Introduction to superspace symmetry

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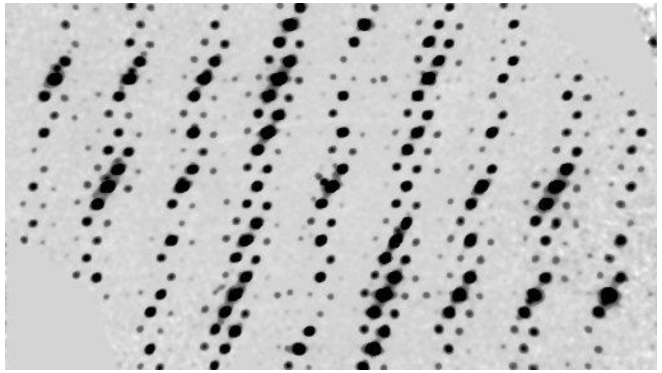
Single Crystal Neutron Diffraction Data Reduction and Analysis
June 22, 2024
ORNL

Diffraction pattern

Diffraction pattern of Na_2CO_3
Reconstructed images (precession-like view)

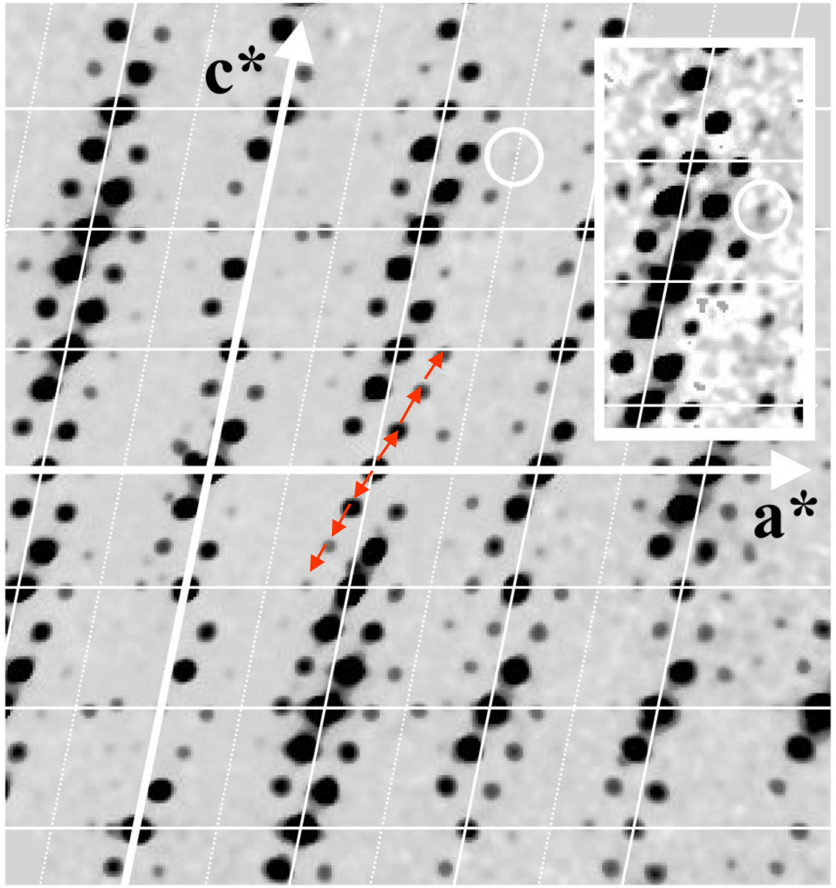
- **The diffraction pattern does not show 3D lattice character anymore: the translation symmetry is violated in a specific, regular way**
- **One or more additional (modulation) vectors must be added to the reciprocal base to index all diffraction spots**



Additional diff spots

$$\mathbf{Q} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^* + m\mathbf{q} = \mathbf{H} + m\mathbf{q}$$

$$\mathbf{q} = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$$



α, β, γ ..... all rational $\rightarrow$ *commensurate structure*

α, β, γ ..... at least one irrational $\rightarrow$ *incommensurate structure*

Diffraction pattern

Additional diffraction spots:

Modulated structures:

"*Gittergeister*" U.Dehlinger, *Z. Kristallogr.* (1927) **65** 615–31.
"*Satellites*" G.D.Preston *Proc. R. Soc.* (1938) **167** 526–38.

$2n+1$. The normal reflexions occur when $c = 2\pi$, 4π, etc., i.e. when $m = 2n+1$, $2(2n+1)$, etc., and each of these is accompanied by two satellites, one on either side, when $c = 2\pi\left(1 \pm \frac{1}{2n+1}\right)$, $2\pi\left(2 \pm \frac{1}{2n+1}\right)$, etc. These are the only spectra which arise. The presence of a pair of satellites associated with each normal reflexion is a consequence of our original assumption involving a simple harmonic distortion. A less simple type of distortion

M. Korekawa (1967) *Theorie der Satellitereflexe Habilitationschrift* (München, Germany: Ludwigs-Maximilians-University).
Korekawa & Jagodzinski (1967), *Schweitz.Miner.Petrogr.Mitt.,* **47**, 269-278.
The theory of satellite reflections due to various types of modulation waves.

Composite crystals:

S. van Smallen, (1991), Phys. Rew. B, **43**, 11330-11341.
E. Makovicky & B.G.Hide, (1992), *Material Science Forum,* **100&101**, 1-100.

Diffraction pattern

Composite character of pure metals under high pressure.

Nelmes, Allan, Mc Mahon & Belmonte, *Phys.Rev.Lett.* (1999), **83**, 4081-4084. Barium IV.
Schwarz, Grzechnik, Syassen, Loa & Hanfland, *Phys.Rev.Lett.* (1999), **83**, 4085-4088. Rubidium IV.

Modulated protein crystals - profilic:actin

C. E. Schutt, U. Lindberg, J. Myslik and N. Strauss, *Journal of Molecular Biology* , (1989), **209,** 735-746.

J. J. Lovelace, K. Narayan, J. K. Chik, H. D. Bellamy, E. H. Snell, U. Lindberg, C. E. Schutt and G. E. O. Borgstahl, *J. Appl. Cryst.* (2004). **37**, 327-330.

Special importance: magnetic materials – helical, cycloidal, skyrmion ordering of magnetic moments

Superspace approach

Diffraction pattern ← **Fourier transform** → **Charge (nuclear) density**

3d lattice

$$\mathbf{h} = \sum_{i=1}^{3} h_i \mathbf{a}_i^*$$

translation symmetry in 3d space

$$\rho(\mathbf{r}) = \rho\left(\mathbf{r} + \sum_{i=1}^{3} n_i \mathbf{a}_i\right)$$

additional satellite spots

$$\mathbf{h} = \sum_{i=1}^{3+d} h_i \mathbf{A}_i^*$$

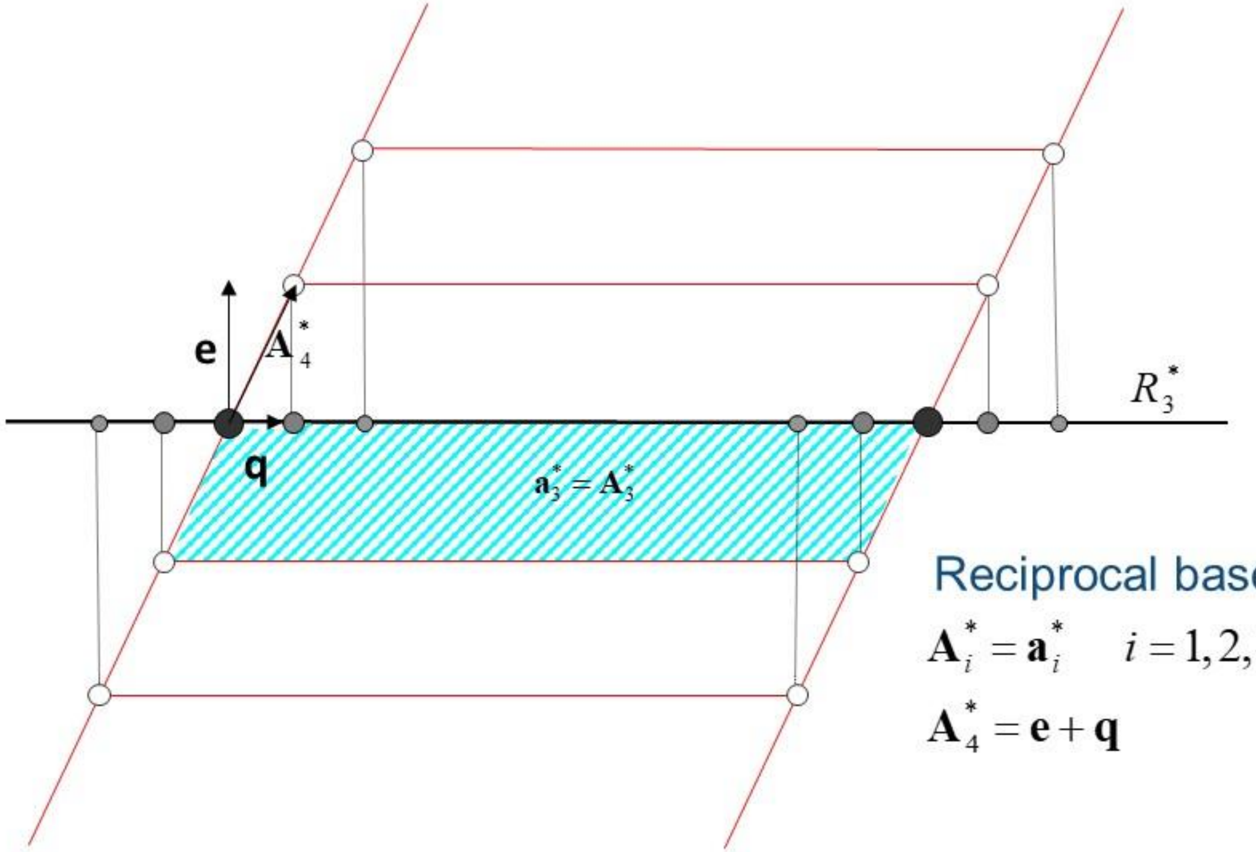
translation symmetry in (3+d) dimensional space

$$\tilde{\rho}(\mathbf{r}) = \tilde{\rho}\left(\mathbf{r} + \sum_{i=1}^{3+d} n_i \mathbf{A}_i\right)$$

$\Rightarrow$ Description in 3+d dimensional superspace

Superspace approach

- **Superspace theory by P.M. De Wolff, A. Janner, T. Jansen**



Reciprocal base:

$$\mathbf{A}_i^* = \mathbf{a}_i^* \qquad i = 1,2,3$$

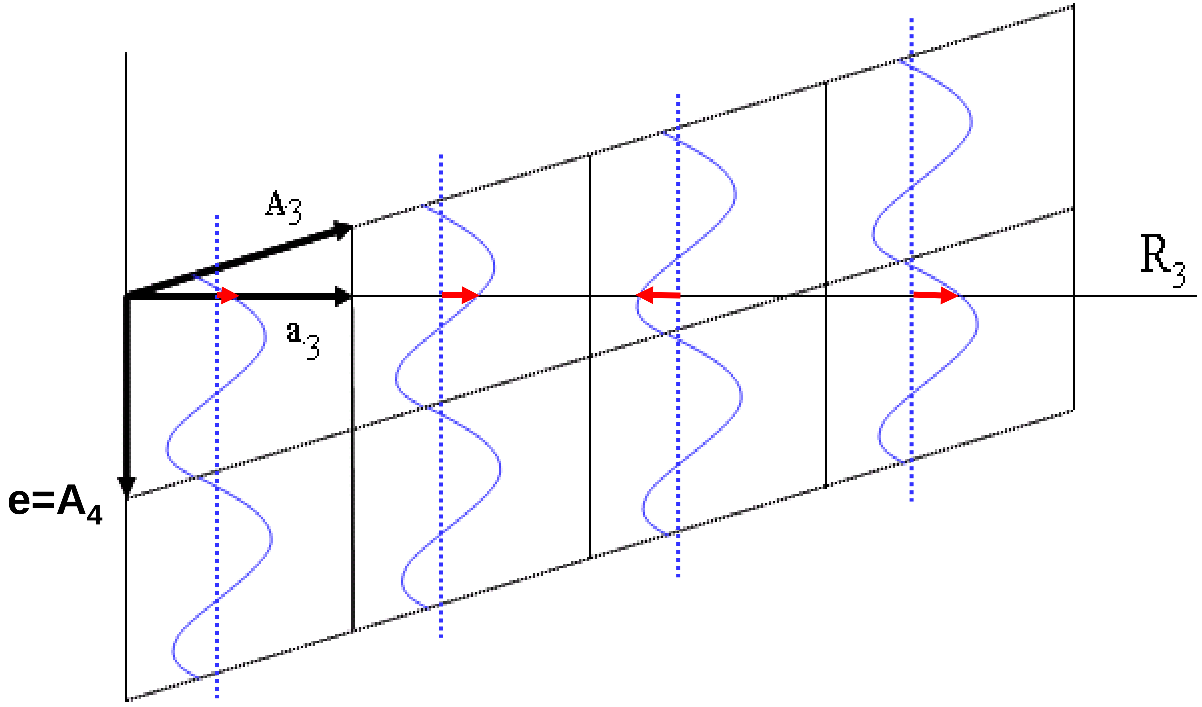
$$\mathbf{A}_4^* = \mathbf{e} + \mathbf{q}$$

Superspace approach

- **The atomic parameters are generally different from cell to cell**
- **It can be described in a superspace by a periodic modulation function**

$$p(x_4) = A_0 + \sum_n A_{s,n} \sin(2\pi n x_4) + \sum_n A_{c,n} \cos(2\pi n x_4)$$

$p(x_4)$ is the modulated parameter or spin, and x_4 is the 4[th] superspace coordinate and $p(x_4+1)= p(x_4)$



Superspace approach

Diffraction pattern	← Fourier transform →	Charge (nuclear) density
$\mathbf{h} = \sum_{i=1}^{3+d} h_i \mathbf{A}_i^*$	Artificial description in (3+d)	$\tilde{\rho}(\mathbf{r}) = \tilde{\rho}\left(\mathbf{r} + \sum_{i=1}^{3+d} n_i \mathbf{A}_i\right)$
Projection from (3+1)d superspace into 3d space		3d section through (3+1)d superspace
↓		↓
Diffraction pattern	Real 3d	Modulated structure

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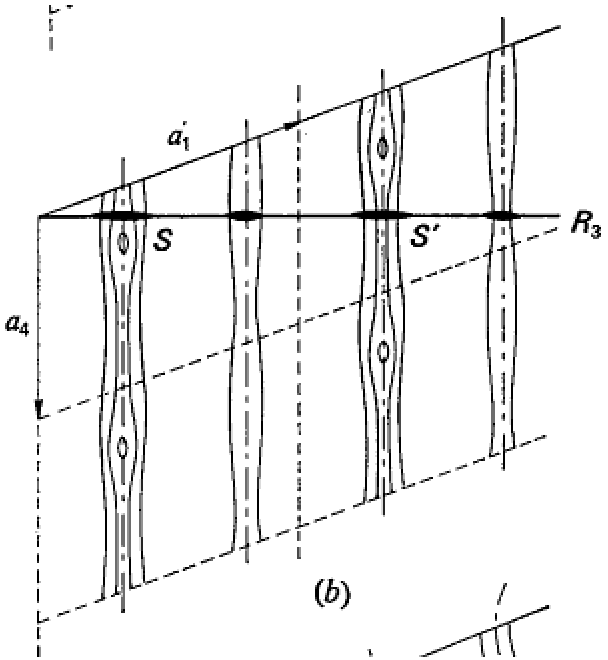
Superspace approach

Superspace theory in solution, refinement, and interpretation of modulated structures:

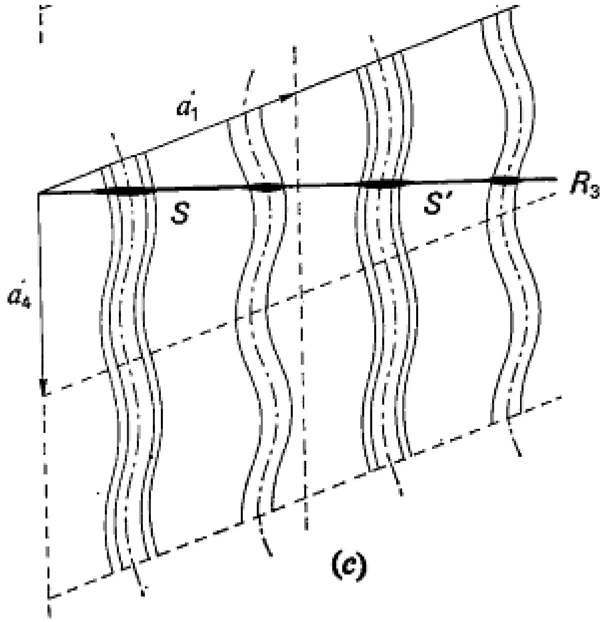
- calculation of structure factors
- Fourier synthesis in (3+d) superspace
- Calculation of geometrical characteristics (distances, angles, BVS) for modulated structures

P.M. de Wolff, *Acta Cryst.* (1974). A30, 777-785 - de Wolff's sections

Substitutional modulation:



Modulation of atomic position:



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Basic types of modulations

Each individual atom having density:

$$\rho_\nu(\mathbf{r}) = \sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\sum_{n_3=0}^{N_3-1}\rho_\nu^A(\mathbf{r})*\delta(\mathbf{r}-\mathbf{r}_\nu - n_1\mathbf{a}_1 - n_2\mathbf{a}_2 - n_3\mathbf{a}_3)$$

makes the following contribution to the structure factor:

$$F_\nu(\mathbf{Q}) = f_\nu(|\mathbf{Q}|)\exp(2\pi i\mathbf{Q}\cdot\mathbf{r}_\nu)\sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\sum_{n_3=0}^{N_3-1}\exp\{2\pi i\mathbf{Q}\cdot(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3)\} =$$

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

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

$f_\nu(|\mathbf{Q}|)$ … atom form factor

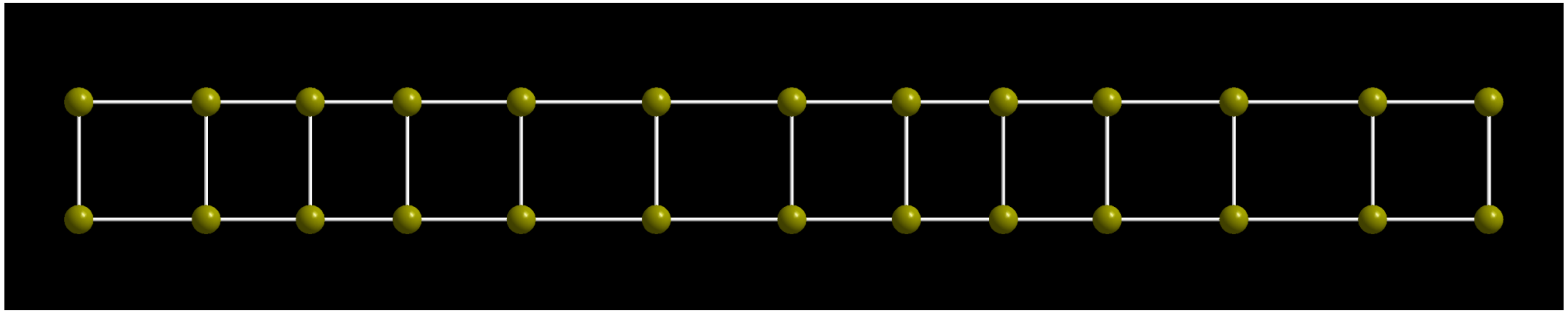
For $N_i >> 1 \rightarrow$ principal maxima for $\mathbf{Q} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*$

h_i … integers

$\mathbf{a}_i \cdot \mathbf{a}_j^* = \delta_{ij}$

Basic types of modulations

Positional modulation – longitudinal, one harmonic wave



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

$$\rho_{\nu}(\mathbf{r}) = \sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\sum_{n_3=0}^{N_3-1}\rho_{\nu}^{A}(\mathbf{r}) * \delta\left(\mathbf{r}-\mathbf{r}_{\nu}(\mathbf{n})-n_1\mathbf{a}_1-n_2\mathbf{a}_2-n_3\mathbf{a}_3\right)$$

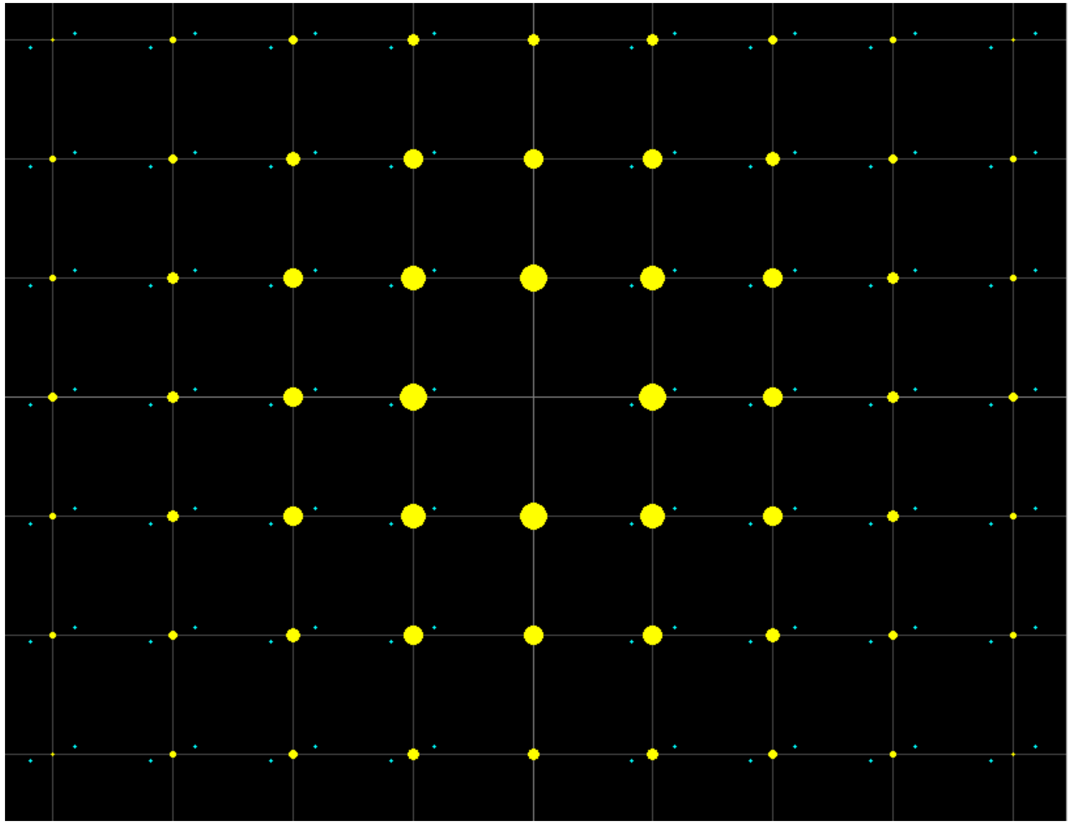
Fourier transform:

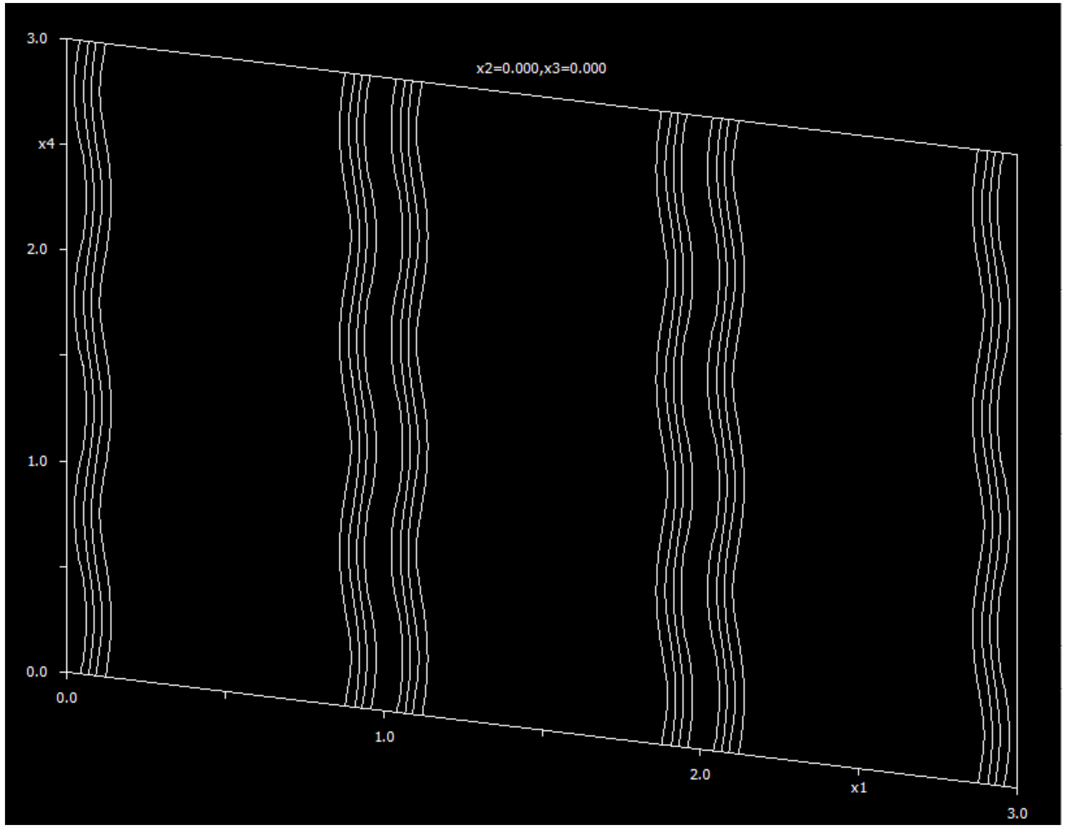
$$F_{\nu}(\mathbf{Q}) = f_{\nu}\left(|\mathbf{Q}|\right)\exp\left(2\pi i\mathbf{Q}\cdot\mathbf{r}_{\nu 0}\right)\sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\sum_{n_3=0}^{N_3-1}\exp\left\{2\pi i\mathbf{Q}\cdot\left(\mathbf{U}_{\nu}\sin\left[2\pi\mathbf{q}\left(\mathbf{r}_{\nu 0}+\mathbf{n}\right)\right]+\mathbf{n}\right)\right\}$$

Basic types of modulations

Positional modulation – longitudinal, one harmonic wave

Weak modulation

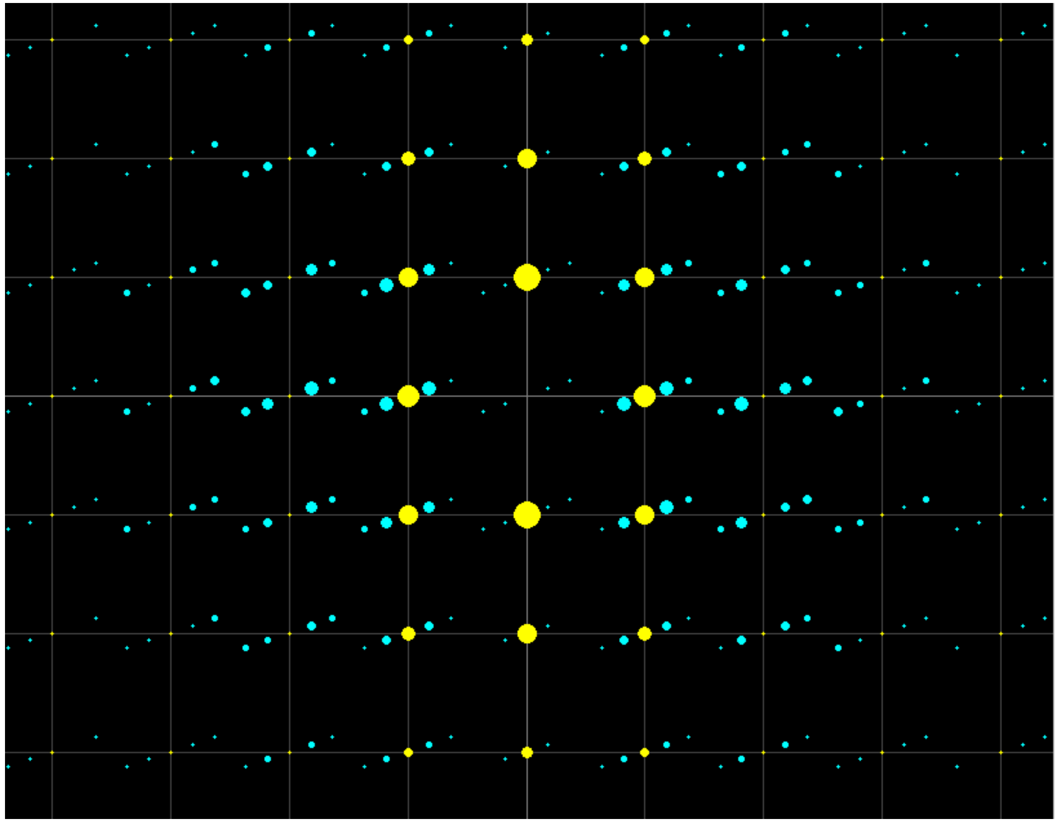


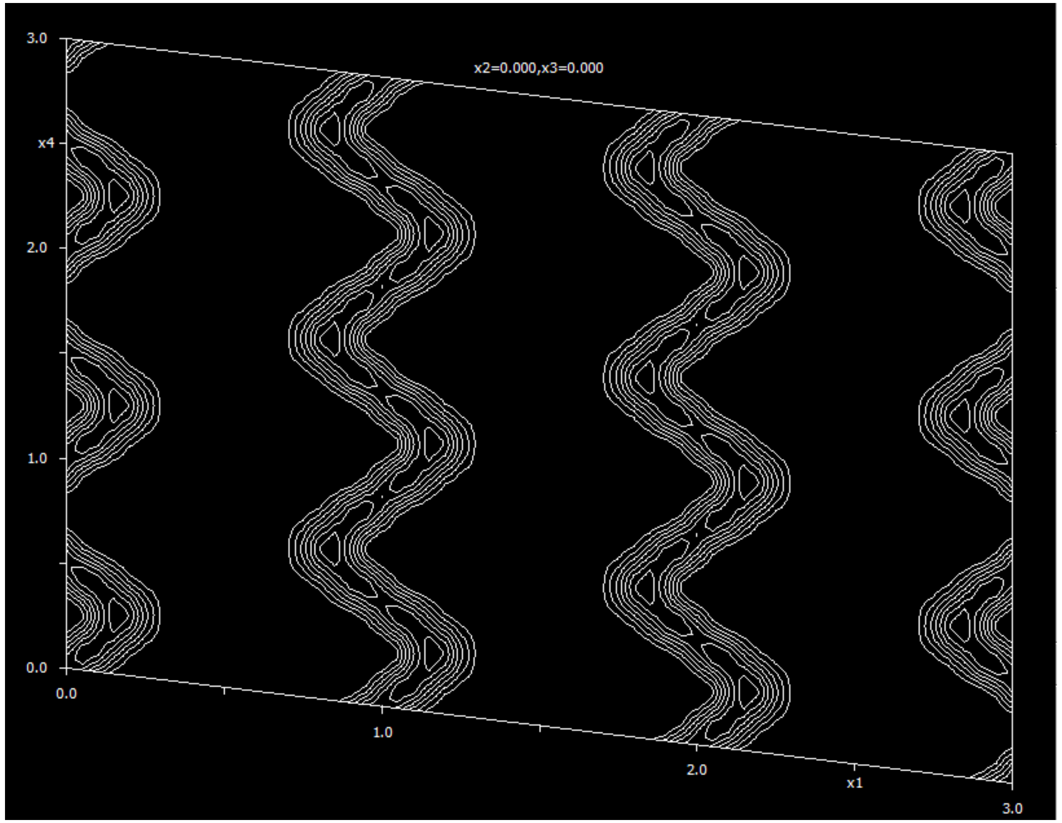


Basic types of modulations

Positional modulation – longitudinal, one harmonic wave

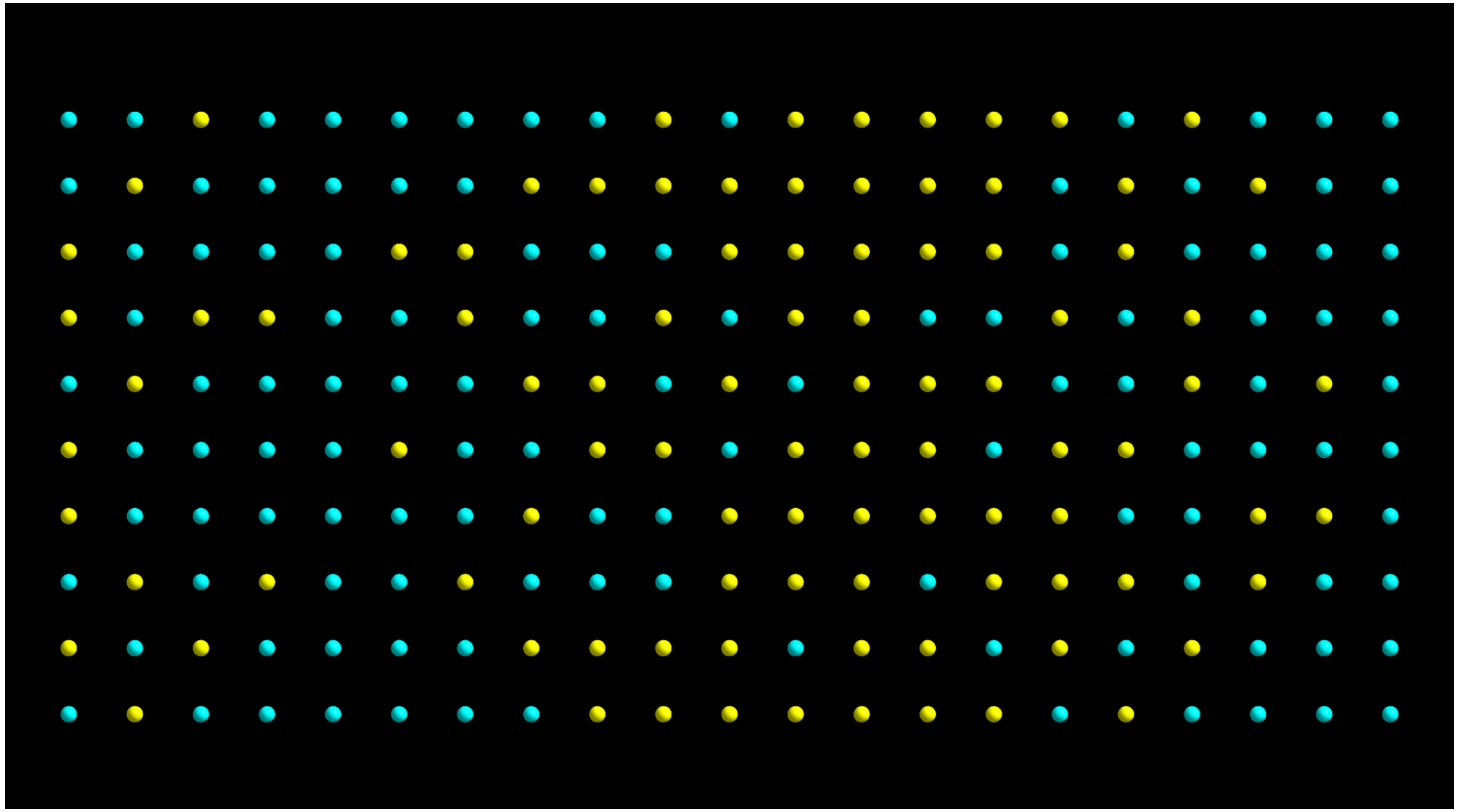
Strong modulation





Basic types of modulations

Occupational modulation – one harmonic wave



Basic types of modulations

Occupational modulation – one harmonic wave

$$\rho^A(\mathbf{r},\mathbf{n}) = \left[1+\cos 2\pi\mathbf{q}\cdot(\mathbf{r}_\nu+\mathbf{n})\right]\rho^A(\mathbf{r})/2 =$$

$$\left[1+1/2\left\{\exp\left(2\pi i\mathbf{q}\cdot(\mathbf{r}_\nu+\mathbf{n})\right)+\exp\left(-2\pi i\mathbf{q}\cdot(\mathbf{r}_\nu+\mathbf{n})\right)\right\}\right]\rho^A(\mathbf{r})/2$$

The contribution to the structure factor is:

$$F_\nu(\mathbf{Q}) = \frac{f_\nu(|\mathbf{Q}|)}{2}\exp(2\pi i\mathbf{Q}\cdot\mathbf{r}_\nu)\sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\sum_{n_3=0}^{N_3-1}\exp\left\{2\pi i\mathbf{Q}\cdot(n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\right\}+$$

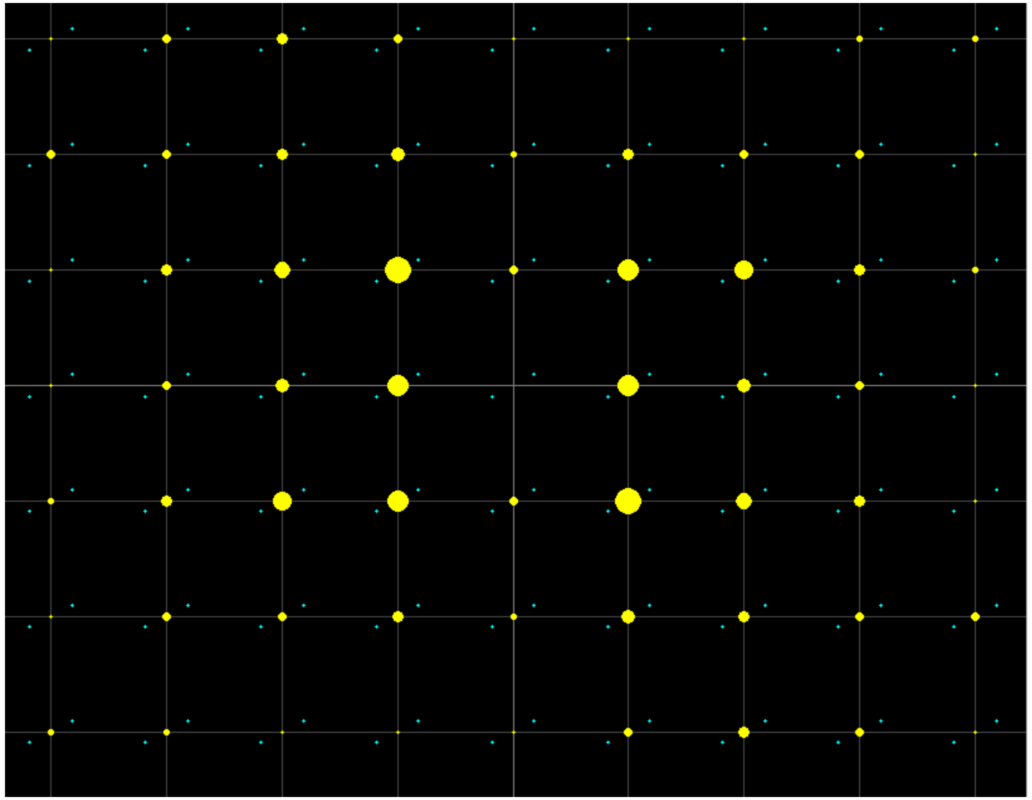
$$\frac{f_\nu(|\mathbf{Q}|)}{2}\exp\left(2\pi i(\mathbf{Q}\pm\mathbf{q})\cdot\mathbf{r}_\nu\right)\sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\sum_{n_3=0}^{N_3-1}\exp\left\{2\pi i(\mathbf{Q}\pm\mathbf{q})\cdot(n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\right\}$$

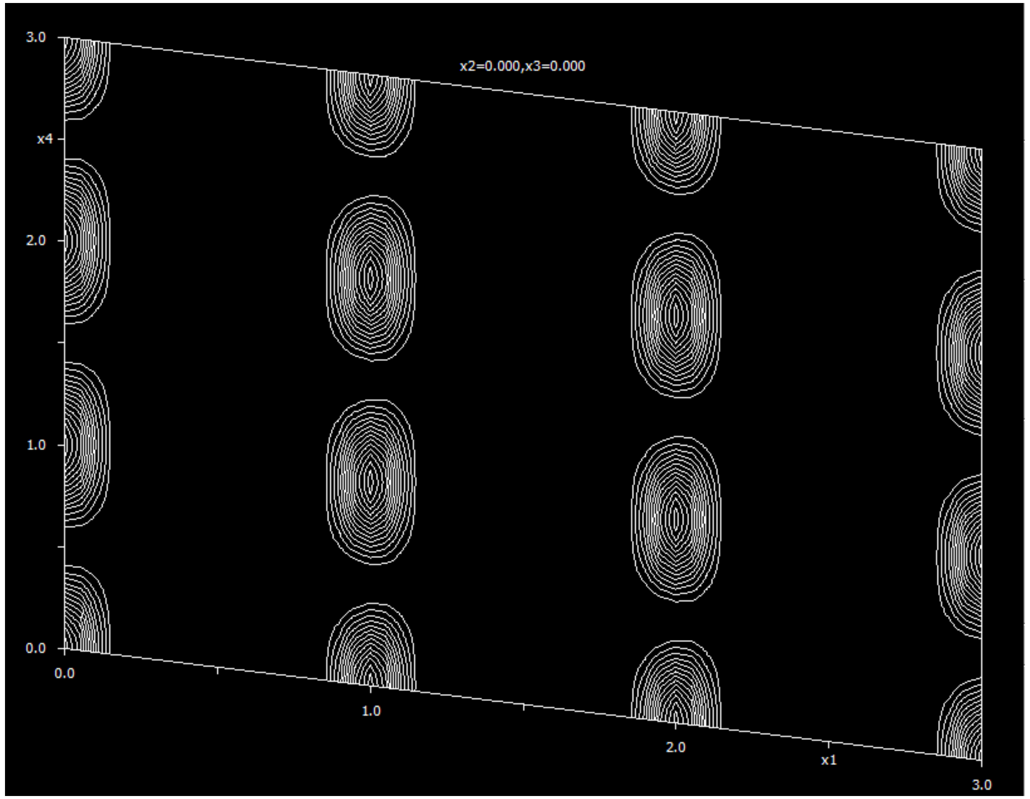
Main reflections at $\mathbf{Q} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*$

Satellite reflections at $\mathbf{Q} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^* \pm \mathbf{q}$

Basic types of modulations

Occupational modulation – one harmonic wave





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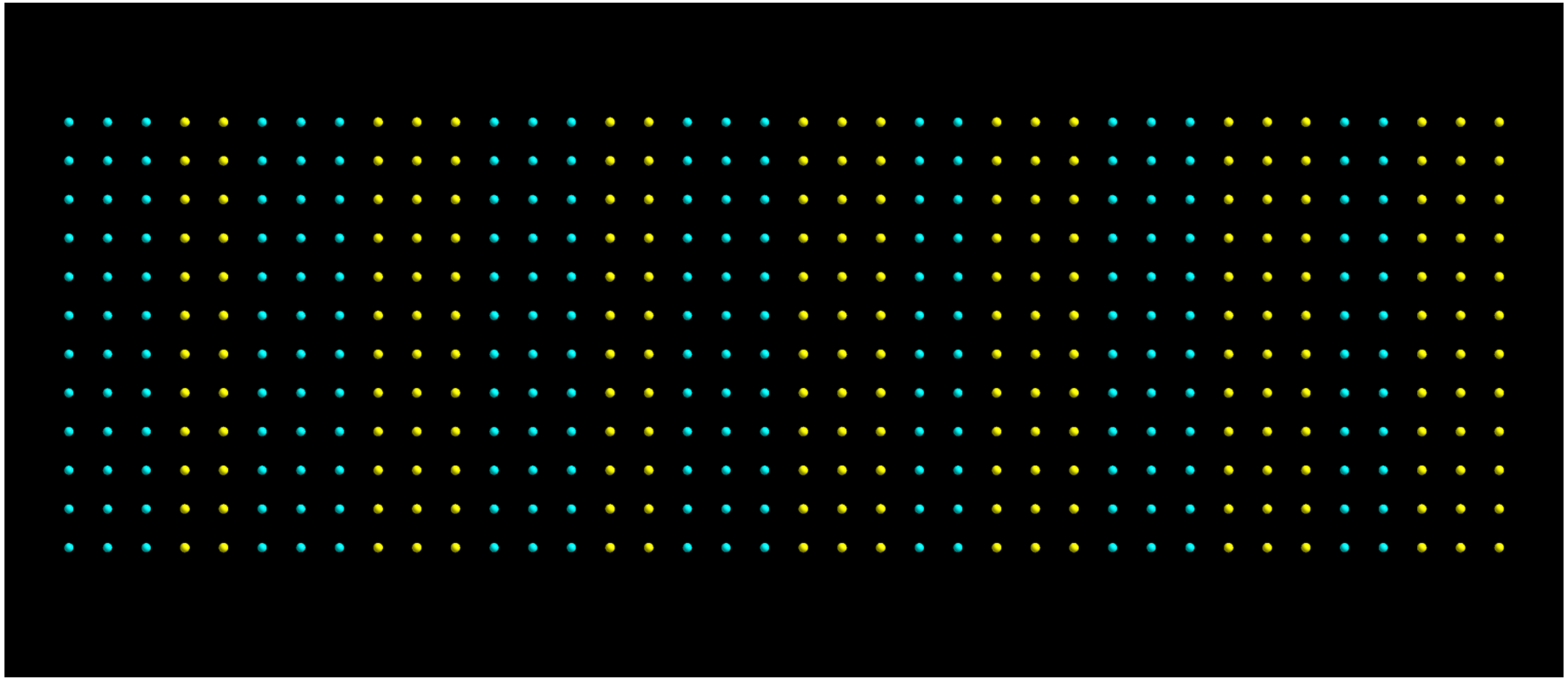
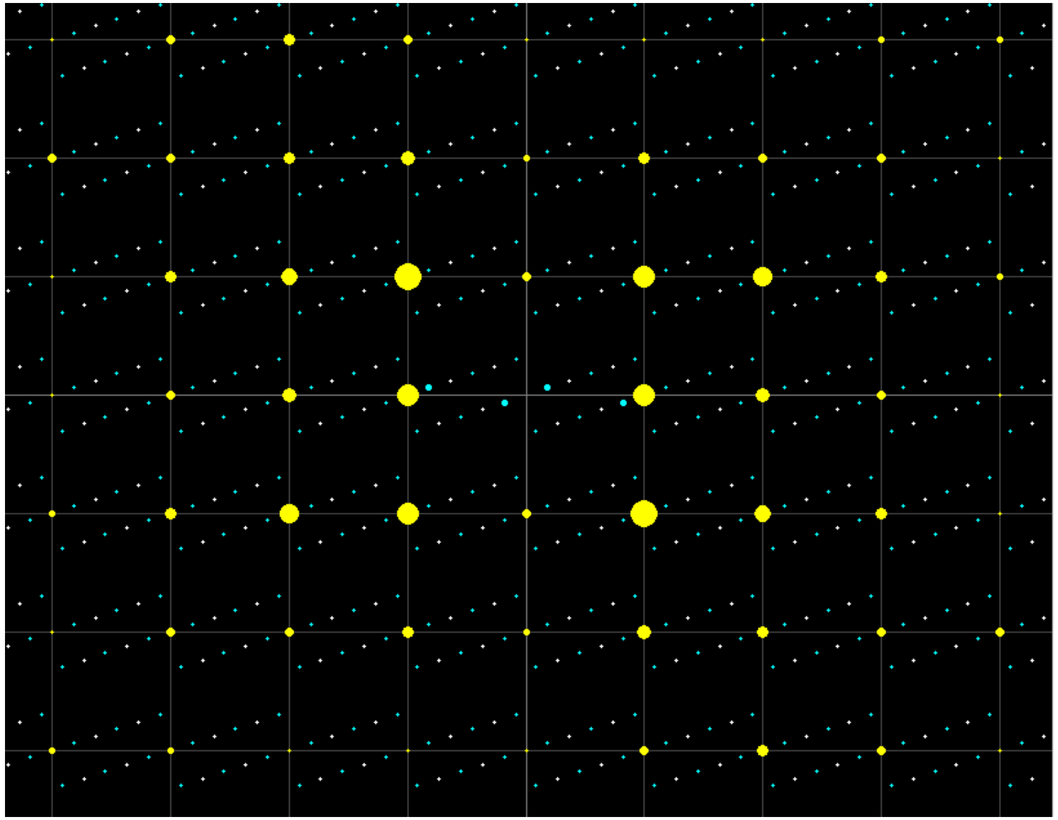
Basic types of modulations

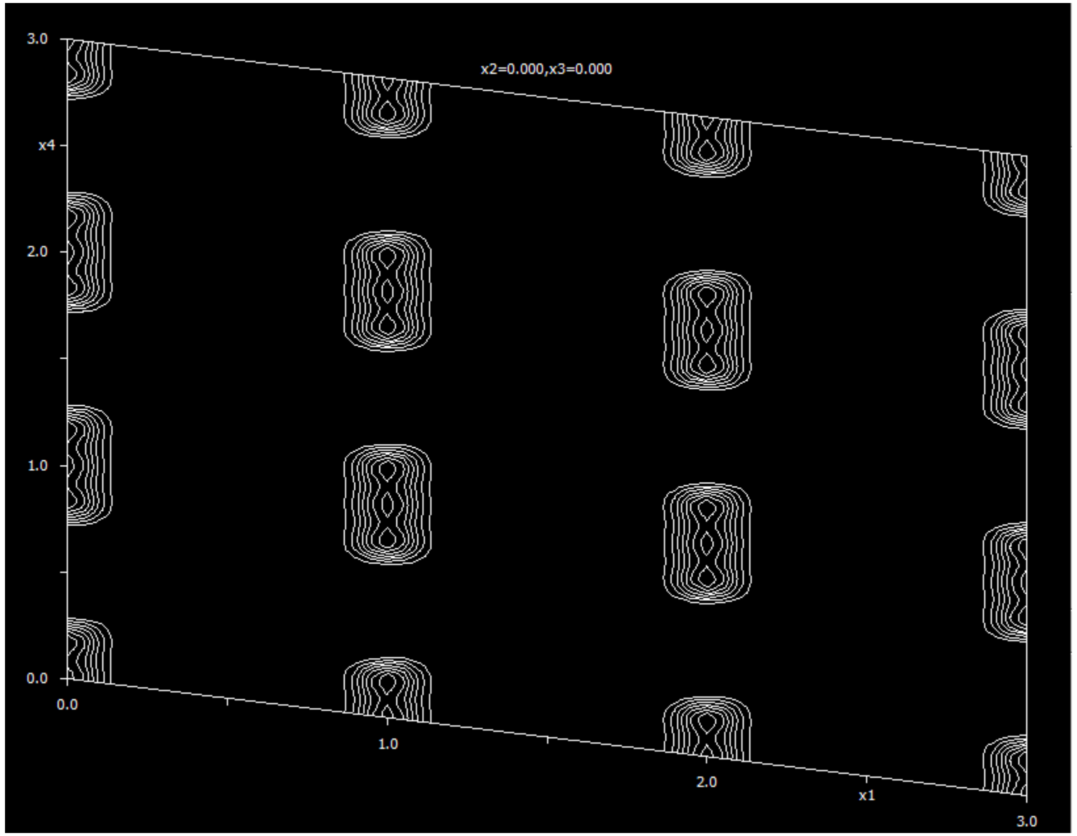
Occupational modulation – crenel function



Basic types of modulations

Occupational modulation – crenel function





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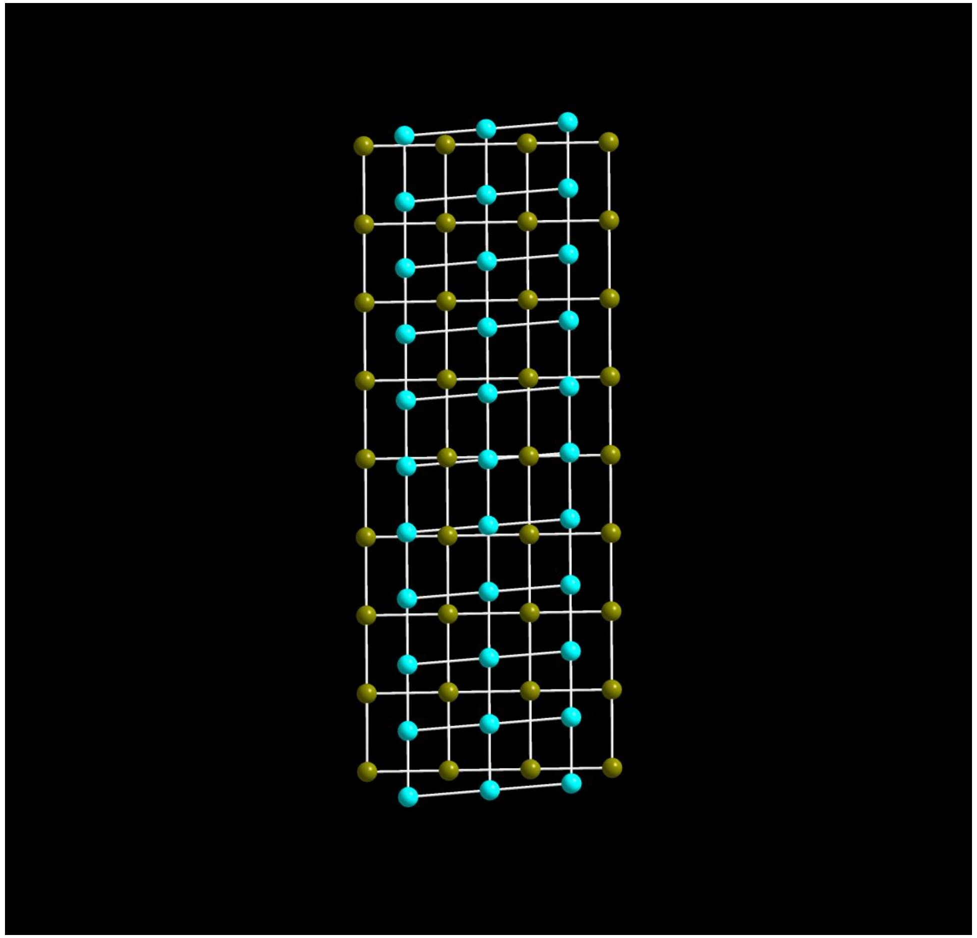
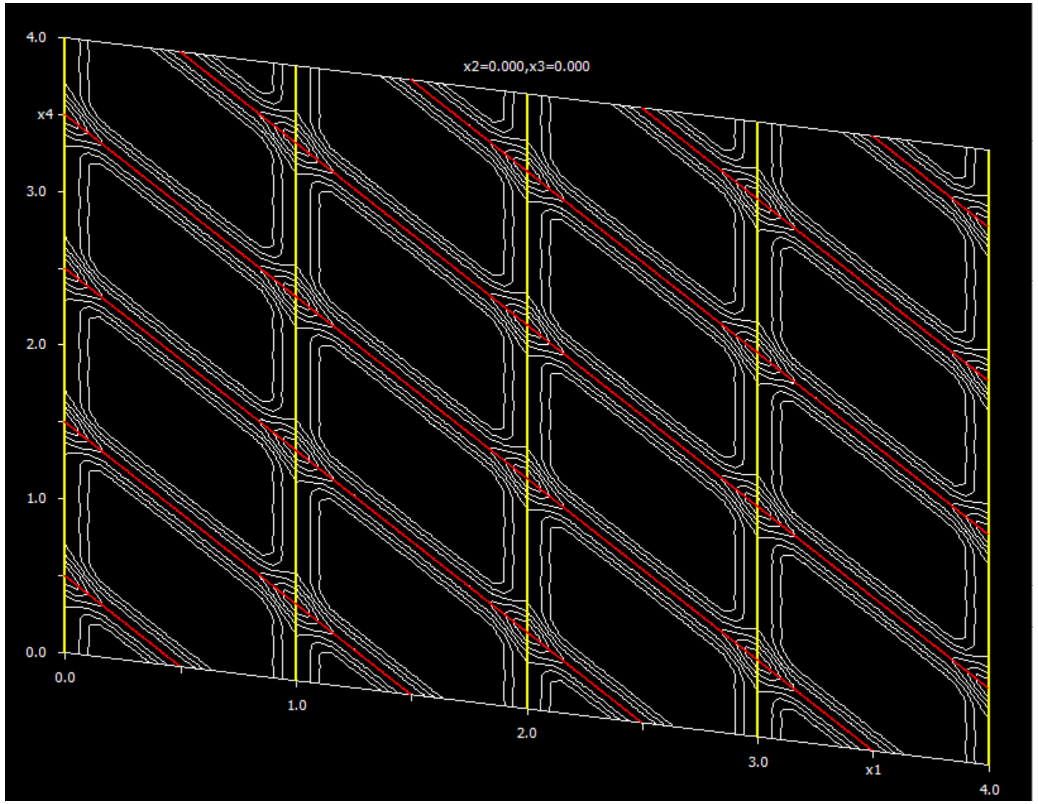
Basic types of modulations

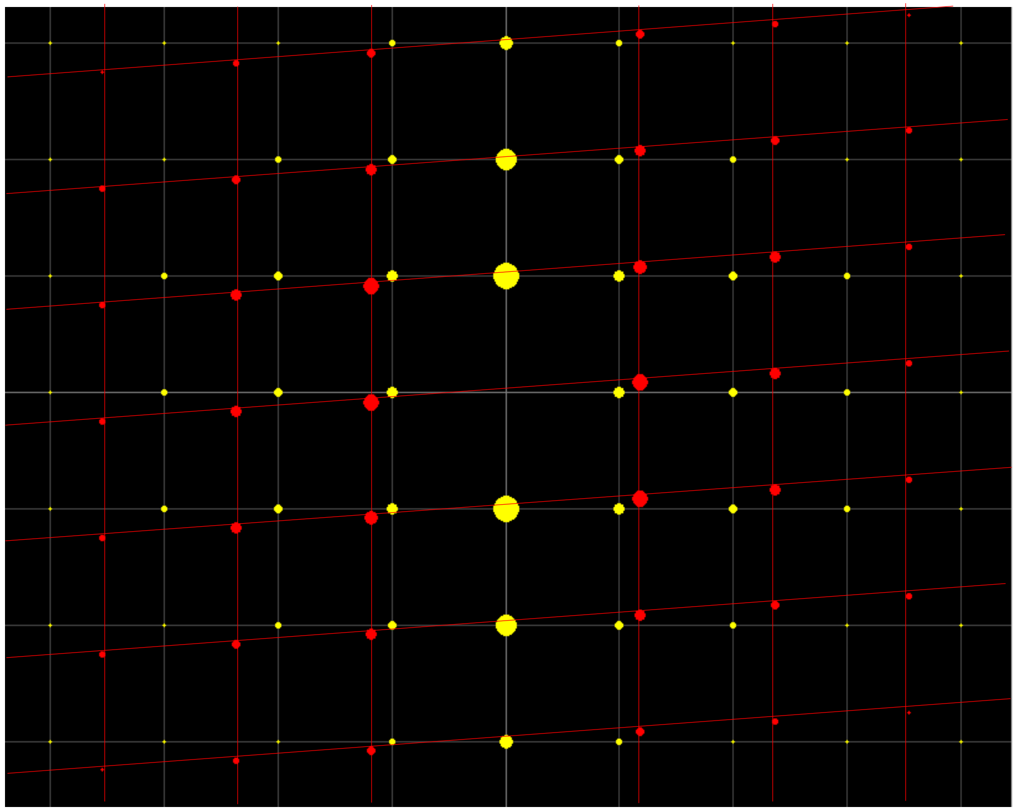
Composite structure – no mutual modulation



Basic types of modulations

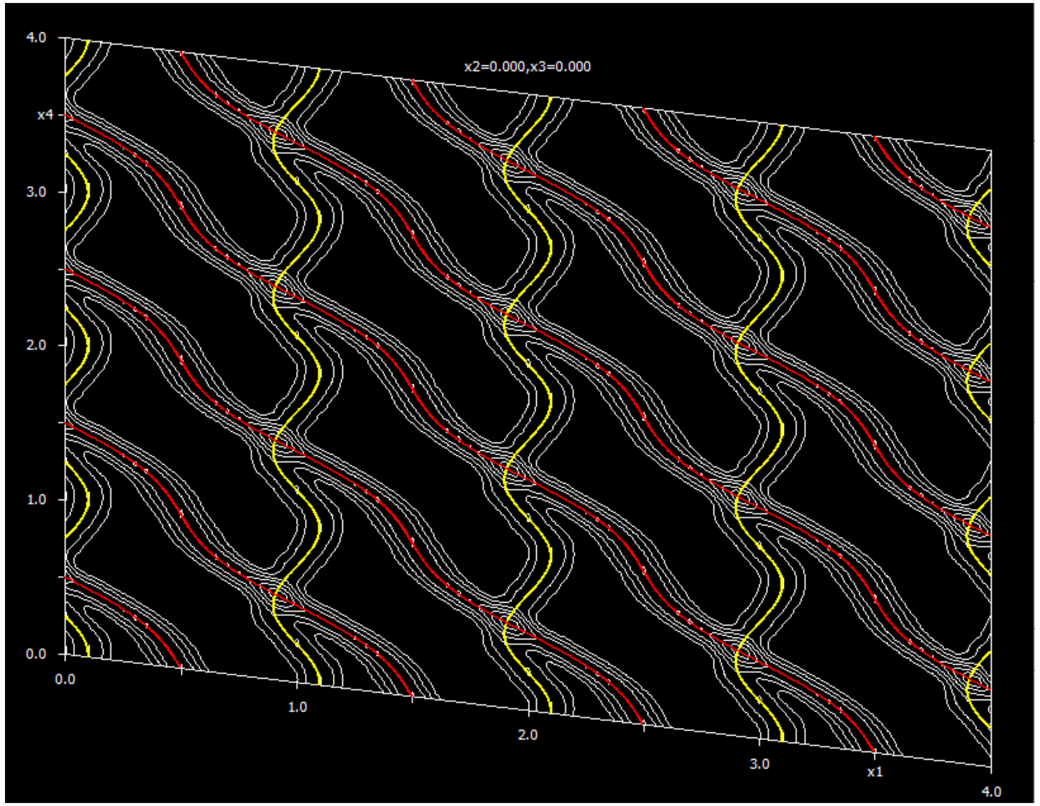
Composite structure – no mutual modulation

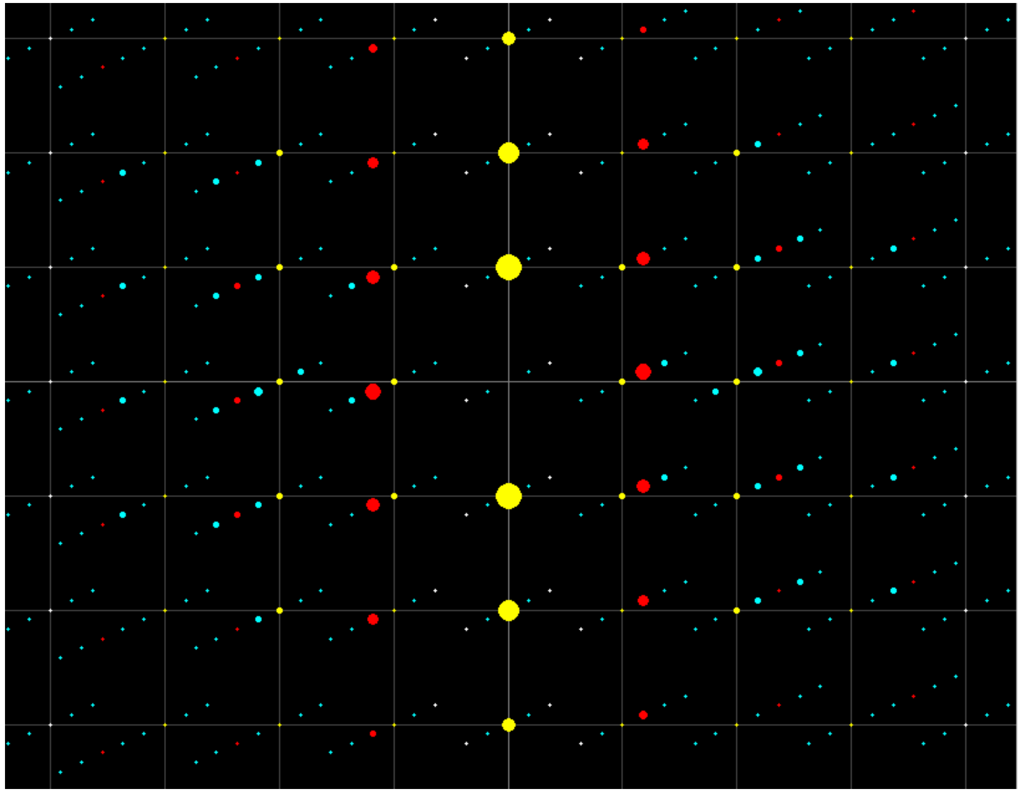




Basic types of modulations

Composite structure – mutual modulation





Superspace symmetry

$$\tilde{\rho}(\hat{S}\mathbf{r}) = \tilde{\rho}(\mathbf{r})$$
↓
basic property

$$\hat{S}\mathbf{r} \cdot \hat{S}\mathbf{r} = \mathbf{r} \cdot \mathbf{r}$$
↓
unitary operator

$$\hat{S} = (\mathbf{R}\,,\,\mathbf{t})$$
↓
matrix representation

Trivial symmetry operator - translation symmetry :

$$\mathbf{R} = \mathbf{E}, \quad \mathbf{t} = \sum_{i=1}^{3+d} n_i \mathbf{A}_i$$

Generally, these conditions are also used for space group in (3+d) dimensional space.

de Wolff construction leads to a specific simplification: superspace groups are in fact 3+d reducible subgroups of more general (3+d) dimensional space groups

Superspace symmetry

Superspace symmetry operation: $\boldsymbol{\Gamma} = \left(\left[\begin{array}{c|c} \boldsymbol{\Gamma}_E & 0 \\ \hline \boldsymbol{\Gamma}_M & \boldsymbol{\Gamma}_I \end{array} \right], \left[\begin{array}{c} \mathbf{s}_E \\ \hline \mathbf{s}_I \end{array} \right] \right)$

$\boldsymbol{\Gamma}_E, \boldsymbol{\Gamma}_M, \boldsymbol{\Gamma}_I$ (3x3) external, (dx3) mixed and (dxd) internal blocks of the rotational part of the superspace symmetry operation

$\mathbf{s}_E, \mathbf{s}_I$ 3x1 external and (dx1) internal block of the translation part of the superspace symmetry operation

Application of superspace operation to a point **x:**

$$\boldsymbol{\Gamma}\mathbf{x} = \left[\begin{array}{c|c} \boldsymbol{\Gamma}_E & 0 \\ \hline \boldsymbol{\Gamma}_M & \boldsymbol{\Gamma}_I \end{array} \right] \left[\begin{array}{c} \mathbf{x}_E \\ \hline \mathbf{x}_I \end{array} \right] + \left[\begin{array}{c} \mathbf{s}_E \\ \hline \mathbf{s}_I \end{array} \right]$$

$\mathbf{x}_E, \mathbf{x}_I$ external and internal coordinates

In the (3+1) dimensional superspace: 4 components (x_1, x_2, x_3, x_4)

Superspace symmetry

Superspace symmetry operation: $\mathbf{\Gamma} = \left(\begin{bmatrix} \Gamma_E & 0 \\ \Gamma_M & \Gamma_I \end{bmatrix}, \begin{bmatrix} \mathbf{s}_E \\ \mathbf{s}_I \end{bmatrix} \right)$

From the basic symmetry as determined from main reflections

Internal and external spaces do not mix

From the metric properties (unitary conditions) : $\Gamma_M = \boldsymbol{q}\Gamma_E - \Gamma_I \boldsymbol{q}$

q and ***S**$_I$*: New!

***S**$_I$*: the **shift of the modulation** wave in the internal space. It affects reflection conditions for the satellites

q can be split into two parts: rational and irrational: $\boldsymbol{q_i}\Gamma_E - \Gamma_I \boldsymbol{q_i} = 0$ and $\boldsymbol{q_r}\Gamma_E - \Gamma_I \boldsymbol{q_r} = \Gamma_M$

The **rational part** is made of zeros and specific fractions 1/2, 1/3 **fixed by symmetry**.
$\rightarrow$ complete separation of the external and internal case

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Superspace symmetry

The equations $\boldsymbol{q_i}\Gamma_E - \Gamma_I\boldsymbol{q_i} = 0$ and $\boldsymbol{q_r}\Gamma_E - \Gamma_I\boldsymbol{q_r} = \Gamma_M$ can be used to find all possible modulation vectors compatible with a superspace symmetry operation:

Examples for (3+1)d superspace

1- Inversion center:

$$\mathbf{\Gamma}_E = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \mathbf{\Gamma}_I = \pm 1 \quad \Rightarrow \quad [\alpha,\beta,\gamma]\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \mp 1[\alpha,\beta,\gamma] = [0,0,0]$$

For $\mathbf{\Gamma}_I = +1 \Rightarrow \alpha = \beta = \gamma = 0 \rightarrow \mathbf{q} = (0,0,0)$ – no incommensurate modulation

For $\mathbf{\Gamma}_I = -1 \Rightarrow \alpha \neq 0, \beta \neq 0, \gamma \neq 0' \rightarrow \mathbf{q} = (\alpha,\beta,\gamma)$ – all three components can have non-zero values

Superspace symmetry

2- Two-fold axis along b:

$$\mathbf{\Gamma}_E = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \mathbf{\Gamma}_I = \pm 1 \quad \Rightarrow \quad [\alpha,\beta,\gamma]\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \mp 1[\alpha,\beta,\gamma] = [0,0,0]$$

For $\mathbf{\Gamma}_I = +1 \Rightarrow \alpha = \gamma = 0 \quad \beta \neq 0 \rightarrow \mathbf{q} = (0,\beta,0)$ – axial monoclinic case

For $\mathbf{\Gamma}_I = -1 \Rightarrow \alpha \neq 0, \gamma \neq 0, \beta = 0, \rightarrow \mathbf{q} = (\alpha,0,\gamma)$ – planar monoclinic case

What about the rational part of **q**?

$$\mathbf{q}_r\mathbf{\Gamma}_E - \mathbf{\Gamma}_I\mathbf{q}_r = \mathbf{\Gamma}_M \qquad [\alpha,\beta,\gamma]\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \mp 1[\alpha,\beta,\gamma] = [n_1,n_2,n_3]$$

For $\mathbf{\Gamma}_I = +1 \Rightarrow \alpha = 0 \wedge \alpha = 1/2 \quad \gamma = 0 \wedge \gamma = 1/2$ – axial monoclinic case

For $\mathbf{\Gamma}_I = -1 \Rightarrow \beta = 0 \wedge \beta = 1/2$ – planar monoclinic case

Superspace symmetry

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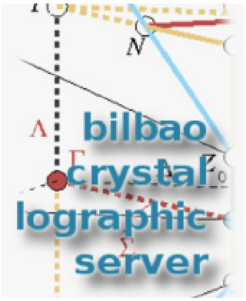

Bilbao Crystallographic Server in forthcoming schools and workshops

News:

- **New Article**
  05/2024: Xu *et al.* "Catalog of topological phonon materials". Science (2024) **384**, 6696

Space-group symmetry	
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

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Superspace symmetry

Bilbao Crystallographic Server → k-vector types and Brillouin zones

The k-vector types of space group *P2/m* (10) [unique axis b]

Unique axis c description is available here

(Table for arithmetic crystal class 2/mP)

P12/m1(P2/m)-C_{2h}^1(10) , P12$_1$/m1(P2$_1$/m)-C_{2h}^2(11),P12/c1(P2/c)-C_{2h}^4(13),P12$_1$/a1(P2$_1$/c)-C_{2h}^5(14)

Reciprocal space group $(P12/m1)^*$, No.10

k-vector description		ITA description			
Label	Coefficients	Wyckoff Position			Coordinates
LD	0,u,0	2	i	2	0,y,0 : 0 < y < 1/2
W	1/2,u,0	2	j	2	1/2,y,0 : 0 < y < 1/2
V	0,u,1/2	2	k	2	0,y,1/2 : 0 < y < 1/2
U	-1/2,u,1/2	2	l	2	-1/2,y,1/2 : 0 < y < 1/2
U~U_1		2	l	2	1/2,y,1/2 : 0 < y < 1/2
F	v,0,u	2	m	m	x,0,z : 0 < z < 1/2; -1/2 < x <= 1/2 U U x,0,0 : 0 < x < 1/2 U U x,0,1/2 : 0 < x < 1/2
G	v,1/2,u	2	n	m	x,1/2,z : 0 < z < 1/2; -1/2 < x <= 1/2 U U x,1/2,0 : 0 < x < 1/2 U U x,1/2,1/2 : 0 < x < 1/2
GP	u,v,w	4	o	1	x,y,z : 0 < z < 1/2; -1/2 < x <= 1/2; 0 < y < 1/2 U U x,y,0 : 0 < x < 1/2; 0 < y < 1/2 U U x,y,1/2 : 0 < x < 1/2; 0 < y < 1/2

parameter relations: x=u, y=v, z=w

Unique axis b description has been calculated using CDML's description.

Superspace symmetry in reciprocal space

Invariance with respect to the superspace symmetry operation:

$$\tilde{\rho}(\boldsymbol{\Gamma}\mathbf{R}+\mathbf{s})=\sum_{\mathbf{H}}F\left(\mathbf{H}\right)\exp\left[-2\pi\left(\boldsymbol{\Gamma}\mathbf{R}+\mathbf{s}\right).\mathbf{H}\right]=\tilde{\rho}(\mathbf{R})\Rightarrow\quad F\left(\mathbf{H}.\boldsymbol{\Gamma}\right)=F\left(\mathbf{H}\right)\exp\left(-2\pi\mathbf{H}\cdot\mathbf{s}\right)$$

The effect of superspace symmetry on the structure factor of a modulated crystal is a direct generalization of the effect of space groups symmetry on periodic 3d crystals.

Laue symmetry: $\left|F\left(\mathbf{H}.\boldsymbol{\Gamma}\right)\right|=\left|F\left(\mathbf{H}\right)\right|\left|\exp\left(-2\pi\mathbf{H}\cdot\mathbf{s}\right)\right|=\left|F\left(\mathbf{H}\right)\right|$

The diffraction pattern has pure rotational symmetry according to the point group of the crystal class of the superspace group.

Superspace symmetry in reciprocal space

While the point symmetry of the pattern is independent of the translational parts of the symmetry operator, non zero-intrinsic parts lead to systematic extinctions of Bragg reflections:

$$\mathbf{H}.\mathbf{\Gamma} = \mathbf{H} \;\Rightarrow F(\mathbf{H}) = F(\mathbf{H})\exp(-2\pi\mathbf{H}\cdot\mathbf{s})$$

Reflection present only if the phase factor is 1, that is $\mathbf{H}\cdot\mathbf{s} = n$

Translation part	Symbol	Reflection condition for
$(0,0,0,0)$	$\binom{m}{1}$	–
$(0,0,0,1/2)$	$\binom{m}{s}$	$m = 2n$
$(1/2,0,0,0)$	$\binom{a}{1}$	$h = 2n$
$(1/2,0,0,1/2)$	$\binom{a}{s}$	$h + m = 2n$
$(0,1/2,0,0)$	$\binom{b}{1}$	$l = 2n$
$(0,1/2,0,1/2)$	$\binom{b}{s}$	$l + m = 2n$
$(1/2,1/2,0,0)$	$\binom{n}{1}$	$h + k = 2n$
$(1/2,1/2,0,1/2)$	$\binom{n}{s}$	$h + k + m = 2n$

Superspace groups

For (3+1) dimensional superspace groups

Originally proposed by P.M.de Wolff, T. Janssen and A. Janner, *Acta Cryst.* (1981). A37, 625-636
Later modified and included into International Tables for Crystallography, volume C.

For (3+1), (3+2) and (3+3) dimensional space groups

H.T. Stokes, B. Campbell and S. van Smaalen, Acta Cryst. A47, 45-55.

Examples:

$$Pmna(0,0,\gamma)s00$$

$$Pmna(0,1/2,\gamma)s00$$

$$Pmna(0,1/2,\gamma_1)s00(0,0,\gamma_2)000$$

$$Pmna(1/2,\beta_1,\gamma_1)q0q(1/2,\bar{\beta}_1,\gamma_1)qq0(0,1/2,\gamma_2)000$$

s_I	1/2	1/3	1/4	1/6
Symbol	*s*	*t*	*q*	*h*

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Superspace symmetry in direct space

Two symmetry-related atoms in the unit cell: (Xe,Xi) $\rightarrow$ (Xe', Xi')

$$\boldsymbol{\Gamma}\mathbf{x} = \left[\begin{array}{c|c} \boldsymbol{\Gamma}_E & 0 \\ \hline \boldsymbol{\Gamma}_M & \boldsymbol{\Gamma}_I \end{array}\right]\left[\begin{array}{c} \mathbf{x}_E \\ \hline \mathbf{x}_I \end{array}\right] + \left[\begin{array}{c} \mathbf{s}_E \\ \hline \mathbf{s}_I \end{array}\right] \quad \Rightarrow \quad \mathbf{x}'_E = \boldsymbol{\Gamma}_E\mathbf{x}_E + \mathbf{s}_E \qquad \mathbf{x}'_I = \boldsymbol{\Gamma}_I\mathbf{x}_I + \boldsymbol{\Gamma}_M\mathbf{x}_E + \mathbf{s}_I$$

The modulation function of a symmetry related atom is derived from the original one.

For a displacement modulation:

$$\mathbf{u}'(\mathbf{x}'_I) = \boldsymbol{\Gamma}_E\mathbf{u}(\mathbf{x}_I) \quad \Rightarrow \quad \mathbf{u}'(\mathbf{x}'_I) = \boldsymbol{\Gamma}_E\mathbf{u}\left[\boldsymbol{\Gamma}_I^{-1}\left(\mathbf{x}'_I - \boldsymbol{\Gamma}_M\mathbf{x}_E - \mathbf{s}_I\right)\right]$$

It simplifies for (3+1)d superspace!

Superspace symmetry in direct space

For the (3+1)d case (general position):

$$\Gamma = \left(\left[\begin{array}{c|c} \mathbf{R} & \mathbf{0} \\ \hline \mathbf{m}^T & \varepsilon \end{array} \right], \left[\begin{array}{c} \mathbf{s} \\ \hline \delta \end{array} \right] \right)$$

where $\varepsilon=\pm1$ and $\varepsilon^{-1}=\varepsilon$;
m: rational part of **q**

Modulation functions of a symmetry related atom:

Occupational modulation: $o(x_4) = o_0 + \sum_n (o_{ns} \sin 2\pi n x_4 + o_{nc} \cos 2\pi n x_4)$ $\quad o'[x_4] = o[\varepsilon(x_4 - \mathbf{m.r} - \delta)]$

Position modulation: $\mathbf{r}(x_4) = \mathbf{r}_0 + \mathbf{u} = \mathbf{r}_0 + \sum_n (\mathbf{U}_{ns} \sin 2\pi n x_4 + \mathbf{U}_{nc} \cos 2\pi n x_4)$ $\quad \mathbf{r}'[x_4] = \mathbf{R}\mathbf{r}_0 + \mathbf{R}\mathbf{u}[\varepsilon(x_4 - \mathbf{m.r} - \delta)]$

Superspace symmetry in direct space

For the (3+1)d case (special positions):

$$\boldsymbol{\Gamma} = \left(\left[\begin{array}{c|c} \mathbf{R} & \mathbf{0} \\ \hline \mathbf{m}^T & \varepsilon \end{array} \right], \left[\begin{array}{c} \mathbf{s} \\ \hline \delta \end{array} \right] \right)$$

where ε=±1

Modulation functions of a symmetry related atom:

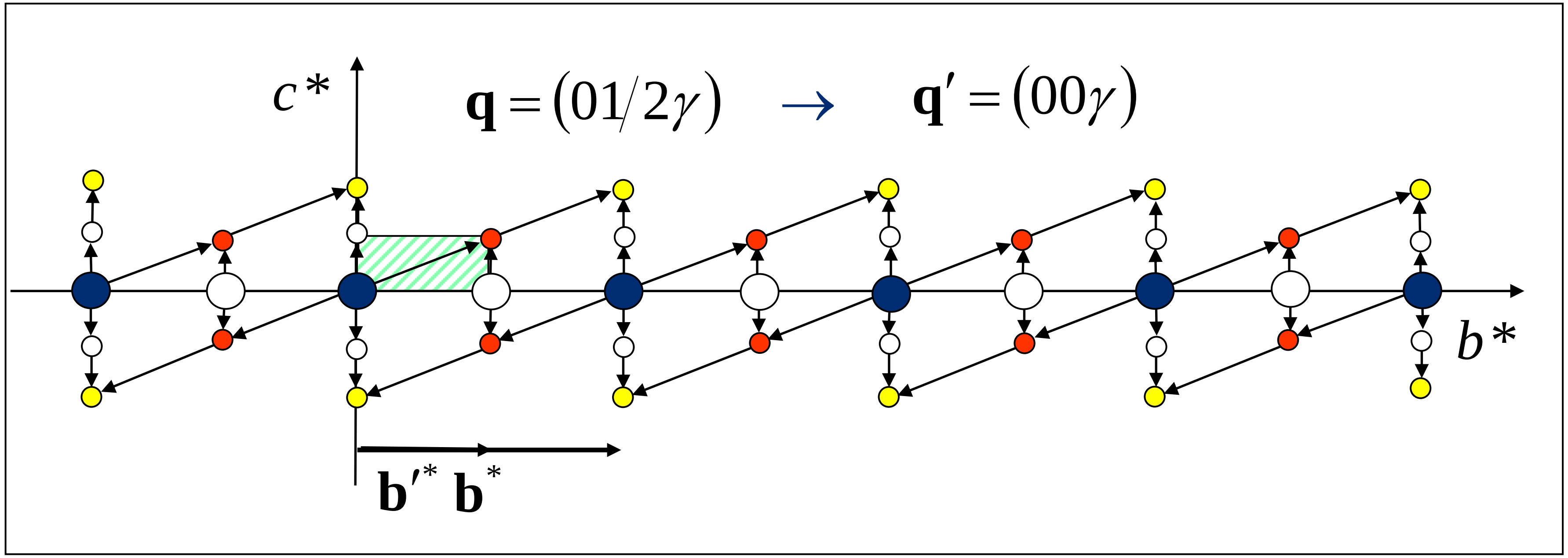
Occupational modulation: $o(x_4) = o_0 + \sum_n (o_{ns} \sin 2\pi n x_4 + o_{nc} \cos 2\pi n x_4)$ $o[x_4] = o[\varepsilon(x_4 - \mathbf{m}.\mathbf{r} - \delta)]$

Position modulation: $\mathbf{u}(x_4) = \sum_n (\mathbf{U}_{ns} \sin 2\pi n x_4 + \mathbf{U}_{nc} \cos 2\pi n x_4)$ $\mathbf{u}[x_4] = \mathbf{R}\mathbf{u}[\varepsilon(x_4 - \mathbf{m}.\mathbf{r} - \delta)]$

Superspace symmetry

Example : $Pmna(01/2\gamma)s00$

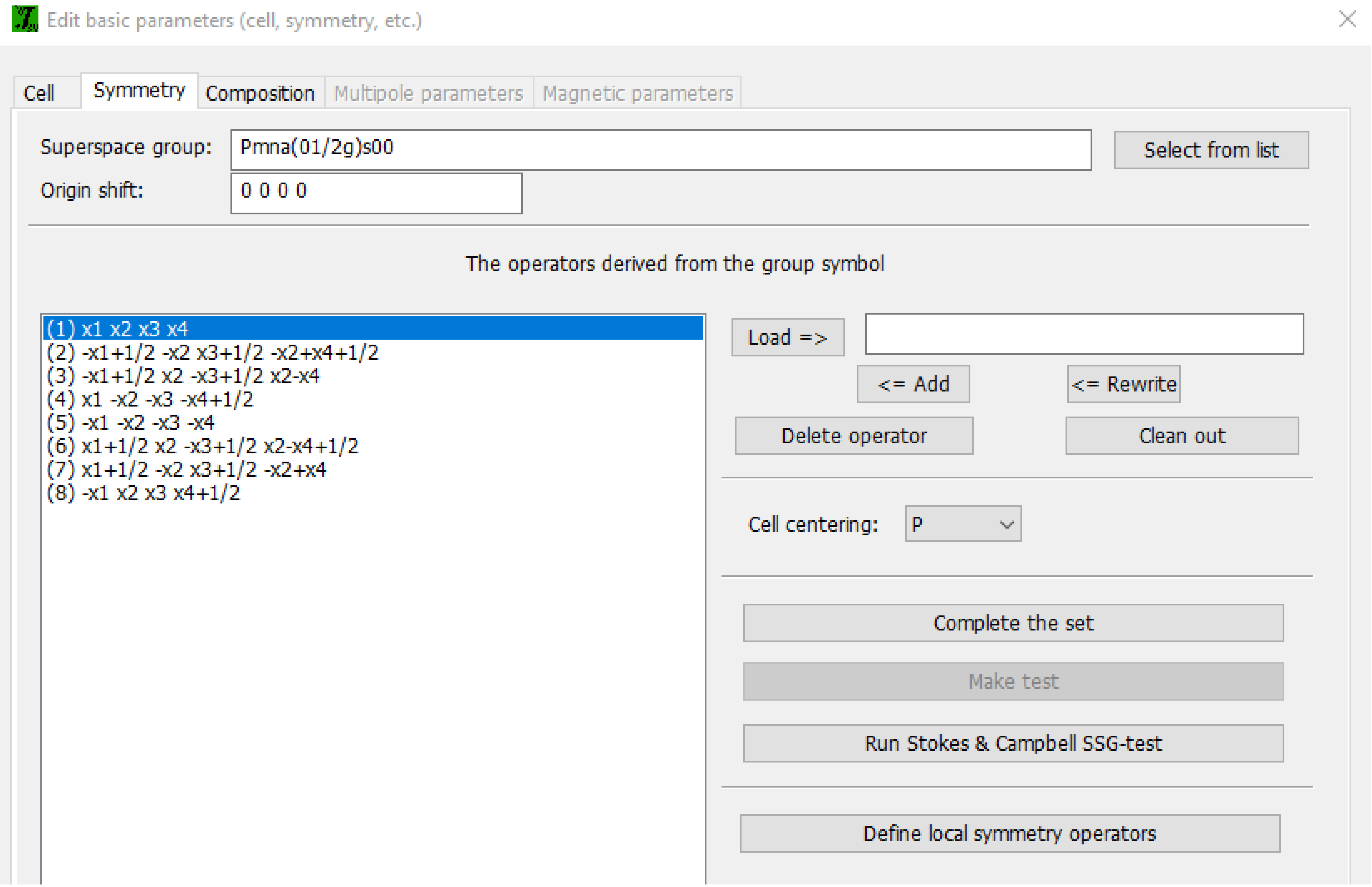
The rational part of the modulation vector represents an additional centring. It is much more convenient to use the supercentred cell instead of the explicit use of the rational part of the modulation vector.



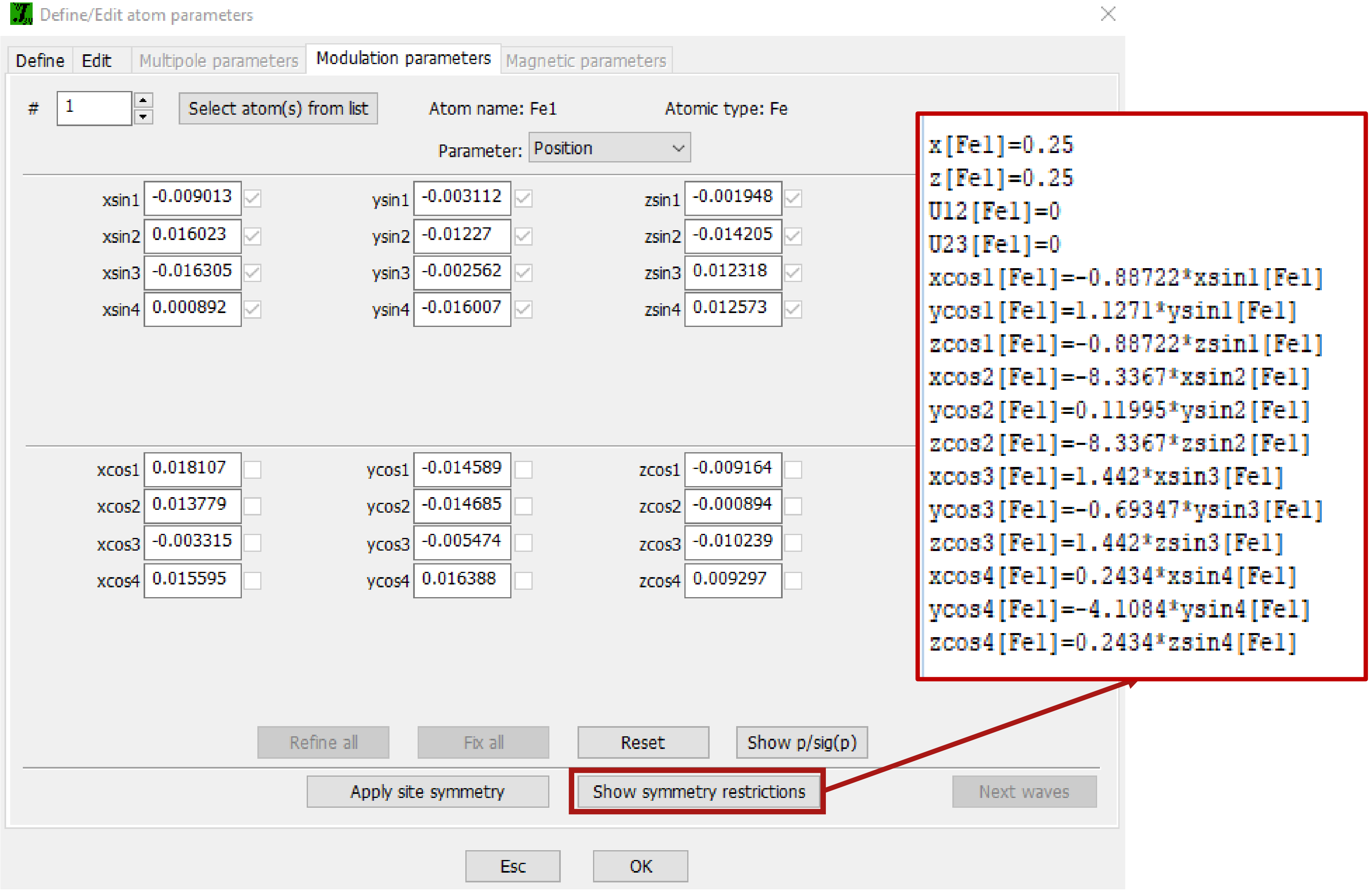
$$\mathbf{u}[x_4] = \mathbf{Ru}[\varepsilon(x_4 - \mathbf{m.r} - \delta)]$$

$$\mathbf{u}[x_4] = \mathbf{Ru}[\varepsilon(x_4 - \delta)]$$

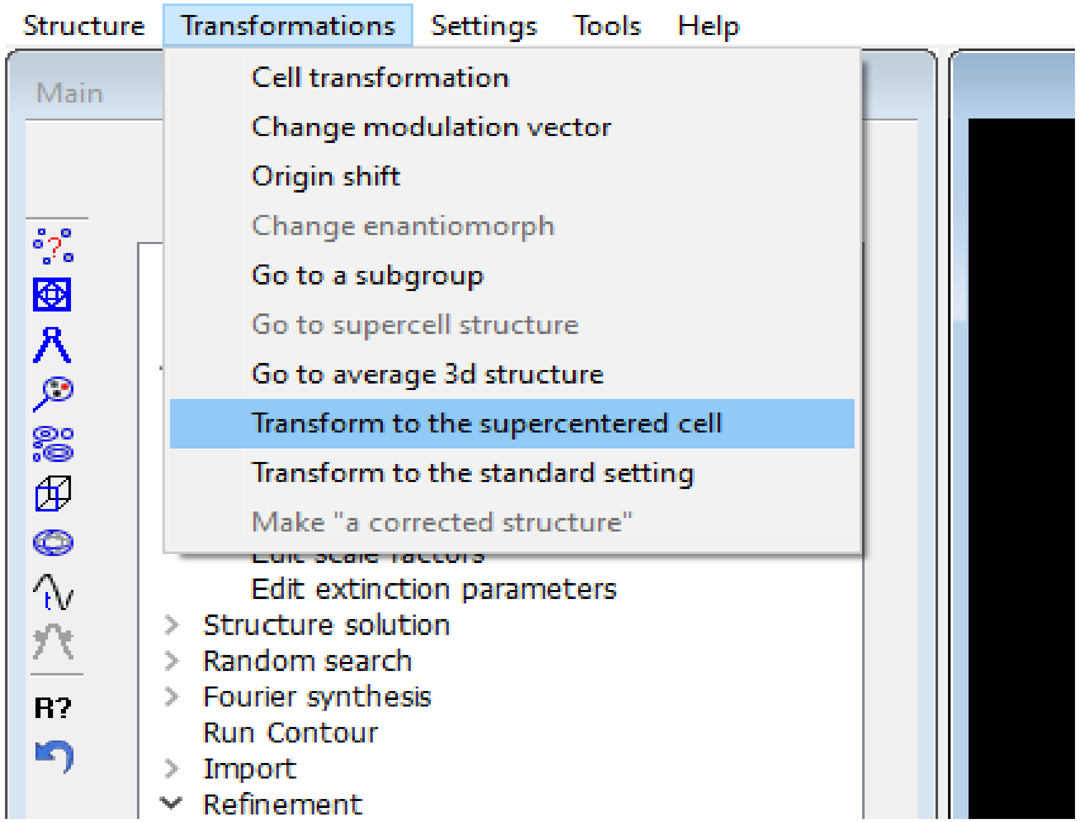
Superspace symmetry in Jana2020



Superspace symmetry in Jana2020



Superspace symmetry in Jana2020



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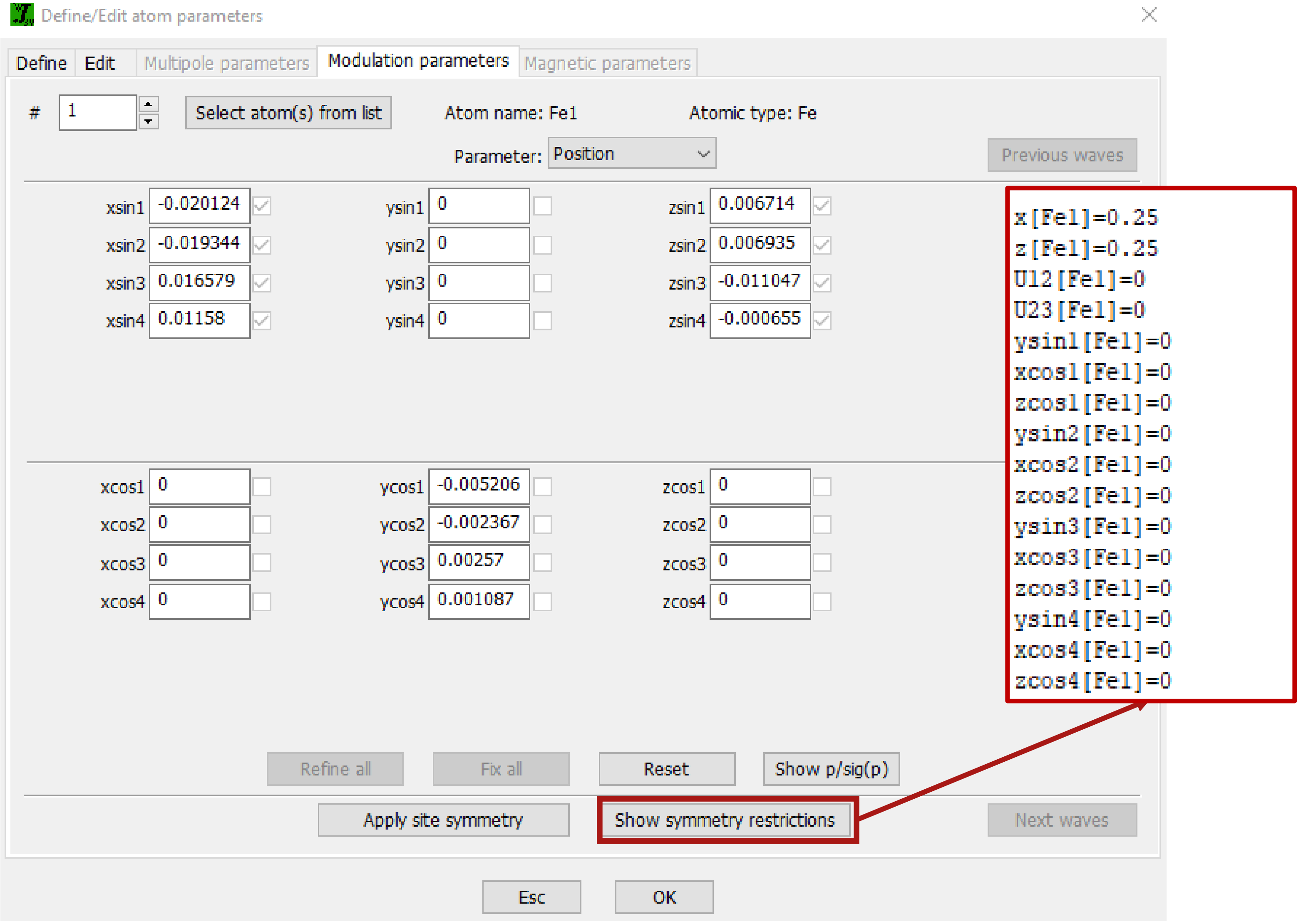
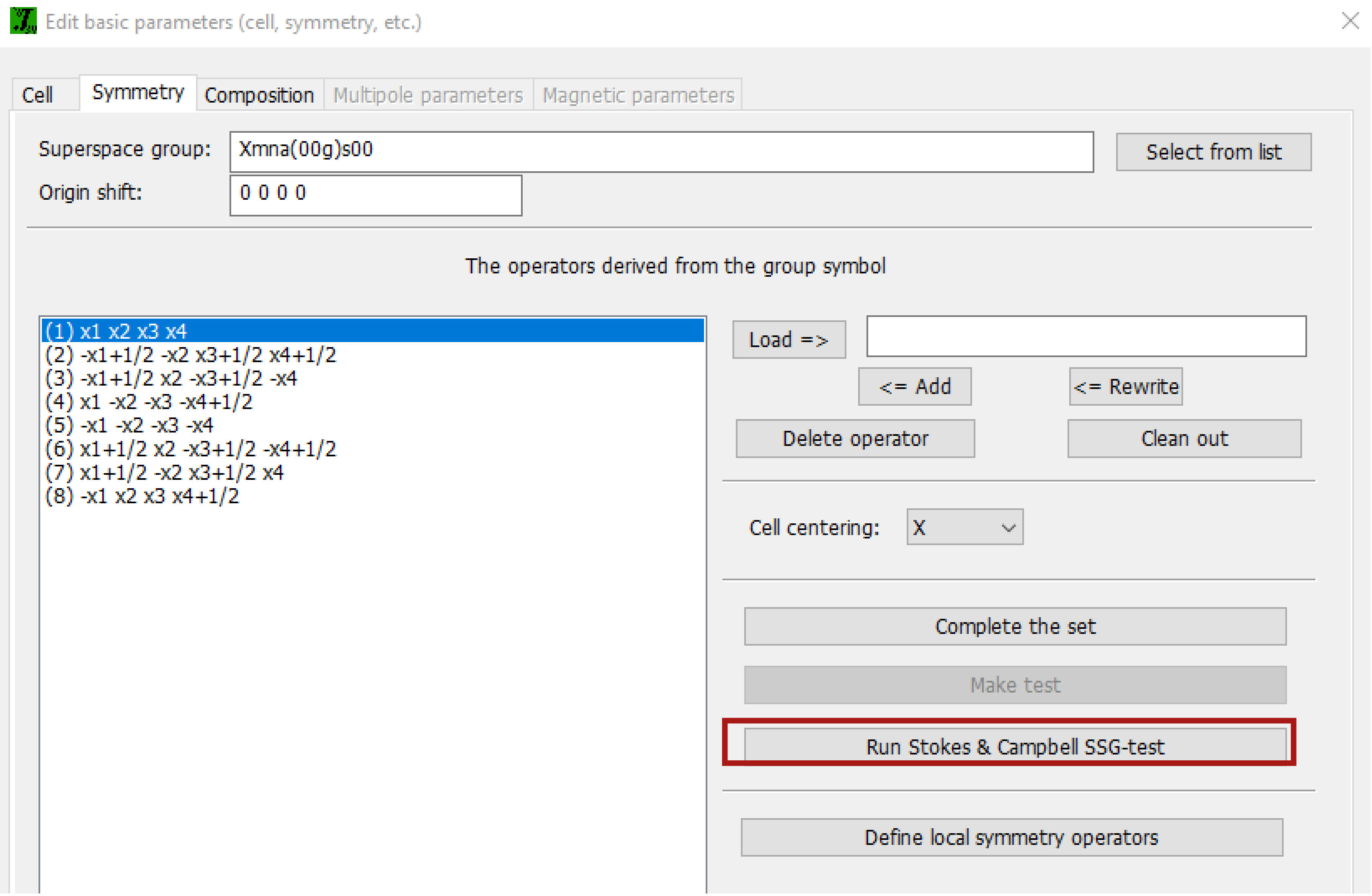
Superspace symmetry in Jana2020



Superspace symmetry in Jana2020



Superspace symmetry in Jana2020

Input setting

Centering
none
Operators
(-x+1/2,-y,z+1/2,-y+t+1/2); (-x+1/2,y,-z+1/2,y-t); (x,-y,-z,-t+1/2); (-x,-y,-z,-t); (x+1/2,y,-z+1/2,y-t+1/2); (x+1/2,-y,z+1/2,-y+t); (-x,y,z,t+1/2); (x,y,z,t)

Standard settings

Superspace group: 53.1.10.10 Pmna(0,1/2,g)s00 [Y:1.369]
Bravais class: 1.10 Pmmm(0,1/2,g) [JJdW:1.10]
Transformation to supercentered setting: As1=as1, As2=2as2+as4, As3=as3, As4=as4

BASIC SPACE GROUP SETTING
Modulation vectors: q1=(0,1/2,g)
Centering: (0,0,0,0)
Non-lattice generators: (-x,y,z,t+1/2); (x+1/2,-y,z+1/2,-y+t); (x+1/2,y,-z+1/2,y-t+1/2)
Non-lattice operators: (x,y,z,t); (x,-y,-z,-t+1/2); (-x+1/2,y,-z+1/2,y-t); (-x+1/2,-y,z+1/2,-y+t+1/2); (-x,-y,-z,-t); (-x,y,z,t+1/2); (x+1/2,-y,z+1/2,-y+t); (x+1/2,y,-z+1/2,y-t+1/2)

SUPERCENTERED SETTING
Modulation vectors: Q1=(0,0,G), where G=g
Centering: (0,0,0,0); (0,1/2,0,1/2)
Non-lattice generators: (-X,Y,Z,T+1/2); (X+1/2,-Y,Z+1/2,T); (X+1/2,Y,-Z+1/2,-T+1/2)
Non-lattice operators: (X,Y,Z,T); (X,-Y,-Z,-T+1/2); (-X+1/2,Y,-Z+1/2,-T); (-X+1/2,-Y,Z+1/2,T+1/2); (-X,-Y,-Z,-T); (-X,Y,Z,T+1/2); (X+1/2,-Y,Z+1/2,T); (X+1/2,Y,-Z+1/2,-T+1/2)
Reflection conditions: HKLM:K+M=2n; H0LM:H+L=2n; 0KLM:M=2n; HK00:H=2n

Thank you!

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