{r}_{\nu,0}+\mathbf{n}\right)\right] =$$

$$f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0}\right)\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{n}\right)\sum_{l=-\infty}^{\infty} J_l\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)\exp\left(2\pi il\mathbf{q}\mathbf{r}_{\nu,0}\right)\exp\left(2\pi il\mathbf{q}\mathbf{n}\right) =$$

$$f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0}\right)\sum_{l=-\infty}^{\infty} J_l\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)\exp\left(2\pi il\mathbf{q}\mathbf{r}_{\nu,0}\right)\exp\left[2\pi i\left(\mathbf{Q}+l\mathbf{q}\right)\mathbf{n}\right]$$

Summation for all $\mathbf{n}$:

$$F_\nu(\mathbf{Q}) = f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0}\right)\sum_{l=-\infty}^{\infty} J_l\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)\exp\left(2\pi il\mathbf{q}\mathbf{r}_{\nu,0}\right)\sum_{\mathbf{n}}\exp\left[2\pi i\left(\mathbf{Q}+l\mathbf{q}\right)\mathbf{n}\right]$$

Contribution of atom ν to the structure factor for 3d crystal :

$$F_\nu(\mathbf{Q}) = f_\nu(|\mathbf{Q}|)\exp(2\pi i\mathbf{Q}\cdot\mathbf{r}_\nu)\sum_{\mathbf{n}}\exp\{2\pi i\mathbf{Q}\cdot\mathbf{n}\} =$$

$$f_\nu(|\mathbf{Q}|)\exp(2\pi i\mathbf{Q}\cdot\mathbf{r}_\nu)\frac{\sin\pi N_1\mathbf{Q}\cdot\mathbf{a}_1}{\sin\pi\mathbf{Q}\cdot\mathbf{a}_1}\frac{\sin\pi N_2\mathbf{Q}\cdot\mathbf{a}_2}{\sin\pi\mathbf{Q}\cdot\mathbf{a}_2}\frac{\sin\pi N_3\mathbf{Q}\cdot\mathbf{a}_3}{\sin\pi\mathbf{Q}\cdot\mathbf{a}_3}$$

$$\exp\{\pi i\mathbf{Q}\cdot((N_1-1)\mathbf{a}_1+(N_2-1)\mathbf{a}_2+(N_3-1)\mathbf{a}_3)\}$$

This function has maxima if $\mathbf{Q}\cdot\mathbf{a}_1$, $\mathbf{Q}\cdot\mathbf{a}_2$ and $\mathbf{Q}\cdot\mathbf{a}_3$ are integers. This occurs if

$$\mathbf{Q} = \mathbf{H} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*, \quad h_i \text{ integers}, \quad \mathbf{a}_i\cdot\mathbf{a}_j^* = \delta_{ij}$$

Contribution of atom ν to the structure factor in case of simple harmonic modulation :

$$F_\nu(\mathbf{Q}) = f_\nu^T(\mathbf{Q})\exp(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0})\sum_{l=-\infty}^{\infty}J_l(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1})\exp(2\pi il\mathbf{q}\mathbf{r}_{\nu,0})\sum_{\mathbf{n}}\exp[2\pi i(\mathbf{Q}+l\mathbf{q})\mathbf{n}]$$

This function has maxima if $(\mathbf{Q}+l\mathbf{q}_1)\cdot\mathbf{a}_1$, $(\mathbf{Q}+l\mathbf{q}_2)\cdot\mathbf{a}_2$ and $(\mathbf{Q}+l\mathbf{q}_3)\cdot\mathbf{a}_3$ are integers.

This occurs if

$$\mathbf{Q}+l\mathbf{q} = \mathbf{H} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*, \quad h_i \text{ integers}, \quad \mathbf{a}_i\cdot\mathbf{a}_j^* = \delta_{ij}$$

$$\mathbf{Q} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^* + m\mathbf{q} = \mathbf{H} + m\mathbf{q} \qquad l = -m$$

$$F_\nu(\mathbf{Q}) = f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu,0}\right)\sum_{l=-\infty}^{\infty} J_l\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)\exp\left(2\pi il\mathbf{q}\mathbf{r}_{\nu,0}\right)\sum_{\mathbf{n}}\exp\left[2\pi i\left(\mathbf{Q}+l\mathbf{q}\right)\mathbf{n}\right]$$

This function has maxima at

$$\mathbf{Q} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^* + m\mathbf{q} = \mathbf{H} + m\mathbf{q} \qquad l = -m$$

Contribution of atom ν to the reflection (h,k,l,m):

$$F_\nu(\mathbf{Q}) =$$

$$f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{H}\cdot\mathbf{r}_{\nu,0}\right)\exp\left(-2\pi il\mathbf{q}\cdot\mathbf{r}_{\nu,0}\right)J_{-m}\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)\exp\left(2\pi il\mathbf{q}\mathbf{r}_{\nu,0}\right)S =$$

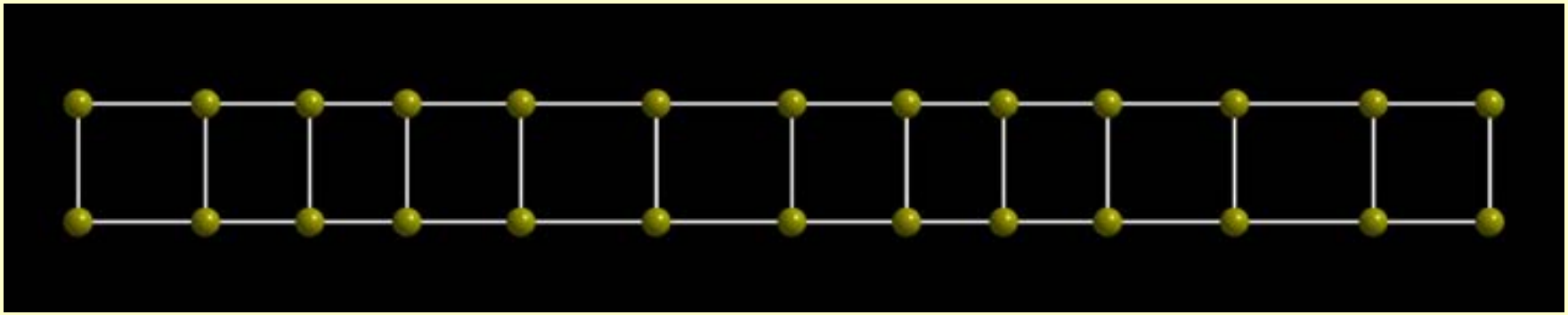
$$f_\nu^T(\mathbf{Q})\exp\left(2\pi i\mathbf{H}\cdot\mathbf{r}_{\nu,0}\right)J_{-m}\left(2\pi\mathbf{Q}\cdot\mathbf{U}_{\nu s1}\right)S$$

where S is result of summation over $\mathbf{n}$.

Conclusions:

1. One harmonic wave generates satellites up to the "infinite" order.
2. Intensity of the satellite (h,k,l,m) is proportional to the square of the Bessel function of the order m
3. Intensity of satellites grows with $\mathbf{Q}\cdot\mathbf{U}_\nu$

Simulation of a simple longitudinal modulation



$$\mathbf{q} = (\alpha, \beta, 0)$$

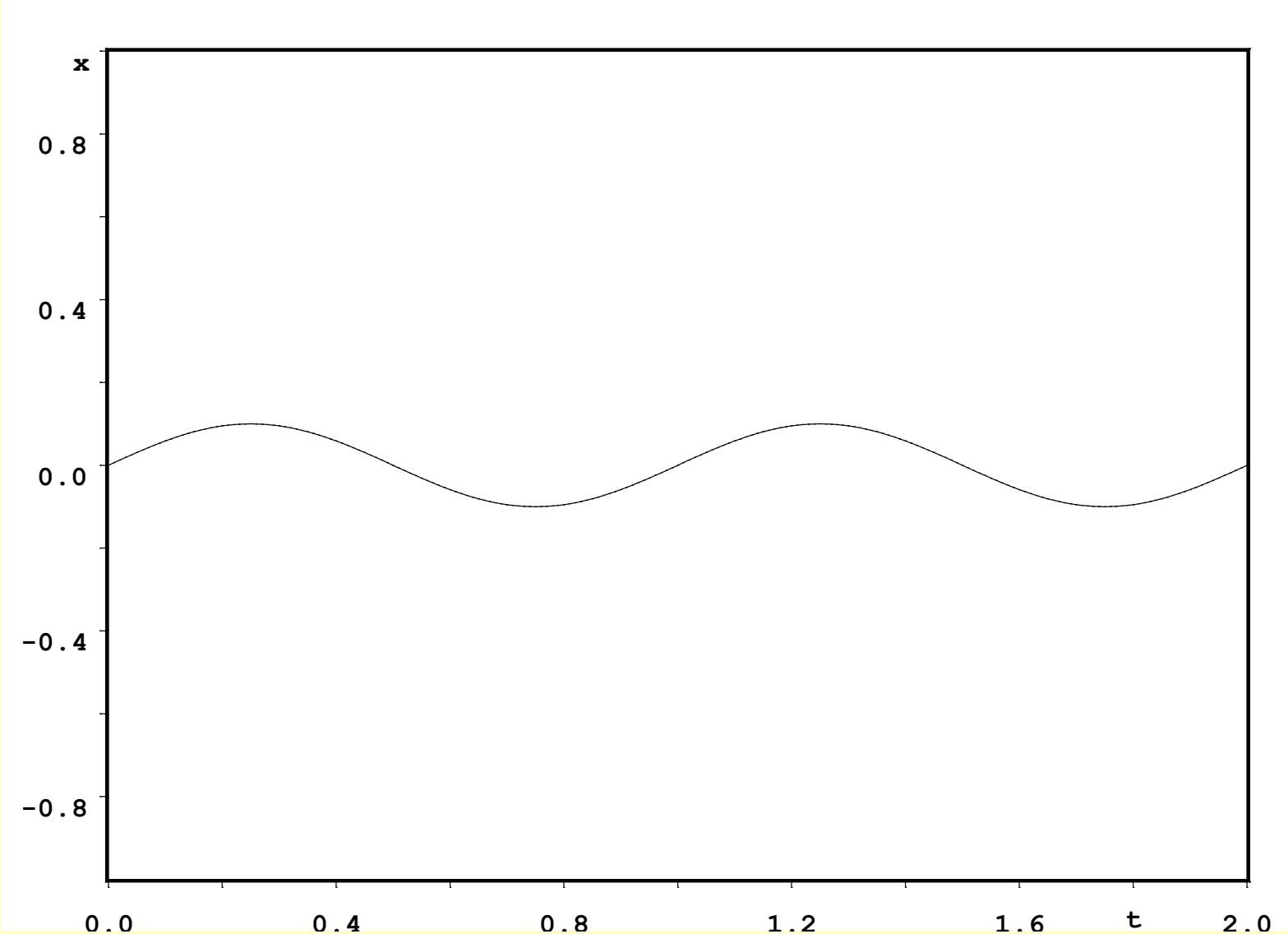
$$\mathbf{u} = \mathbf{U}\cos(2\pi\,\mathbf{q}\cdot\mathbf{r})$$

$$F = f\exp(2\pi i\mathbf{H}\cdot\mathbf{r})J_{-m}(2\pi\,\mathbf{U}\cdot\mathbf{Q})$$

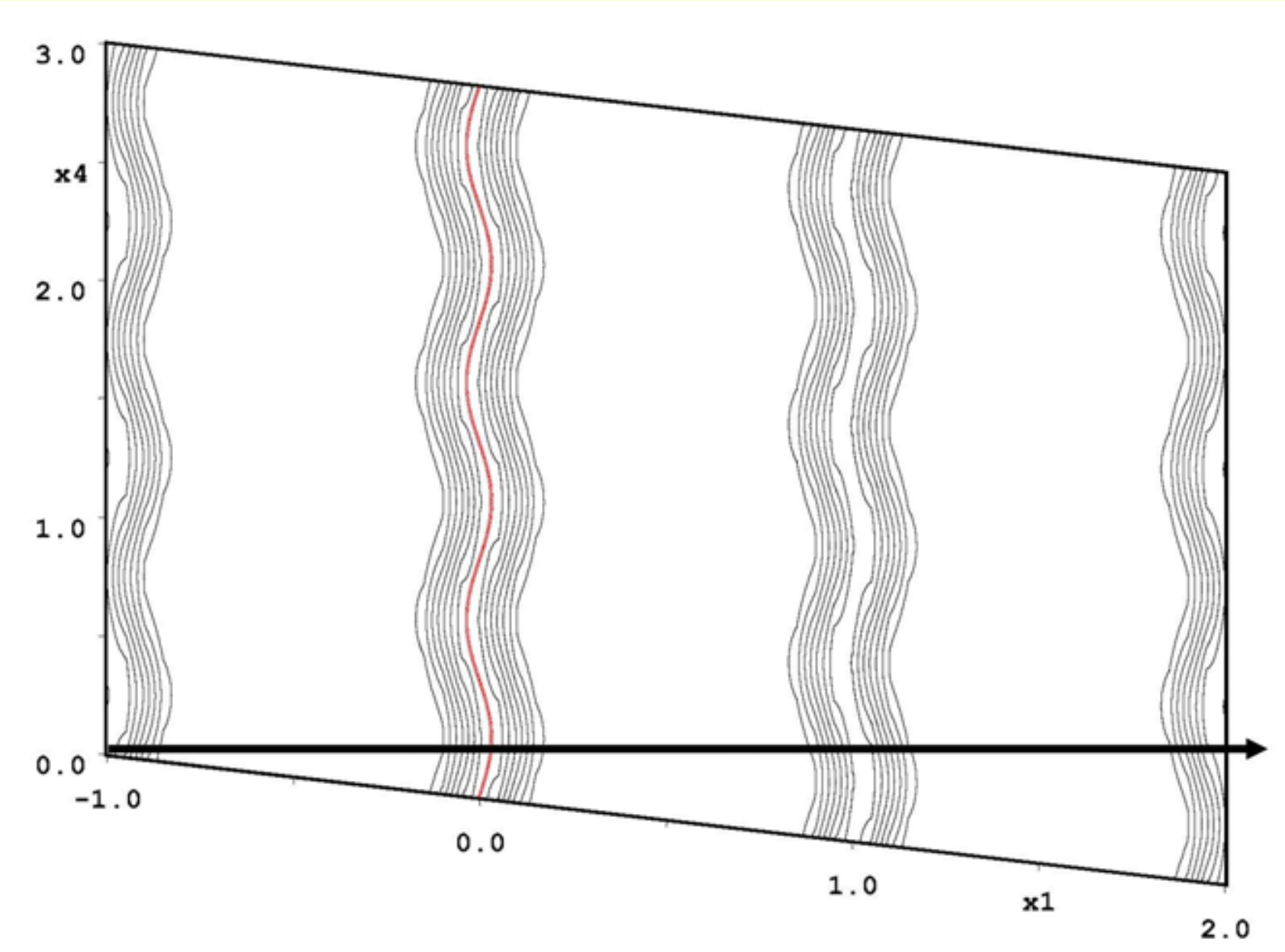
$$\mathbf{U} = (U_x, 0, 0)$$

We shall show how the simulated diffraction pattern depends on the modulation amplitude, i.e. U_x, and that with a large amplitude we can see higher order satellites generated with the first modulation wave.
The cos term can be replaced by sin term used in the previous calculations. This would only shift the figures.

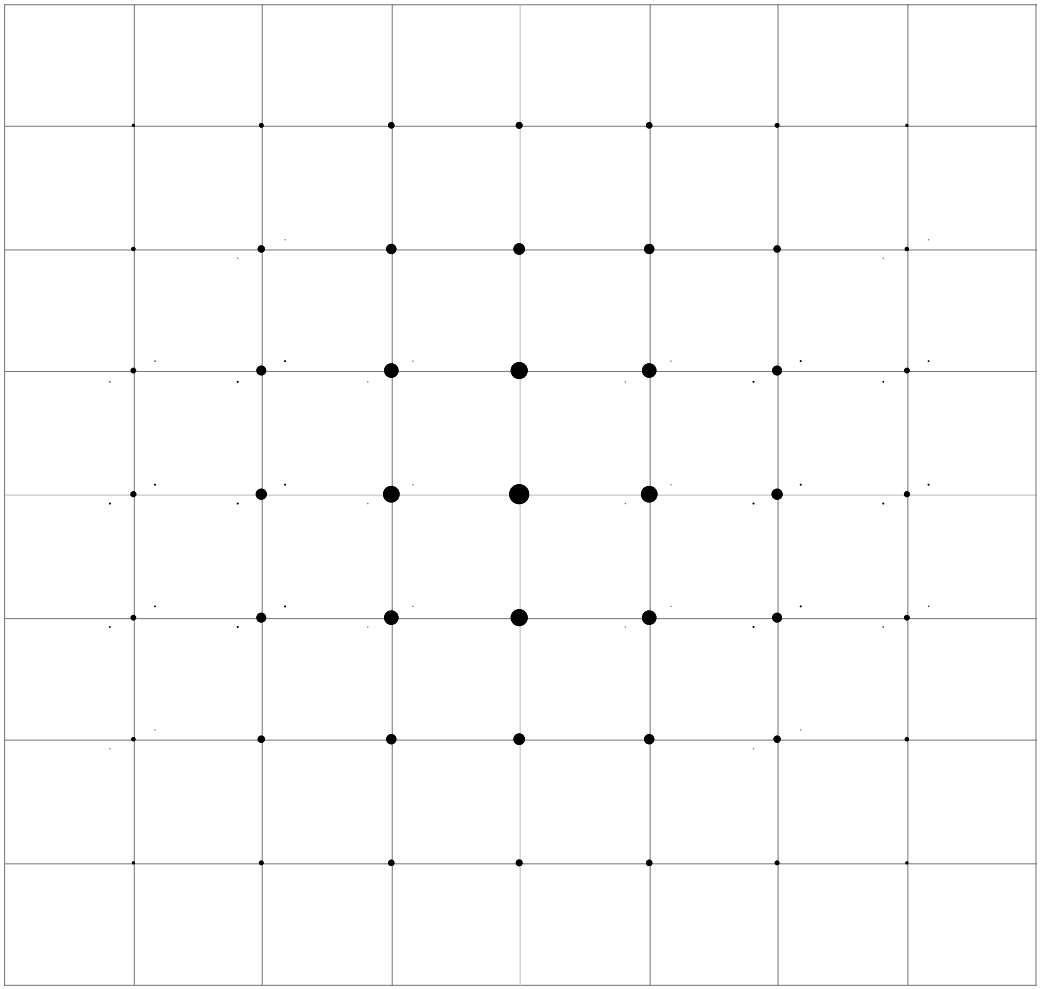
Positional modulation longitudinal
1st harmonic 0.1Å
Modulation function



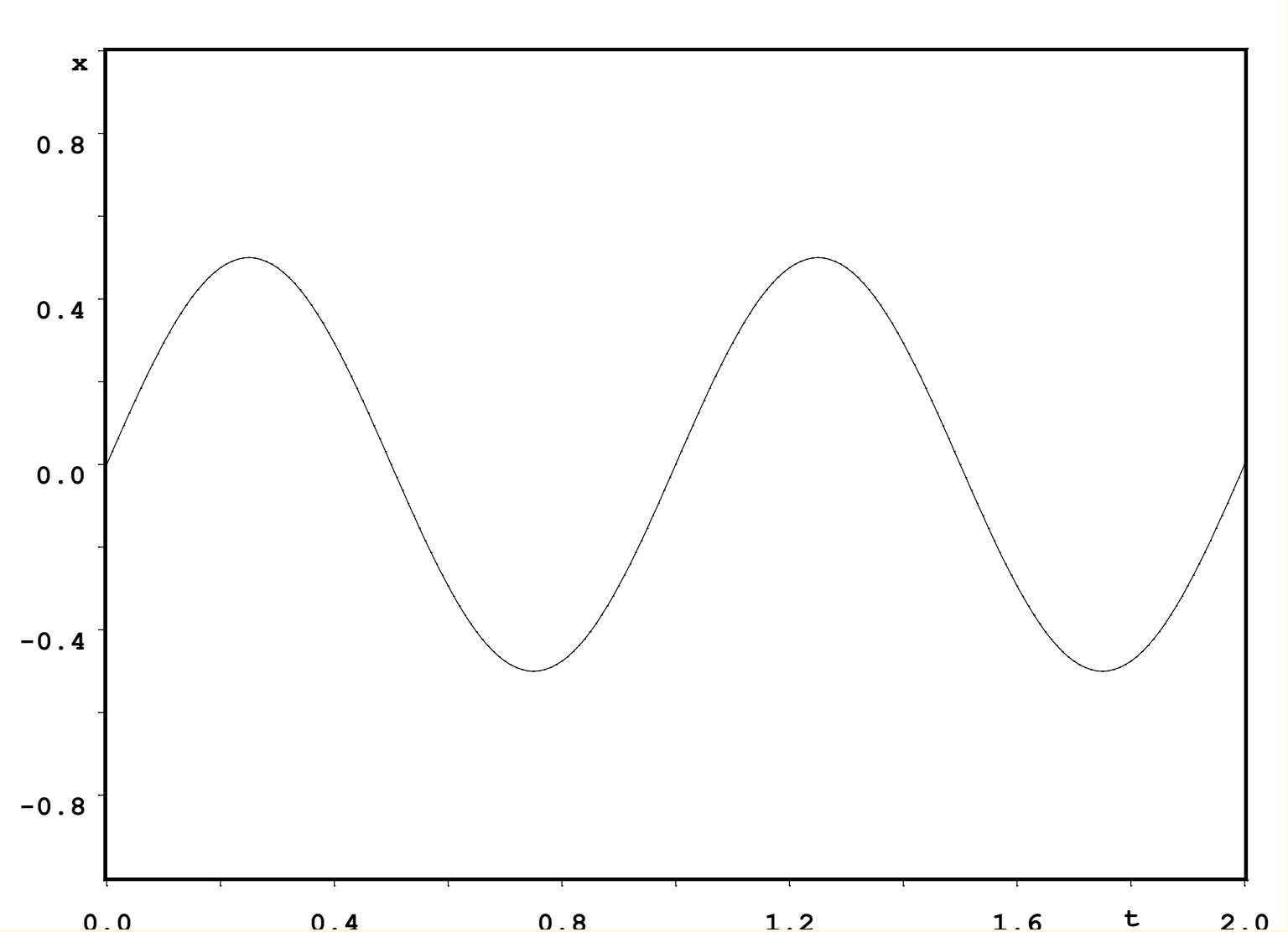
Positional modulation longitudinal
1st harmonic 0.1Å
Fourier map



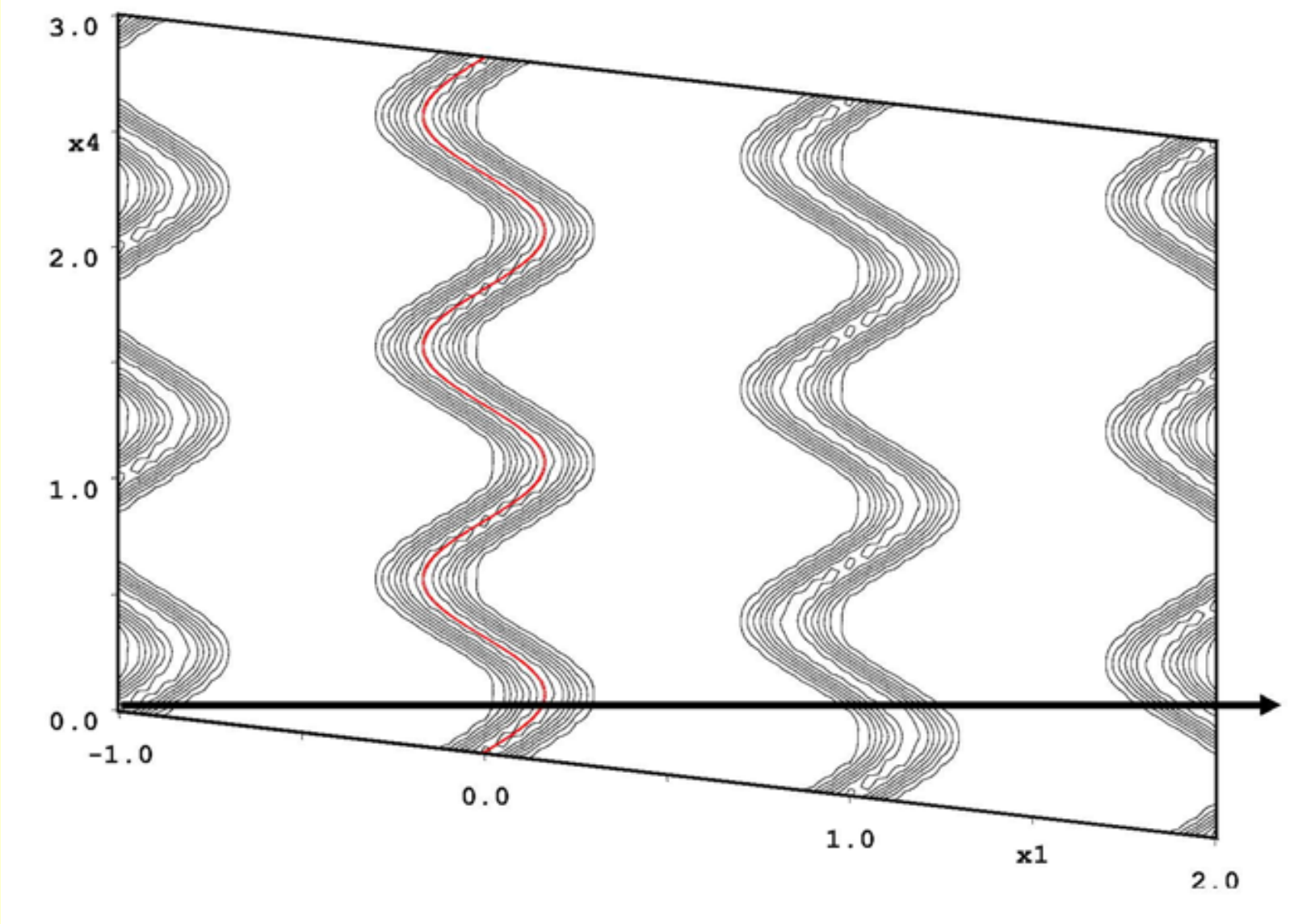
Positional modulation longitudinal
1st harmonic 0.1Å
Diffraction pattern



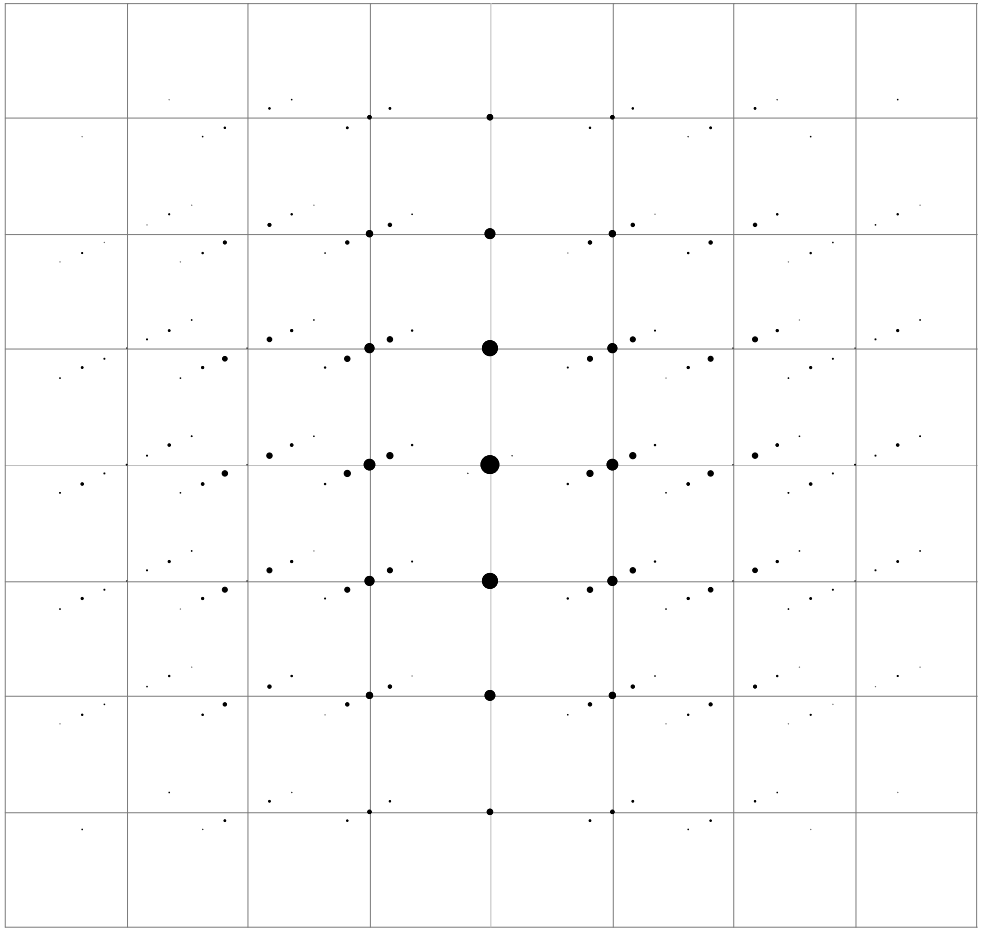
Positional modulation longitudinal
1st harmonic 0.5Å
Modulation function



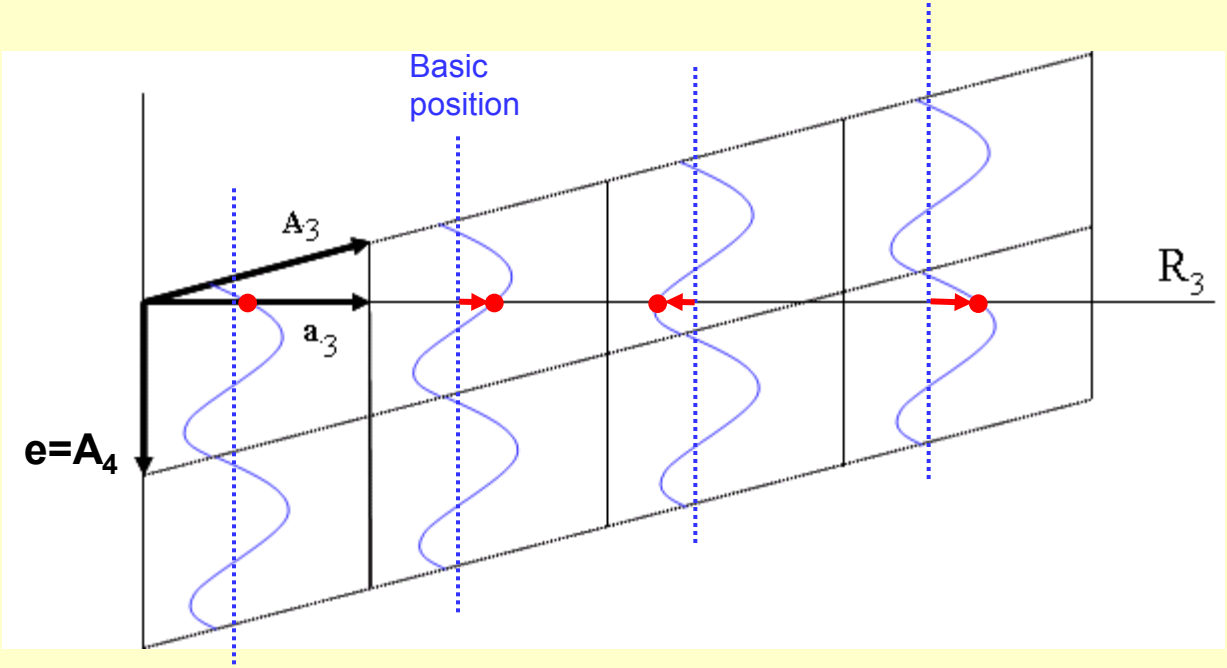
Positional modulation longitudinal
1st harmonic 0.5Å
Fourier map



Positional modulation longitudinal
1st harmonic 0.5Å
Diffraction pattern



Parameters for position modulation



Basic position
x
average position

The same fractional coordinates in A3 and a3.

The atom is displaced from its basic position by a periodic modulation function that can be expressed as a Fourier expansion. In the first approximation intensities of satellites reflections up to order m are determined by modulation waves of the same order.

$$\mathbf{r} = \overline{\mathbf{r}} + \mathbf{u}$$

$$\mathbf{u}(\overline{x}_4) = \sum_{n=1}^{m} \mathbf{U}_{s,n} \sin(2\pi n \overline{x}_4) + \sum_{n=1}^{m} \mathbf{U}_{c,n} \cos(2\pi n \overline{x}_4)$$

What can be modulated *(in Jana2006)*

positions of individual atoms

positions of rigid bodies

ADP of individual atoms (harmonic or anharmonic)

Displacement parameters of rigid bodies -TLS tenzors (harmonic or anharmonic)

occupation of individual atoms

occupation of rigid bodies

magnetic moments

Jana2006

Program for structure analysis of crystals periodic in three or more dimensions from diffraction data

Václav Petříček, Michal Dušek & Lukáš Palatinus
Institute of Physics, Prague, Czech Republic

1980 SDS: *Program for solution and refinement of 3d structures*

1984 Jana : *Refinement program for modulated structures*

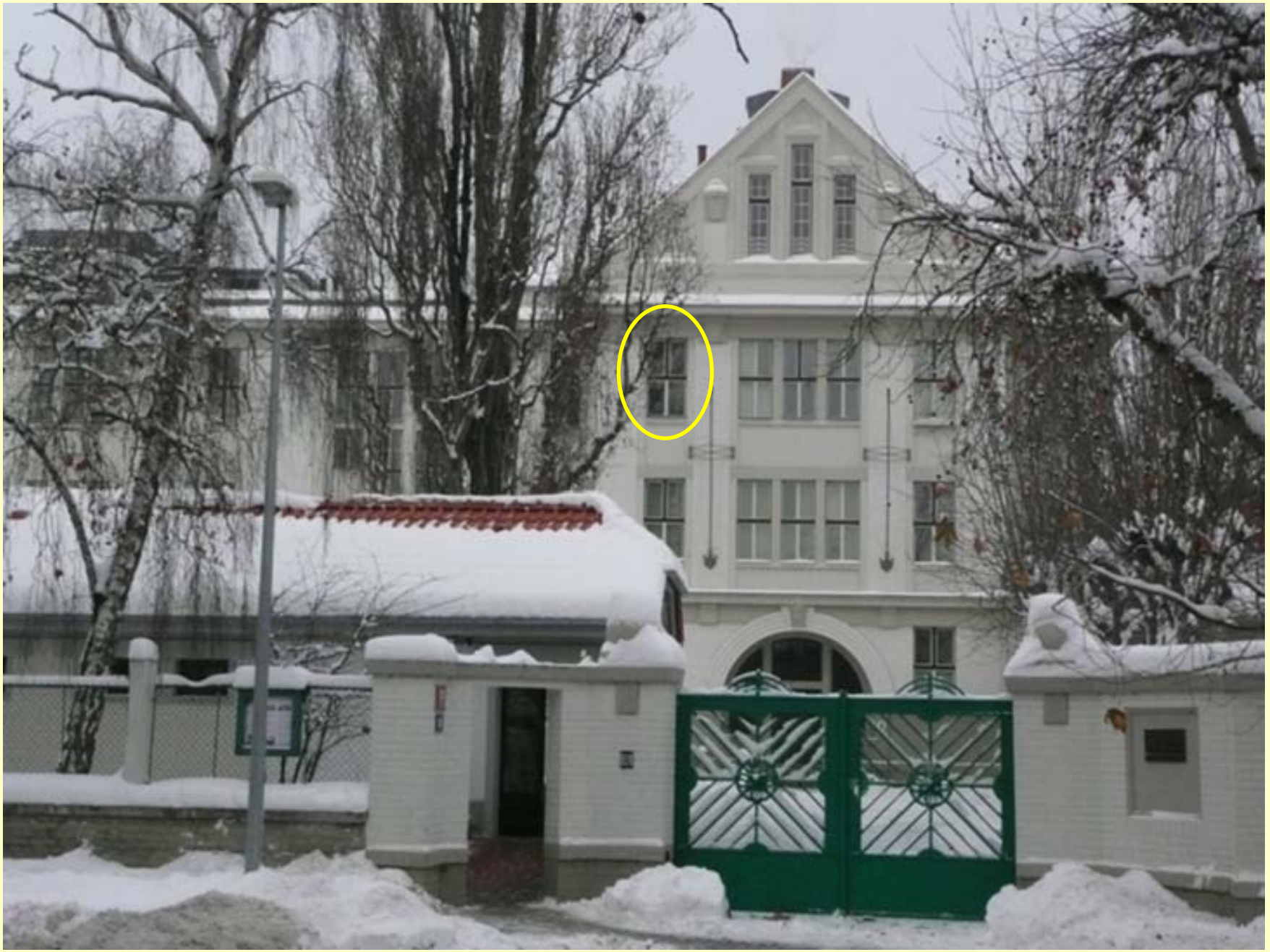
1996 J**ana96**: *Modulated and 3d structures in one program. Graphical interface for DOS and UNIX X11.*

1998 Jana98 :*Improved Jana96. First widely used version. Graphical interface for DOS, DOS emulation and UNIX X11*

2000 Jana2000: *Support for powder data and multiphase refinement. Graphical interface for Win32 and UNIX X11*.

2006 Jana2006: *Combination of data sources, magnetic structures, TOF data. Dynamical allocation of memory. Only for Windows.*

Institute of Physics, Prague 6, Cukrovarnická street



Data input

X-rays **OR** neutrons **OR** electrons

↓

Powder data of one or more phases

OR

Single crystal data of one or more domains

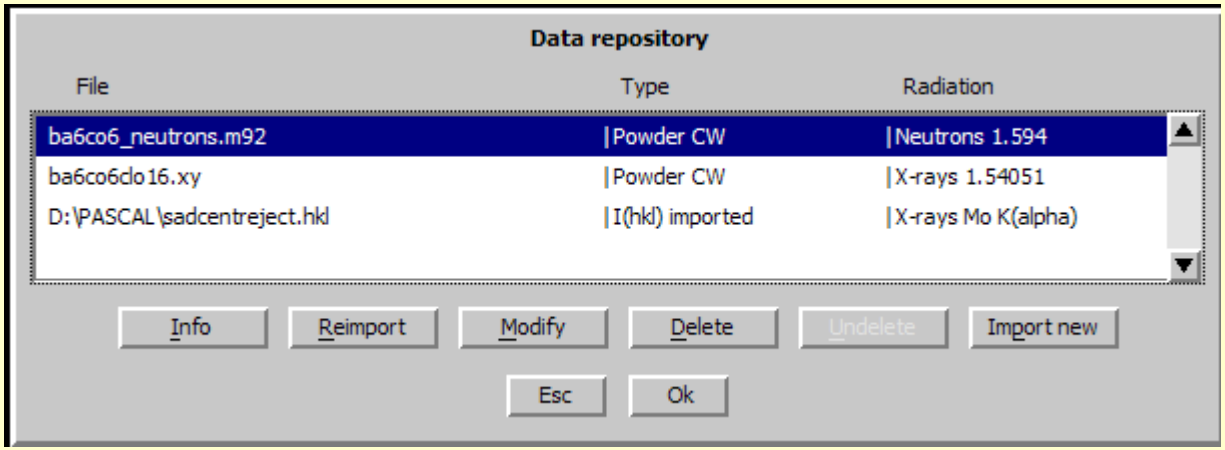
↓

Import Wizard

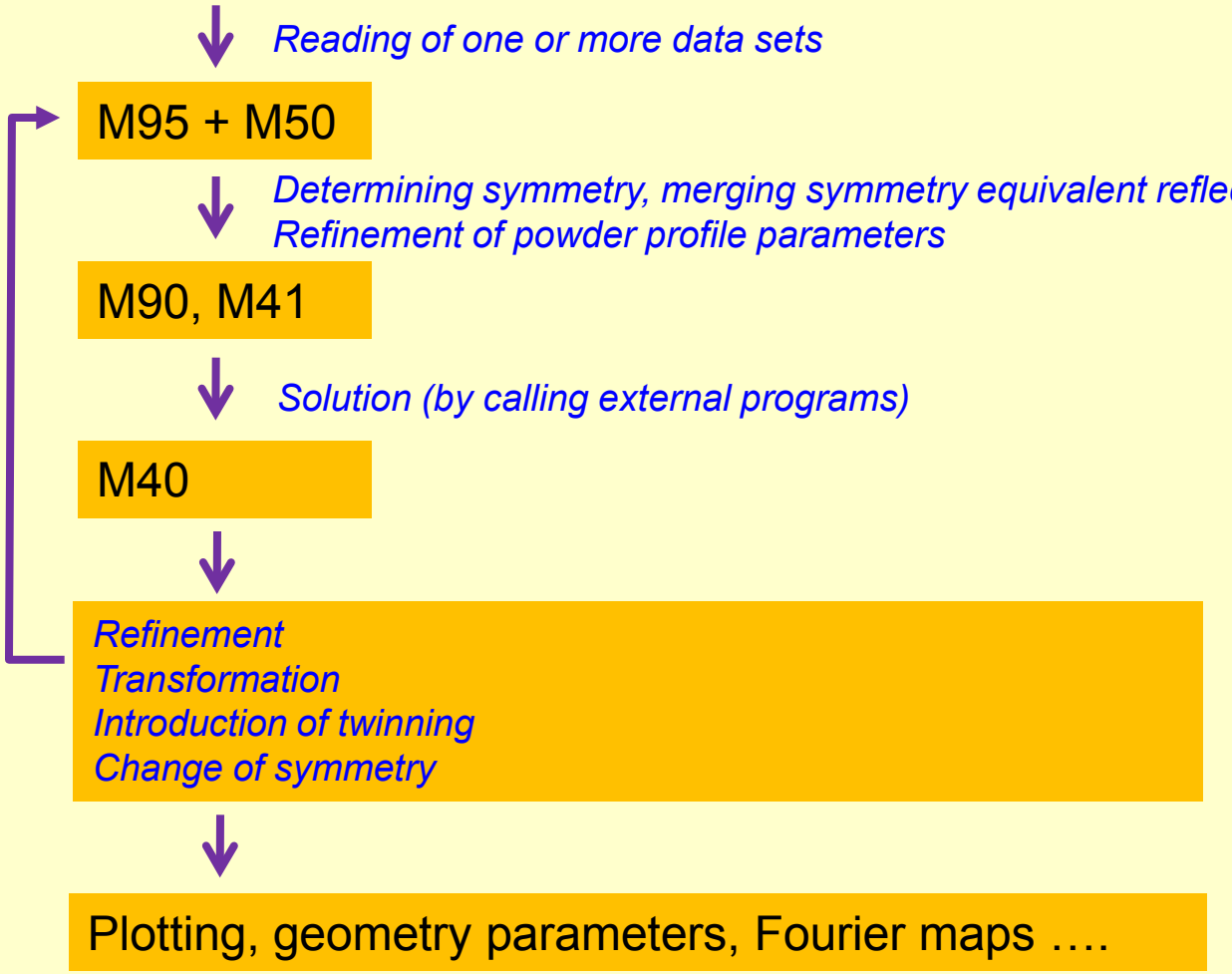
Format conversion, cell transformation, sorting reflections to twin domains

↓

Data Repository



Program Scheme



M95	data repository
M90	refinement reflection file
M50	basic crystal information, form factors, program options
M40	structure model

Topics covered by Jana2006

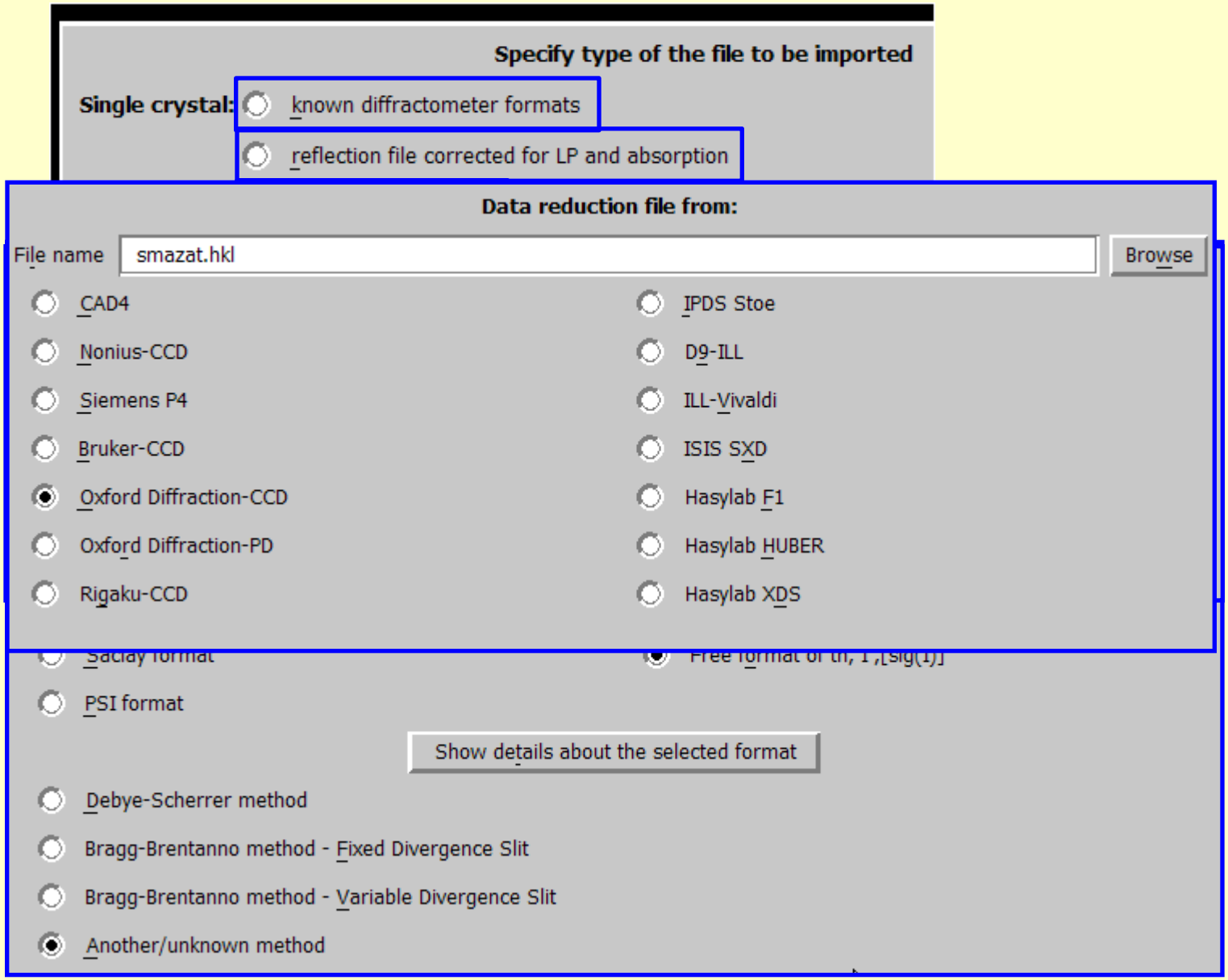
Service crystallography
Advanced tools
Incommensurate structures
Commensurate structures
Composite structures
Magnetic structures

Jana2006 is still old fashioned: written in Fortran; not using external libraries (except basic graphics); not written by a team of programmers → flexibility

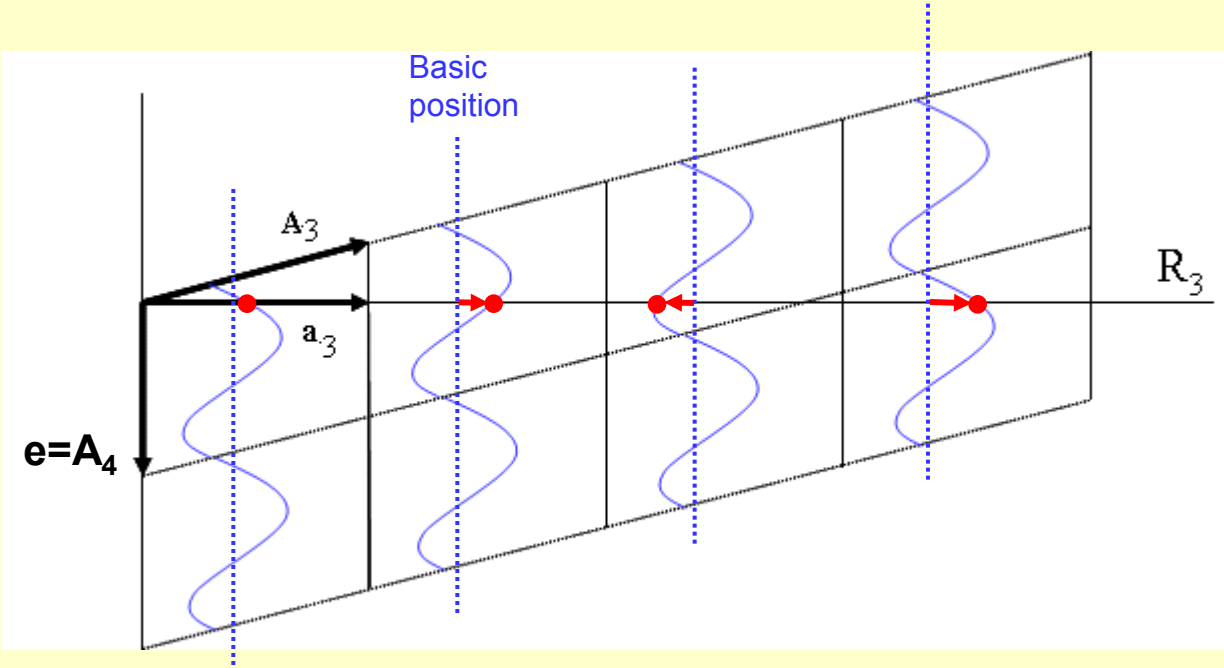
NOT included in Jana2006:

Phase problem solution: calls SIR97,2000,2004; EXPO, EXPO2004, Superflip
Plotting: calls Diamond, Vesta, MC (marching cube) and other plotting software
Validations and geometry analysis: relies on Platon

Where to start?



Two ways how to solve modulated structure



1. Through average structure solved from main reflections. The modulation is then refined from small arbitrary displacements

2. Directly using charge flipping. It yields 3+d electron density map which can be interpreted in terms of basic positions and their modulations

Simple example: δ-Na_2CO_3 solved by classical way

Alpha	757K	Beta	628K	Gamma	170K	Delta
9.02, 5.21, 6.50 90, 90, 90 $P6_3/mmm$		8.98, 5.25, 6.21 90, 90.33, 90 C2/m		8.92, 5.25, 6.05 90, 101.35, 90 C2/m(α0γ) q=(0.182,0,0.322)		8.90, 5.24, 6.00 90, 101.87, 90 C2/m(α0γ) q=(1/6,0,1/3)

Change of rotation symmetry

Change of translation symmetry

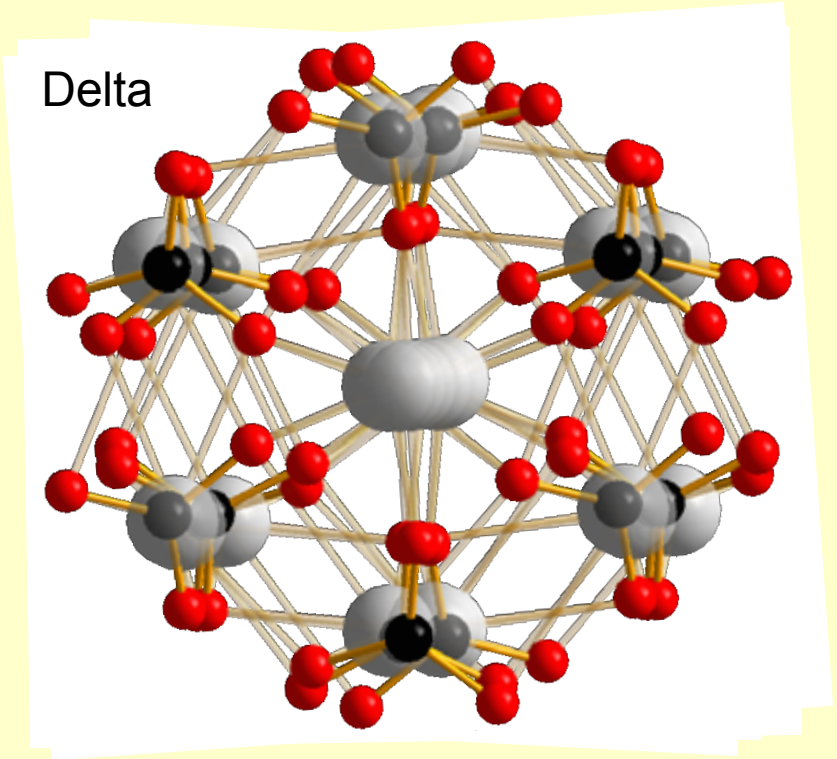
Average structure from main reflections

Arbitrary displacement for the first position modulation wave for all atoms

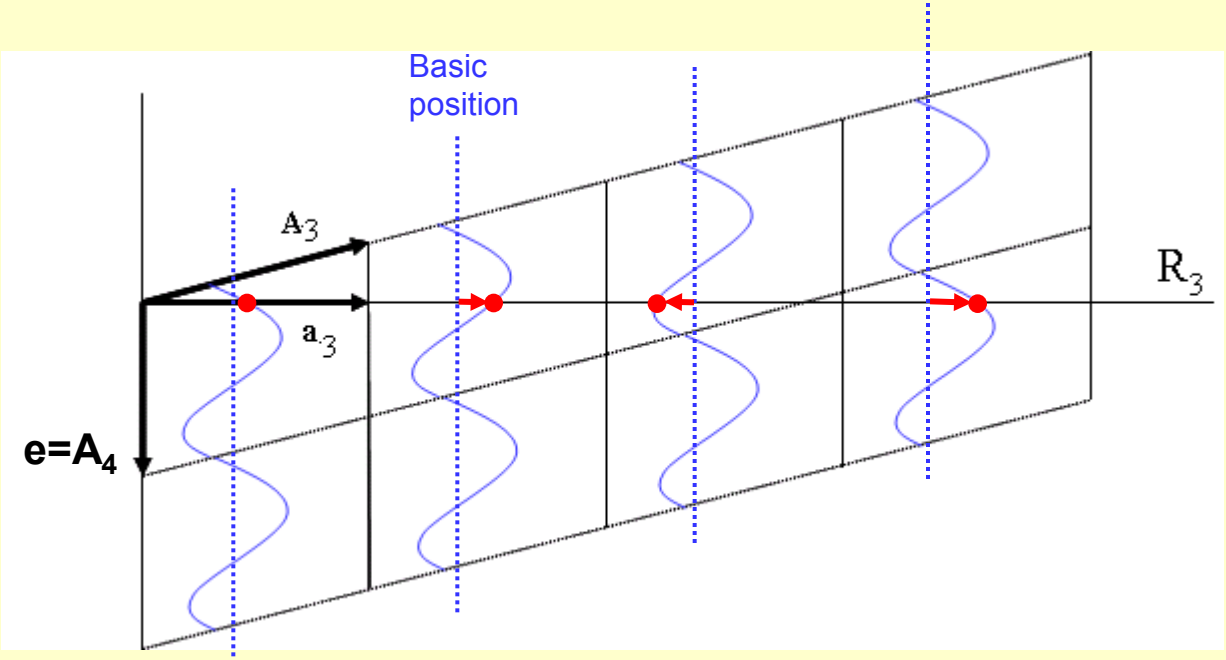
More position modulation waves for all atoms

ADP modulation

← *this launches Jana2006*



Verification of results from Fourier maps

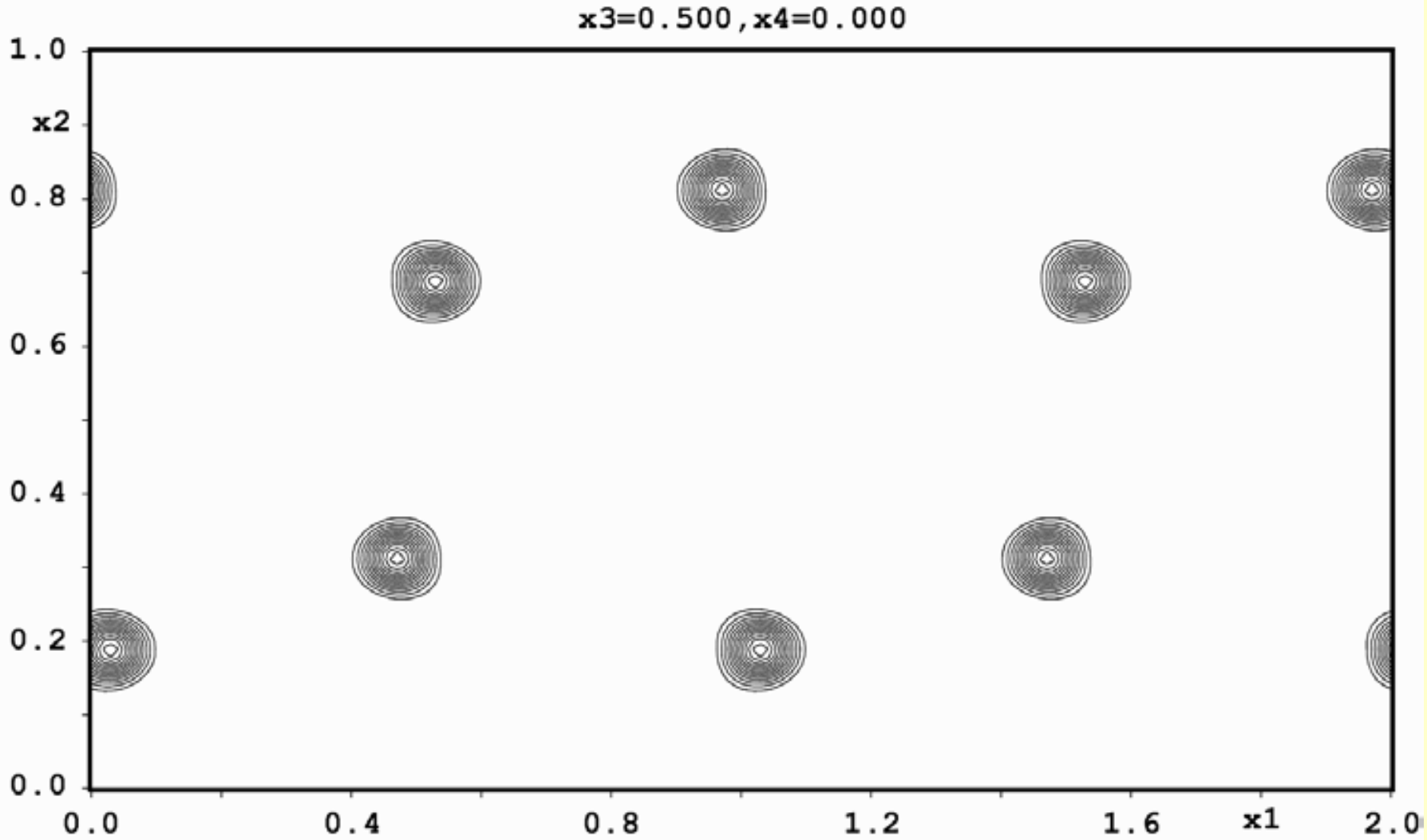


The $\mathbf{A}_3 - \mathbf{A}_4$ sections show modulation functions.

The $\mathbf{A}_3 - \mathbf{A}_3$ sections show periodicity and symmetry.

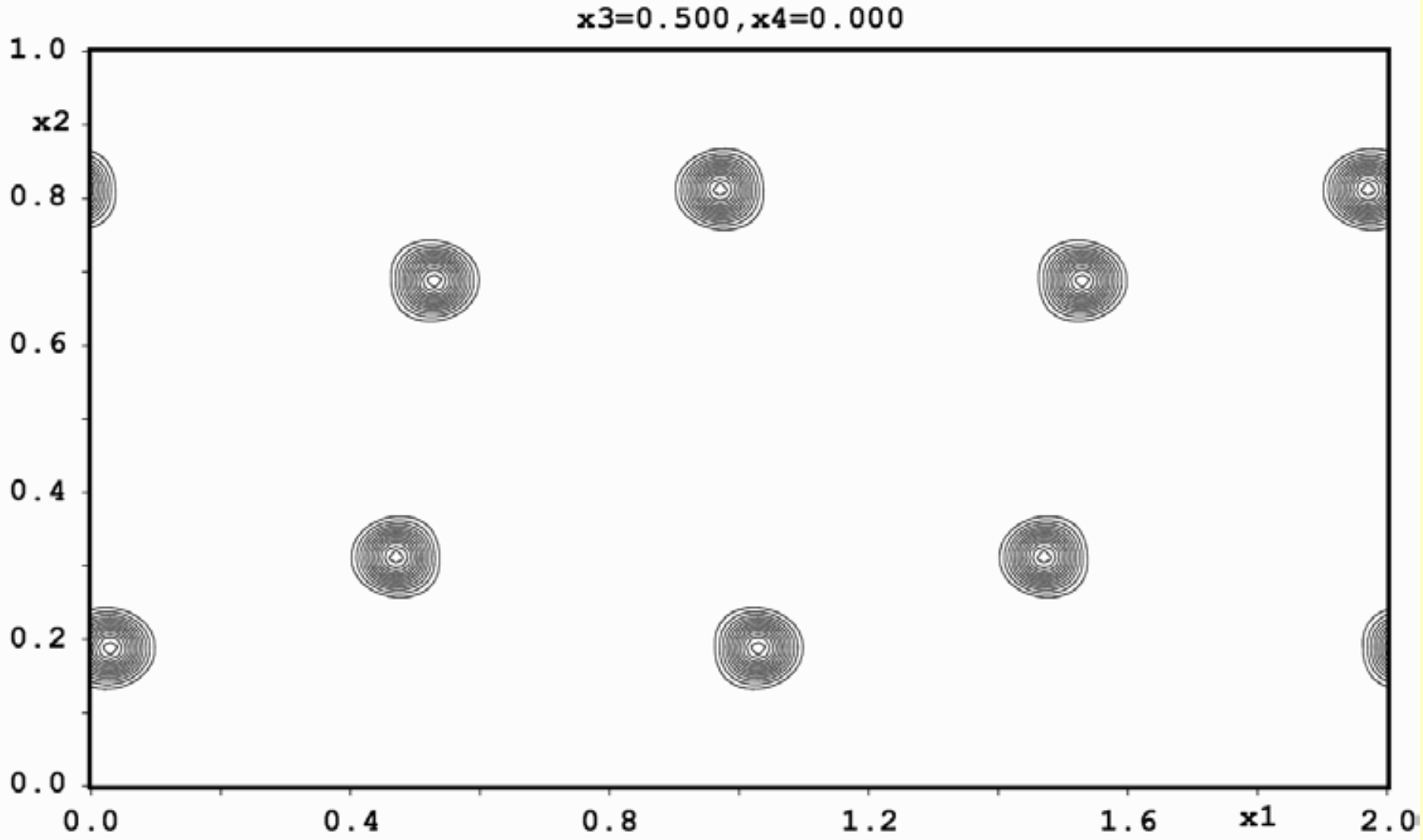
The $\mathbf{R}_3 - \mathbf{R}_3$ sections show real space electron density.

$\mathbf{A}_3 - \mathbf{A}_3$ sections

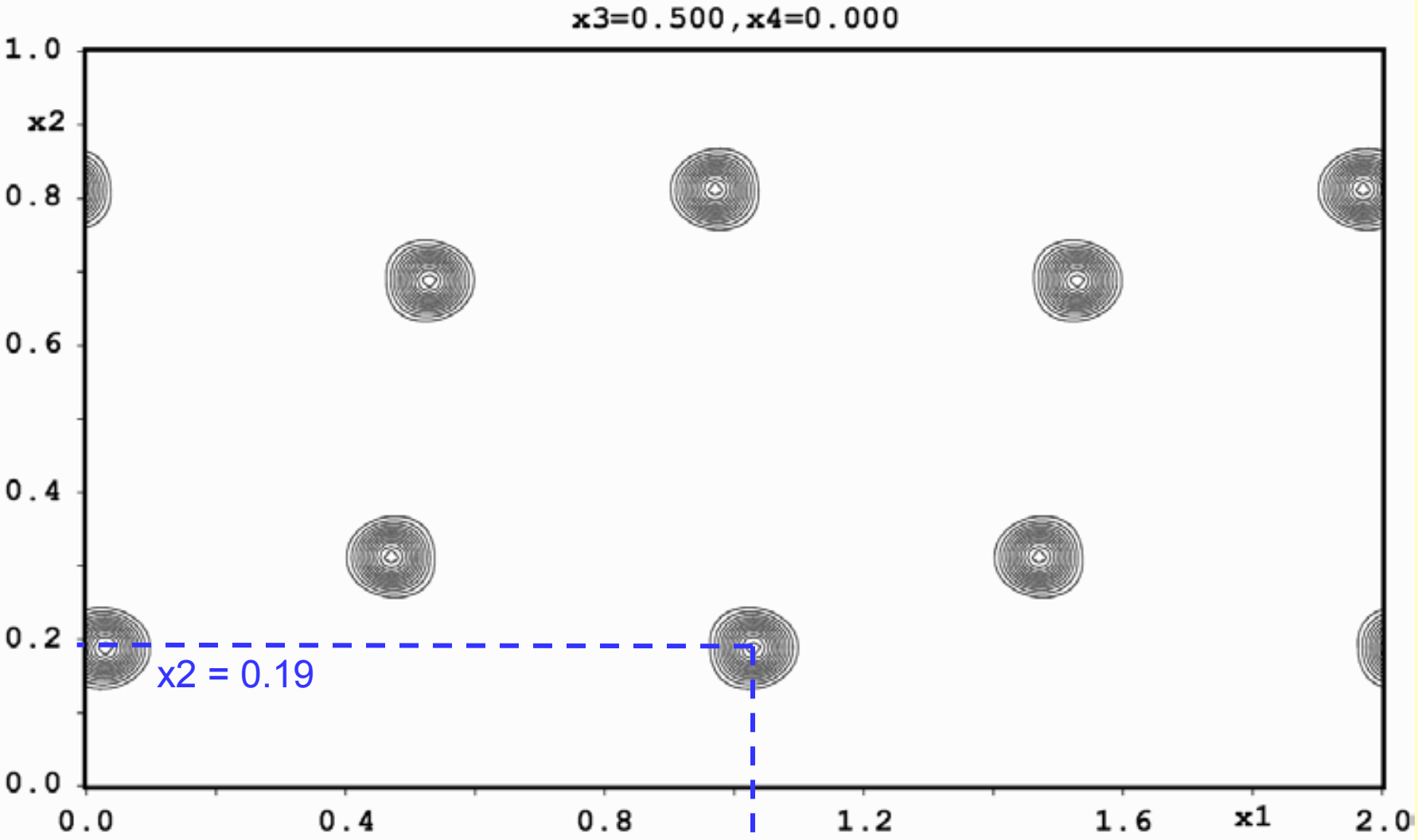


Jana notation: $\mathbf{A}_1$=x1, $\mathbf{A}_2$=x2, $\mathbf{A}_3$=x3, $\mathbf{A}_4$=x4

$\mathbf{A}_3 - \mathbf{A}_3$ sections

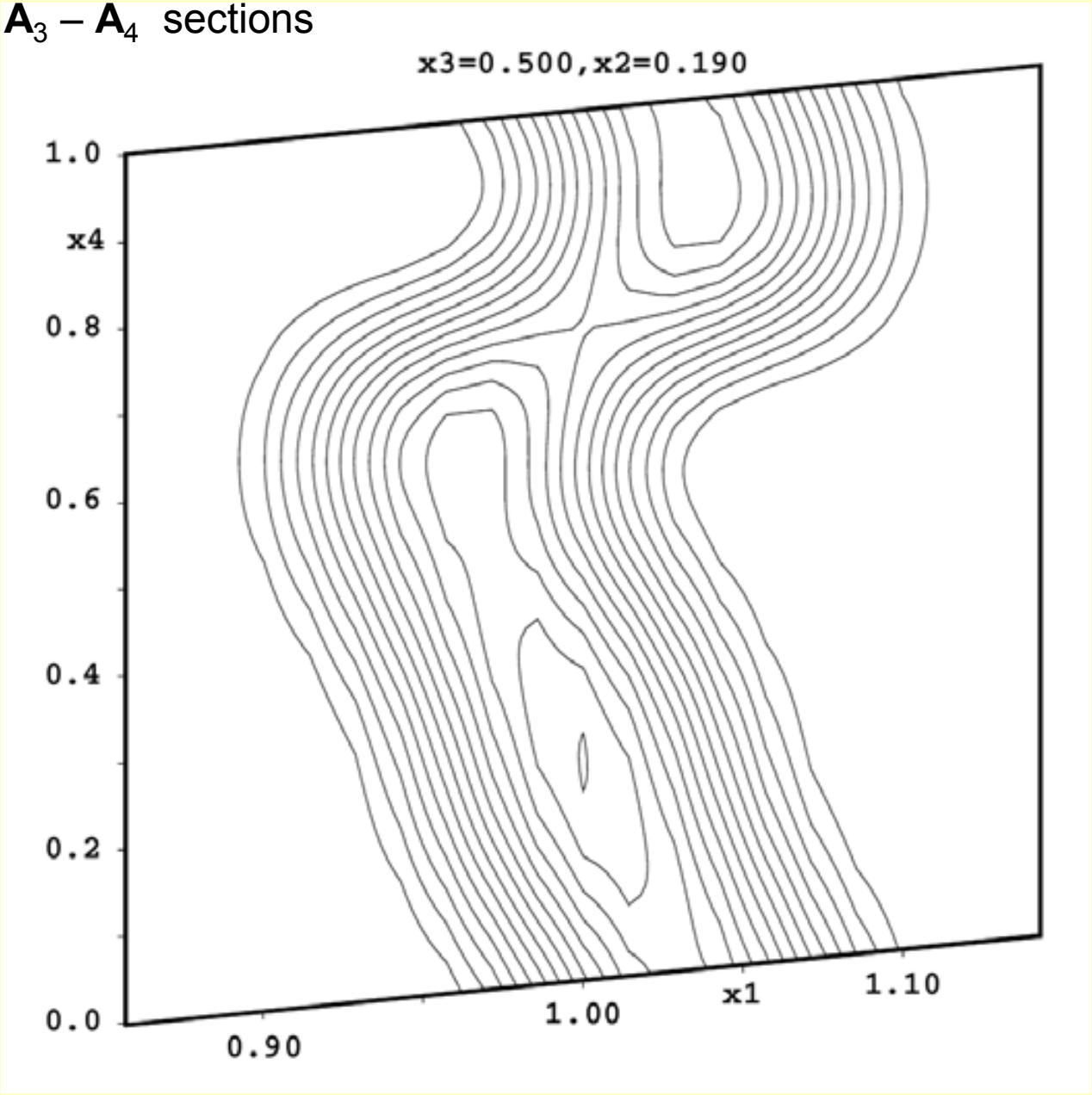


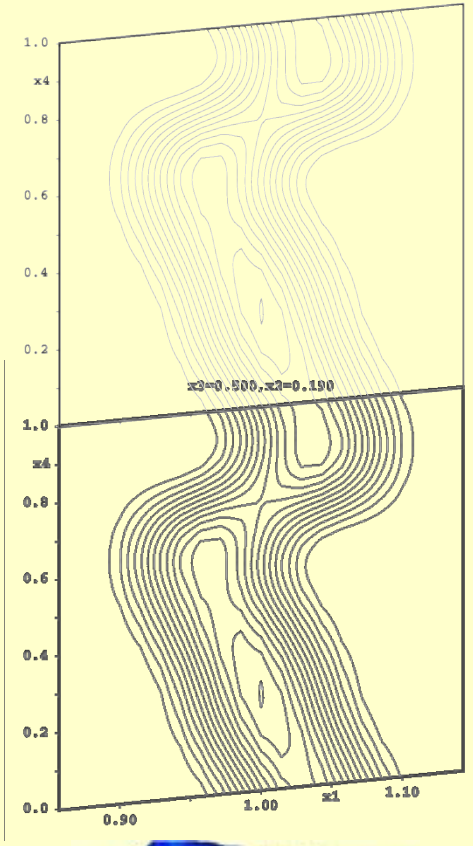
$A_3 - A_3$ sections

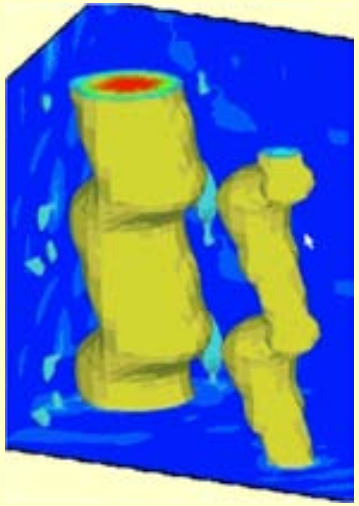


x1 between 0.97
and 1.03

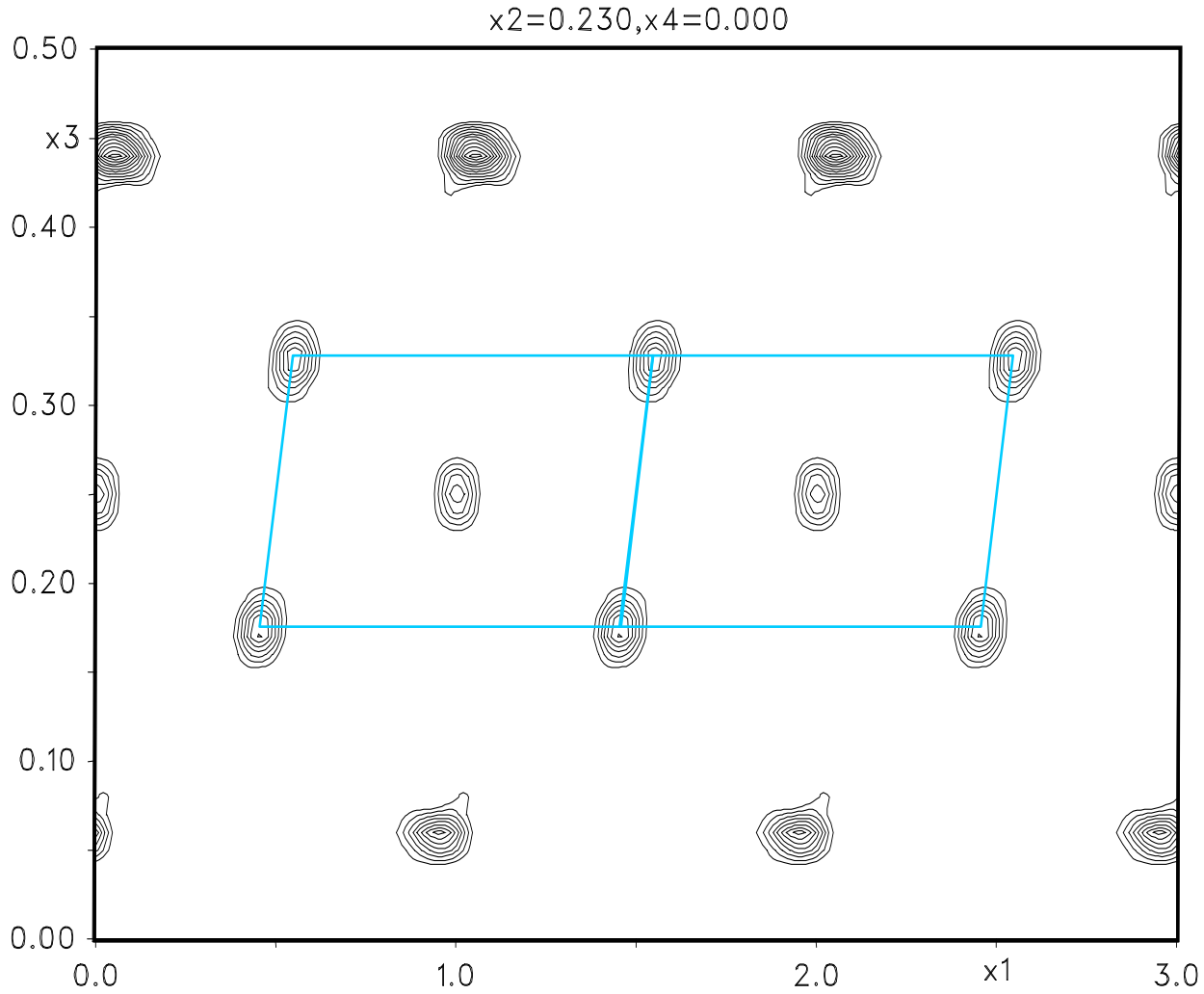
$A_3 - A_4$ sections





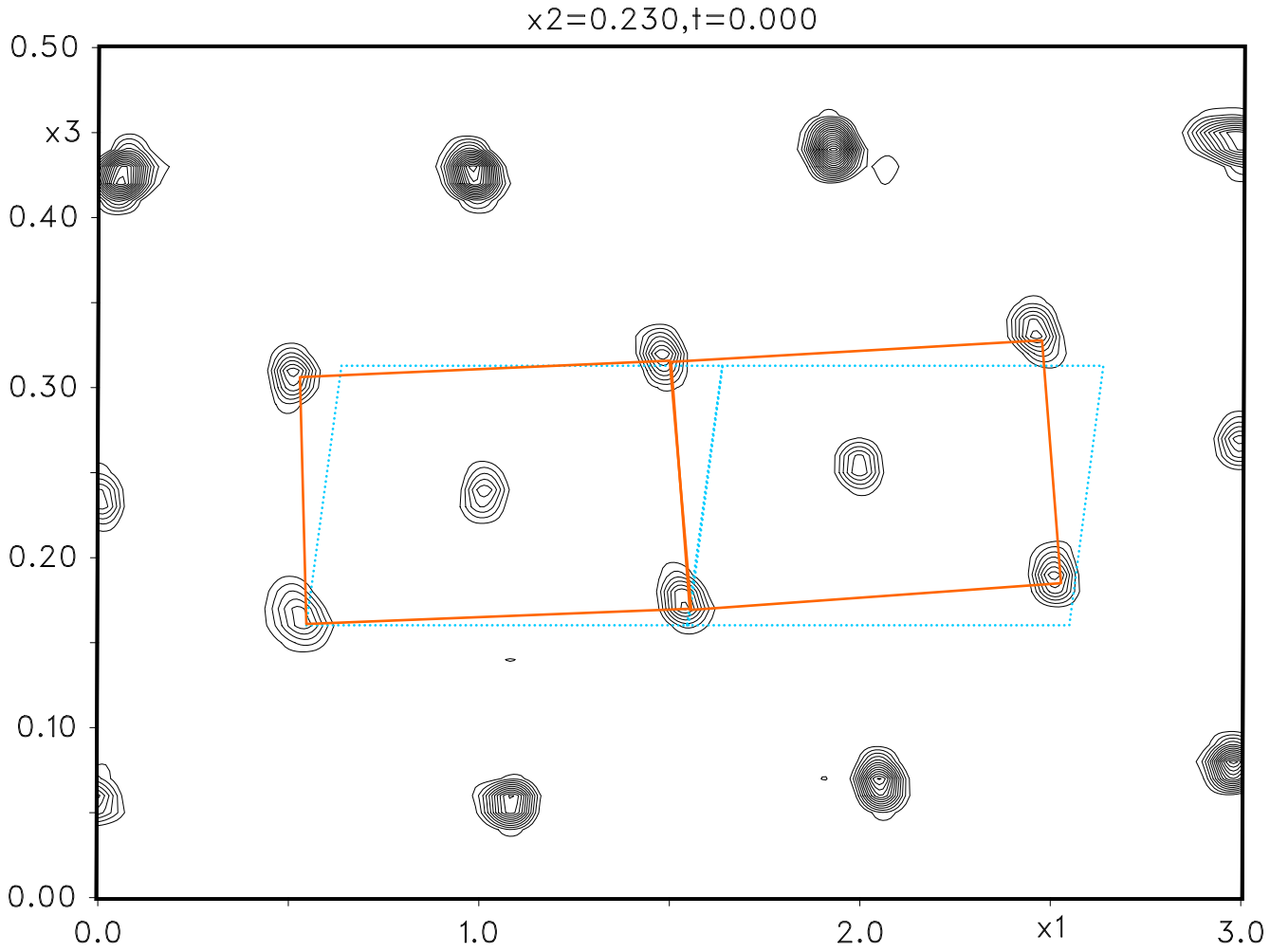


The difference between $\mathbf{A}_3 - \mathbf{A}_3$ and $\mathbf{R}_3$-$\mathbf{R}_3$



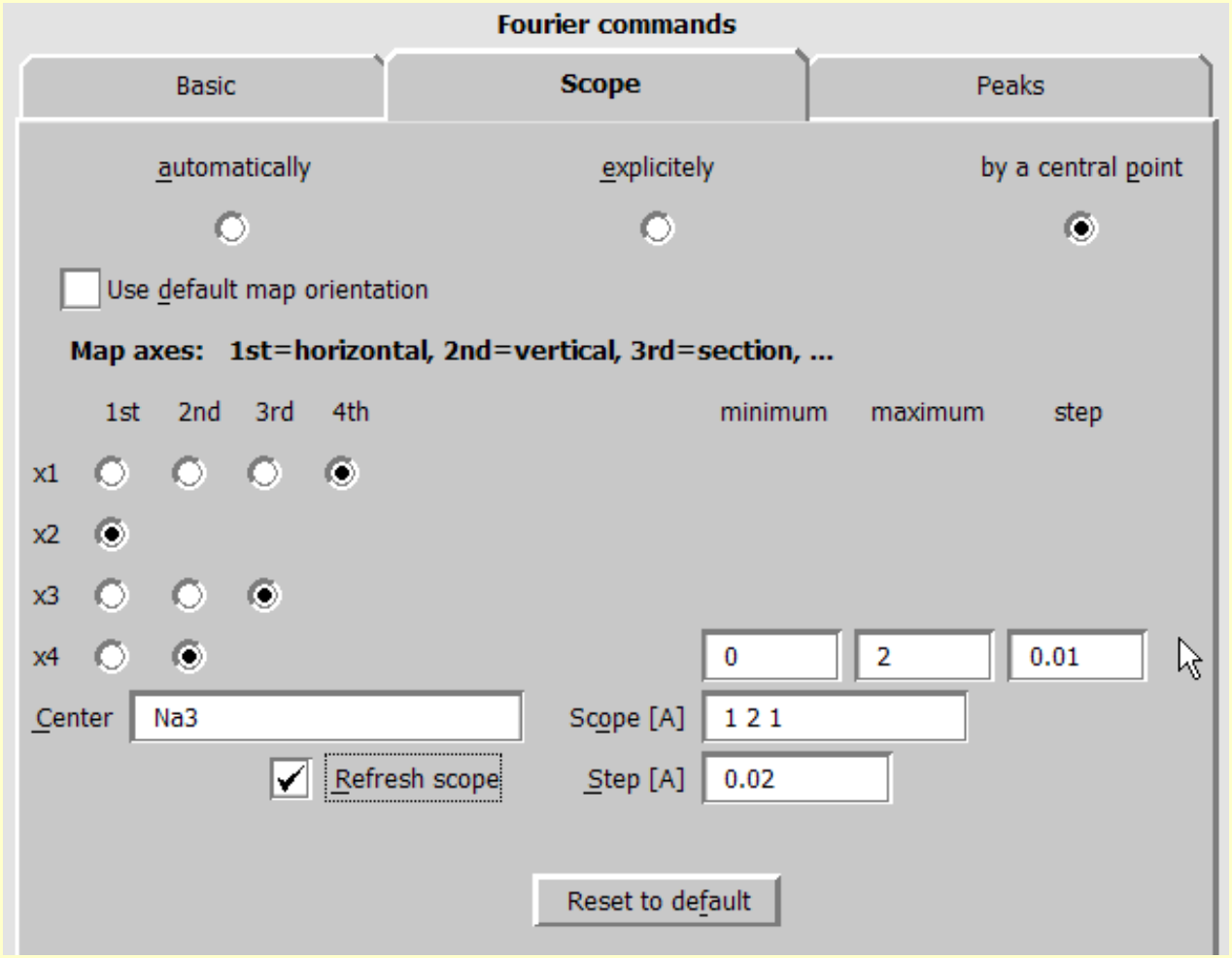
$\mathbf{A}_3$-$\mathbf{A}_3$ sections show periodicity. Geometry is distorted.

The difference between $\mathbf{A}_3 - \mathbf{A}_3$ and $\mathbf{R}_3$-$\mathbf{R}_3$



$\mathbf{R}_3$-$\mathbf{R}_3$ sections show proper geometry. Periodicity is broken.

How Fourier works for δ-Na_2CO_3 ; what does it say about number of modulation waves and about modulation of ADP?



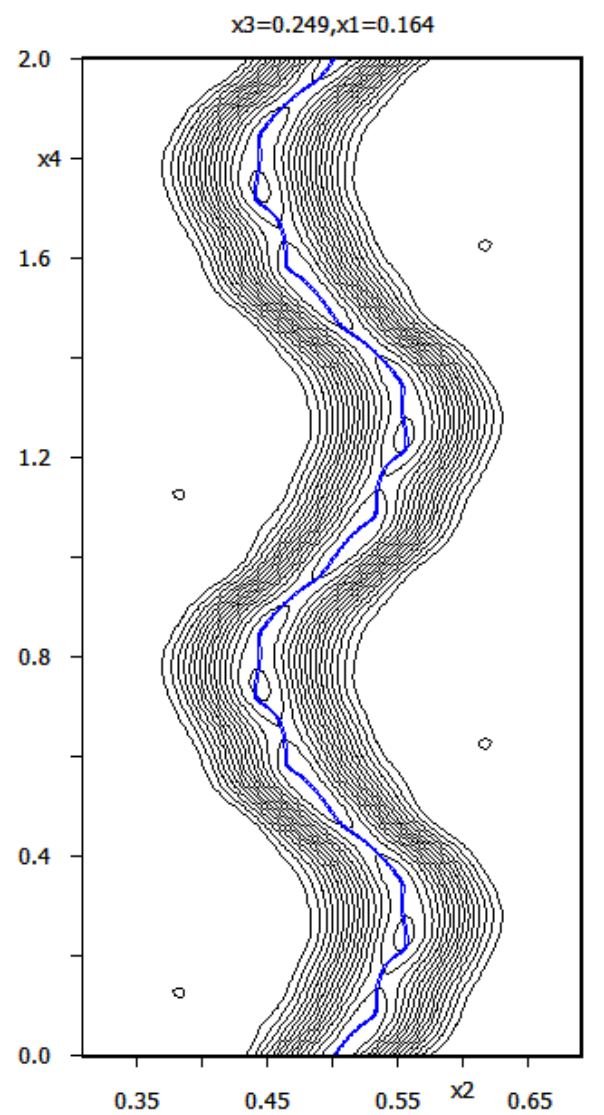
This will calculate a parallelepiped 1x2x1 Å centered at the basic position of Na3.

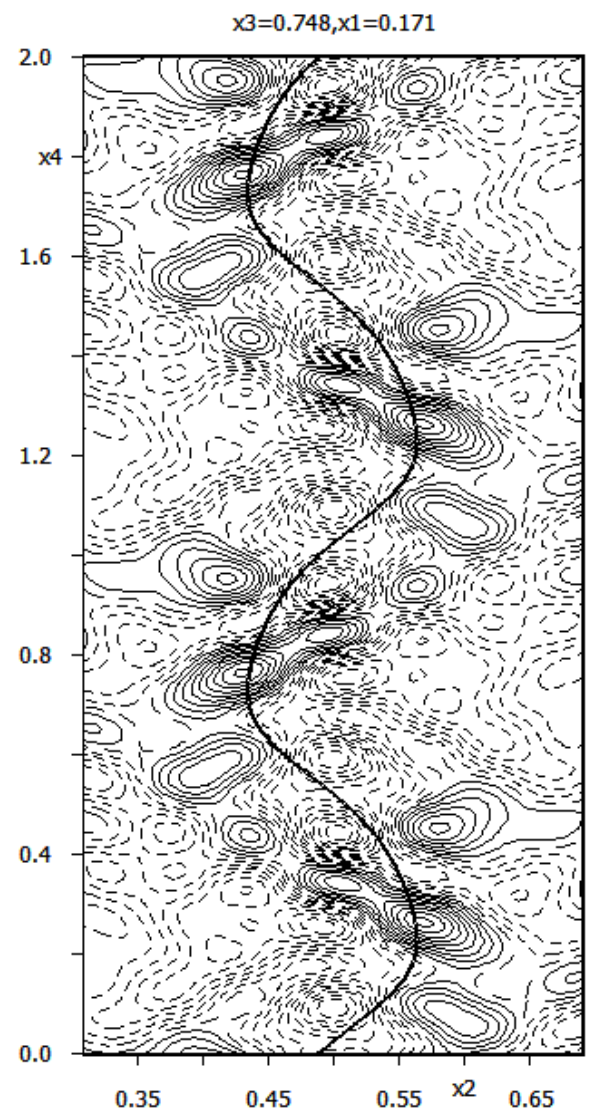
The two dimensional sections x2-x4 will be stacked along x1 and x3.

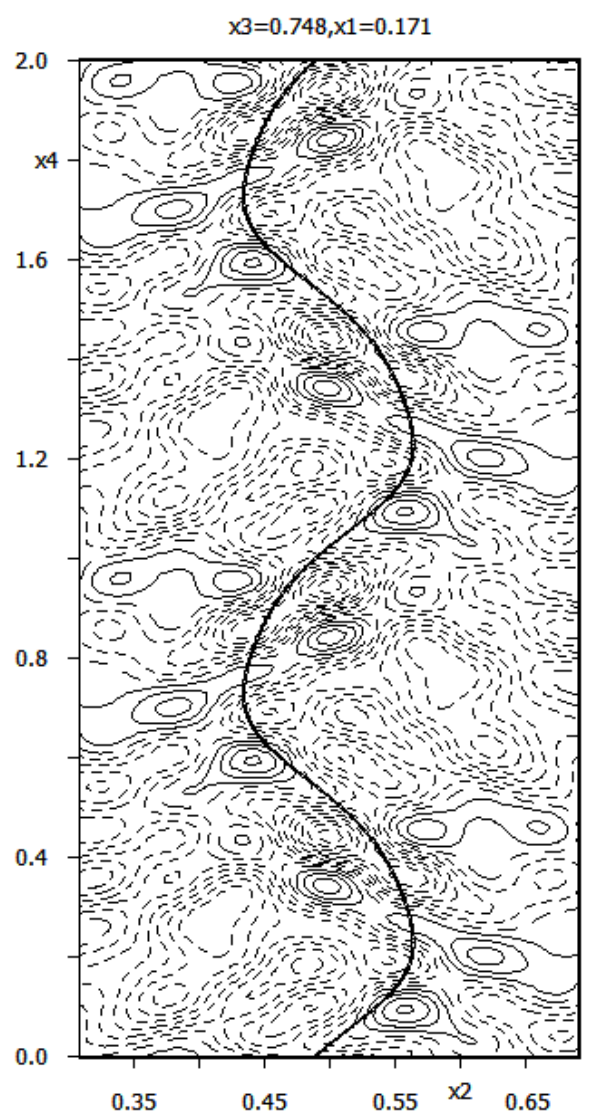
The number of sections will be 1/0.02 along x1 and 1/0.02 along x3.

The physical dimension of the plot along x4 will be 2 Å

← *this launches Jana2006*





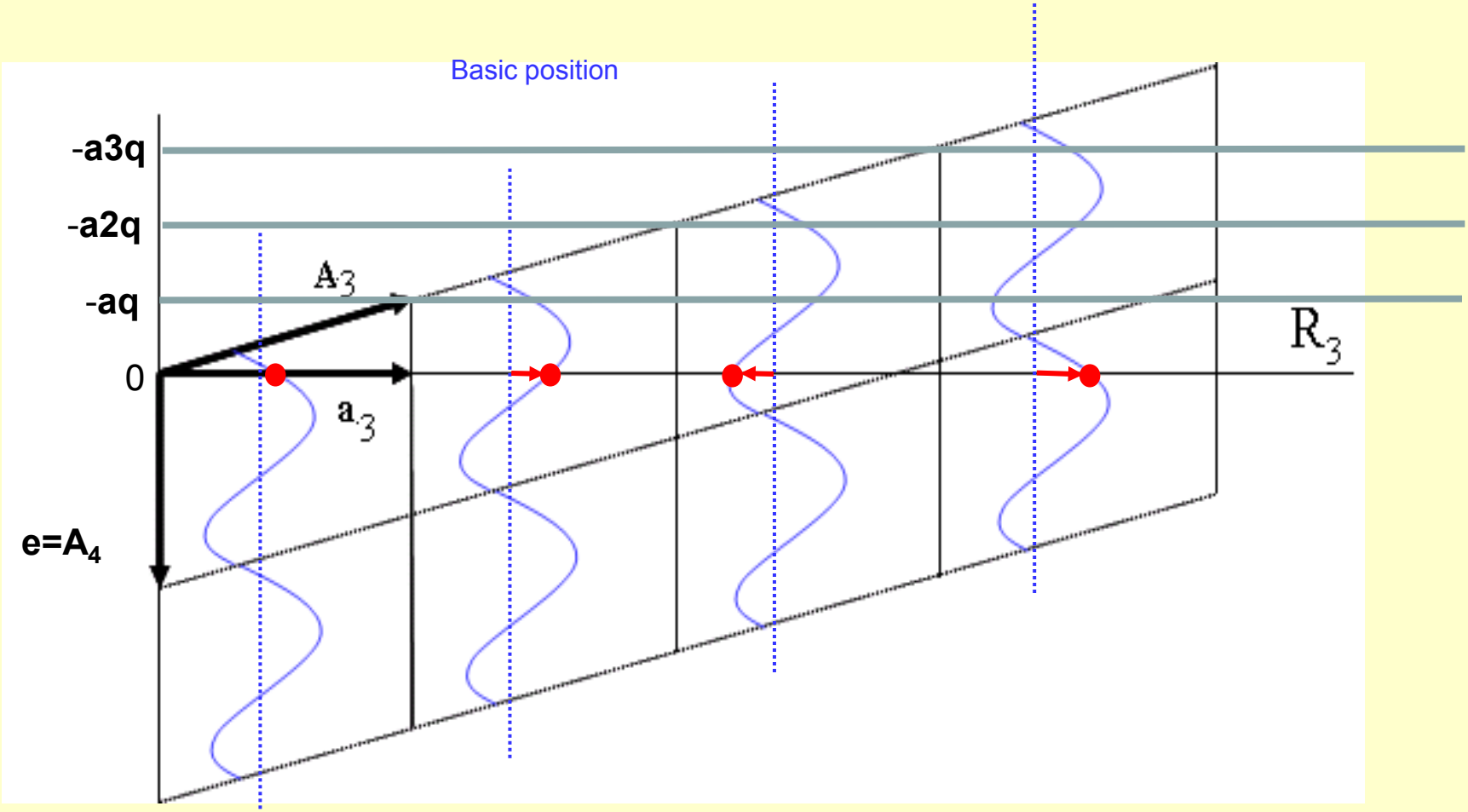


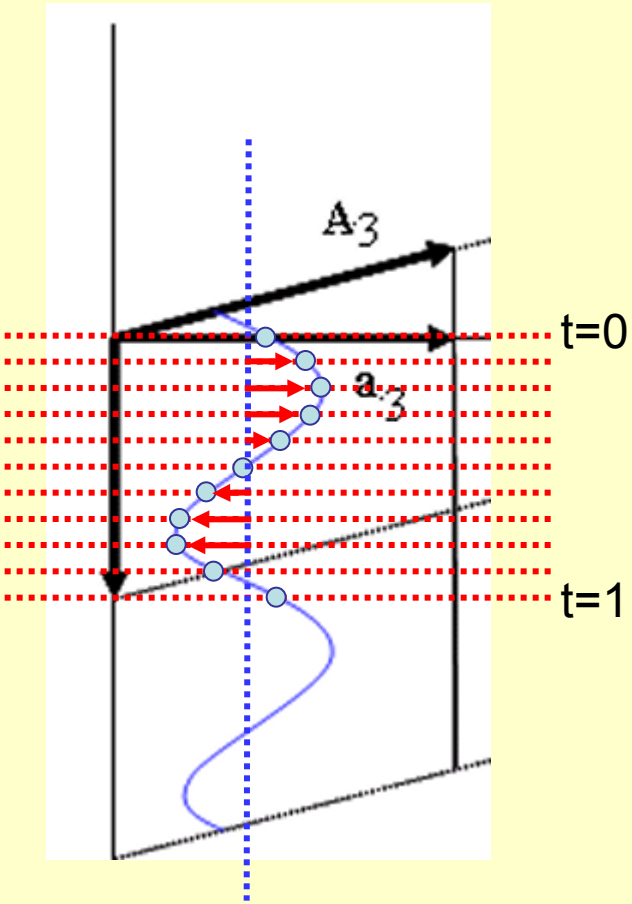
Carbon with eight position modulation waves. This causes also problem with ADP modulation.

Sodium (Na3) without (left) and with modulation of ADP. Contour step 0.1

Distances and t-plots

Changing t by n**aq** shifts origin by n unit cells. This can be used to visualize modulated structure from cell to cell.





Changing t from 0 to 1 can be used to visualize all possible (but not neighboring) configurations of modulated structure.

Applications:

“Animated” Fourier sections

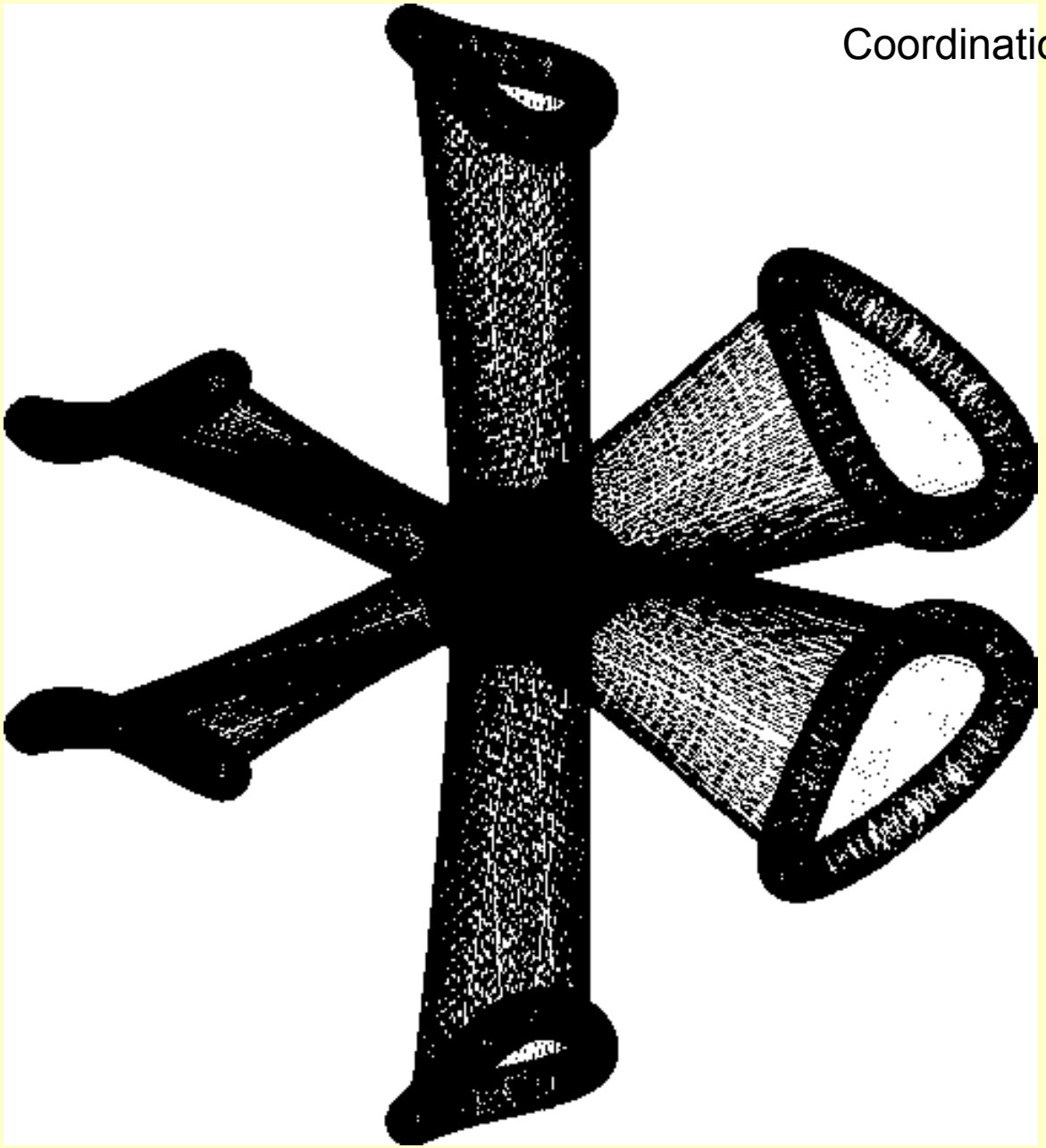
“Animated” plots of the structure

Graphical representation of modulated parameters (so-called t-plots)

Calculation of distances

Examples with sodium carbonate:

← *this launches Jana2006*

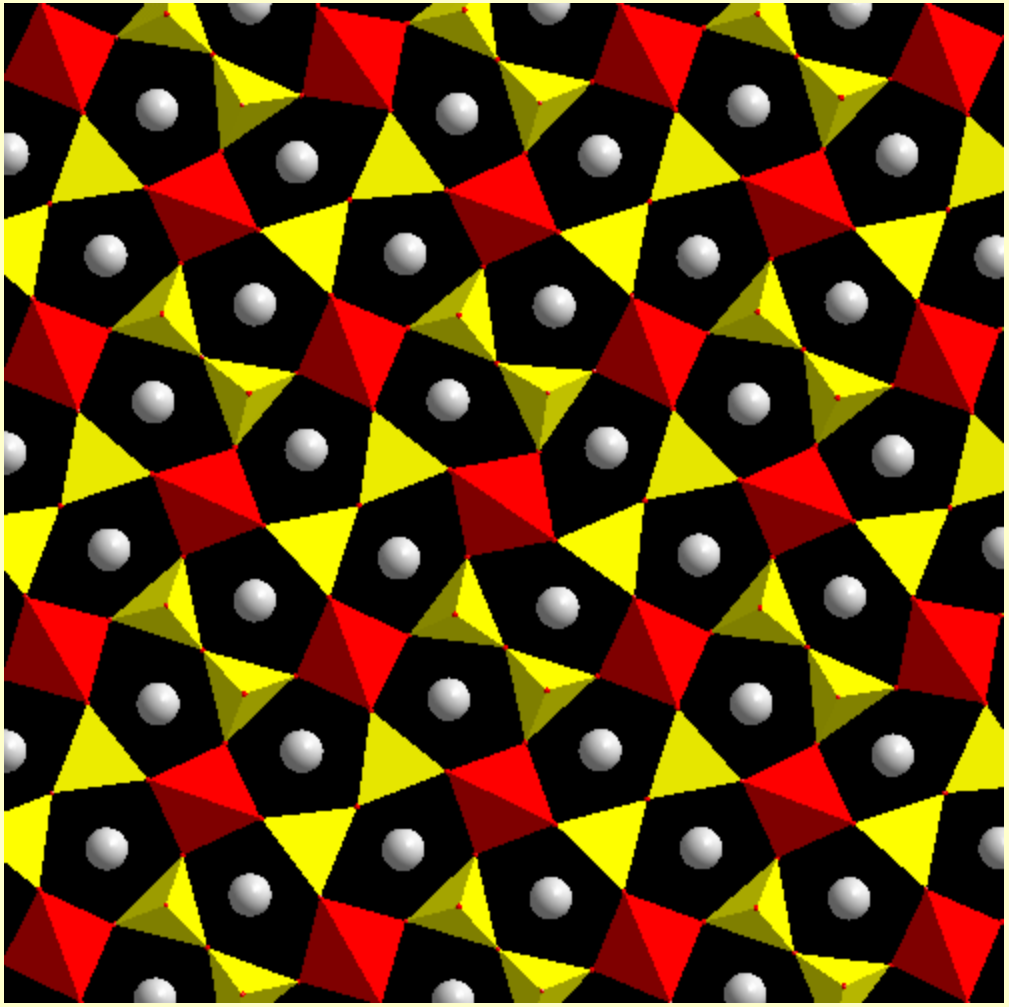


Coordination of As in KAsF4(OH)2

(logo Jana2006)

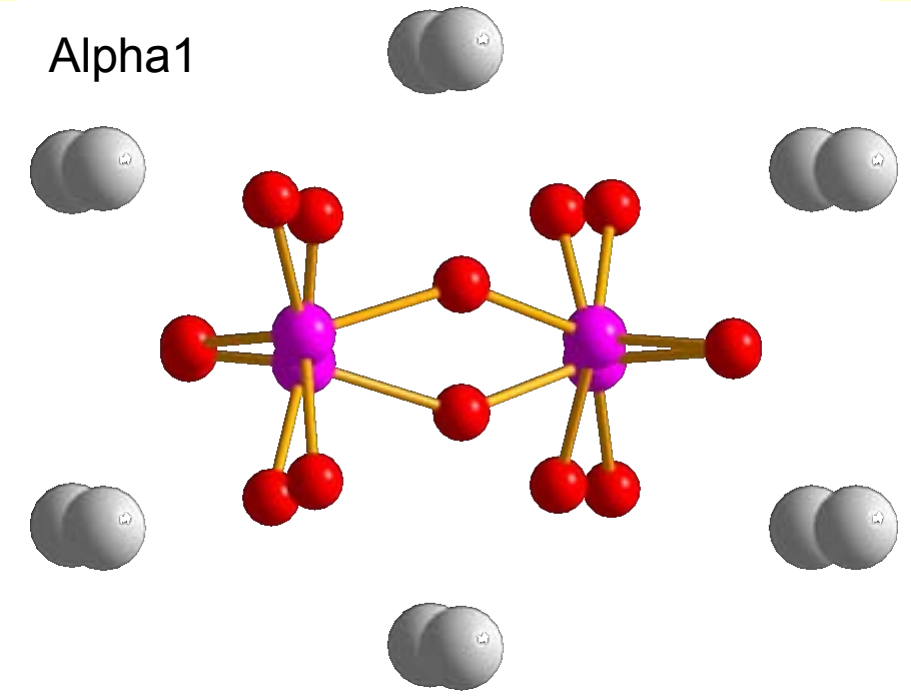
Natural melilite from San Venanzo, Umbria, Italy

Formula: $(Ca_{1.89}Sr_{0.01}Na_{0.08}K_{0.02})(Mg_{0.92}Al_{0.08})(Si_{1.98}Al_{0.02})O_7$



Chromium diphosphate

Beta		Alpha3		Alpha2		Alpha1
6.97, 8.45, 4.60 90, 107.90, 90 C2/m	364K	7.05, 8.41, 4.64 90, 108.71, 90 C2/m(α0γ)0s q=(-1,0,0.5)	345K	7.02, 8.40, 4.62 90, 108.59, 90 C2/m(α0γ)0s q=(0.361,0,-0.471)	285K	7.05, 8.41, 4.64 90, 108.71, 90 C2/m(α0γ) q=(-1/3,0,1/2)

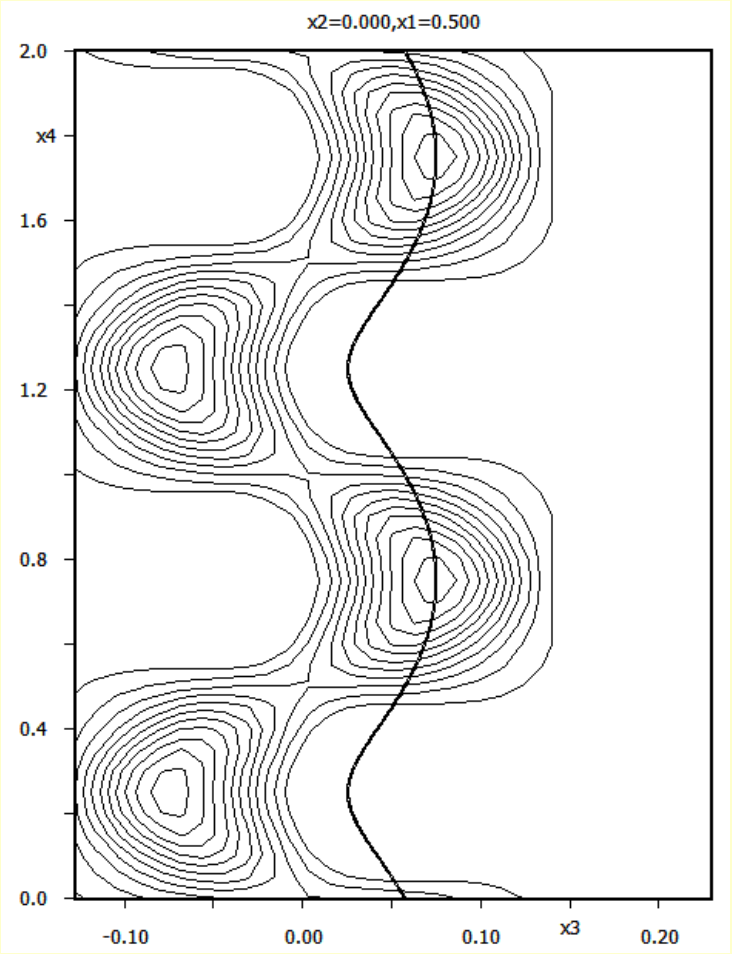


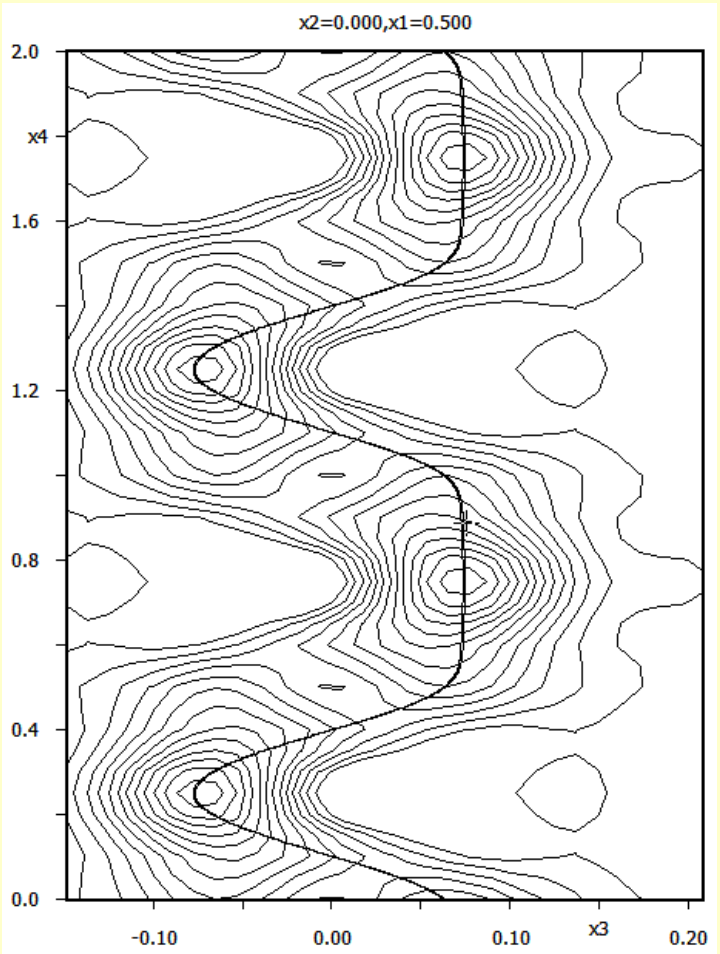
In case of Cr2P2O7 no change of rotation symmetry occurs. The phases alpha1, alpha2 and alpha3 represent various ways how to resolve the disorder observed in the phase beta.

Lukas Palatinus et al., Acta Cryst. (2006). B62, 556–566

Solution of chromium diphosphate by Charge flipping

← *this launches Jana2006*

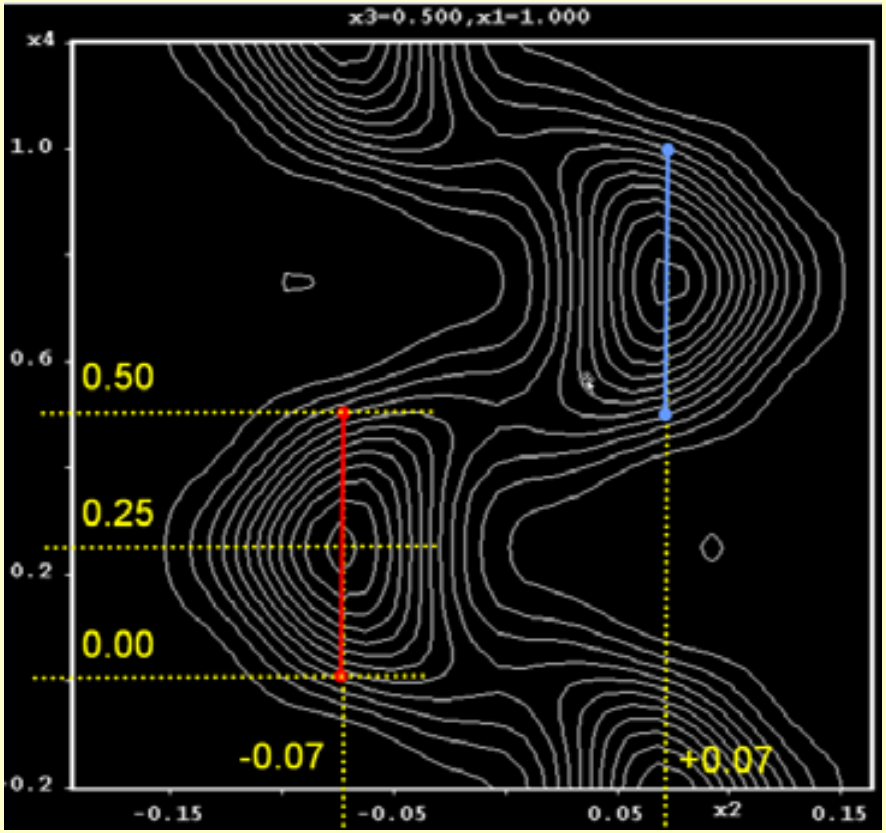




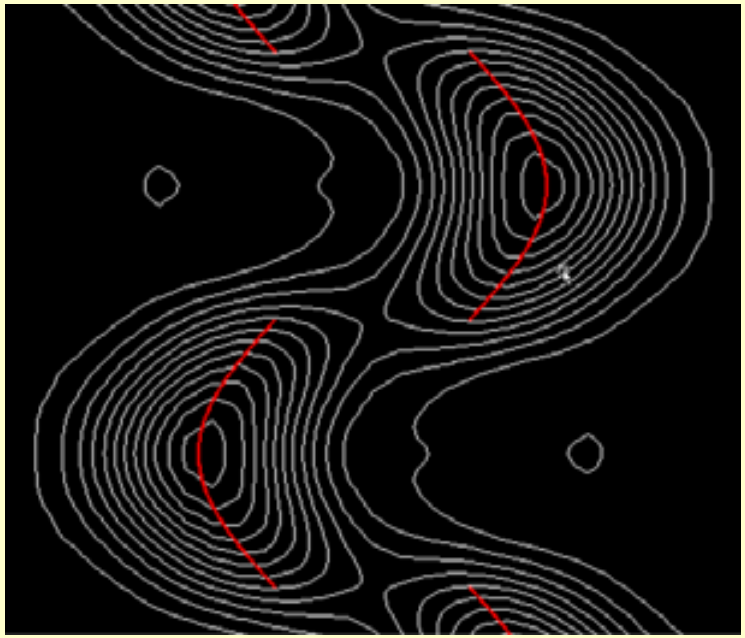
Bridging oxygen from charge flipping

refined with three position modulation waves

Crenel function



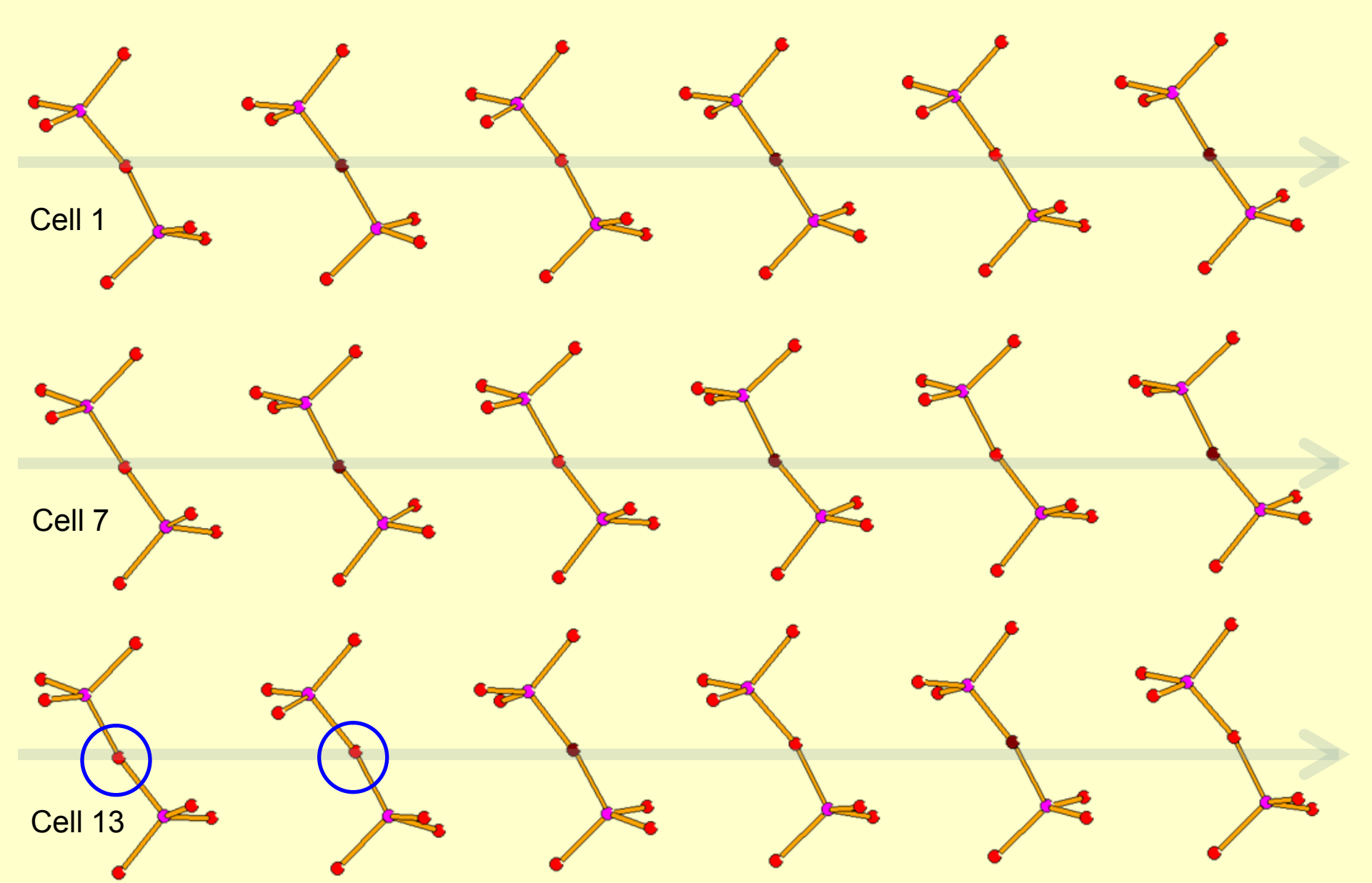
Definition of crenel function from Fourier map



Crenel function combined with modulation of position

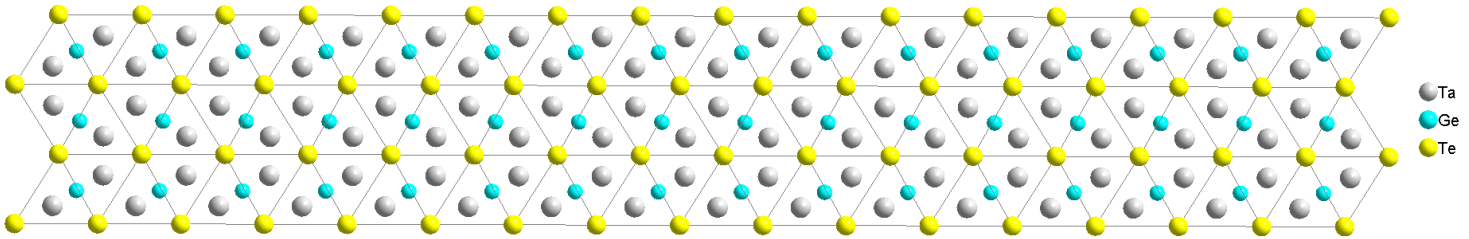
Crenel function describes definition interval for an atom. Crenel reduces occupancy but two crenel functions may together describe full occupancy.

For combining crenel function with position modulations Jana2006 uses Legendre polynomials

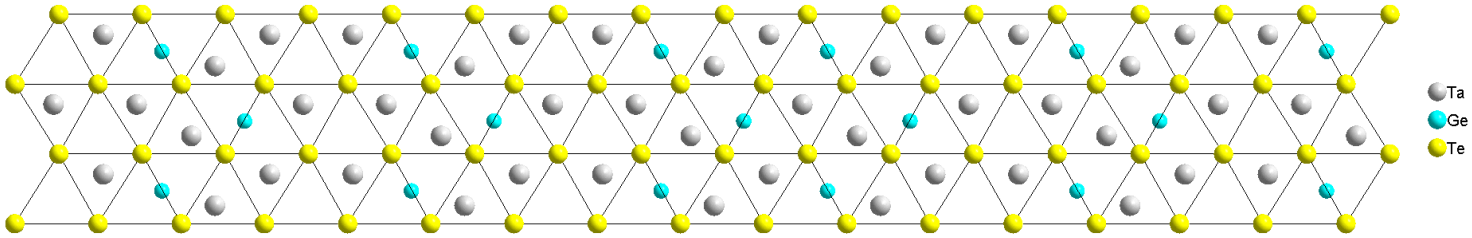


Modulated structure of $Cr_2P_2O_7$ expanded in the c direction

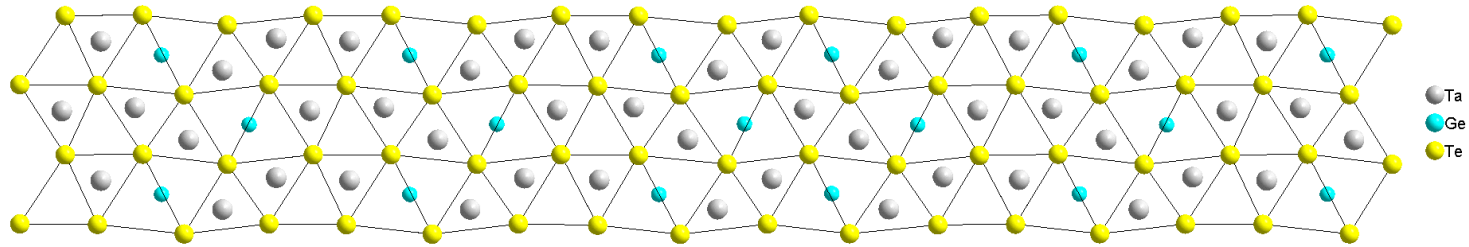
$TaGe_{0.354}Te$ – Acta Cryst.,B52, 100, (1996).



Average structure



Crenel occupation modulation

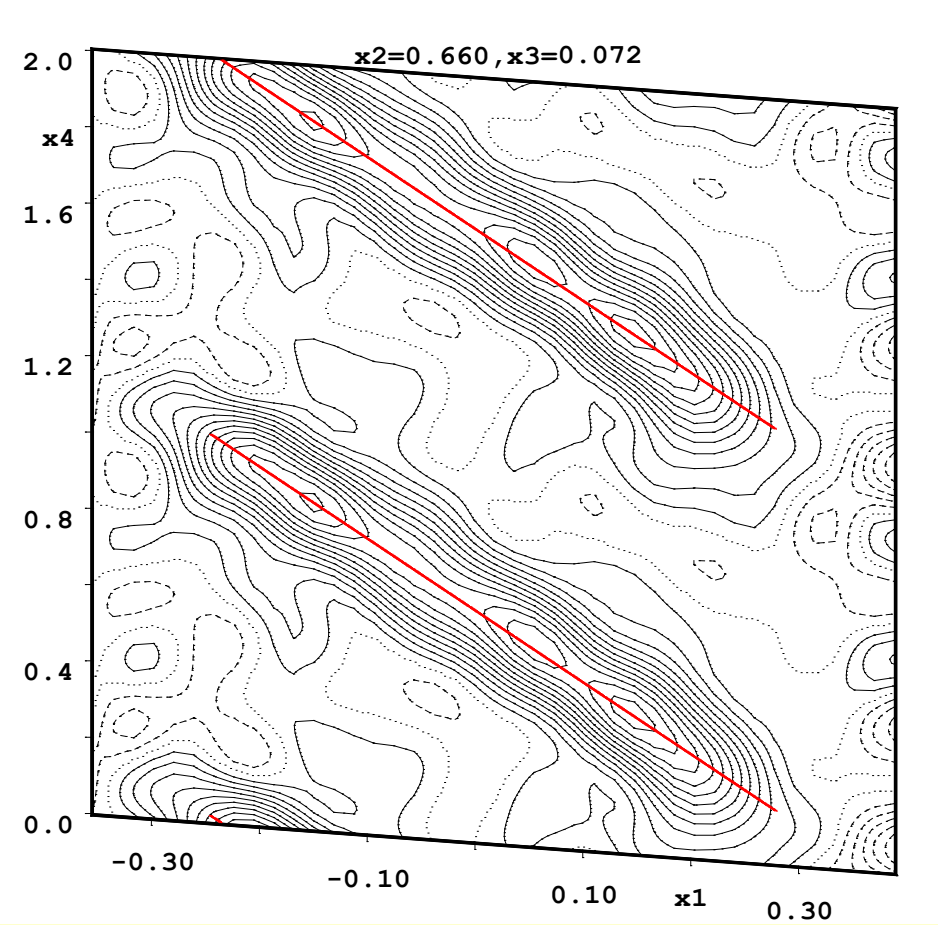


Crenel occupation modulation and harmonic positional modulation

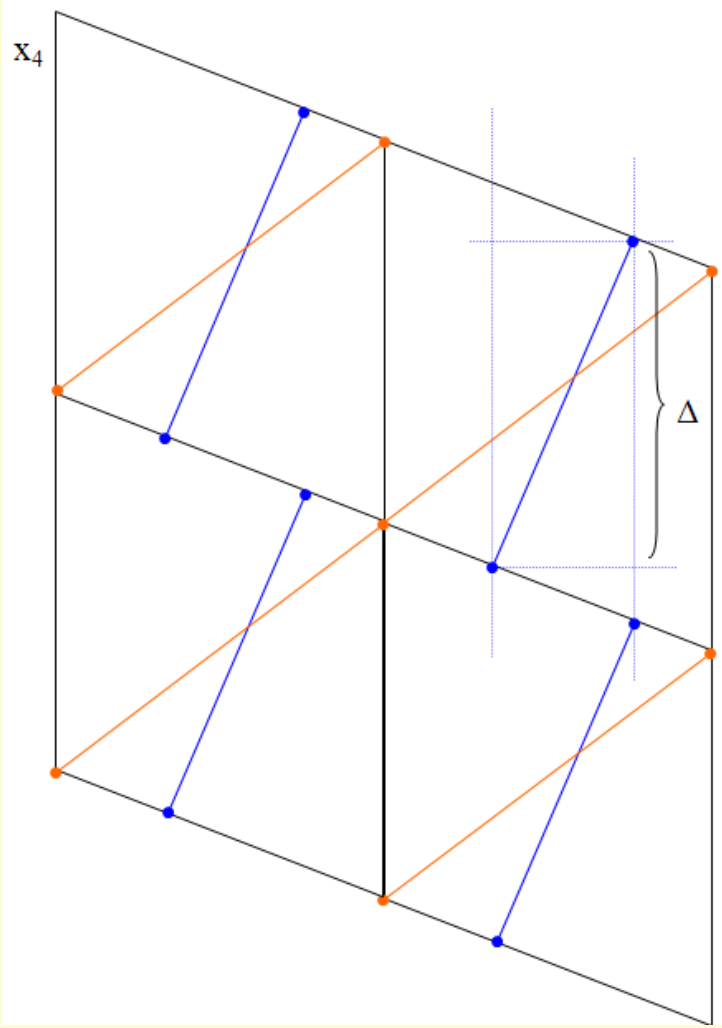
Sawtooth function

$Bi_2Sr_2CaCu_2O_8$

*V.Petříček, Y.Gao, P.Lee & P.Coppens, Phys.Rew.B, **42**, 387-392, (1990)*

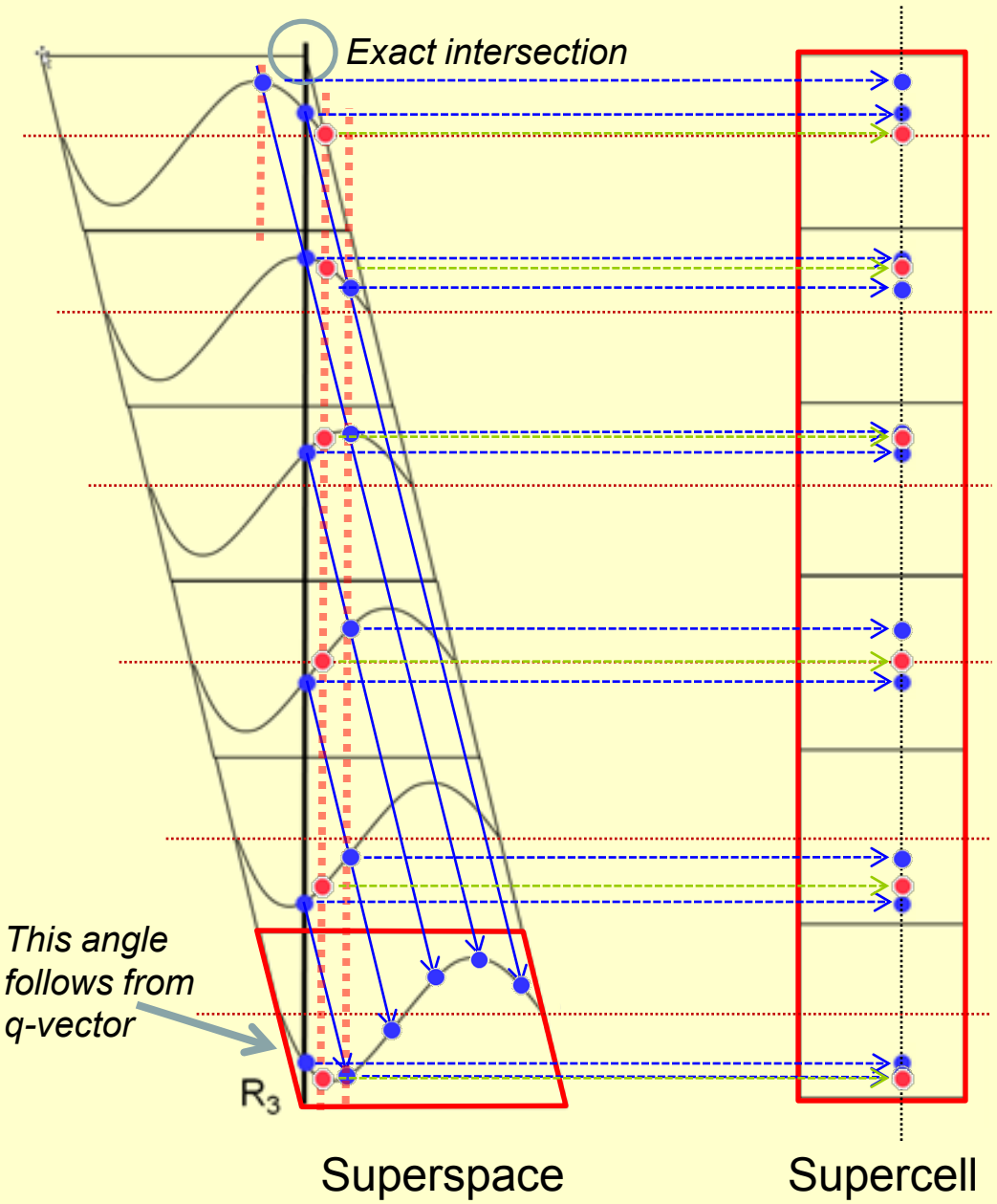


Oxygen atom at Bi layer



Relationship to composite structures

Commensurate structures



Example of a six-fold commensurate structure

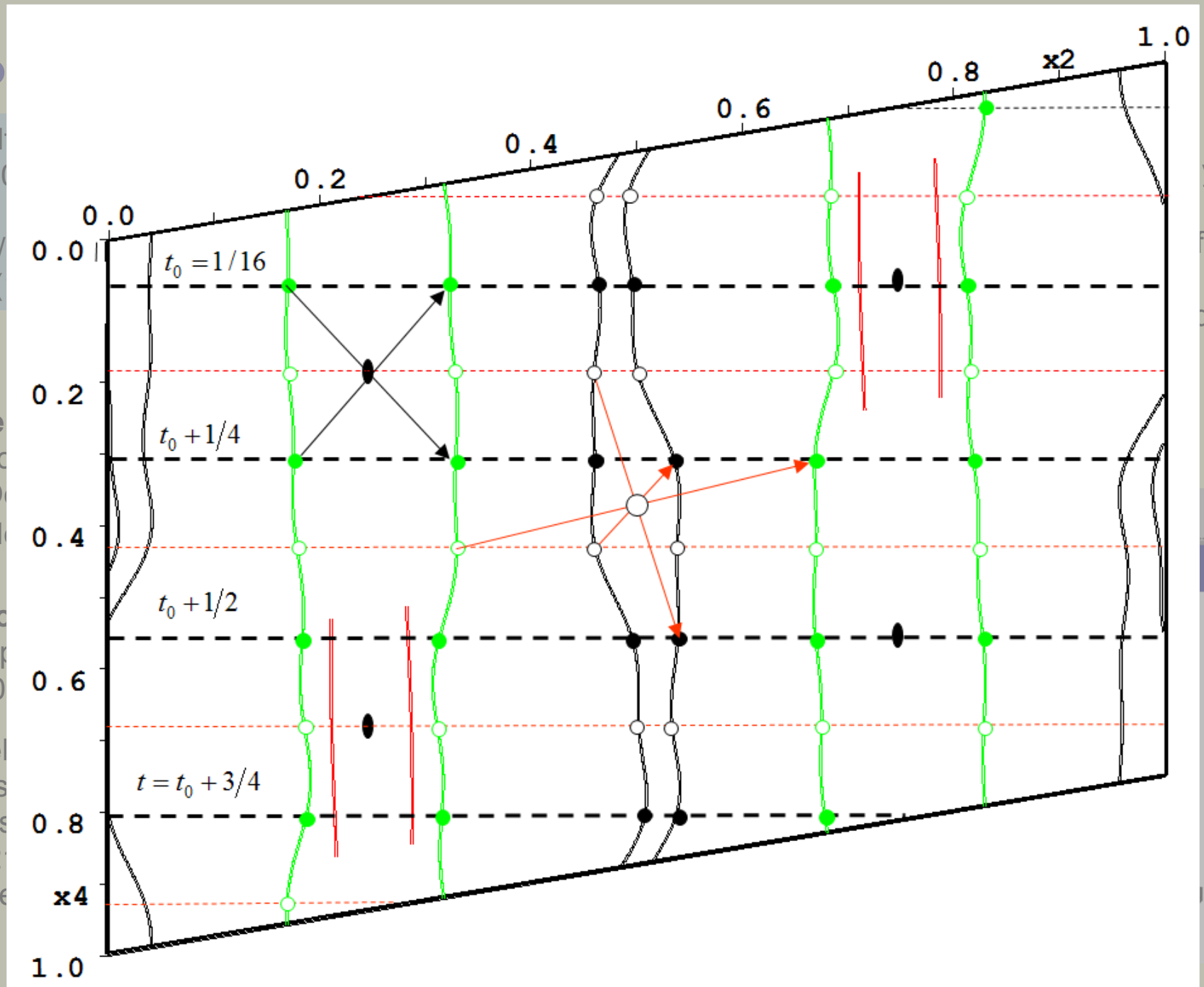
Gamma-Na_2CO_3	170K	Delta-Na_2CO_3
8.92, 5.25, 6.05		8.90, 5.24, 6.00
90, 101.35, 90		90, 101.87, 90
C2/m(α0γ)		C2/m(α0γ)
q=(0.182,0,0.322)		q=(1/6,0,1/3)

Superspace description: 4d cell, atomic position + modulation function, superspace symmetry

Supercell description: 3d six-fold supercell, atomic positions in six cells, 3d symmetry

Both descriptions are equivalent.

Origin of R_3 section may influence symmetry in the supercell.


0.0
0.2
0.4
0.6
0.8
x2
1.0
0.0
0.2
0.4
0.6
0.8
x4
1.0
$t_0 = 1/16$
$t_0 + 1/4$
$t_0 + 1/2$
$t = t_0 + 3/4$

Commensurate families

Commensurate family can be derived from the parent incommensurate structure by changing q-vector and t-zero. By this way we can relate three-dimensional structures which are at the first glance very different.

Example: $M_2P_2O_7$ diphosphates are derived from the parent phase alpha2.

Alpha2-$Cr_2P_2O_7$
7.02, 8.40, 4.62
90, 108.59, 90
C2/m(α0γ)0s
q=(0.361,0,-0.471)

285K

Alpha1-$Cr_2P_2O_7$
7.05, 8.41, 4.64
90, 108.71, 90
C2/m(α0γ)
q=(-1/3,0,1/2)

Metal (II)	**q-vector**	**t-zero**	**space group in the supercell**
Cr, Zn	(-⅓, 0, ½)	0	I2/c
Co, Mg, Ni	(½, 0, ½)	⅛	$B2_1/c$
Cu	(0, 0, ½)	0	C2/c

Magnetic structures

Magnetic structure factor:

$$\vec{\mathbf{F}}_M(\mathbf{h}) = p\sum_i f_i(h)T_i(\mathbf{h})\vec{\mathbf{S}}_i \exp(2\pi i\mathbf{h}\cdot\mathbf{r}_i)$$

f_i magnetic form factor

T_i temperature factor

$\vec{\mathbf{S}}_i$ magnetic moment

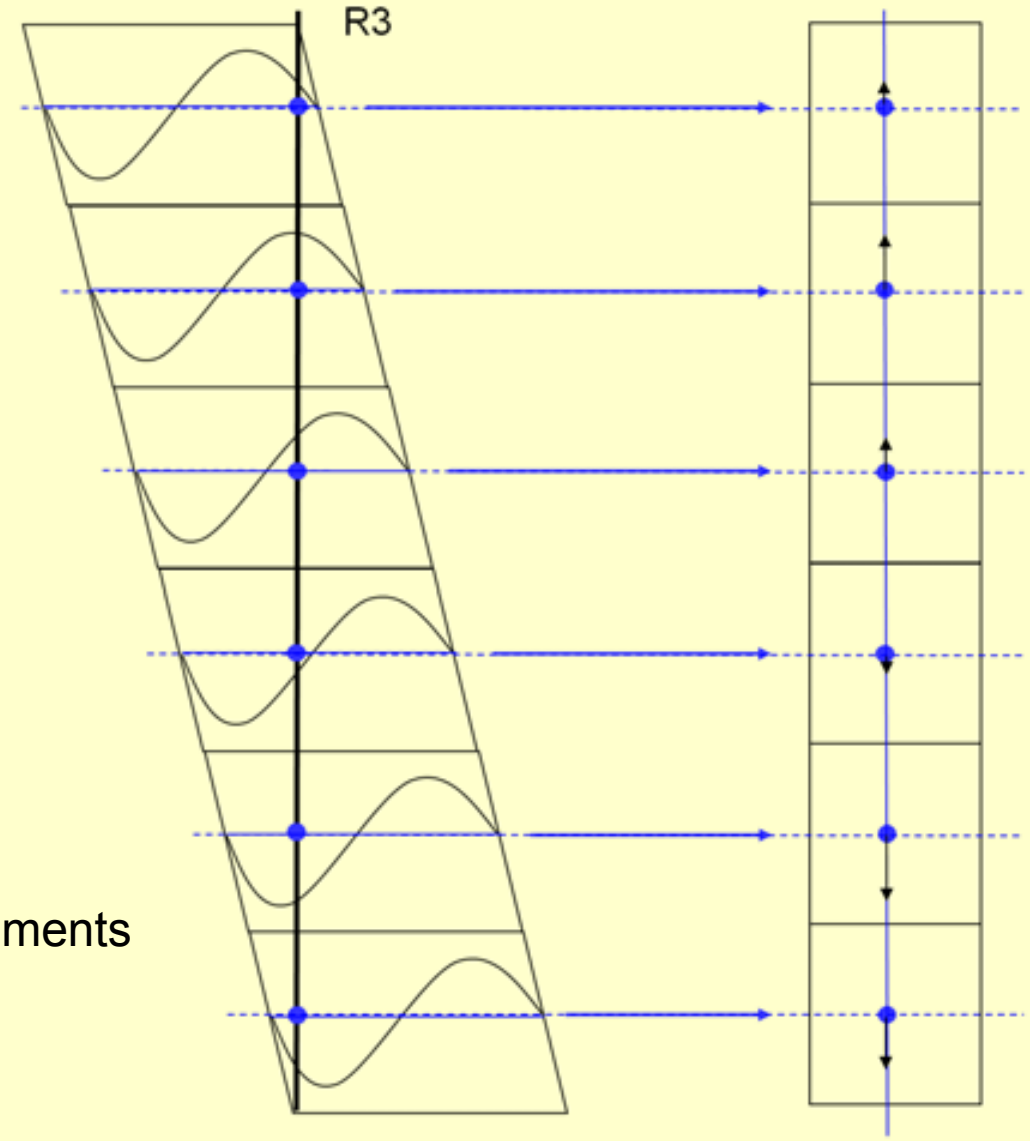
$\mathbf{r}_i$ atomic position

Intensity of magnetic diffraction:

$$I_M(\mathbf{h}) = \vec{\mathbf{F}}_M^2(\mathbf{h}) - \left[\mathbf{h}/h\cdot\vec{\mathbf{F}}_M(\mathbf{h})\right]^2$$

Total intensity:

$$I(\mathbf{h}) = I_N(\mathbf{h}) + I_M(\mathbf{h})$$



The distribution of the magnetic moments over the nuclear structure can be described by a modulation wave:

$$\mathbf{S}_i(x_4) = \mathbf{S}_{i0} + \sum_{n=1}^{N}\left[\mathbf{S}_{ins}\sin(2\pi n x_4) + \mathbf{S}_{ikc}\cos(2\pi n x_4)\right]$$

More information

jana.fzu.cz

Institute of Physics
Department of Structure Analysis
Cukrovarnicka 10
16253 Praha 6
Czech Republic

CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES

Vaclav Petricek, Michal Dusek & Lukas Palatinus

Jana2006 is a crystallographic program focused to solution, refinement and interpretation of difficult, especially modulated structures. It calculates structures having up to three modulation vectors from powder as well as single crystal data measured with X-ray or neutron diffraction. The input diffraction data can be unlimitedly combined, the combination of powder neutron data with single crystal X-ray data being a typical example. The structure solution can be done using the built-in charge flipping algorithm or by calling an external direct methods program. Jana can handle multiphase structures (for both powder and single crystal data), merohedric twins as well as twins with partial overlap of diffraction spots, commensurate and composite structures. It contains powerful transformation tools for symmetry (group-subgroup relations), cell parameters and commensurate-supercell relations. Wide scale of constrains and restrains is available including a powerful rigid body approach and possibility to define a local symmetry affecting only part of the structure. The latest development of Jana concerns magnetic structures.

More about Jana2006 (PowerPoint presentation, 10MB)

News

April 1, 2010 **Maintenance release of Jana2006 for Windows** can be obtained in Download area. It cumulates various improvements and bug fixes. More ....

January 26, 2010 **The Third Ad Hoc Workshop on Jana2006**, 8-9 March 2010. More ....

January 06, 2010 **The Second Ad Hoc Workshop on Jana2006**, 18-19 Jan 2010. More ....

January 05, 2010 **International school on aperiodic crystals.** More ....

October 21, 2009 **Maintenance release of Jana2006 for Windows** can be obtained in Download area. It cumulates various improvements and bug fixes. More ....

September 16, 2009 **Ad hoc workshops on Jana.** We offer informal two days workshops on topics selected by paticipants. More ... .

October 23, 2008 **Maintenance release of Jana2006 for Windows** can be obtained in Download area. It cumulates various improvements and bug fixes. More ....

October 14, 2008 Eset NOD32 antivirus slows down Jana2006. More ...

July 25, 2008 **The first stable version of Jana2006 for Windows.** This program is the successor of Jana2000. Currently only Windows version is available, Unix version as well as manual are under development. The Stable version will be changed occassionally, the everyday work will be immediately available in the Latest version. Registered users will be informed about new Stable versions. Jana2006 can be obtained in Download area.

July 22, 2008 **New web page for Jana** contains all information about Jana2006 and the previous version Jana2000. We have partially changed also download locations, please do not use old links.

December 28, 2007 **Final version of Jana2000** - see the Download area. No further development is expected in Jana2000.

Ad hoc workshops on Jana: details here

March 2011: 7th Workshop in Bayreuth

Ad hoc workshops on Jana

Ad hoc workshops are small two days workshops organized in Praha by authors of Jana software. As soon as five people register for one or more topics listed below and some overlap in topics is found we shall create program of the workshop and discuss it with the participants. Then we shall fix the date of the workshop and arrange accomodation. Registration to a workshop with fixed program and/or date is possible for another five participants. Participants pay themselves all their expenses and they are expected to bring their own laptops with **Windows**. The registration fee is zero (in Czech Crowns). Workshop certificates are issued by our skilled artists on demand.

Topics

- (INT1) Introduction to Jana software, solution of simple 3d structures
- (INT2) Introduction to modulated structures, solution of simple 4d structures
- (PWD) Refinement of powder data
- (TW) Twins and multiphases of 3d and modulated structures
- (CHF) Application of charge flipping to 3d and modulated structures
- (DIS) Disorder, mixed sites, application of rigid body refinement for disordered structures
- (RIG) Rigid body refinement and application of local symmetry
- (CRENEL) Discontinuous modulation functions (crenel and sawtooth)
- (COMM) Commensurate structures
- (COMP) Composite structures
- (FIVE) Five dimensional structures
- (MAG) Magnetic structures
- (ELD) Electron diffraction
- any other topic (please specify)

6th Jana2006 ad hoc workshop Two days in December 2010, **registration is open**.

Special jana2006 workshop on electron diffraction Two days in 2011, **registration is open**.

Special jana2006 workshop on magnetic structures Two days in 2011, **registration is open**.

FUTURE jana2006 ad hoc workshops This link serves for collecting requirements for future Jana2006 Ad Hoc workshops. As soon as an overlap in topics is found a new Ad Hoc Workshop is organized.

Contents

Jana cookbook cumulates workshop examples

Institute of Physics, Prague 6, Cukrovarnická street

Still freeware ….
(the driving force are citations)

Jana2006 is continuously supported by Academy of Sciences of the Czech Republic and (occasionally) by (unpredictable) Grant agency of the CR

YPO - $Y(PO_3)_3$

Example for solution of simple modulated structure

janainst.msi (Jana2006 from 14th September or later)

Diamond installation

Diamond licence valid before17 October

Printed cookbook