$Z_2 x Z_2$ magnetic domains and magnetic moment disproportionation in the spin-orbit Mott insulator Sr_2IrO_4

B. J. Kim
Pohang University of Science and Technology (POSTECH)
Center for Artificial Low-Dimensional Electronic System,
Institute for Basic Science (IBS)

IBS-PCS International Workshop on Frustrated Magnetism
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Outline

- A short introduction to Sr_2IrO_4

- $Z_2 x Z_2$ magnetic domain structure

J. W. Kim (APS)

Sunwook Park (POSTECH)

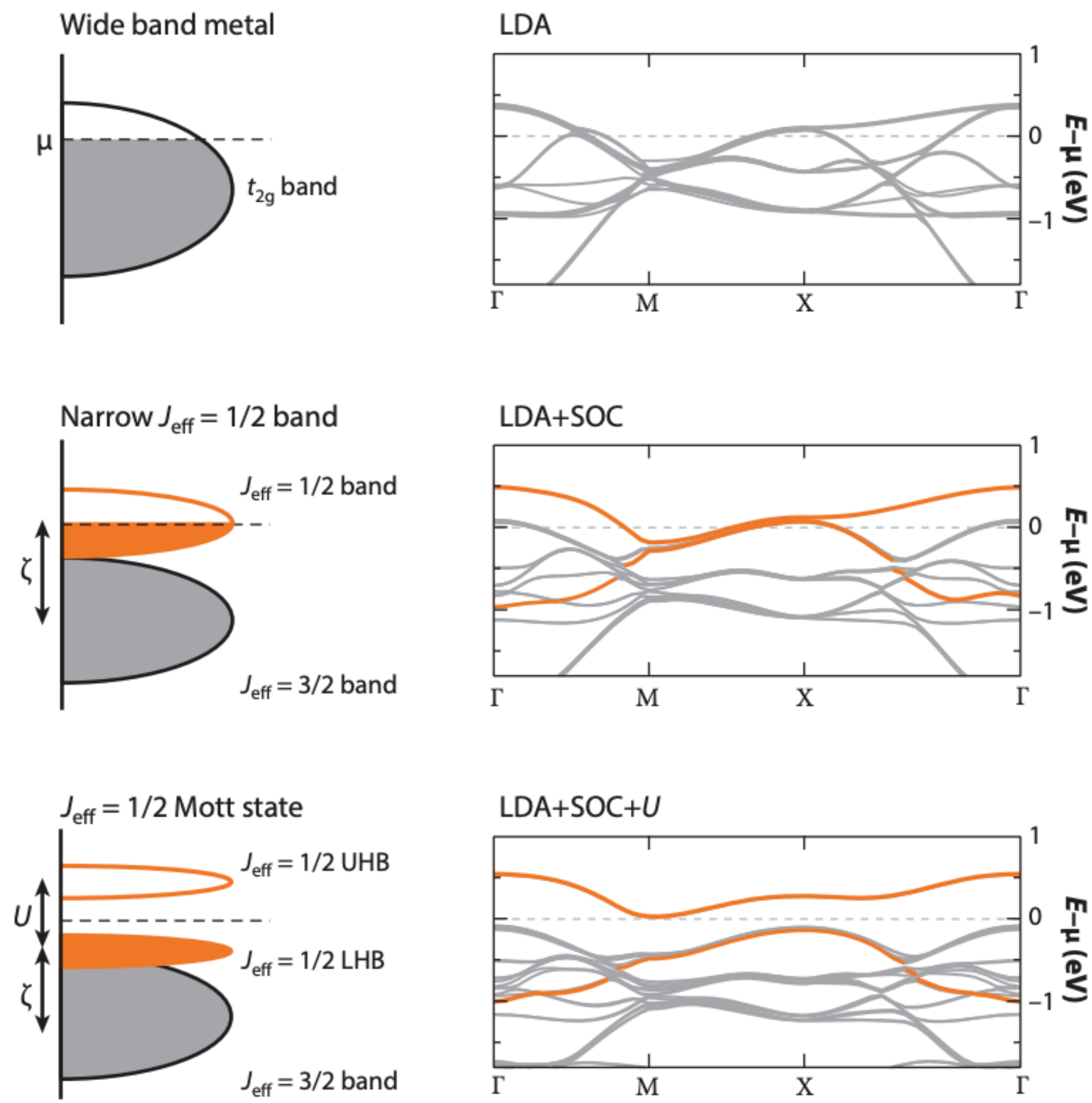
- New magnetic structure from DFT

Alaska Subedi (CNRS)

- Representation analysis

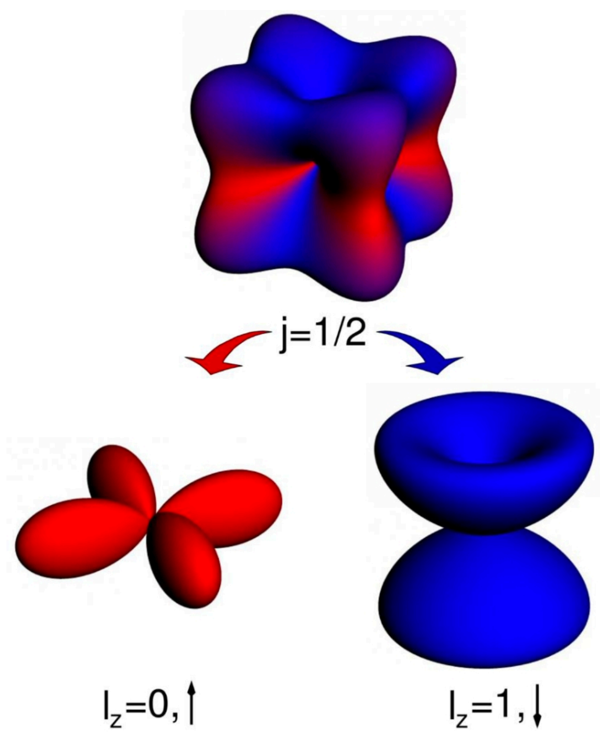
Hoon Kim (POSTECH)

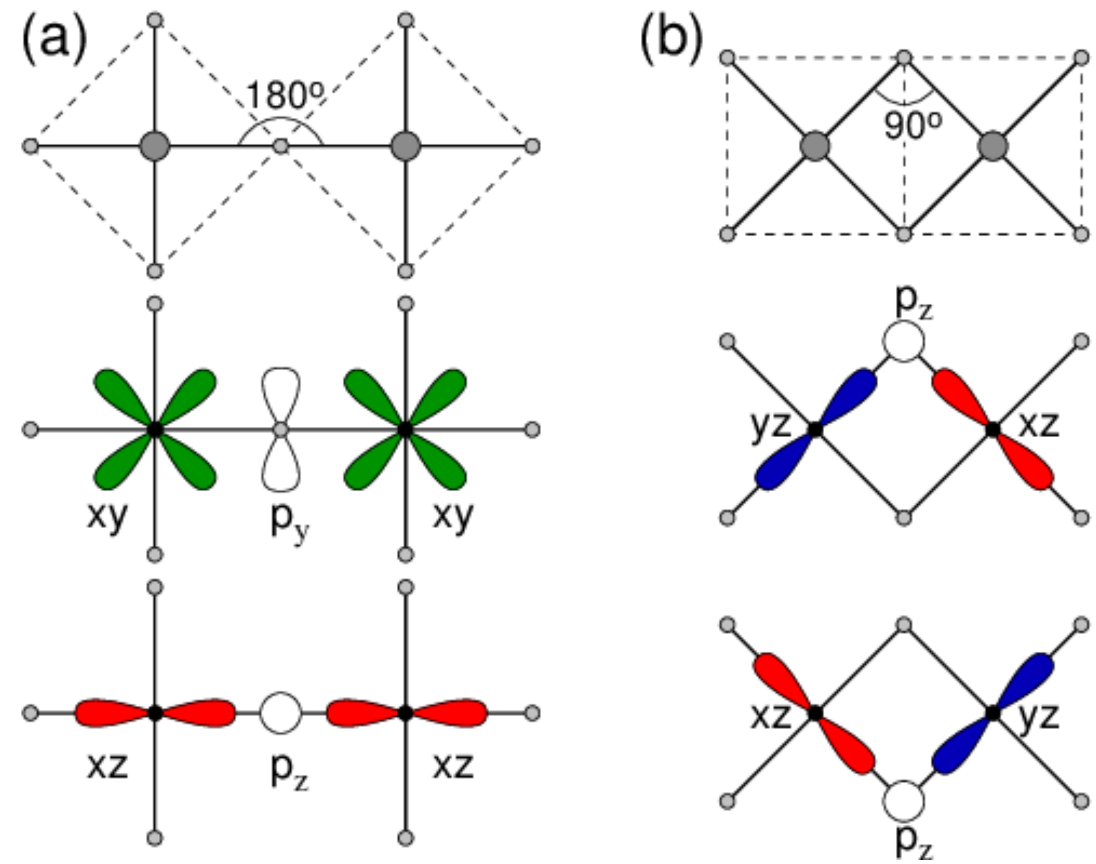
Sr_2IrO_4: Archetypal Spin-Orbit Mott insulator



J. Bertinshaw, Y.-K. Kim, G. Khaliullin, BJK Annu. Rev. Condens. Matter Phys. 2019

J_{eff}=1/2 Kramers doublet





$$|\tilde{\uparrow}\rangle = +\sin\theta\,|0,\uparrow\rangle - \cos\theta\,|+1,\downarrow\rangle,$$

$$|\tilde{\downarrow}\rangle = -\sin\theta\,|0,\downarrow\rangle + \cos\theta\,|-1,\uparrow\rangle.$$

Heisenberg

Kitaev

$|L_z = 0\rangle = |xy\rangle$ and $|Lz = \pm 1\rangle = \mp\frac{1}{\sqrt{2}}(|yz\rangle \pm i|zx\rangle)$,

G. Jackeli and G. Khaliullin, PRL 2009

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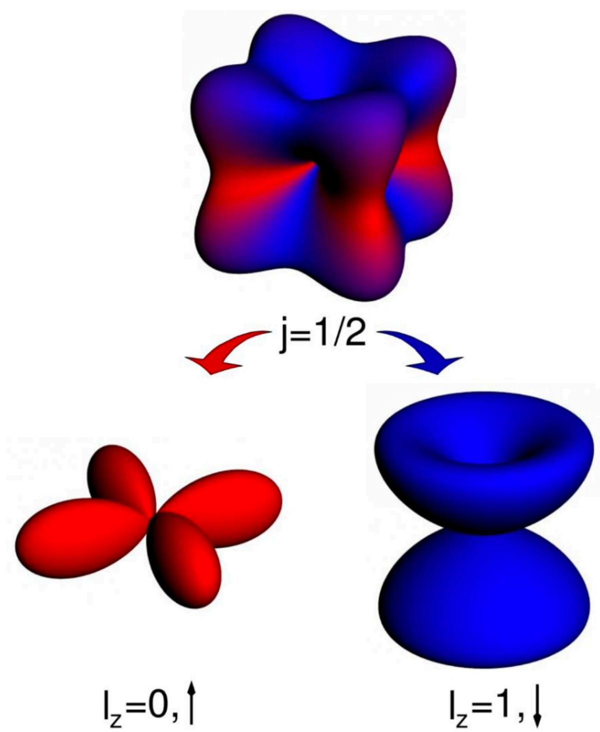

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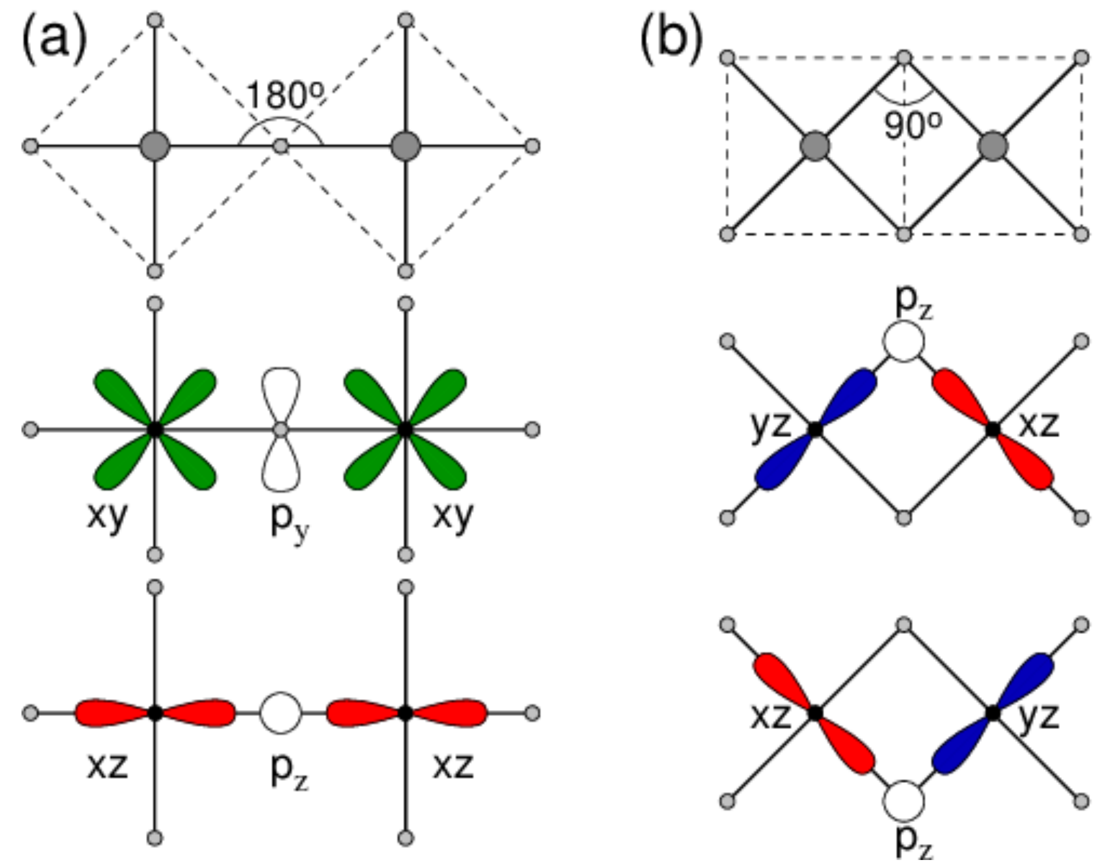
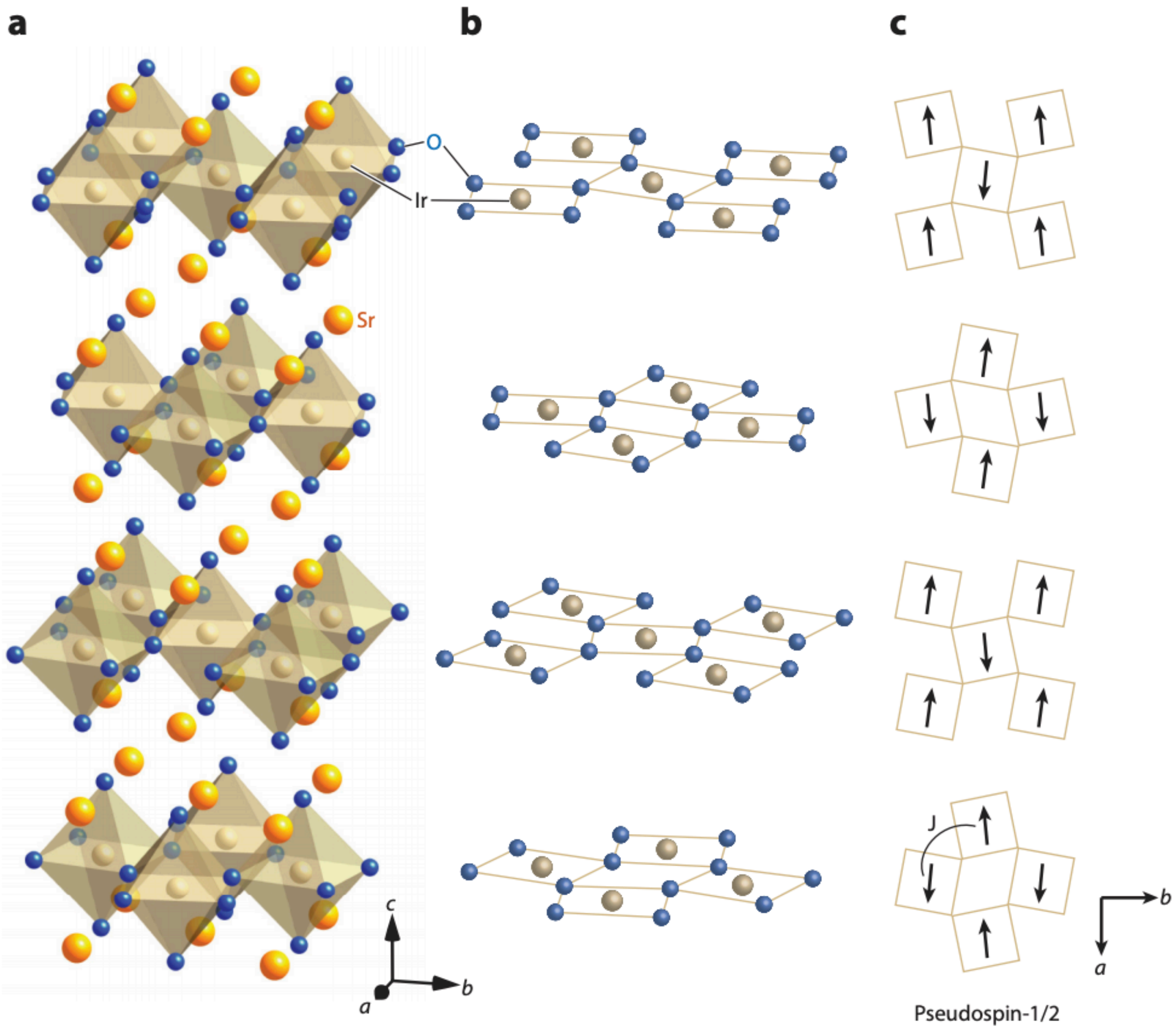


Heisenberg Kitaev

New feature of pseudospins: a propensity to spontaneously disproportionate

➡ possible new instabilities and new magnetic phases!

Sr_2IrO_4: Archetypal Spin-Orbit Mott insulator



- A rare realization of spin-1/2 moments on a square lattice
- Neel order

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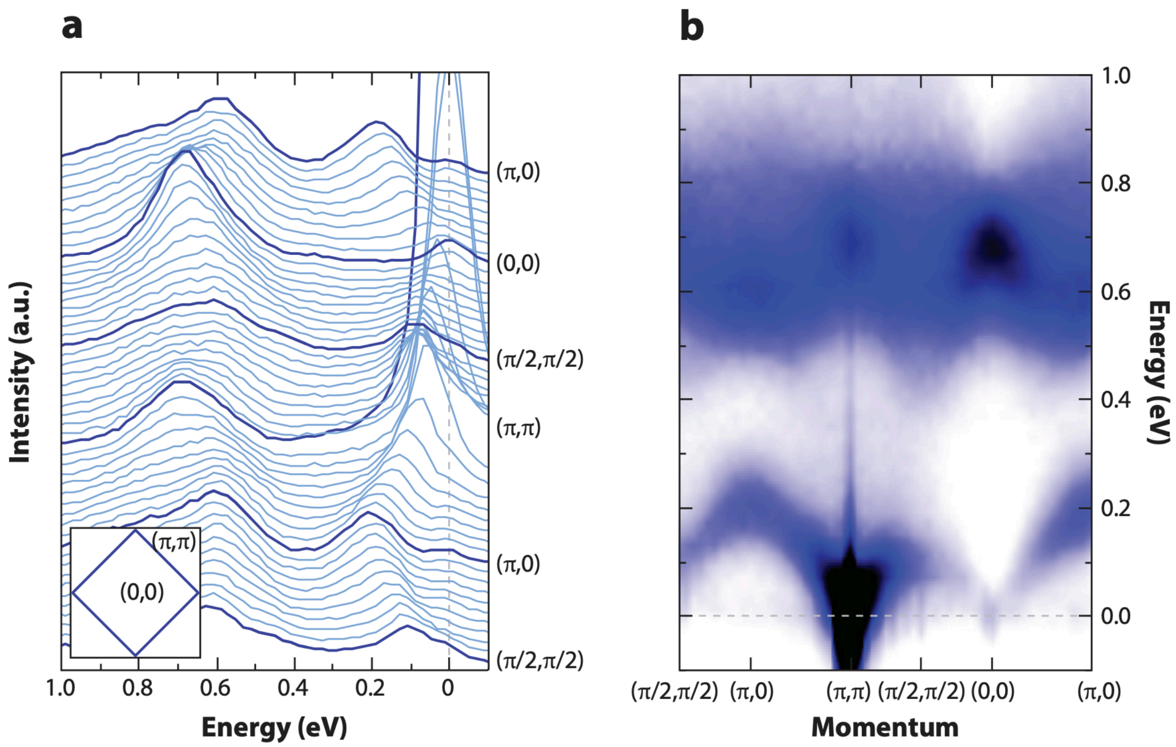

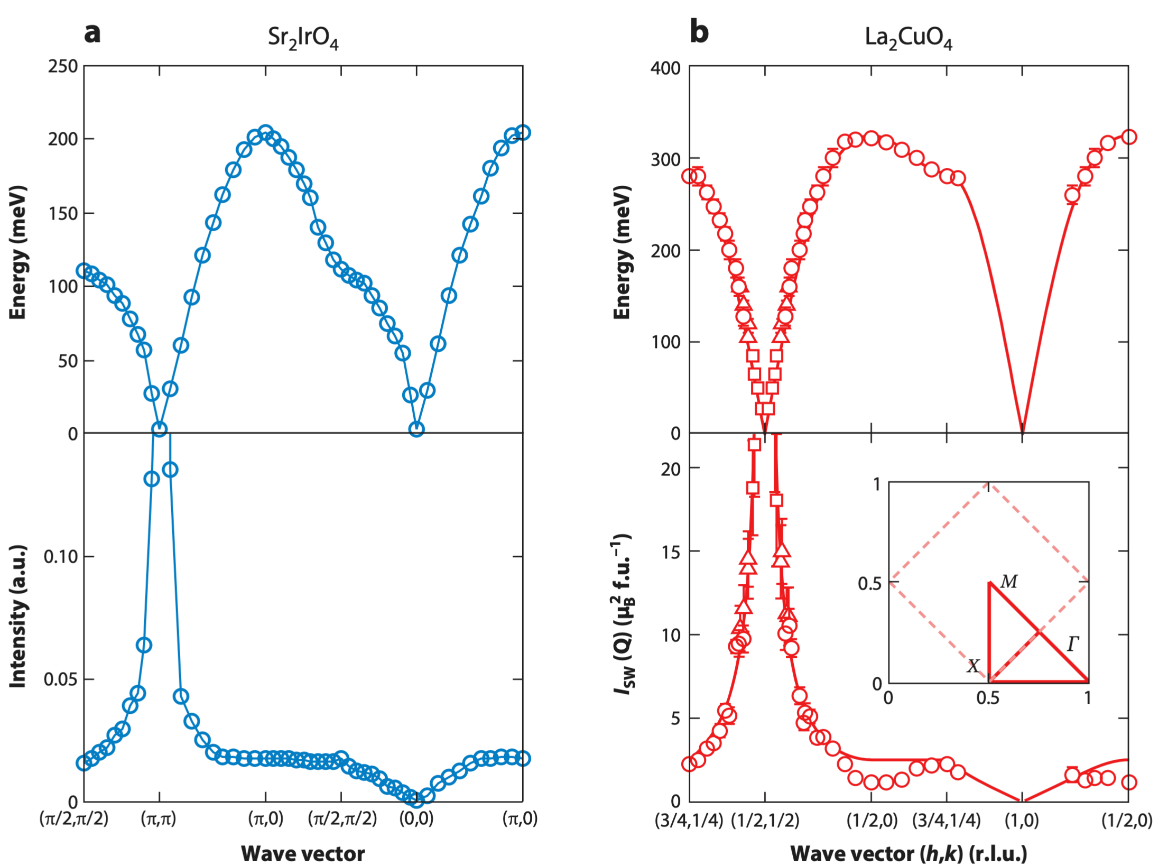

- A rare realization of spin-1/2 moments on a square lattice
- Neel order
- Heisenberg AF

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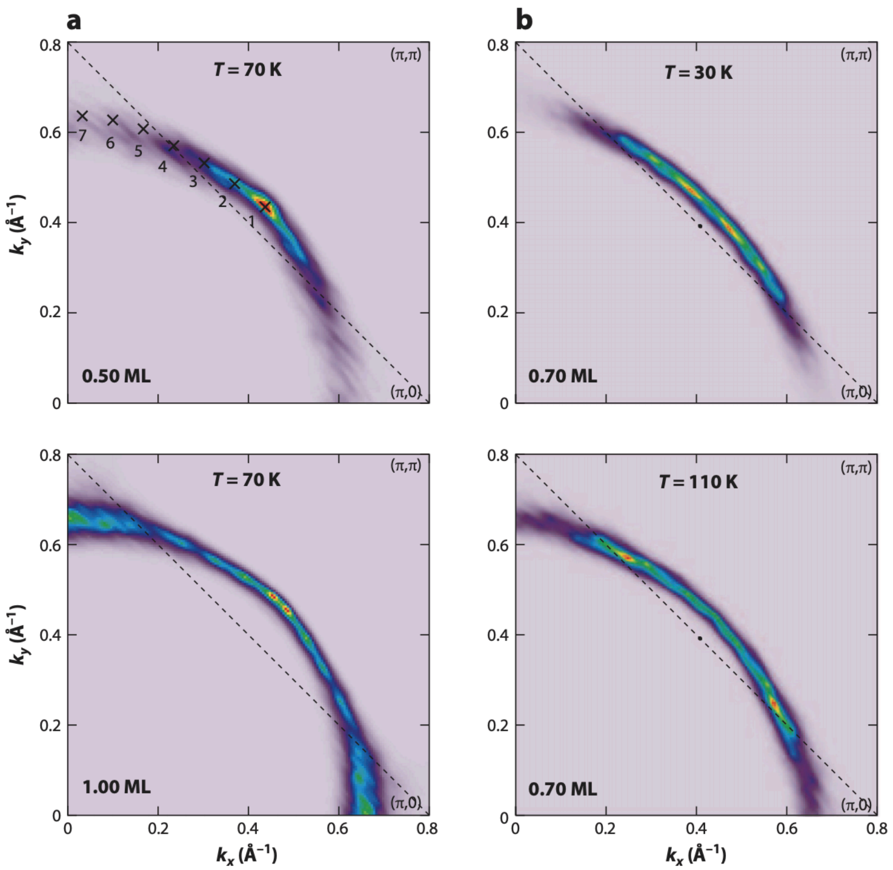
Sr_2IrO_4: Archetypal Spin-Orbit Mott insulator

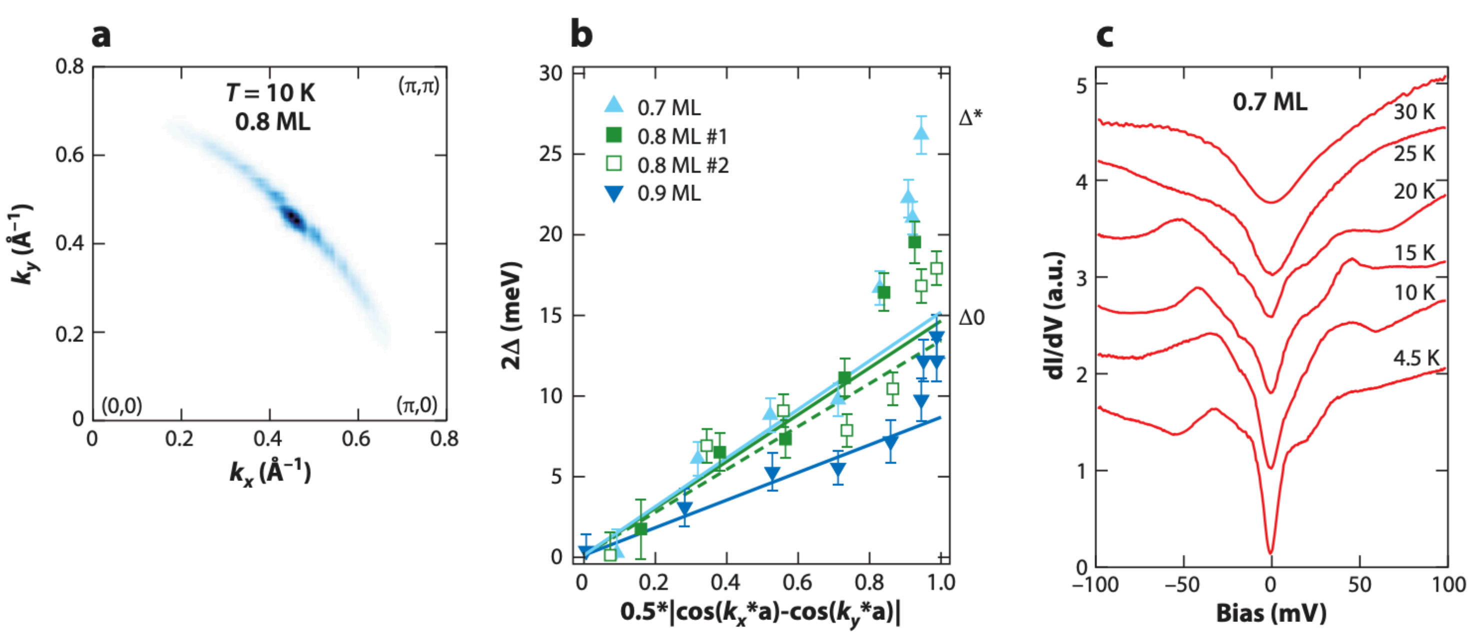
low doping

high doping



low temperature

high temperature



- A rare realization of spin-1/2 moments on a square lattice
- Neel order
- Heisenberg AF
- Reproduces a large part of cuprate phenomenology
- Superconductivity remains to be seen.

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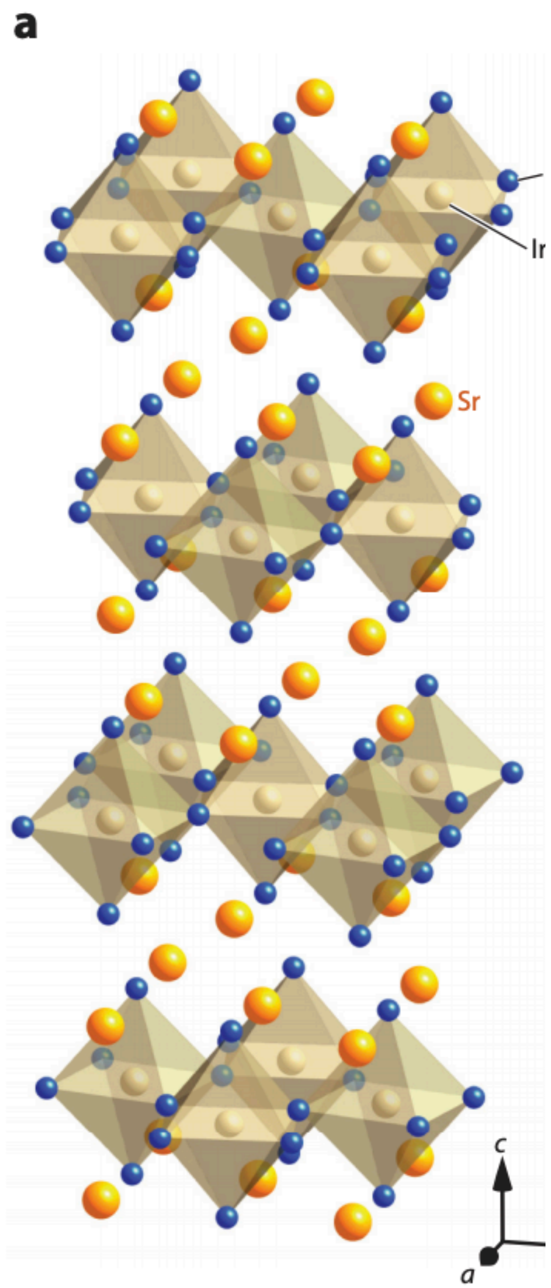
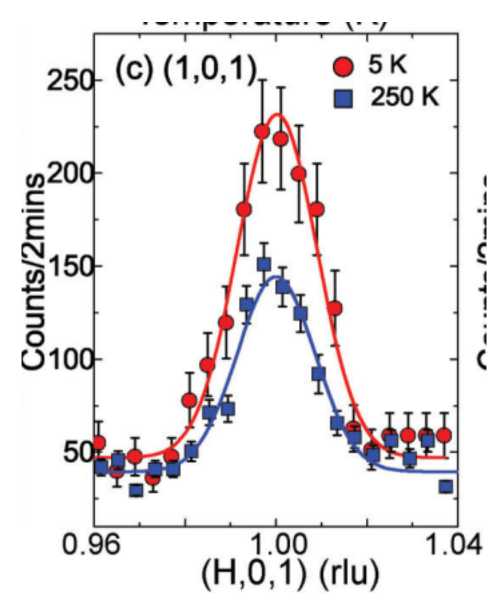
Sr_2IrO_4: Archetypal Spin-Orbit Mott insulator



- Lattice structure still not fully known

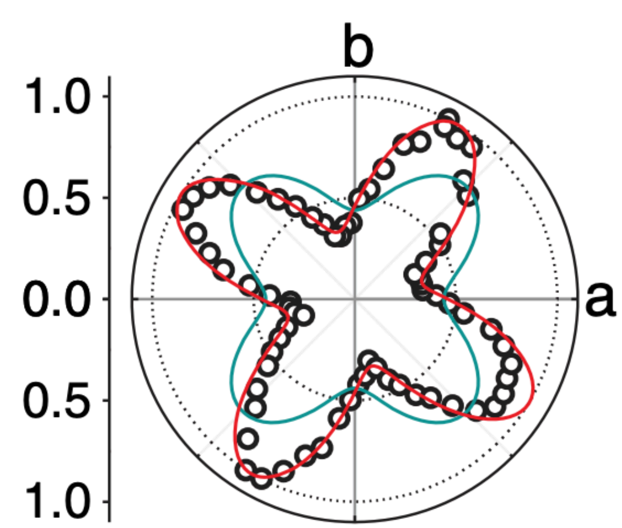
- Long believed to be $I4_1/acd$, but recent studies suggest $14_1/a$
  - Forbidden peaks in ND



F. Ye et al. PRB 2013

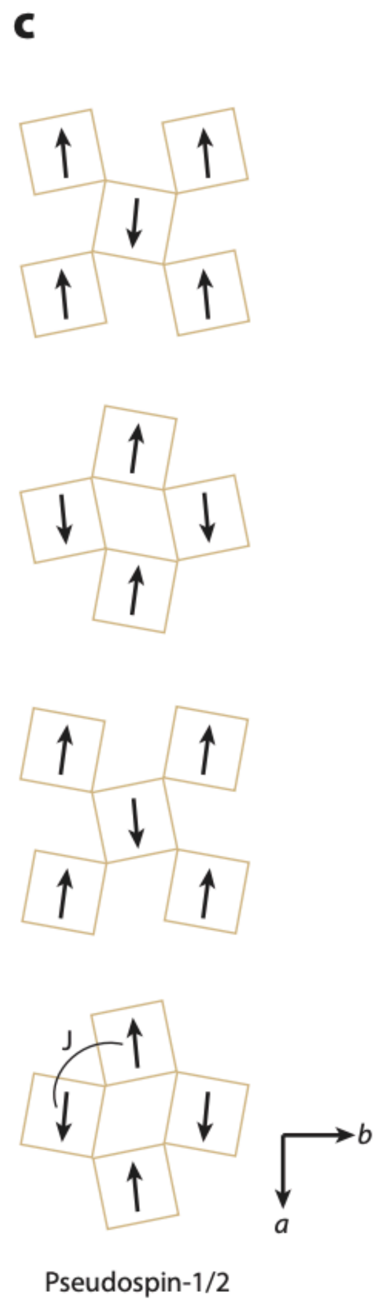
  - SHG indicate 4/m point group

-



D. H. Torchinsky et al. PRL 2015

Sr_2IrO_4: Archetypal Spin-Orbit Mott insulator



- Is the magnetic structure correct?
- In hindsight, the currently known magnetic structure is allowed but unlikely to be the ground state in $I4_1/a$.
- But is the deviation large enough to detect?

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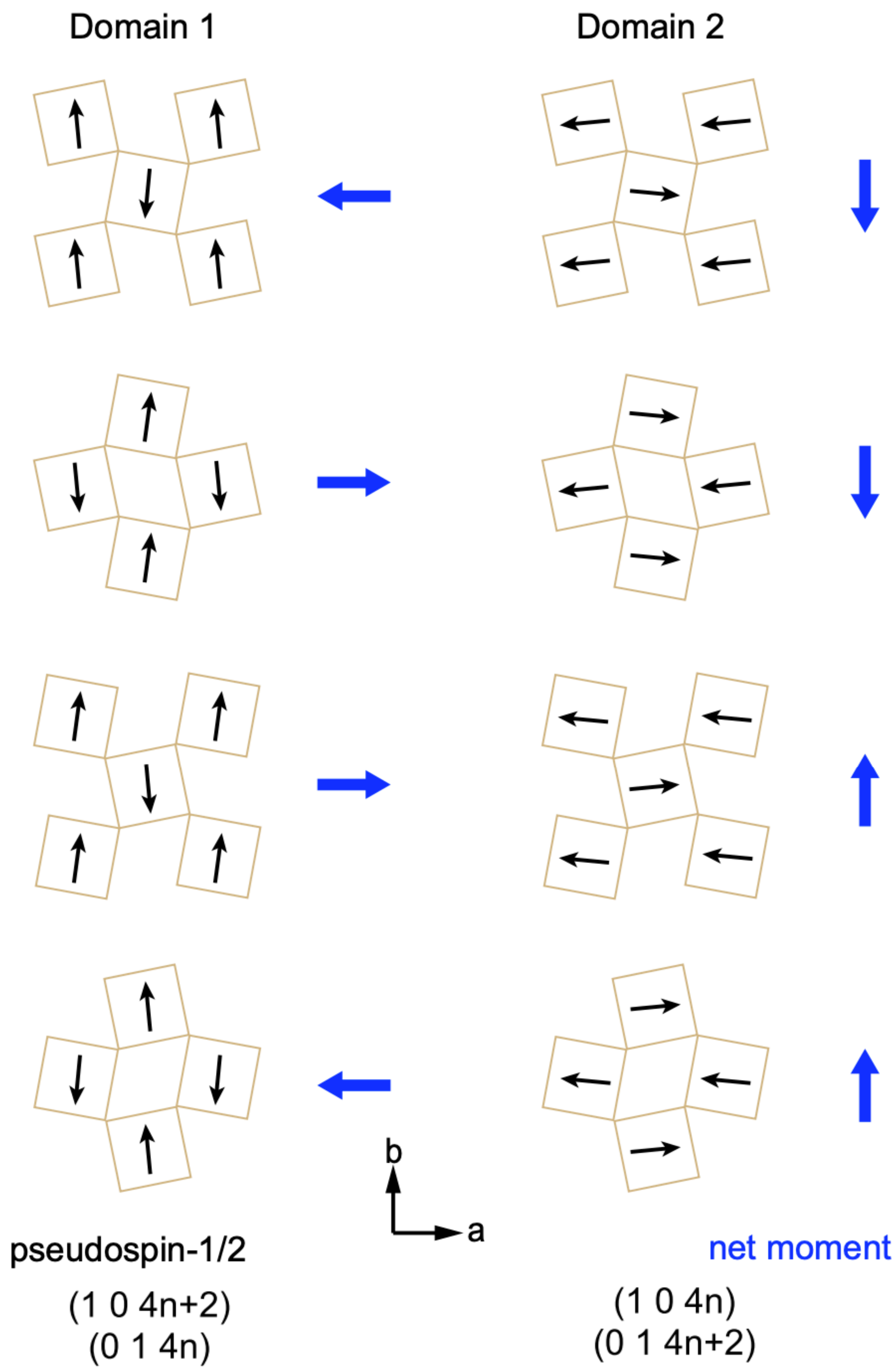
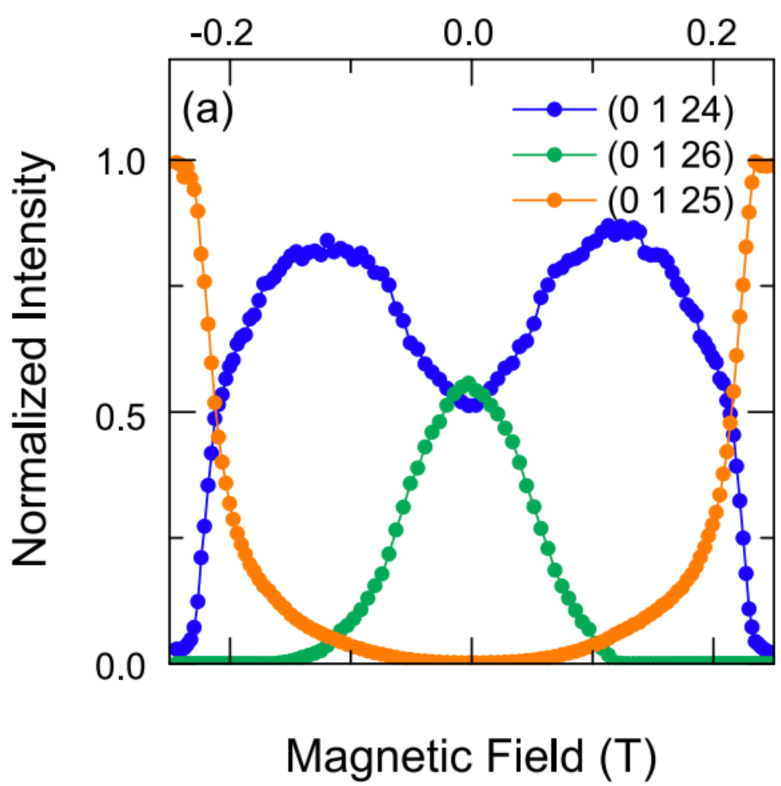
Magnetic domains



- generated by successive 4_1 screw operations
- domain 3 & 4 are just A$\longleftrightarrow$B sublattice switching of domain 1 & 2
- different domains have different stacking patterns
- domain 1: (1 0 4n+2) & (0 1 4n)
  domain 2: (1 0 4n) & (0 1 4n+2)

Magnetic domains

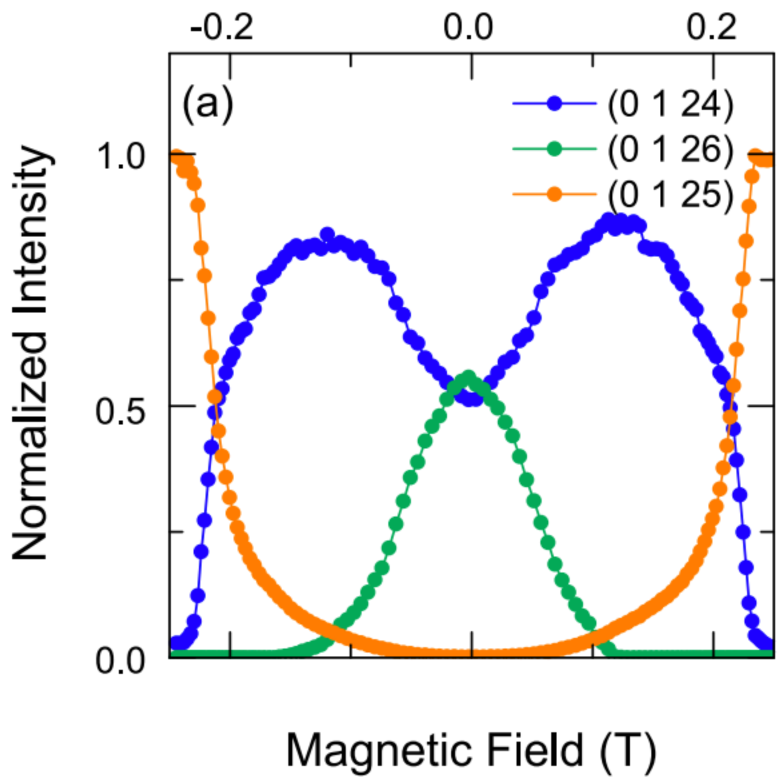


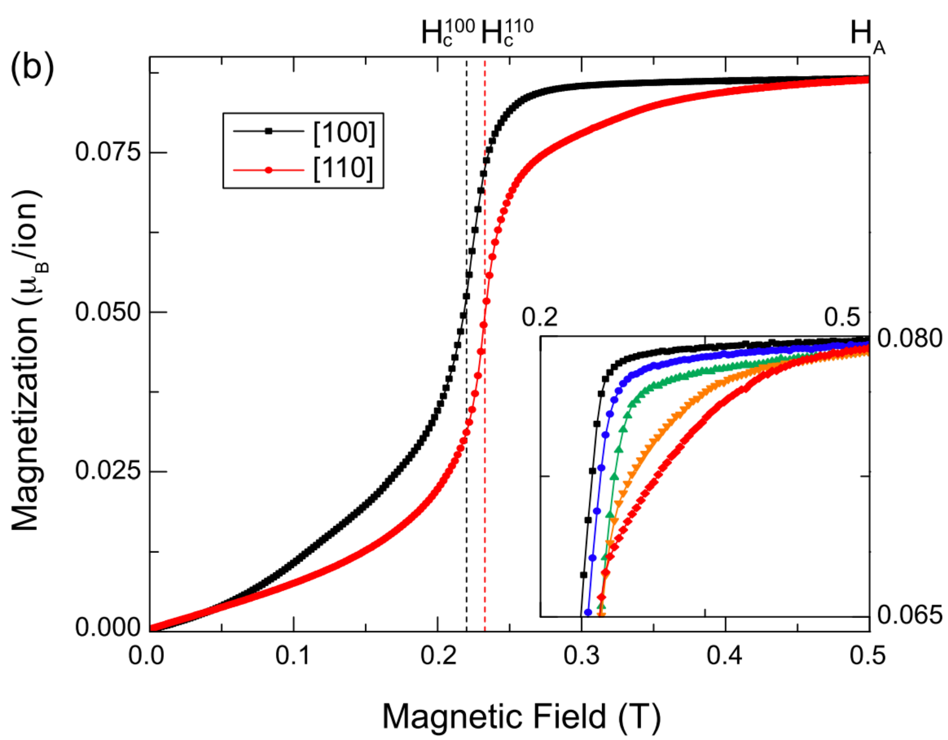
Magnetic domains fully polarized by ~0.1T applied field

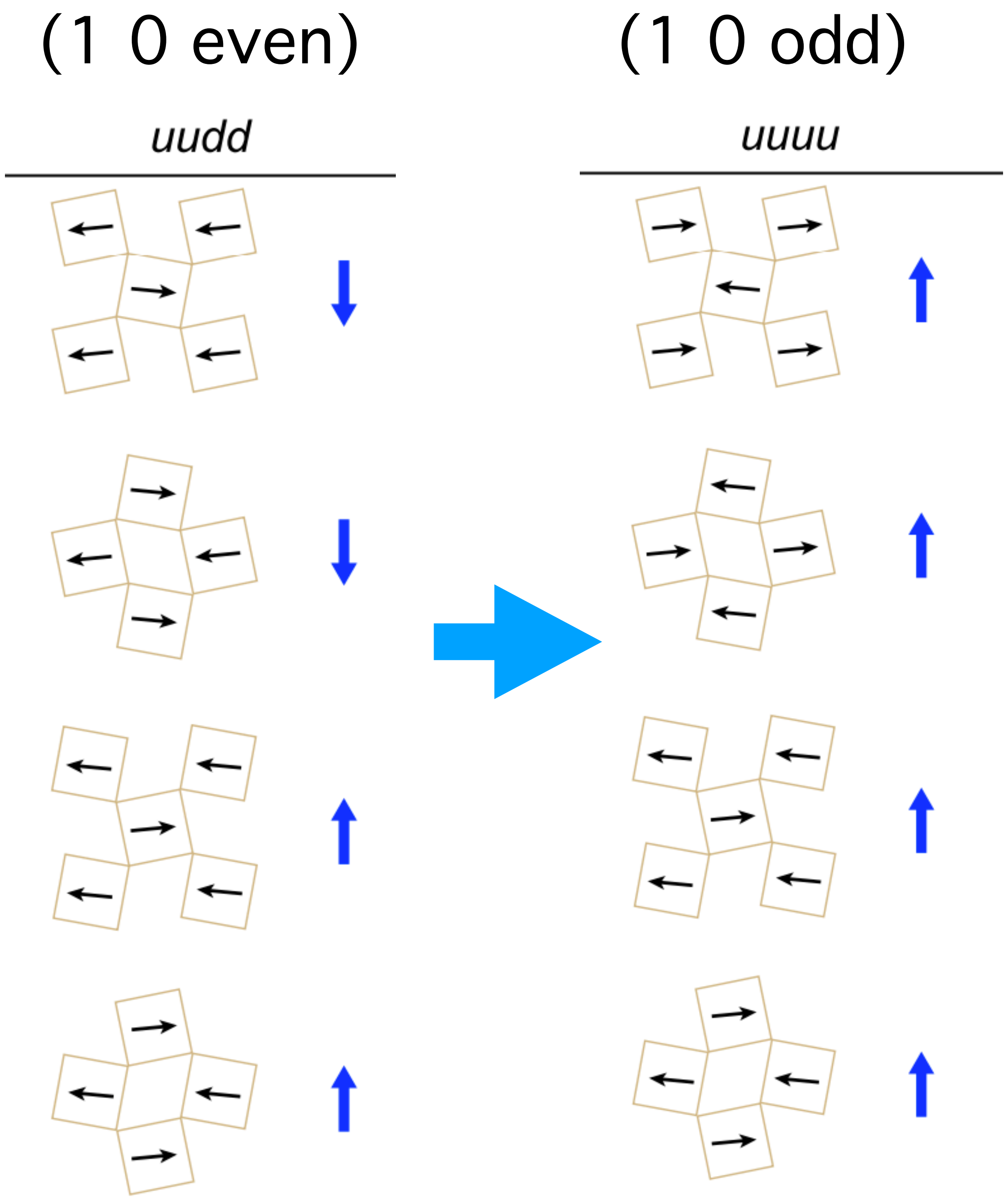
- generated by successive 4_1 screw operations
- domain 3 & 4 are just A$\leftrightarrow$B sublattice switching of domain 1 & 2
- different domains have different stacking patterns
- domains can be easily imaged by going to different q's

J. Porras, BJK et al. PRB 2019

Magnetic domains



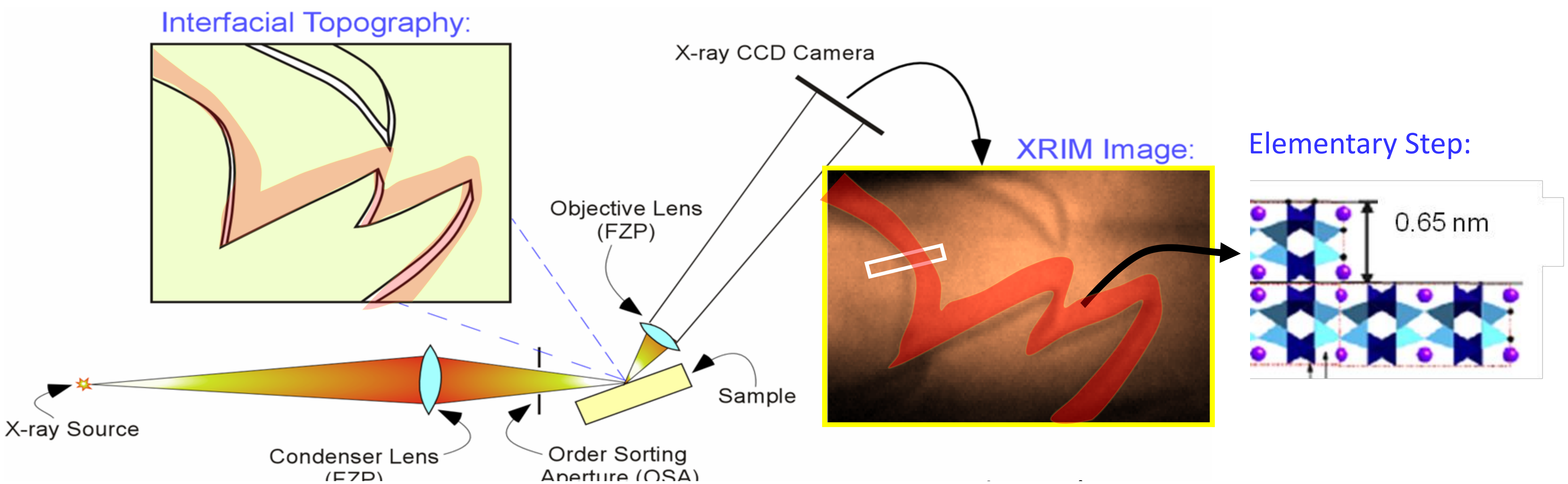




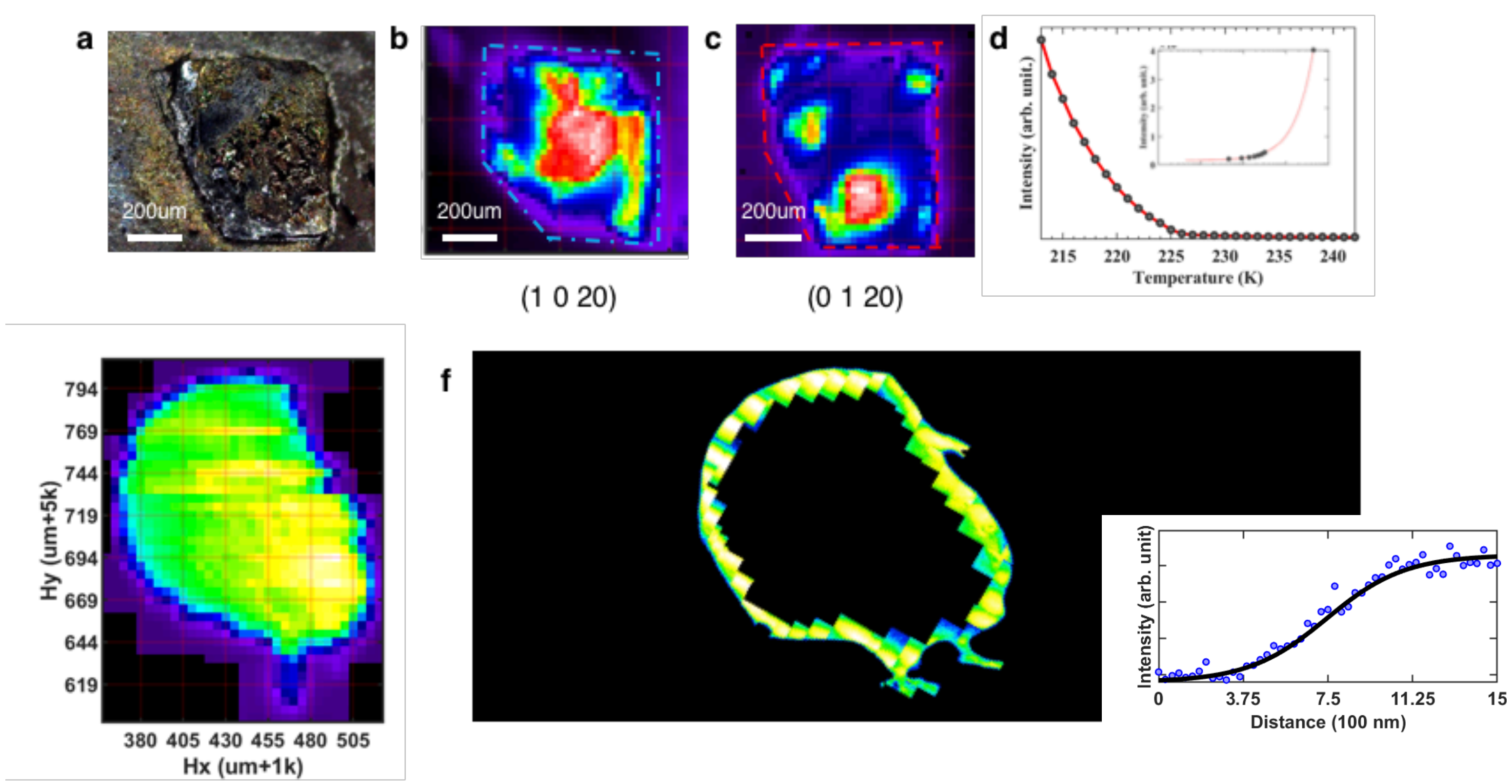
Metamagnetic transition at Hc~0.2 T

J. Porras, BJK et al. PRB 2019

Magnetic Domain Imaging using X-ray Reflection Interference Microscopy (XRIM)



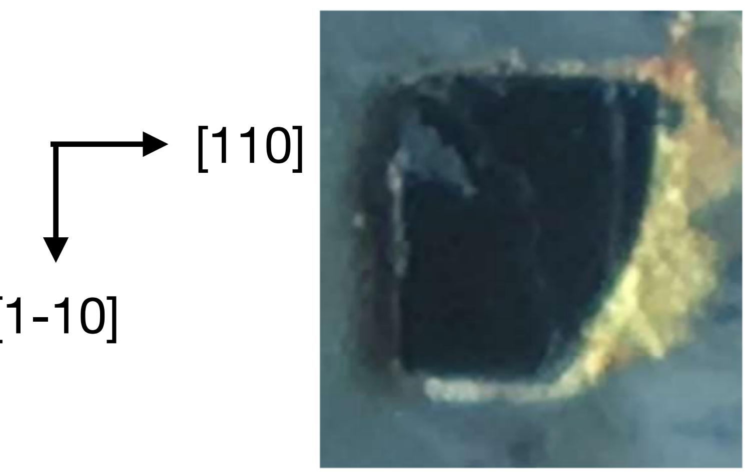
~20 nm Resolution



T. Choi, Z. Zhang, S. H. Chang, BJK et al. to be published

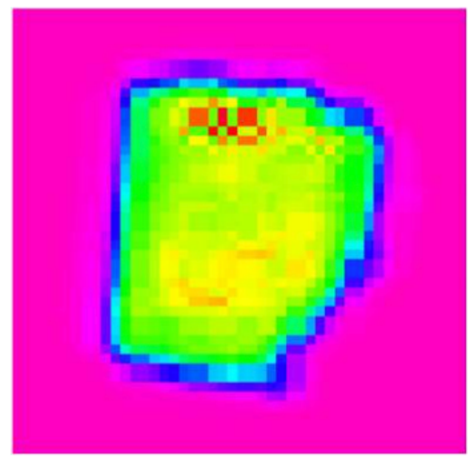
Domain Imaging

Sample picture



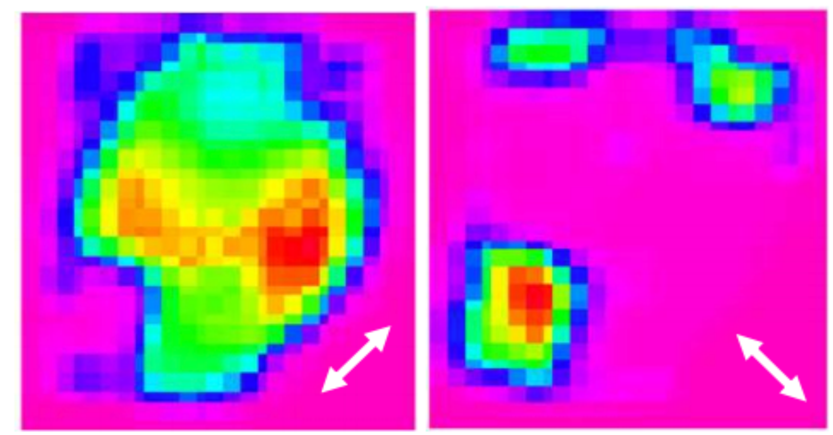
charge

(0 0 20) image

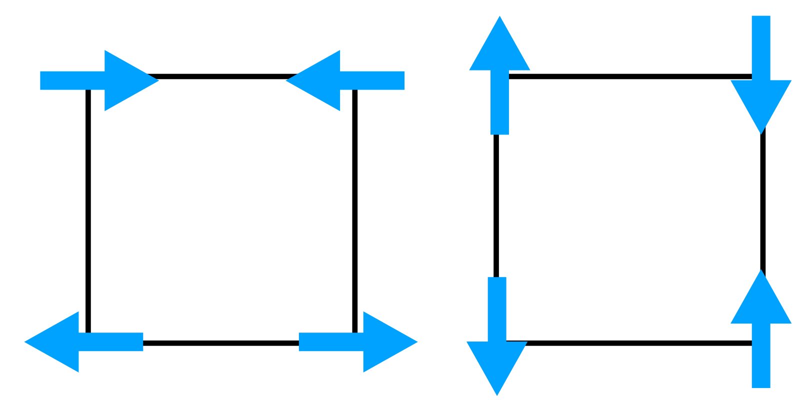


magnetic

(1 0 18) (1 0 20)



domain 1 domain 2

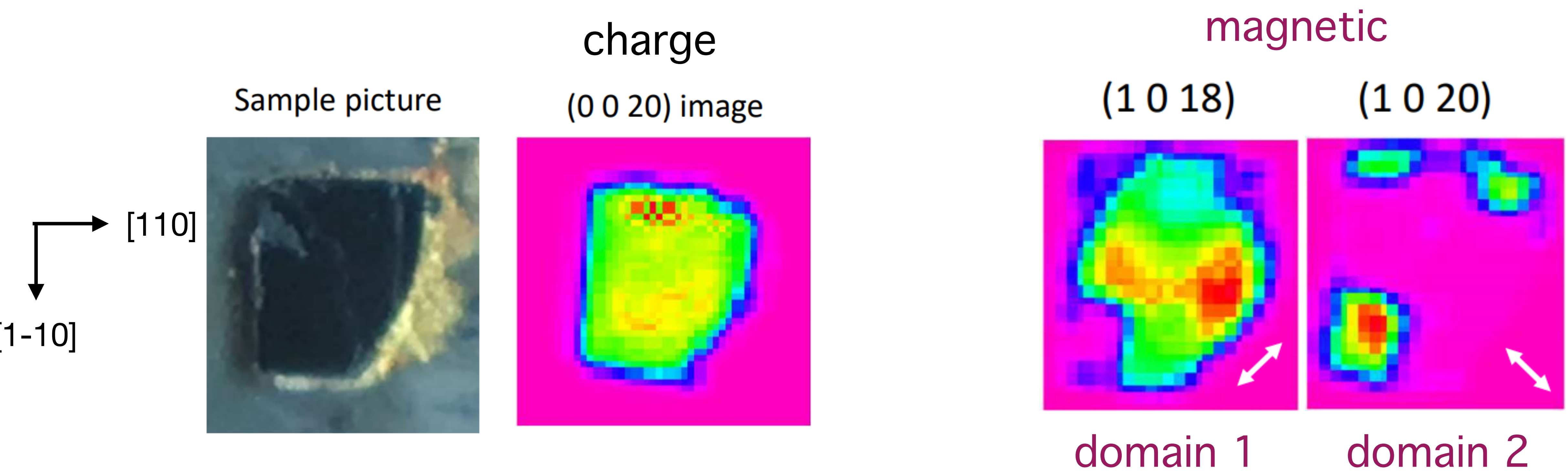


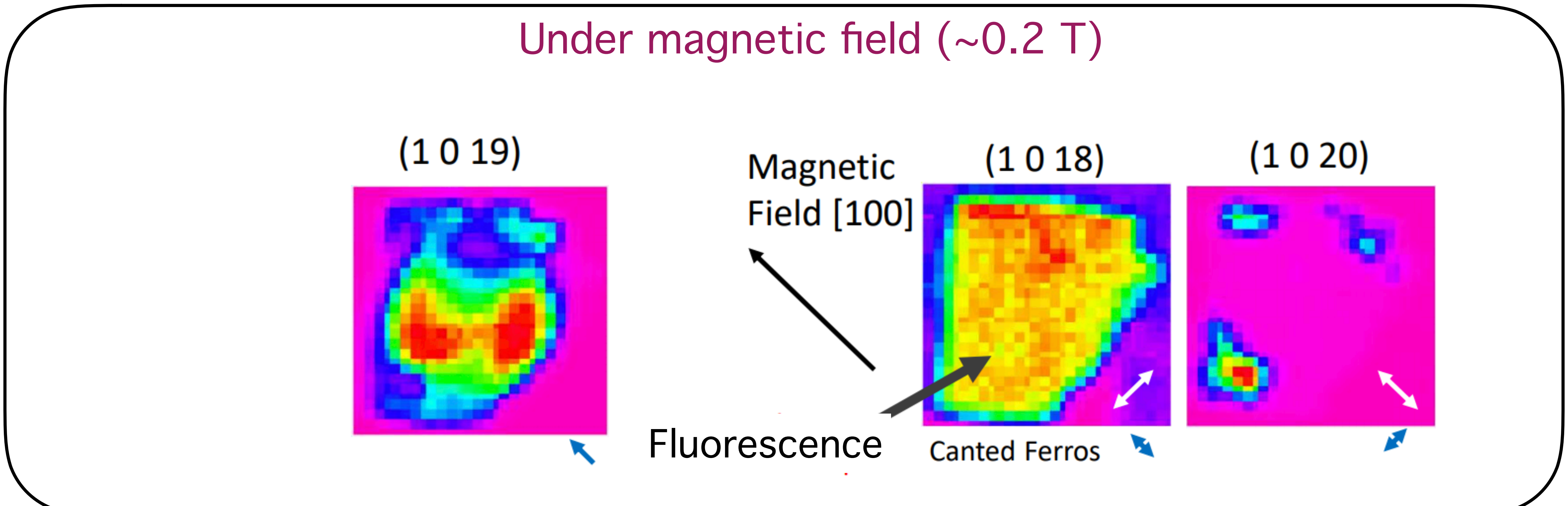
spins along a-axis

spins along b-axis

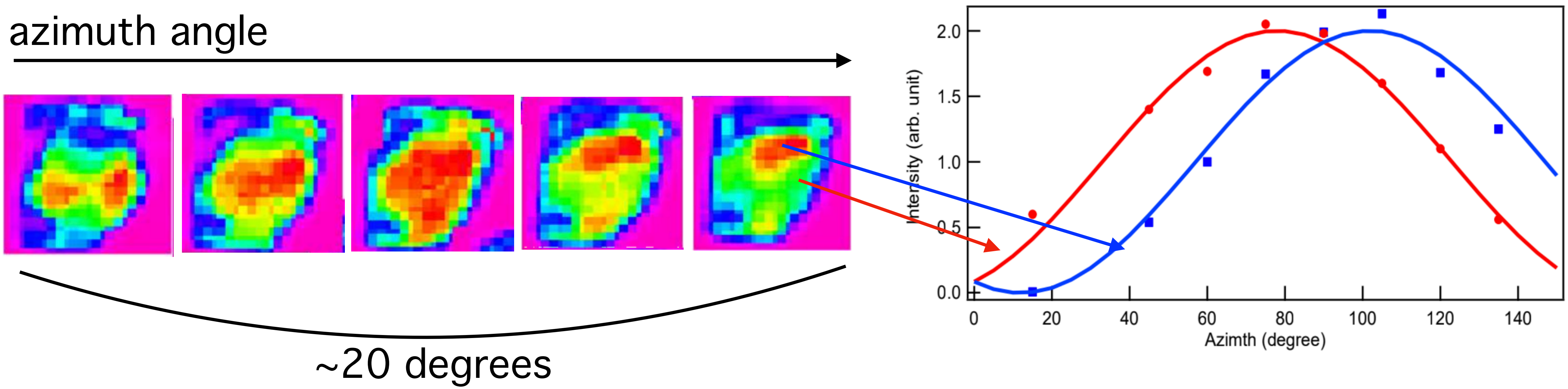
Mostly single domain, but uneven intensity

Domain Imaging

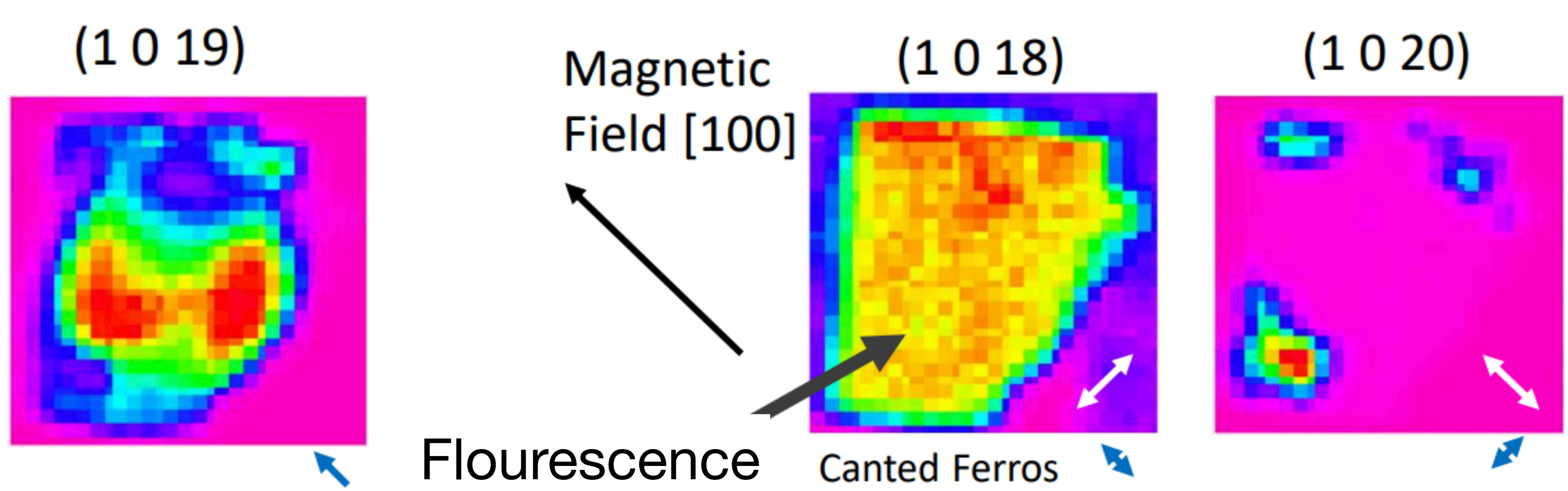




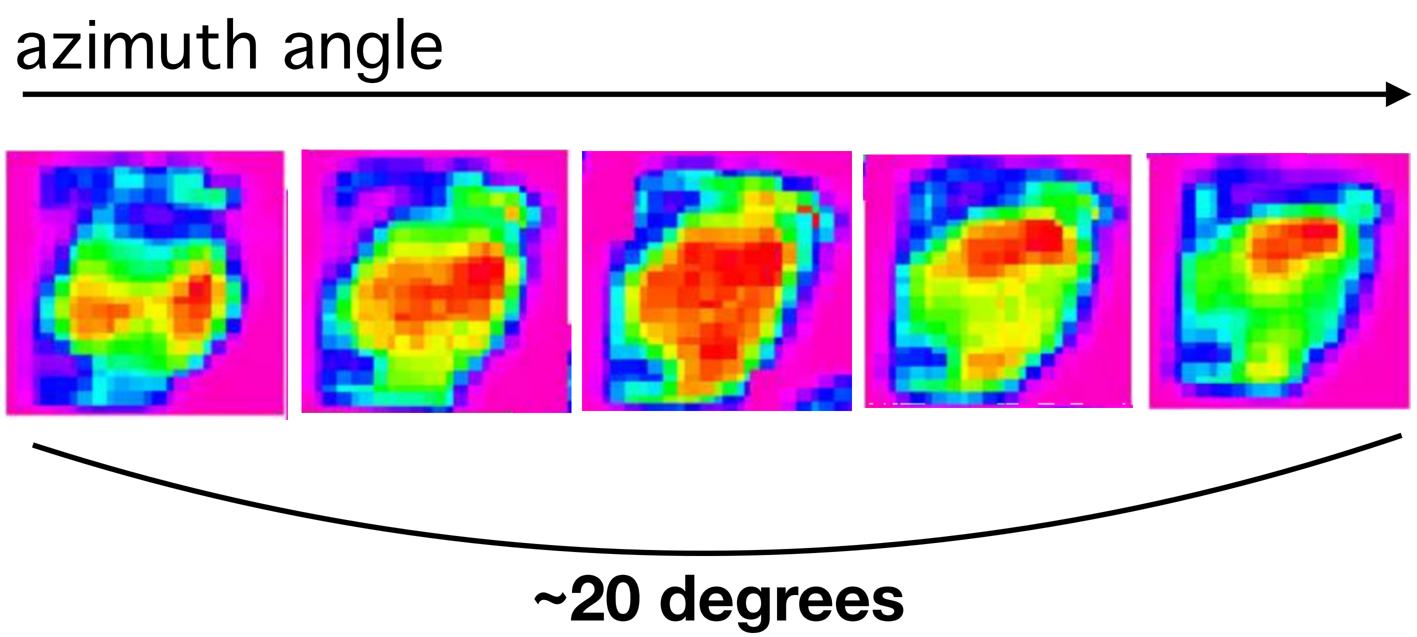
$Z_2 \times Z_2$ Domain Structure

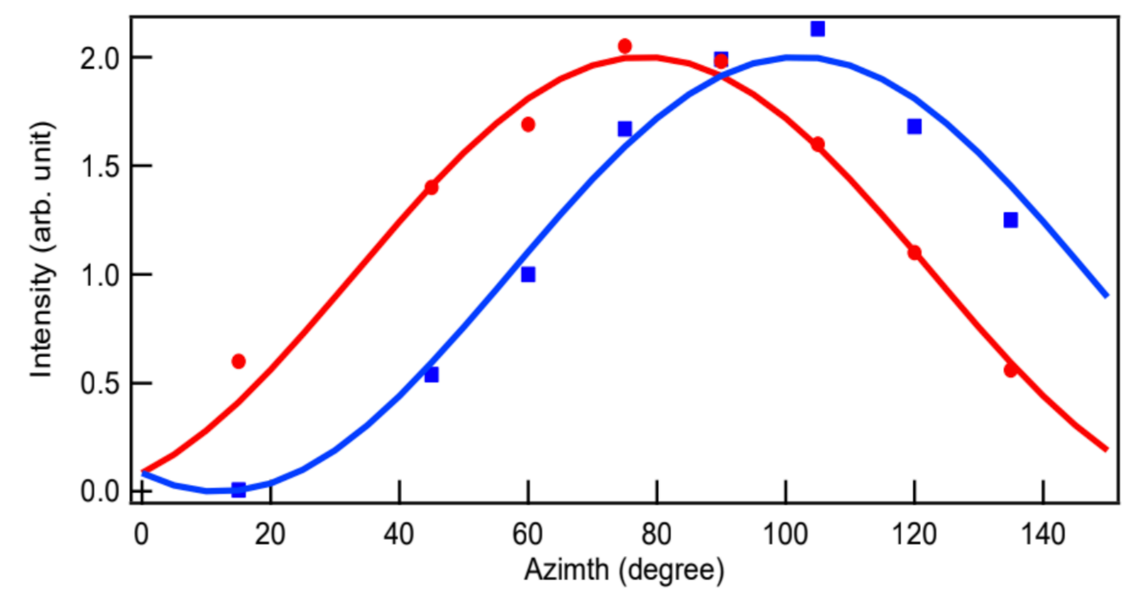


Under magnetic field



Z_2 x Z_2 Domain Structure



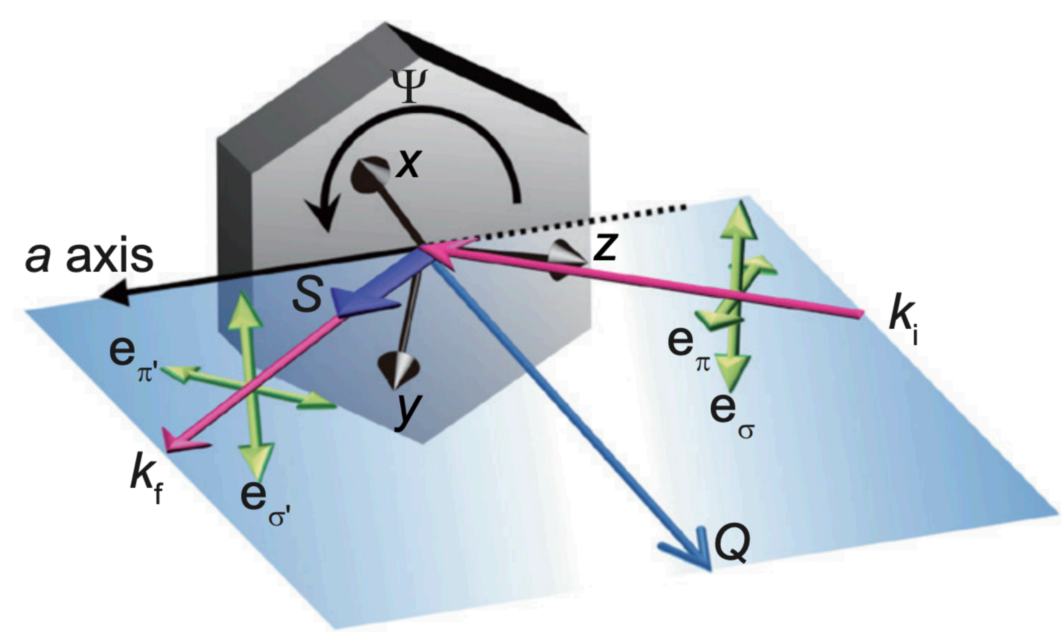


two domains within a domain!

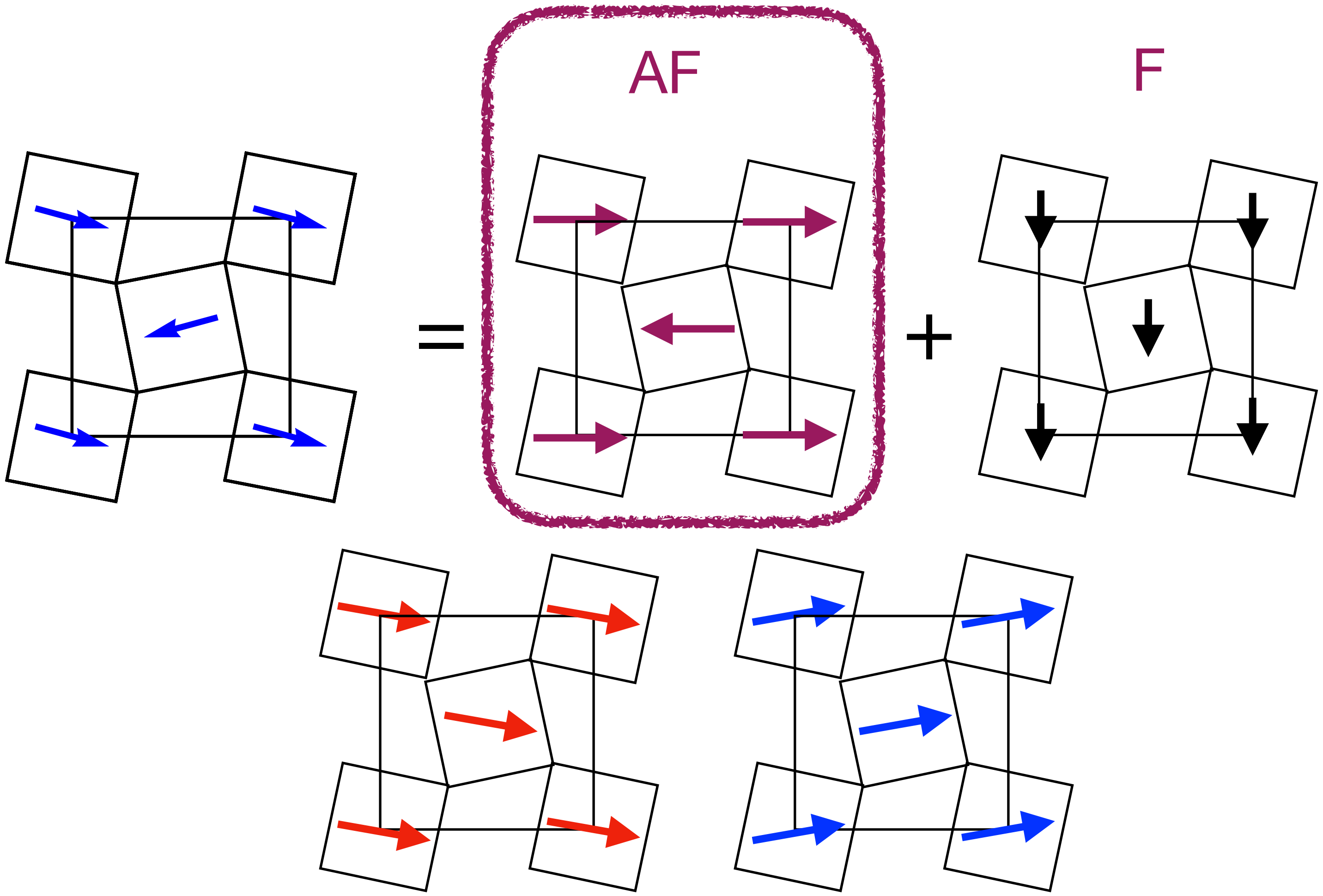
Known magnetic structure cannot explain the domain structure

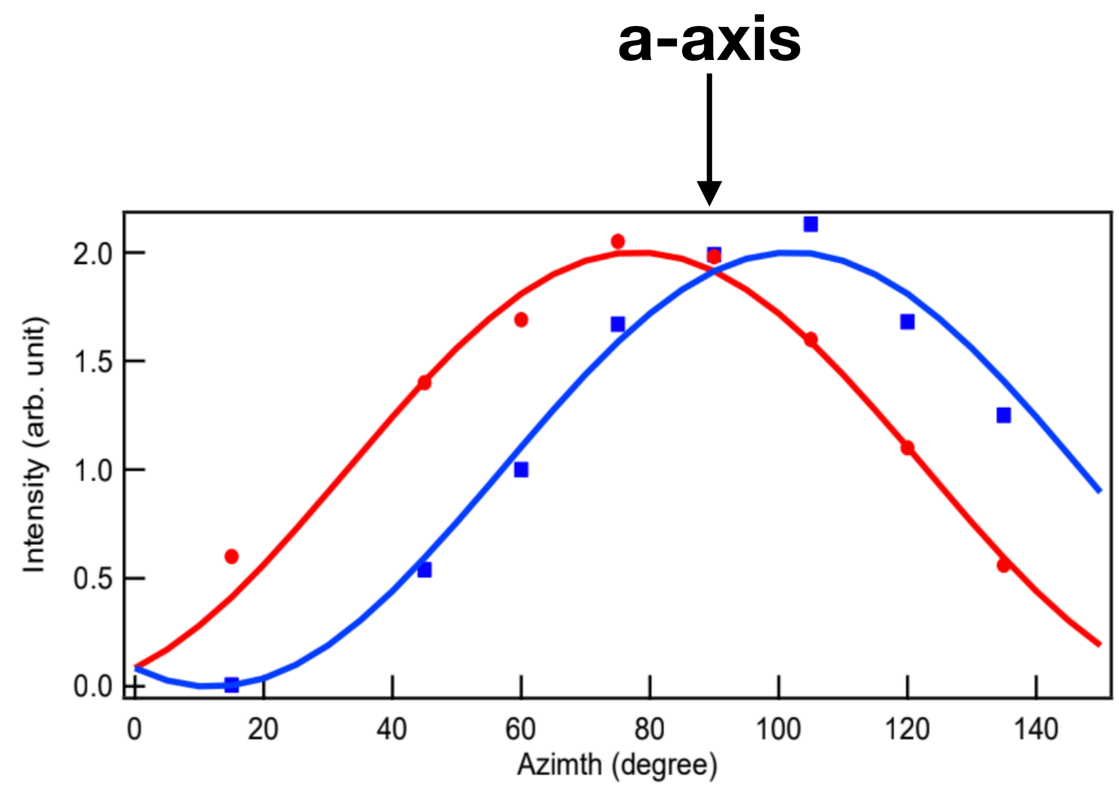
Resonant x-ray diffraction measures
spin component in the scattering plane

$$I \propto |\mathbf{k}_f \cdot \mathbf{S}|^2$$



Z_2 x Z_2 Domain Structure





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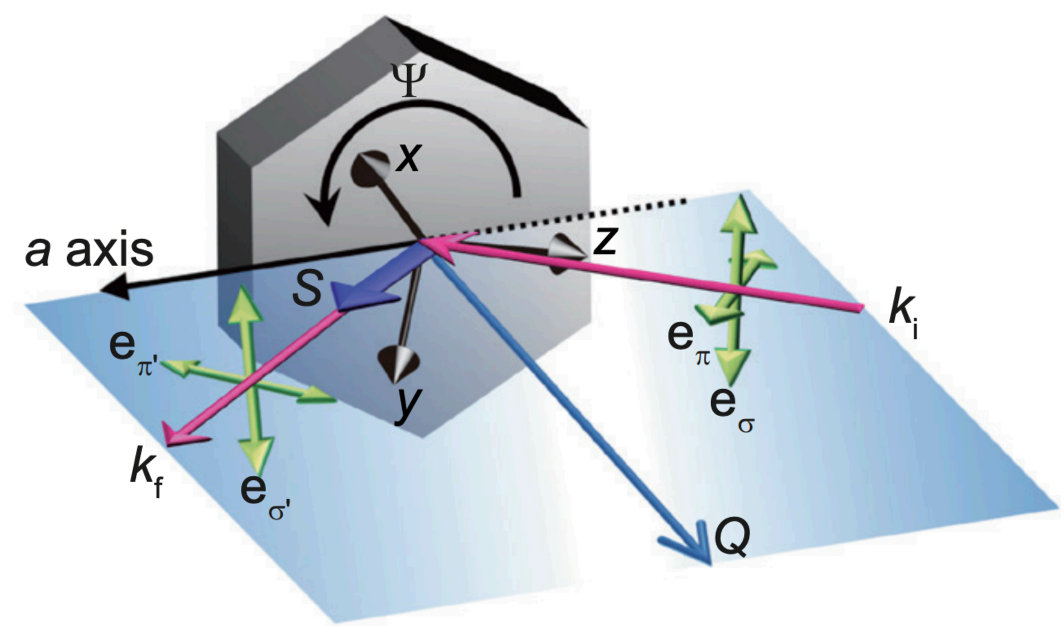
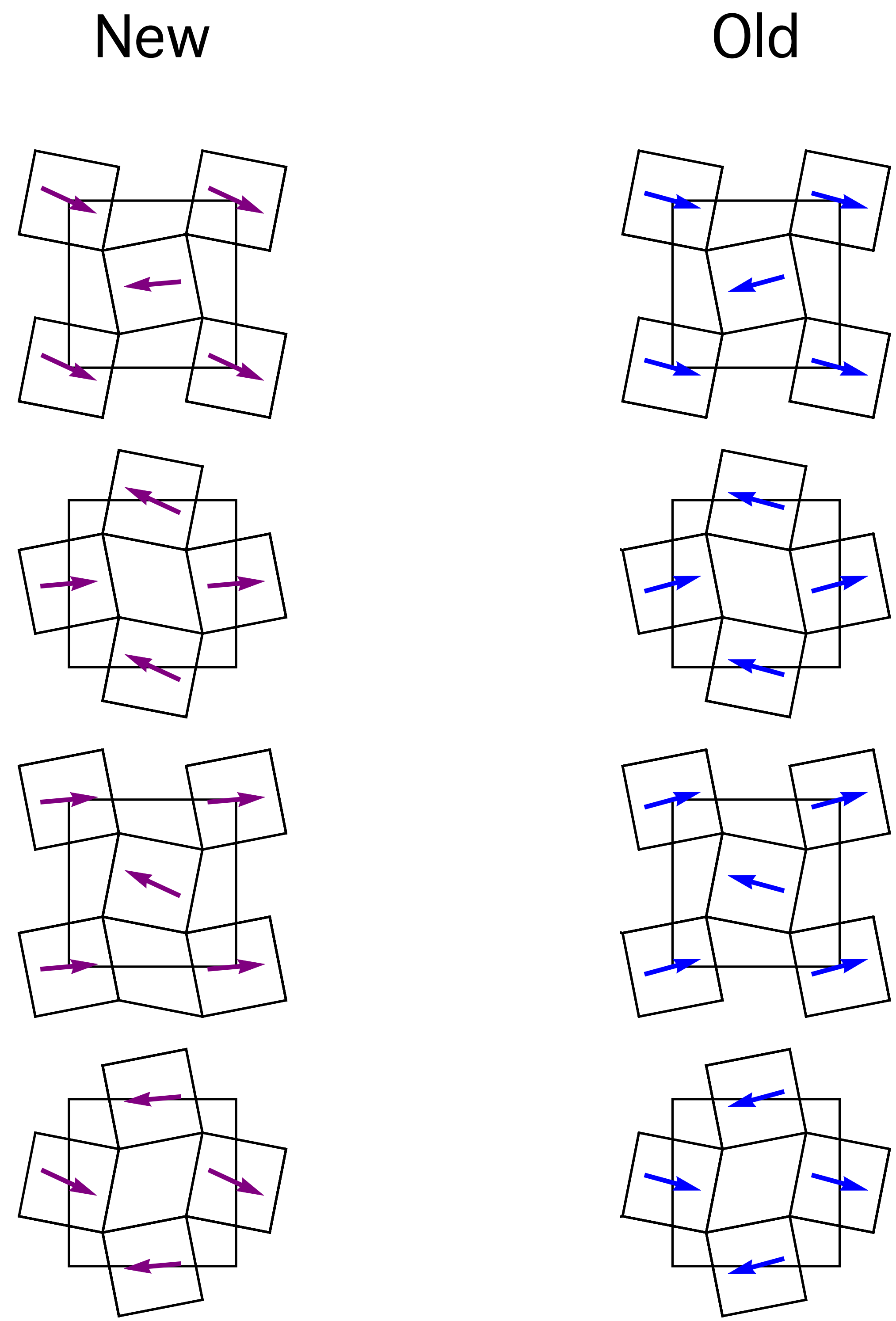


New magnetic solution

- Asymmetric canting angle & moment size
- Unique solution from representation analysis
- Can be stabilized in DFT calculations and has a lower total energy than the previous magnetic solution
- Can be stabilized even in the $I4_1/acd$ space group (instead of the actual $I4_1/a$)

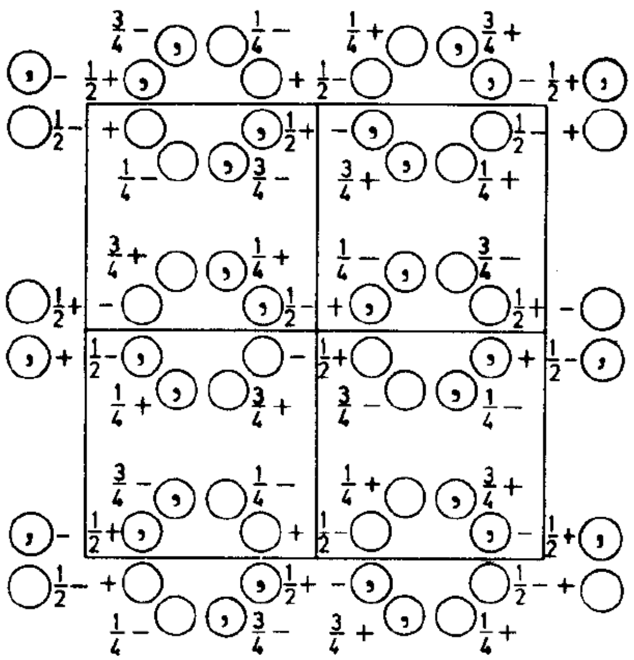


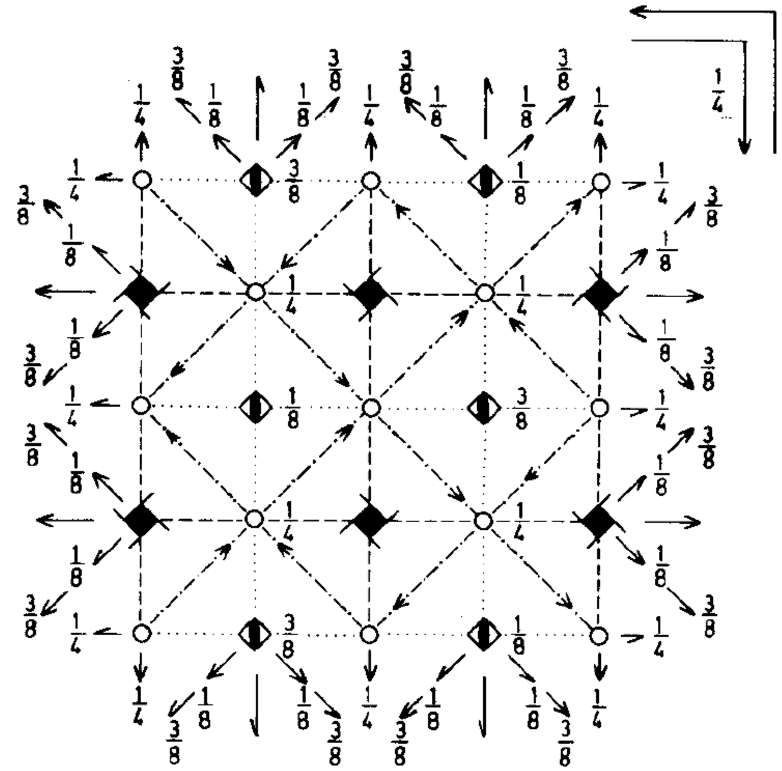
▶ Electronic mechanism of symmetry lowering

$I\,4_1/a\,c\,d$ D_{4h}^{20} $4/m\,m\,m$ Tetragonal

No. 142 $I\,4_1/a\,2/c\,2/d$ Patterson symmetry $I\,4/m\,m\,m$

ORIGIN CHOICE 2





- a body-centered cell.
- has inversion symmetry
- 4_1 screw axis, and a glide plane perpendicular to it.
- two additional glides.

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0\le x\le \frac{1}{2};\ -\frac{1}{4}\le y\le \frac{1}{4};\ 0\le z\le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})\ \ -\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})\ \ \frac{1}{4},0,z$
(5) $\underline{2}\ \ \frac{1}{4},y,0$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{4},\frac{3}{8}$	(8) $\underline{2}\ \ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}\ \ 0,0,0$	(10) $a\ \ x,y,\frac{1}{4}$	(11) $\bar{4}^+\ \ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-\ \ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(13) $a\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})\ \ \frac{3}{4},0,z$
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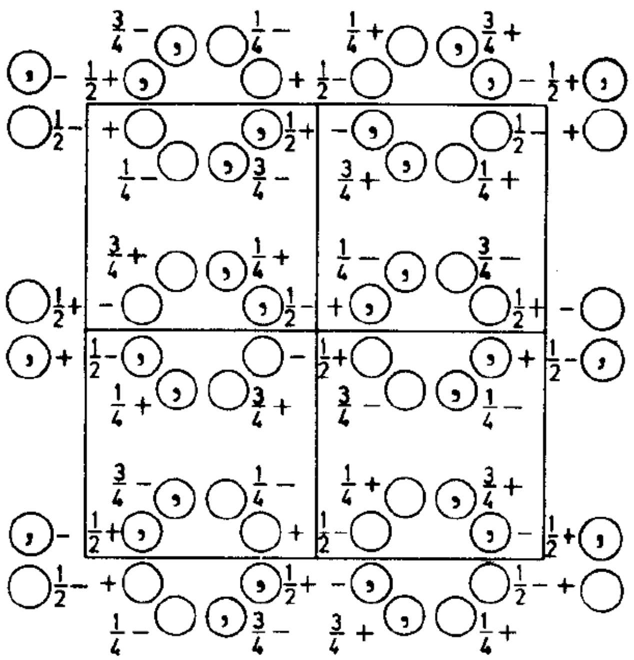
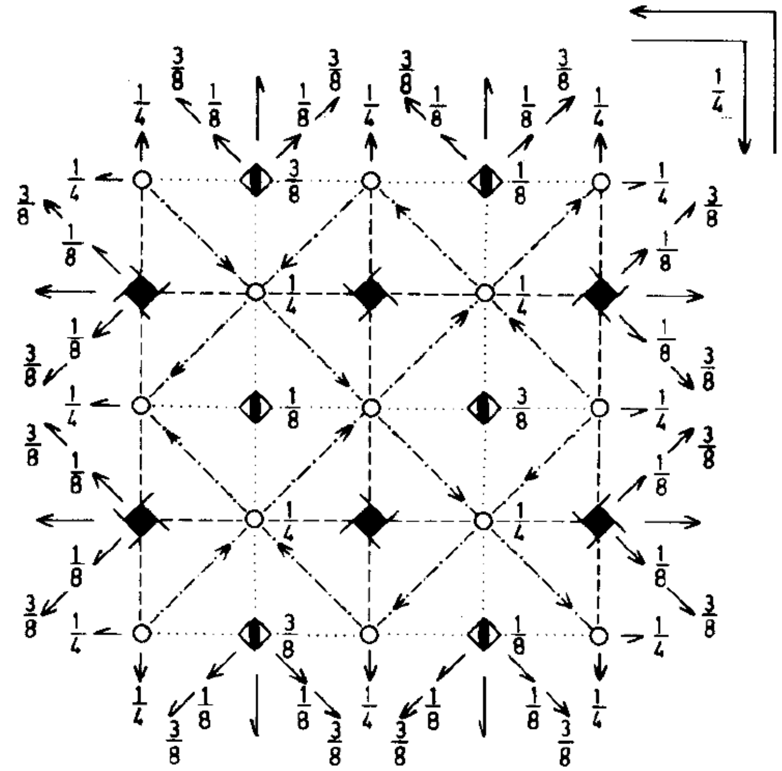
(9) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b\ \ x,y,0$	(11) $\bar{4}^+\ \ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-\ \ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(13) $c\ \ x,\frac{1}{4},z$	(14) $b\ \ \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,x,z$

$I\,4_1/a\,c\,d$ $\quad D_{4h}^{20}$ $\quad 4/m\,m\,m$ $\quad$ Tetragonal

No. 142 $\quad I\,4_1/a\,2/c\,2/d$ $\quad$ Patterson symmetry $I\,4/m\,m\,m$

ORIGIN CHOICE 2





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For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})\ \ \frac{3}{4},0,z$
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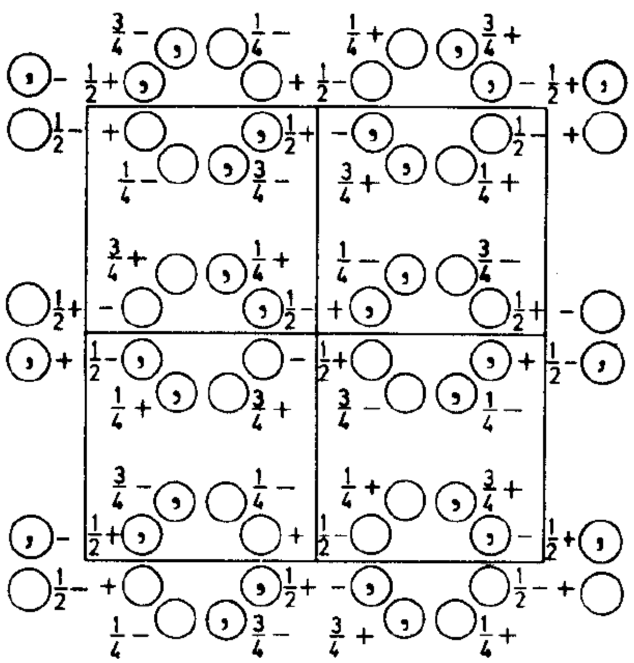
Removing these symmetry elements will lower the symmetry from $I4_1/acd$ to $I4_1/a$

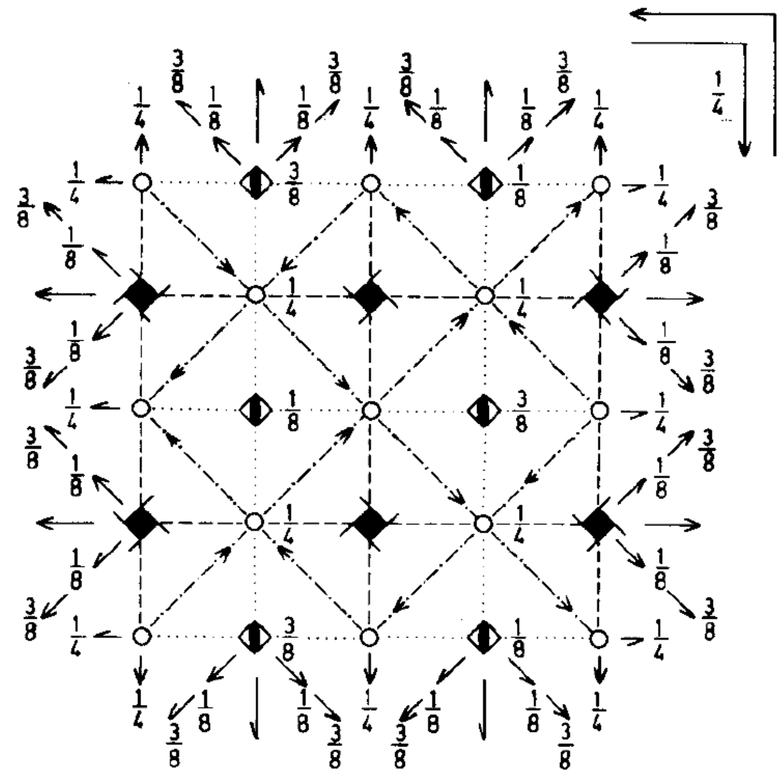
$I\,4_1/a\,c\,d$ D_{4h}^{20} $4/m\,m\,m$ Tetragonal

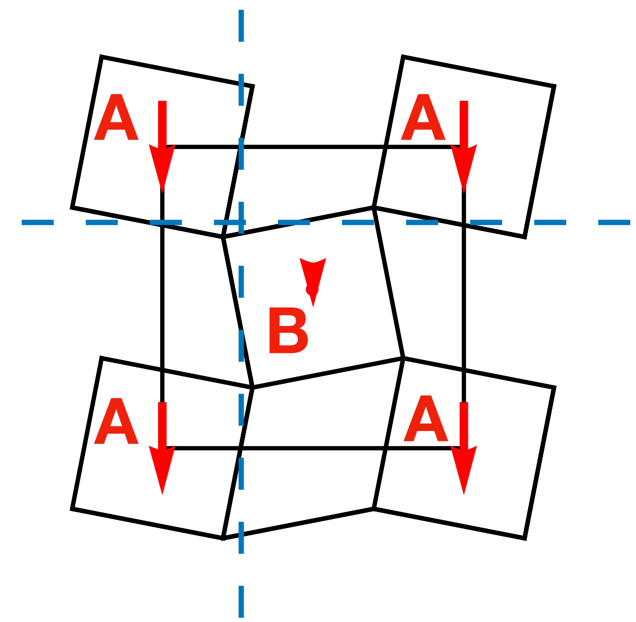
No. 142 $I\,4_1/a\,2/c\,2/d$ Patterson symmetry $I\,4/m\,m\,m$

ORIGIN CHOICE 2

- Ir occupies 8a Wyckoff site, and in-plane O 16f







glide plane

glide plane

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0\le x\le\frac{1}{2};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

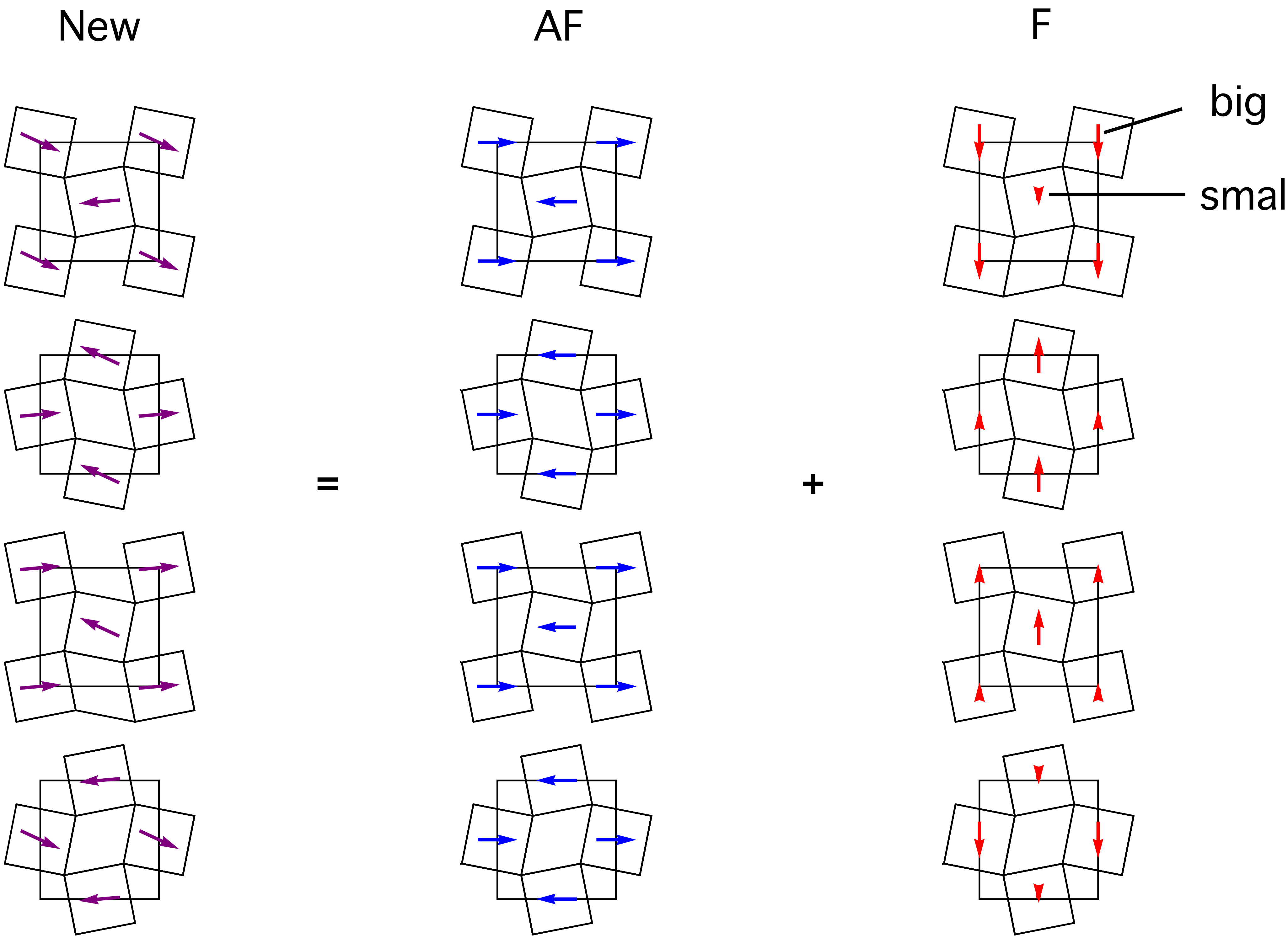
(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
~~(5) 2 $\frac{1}{4},y,0$~~	~~(6) 2 $x,0,\frac{1}{4}$~~	~~(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$~~	~~(8) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$~~
(9) $\bar{1}$ 0,0,0	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
~~(13) a $x,0,z$~~	~~(14) c $0,y,z$~~	~~(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$~~	~~(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z~~

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
~~(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$~~	~~(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$~~	~~(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$~~	~~(8) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$~~
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
~~(13) c $x,\frac{1}{4},z$~~	~~(14) b $\frac{1}{4},y,z$~~	~~(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$~~	~~(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z~~

No symmetry relations between octahedra in the A and B sublattices.

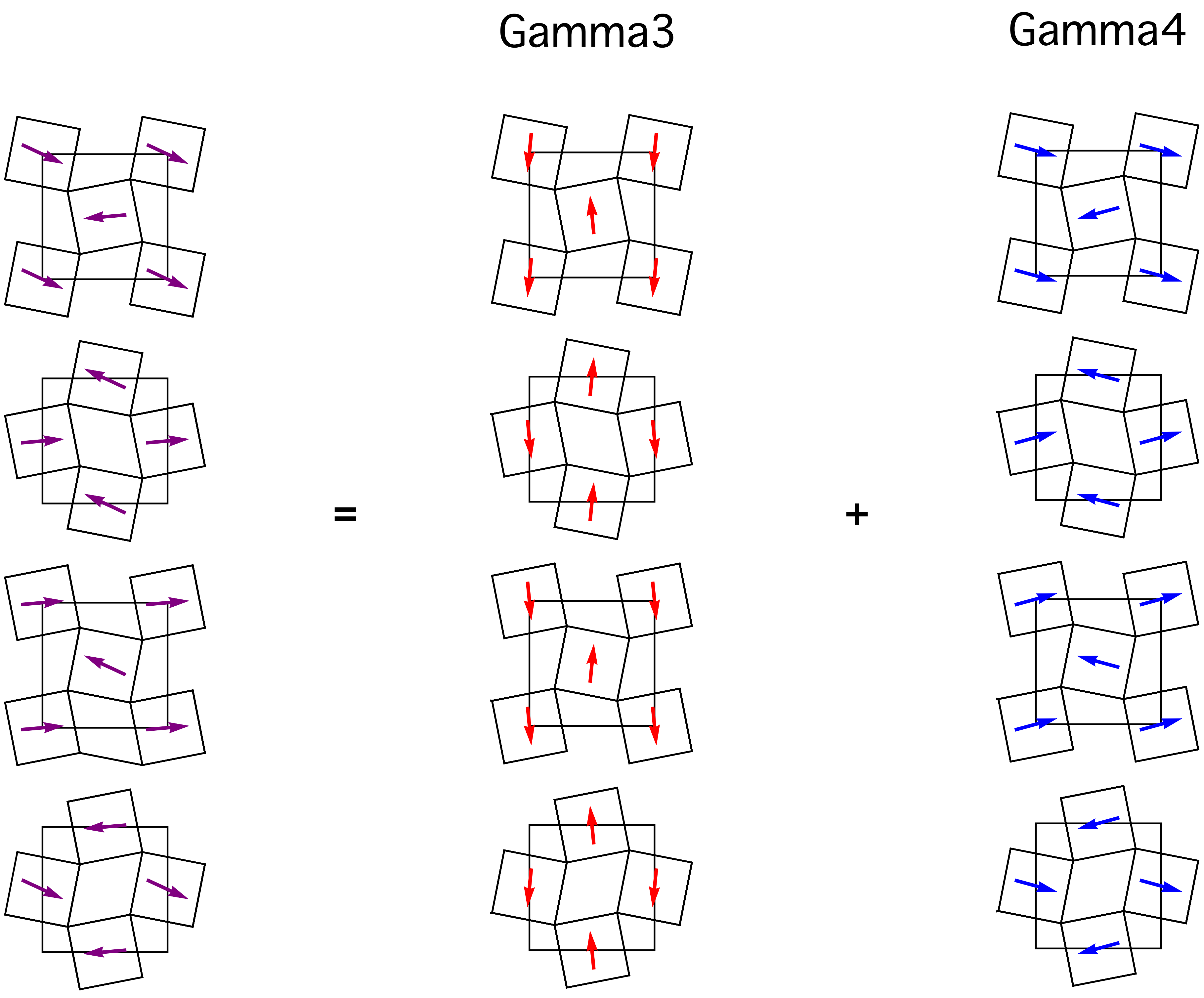
New magnetic solution



Neel order remains
almost unchanged

(pi,pi) modulation
of the moment size!

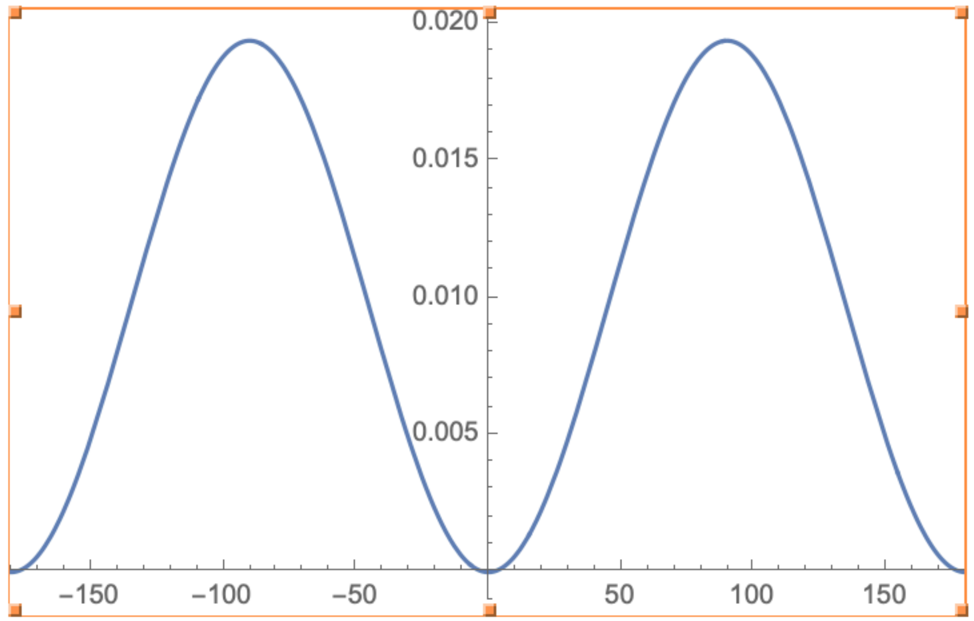
New magnetic solution



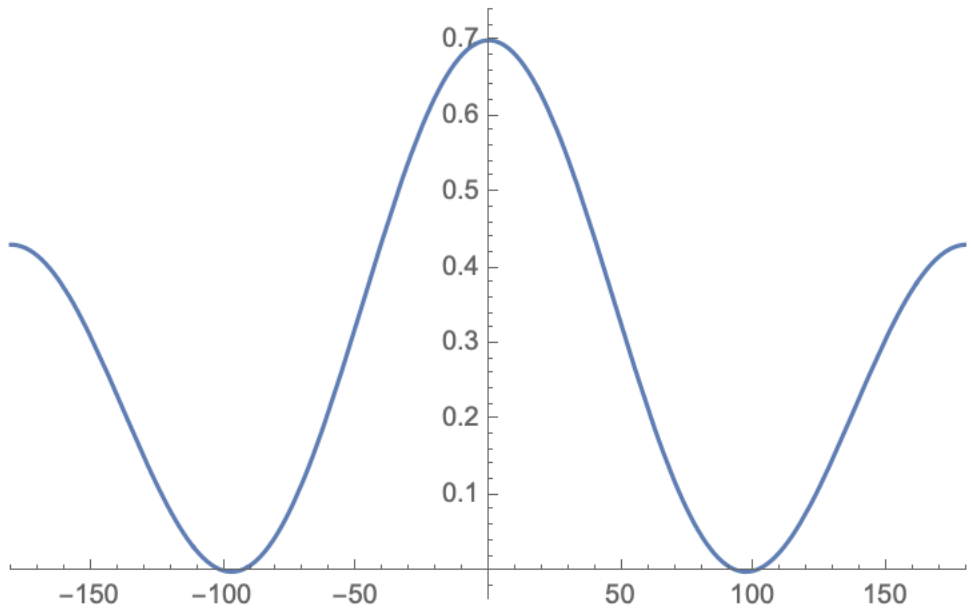
Requires two order parameters of different symmetries

New magnetic solution

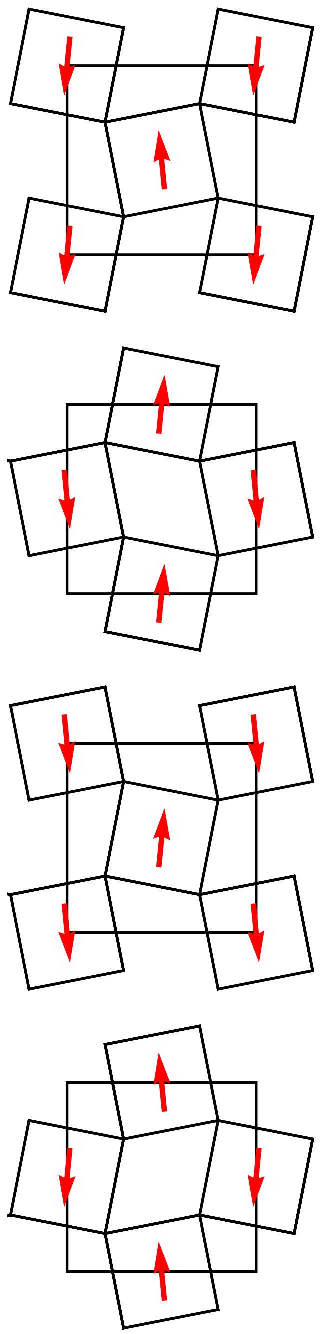
Gamma3



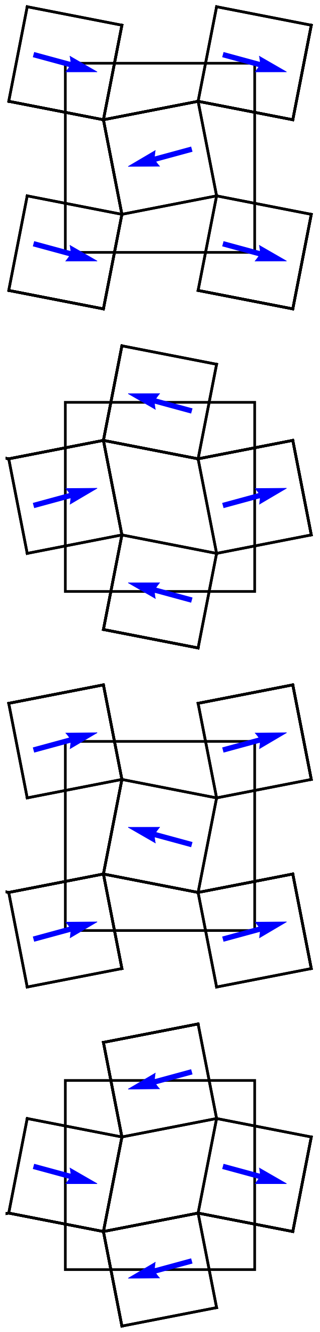
Gamma4



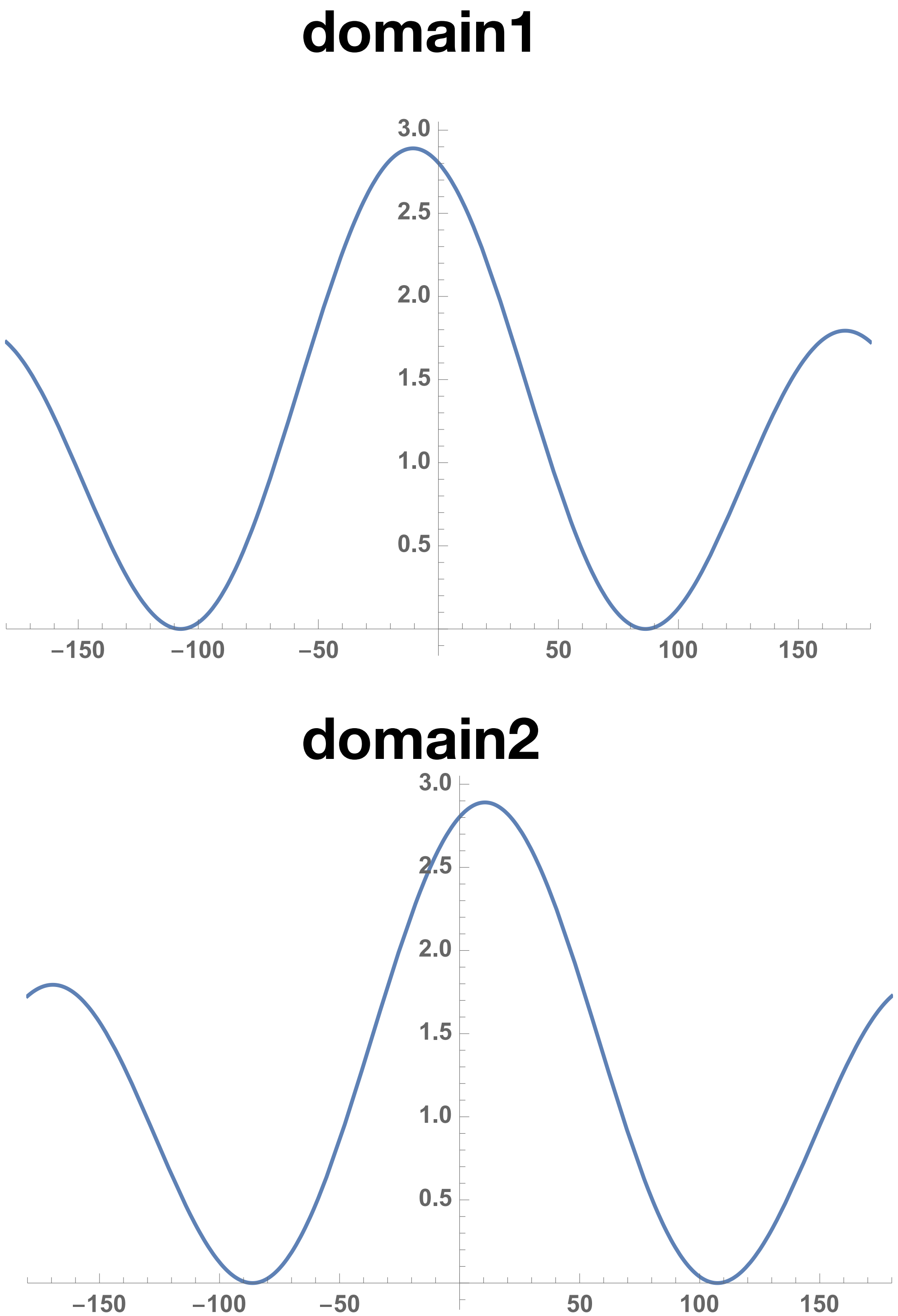
Gamma3

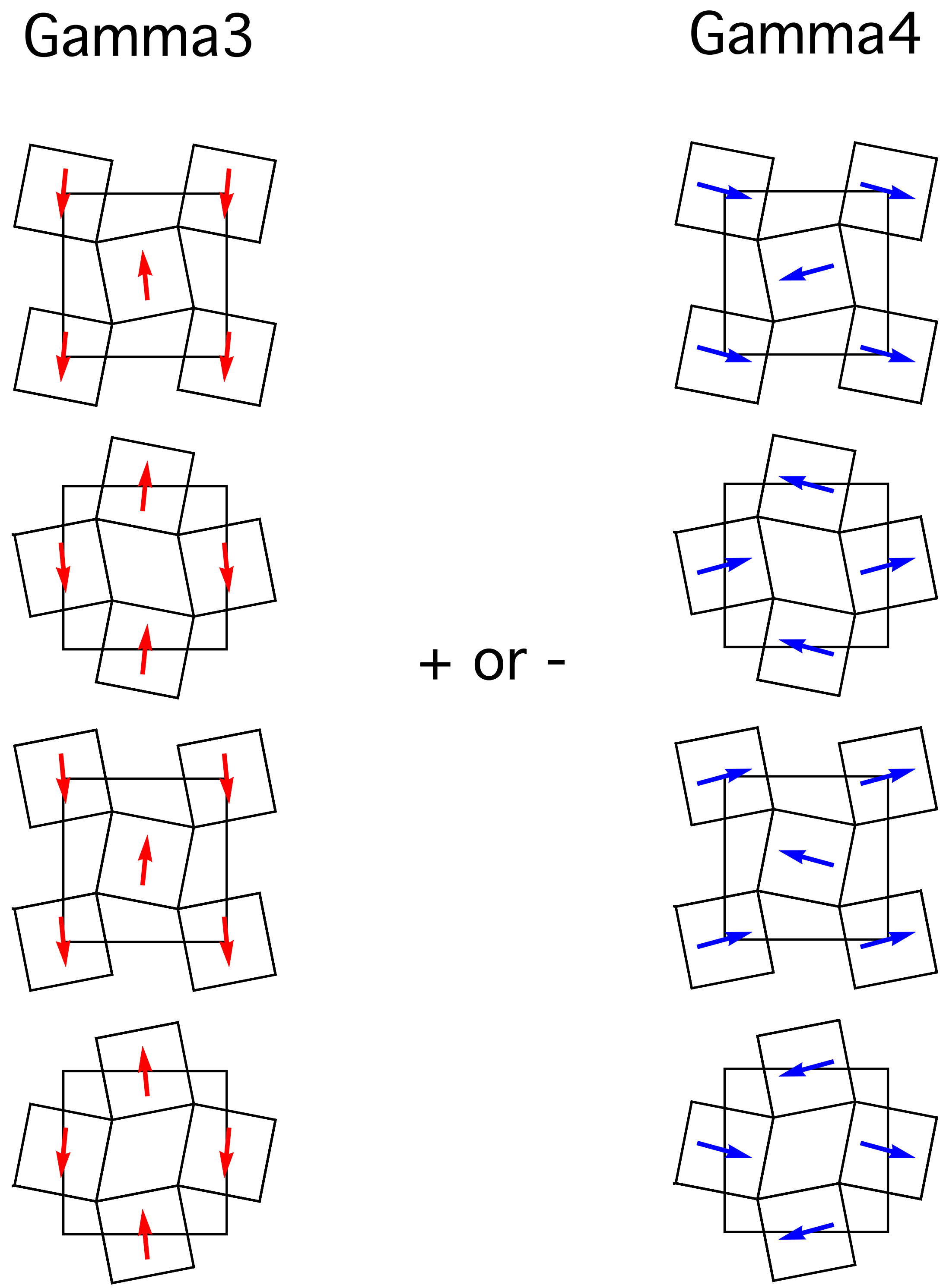


Gamma4



Mixing of two IR's gives $Z_2 x Z_2$





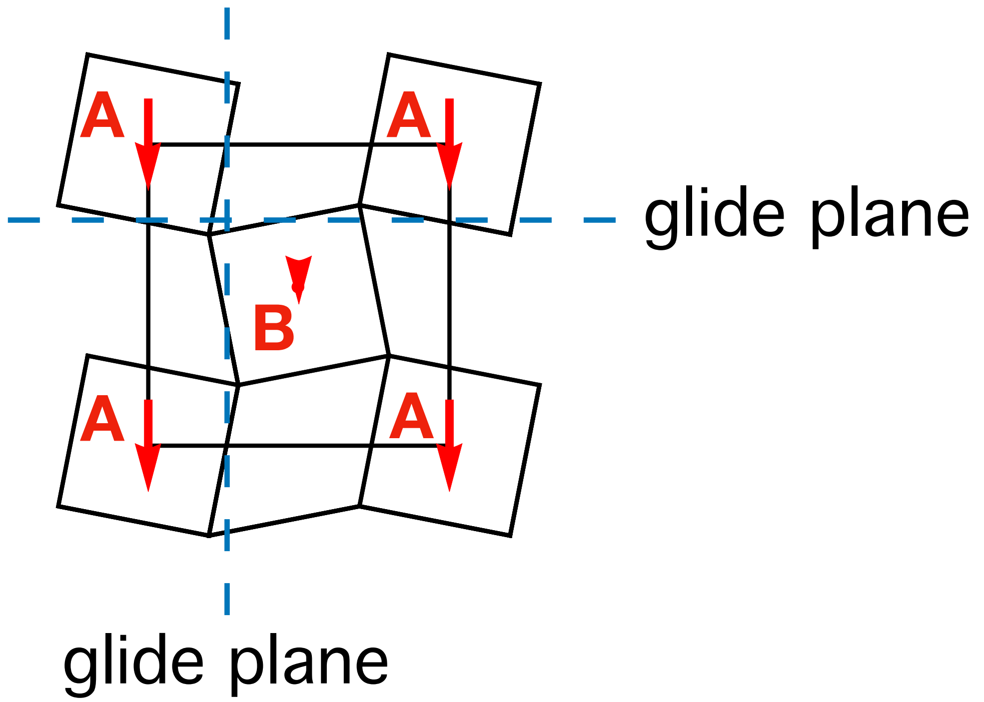
their interference manifests as deviation of the azimuth angle from zero

Spontaneous magnetic moment disproportionation

DFT results from I41/acd
(Sublattice A and B symmetry-wise equivalent)

Spontanesous disproportionation!

Actual space group 141/a
(glide planes c &d removed)



Magnetism drives lattice symmetry lowering!

Modulation of moment size, a new type of instability from pseudospins!

Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^{+}(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(5) $\underline{2}$ $\frac{1}{4},y,0$	(6) 2 $x,0,\frac{1}{4}$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(8) $\underline{2}$ $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}$ $0,0,0$	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^{+}$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^{-}$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(13) a $x,0,z$	(14) c $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(5) $\underline{2}(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$	(8) $\underline{2}$ $x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^{+}$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-}$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(13) c $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z

- 8 distinct Ir sites generated by symmetry operations

(1) {0, 1/4, 3/8}
(2) {1/2, 3/4, 7/8}
(3) {0, 3/4, 5/8}
(4) {1/2, 1/4, 1/8}
(5) {1/2,1/4, 5/8}
(6) {0, 3/4, 1/8}
(7) {1/2, 3/4, 3/8}
(8) {0, 1/4, 7/8}

Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0\leq x\leq\frac{1}{2};\ -\frac{1}{4}\leq y\leq\frac{1}{4};\ 0\leq z\leq\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $4^{+}(0,0,\frac{1}{4})\ \ -\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4})\ \ \frac{1}{4},0,z$
(5) $\underline{2}\ \ \frac{1}{4},y,0$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{4},\frac{3}{8}$	(8) $\underline{2}\ \ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}\ \ 0,0,0$	(10) $a\ \ x,y,\frac{1}{4}$	(11) $\bar{4}^{+}\ \ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^{-}\ \ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(13) $a\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4})\ \ \frac{3}{4},0,z$
(5) $\underline{2}(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)\ \ x,x-\frac{1}{4},\frac{1}{8}$	(8) $\underline{2}\ \ x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b\ \ x,y,0$	(11) $\bar{4}^{+}\ \ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-}\ \ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(13) $c\ \ x,\frac{1}{4},z$	(14) $b\ \ \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,x,z$

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(5) {1/2,1/4, 5/8}
(6) {0, 3/4, 1/8}
(7) {1/2, 3/4, 3/8}
(8) {0, 1/4, 7/8}

- symmetry operations shuffle ir sites

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(5) $\underline{2}$ $\frac{1}{4},y,0$	(6) 2 $x,0,\frac{1}{4}$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(8) $\underline{2}$ $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}$ $0,0,0$	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(13) a $x,0,z$	(14) c $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(5) $\underline{2}(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) $\underline{2}(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$	(8) $\underline{2}$ $x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(13) c $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z

- magnetic moments are rotated under symmetry operations

- symmetry operations shuffle ir sites

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \leq x \leq \frac{1}{2};\ -\frac{1}{4} \leq y \leq \frac{1}{4};\ 0 \leq z \leq \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $4^{+}(0,0,\frac{1}{4})\ \ -\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4})\ \ \frac{1}{4},0,z$
(5) $2\ \ \frac{1}{4},y,0$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{4},\frac{3}{8}$	(8) $2\ \ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}\ \ 0,0,0$	(10) $a\ \ x,y,\frac{1}{4}$	(11) $\bar{4}^{+}\ \ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^{-}\ \ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(13) $a\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4})\ \ \frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x-\frac{1}{4},\frac{1}{8}$	(8) $2\ \ x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b\ \ x,y,0$	(11) $\bar{4}^{+}\ \ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-}\ \ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(13) $c\ \ x,\frac{1}{4},z$	(14) $b\ \ \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,x,z$

- magnetic moments are rotated under symmetry operations
  (M_x,M_y,M_z) -> $(-M_y,M_x,M_z)$

- symmetry operations shuffle ir sites

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $\quad 0\le x\le\frac{1}{2};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $4^{+}(0,0,\frac{1}{4})\ \ -\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4})\ \ \frac{1}{4},0,z$
(5) $2\ \ \frac{1}{4},y,0$	(6) $2\ \ x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{4},\frac{3}{8}$	(8) $2\ \ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}\ \ 0,0,0$	(10) $a\ \ x,y,\frac{1}{4}$	(11) $\bar{4}^{+}\ \ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^{-}\ \ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(13) $a\ \ x,0,z$	(14) $c\ \ 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ \ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ \ 0,\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4})\ \ \frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x-\frac{1}{4},\frac{1}{8}$	(8) $2\ \ x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b\ \ x,y,0$	(11) $\bar{4}^{+}\ \ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-}\ \ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(13) $c\ \ x,\frac{1}{4},z$	(14) $b\ \ \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ \ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \ x,x,z$

- magnetic moments are rotated under symmetry operations $(M_x,M_y,M_z)\ \ \to\ \ (-M_y,M_x,M_z)$
- combining site shuffling and moment rotation

$$
\begin{pmatrix}
0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0
\end{pmatrix}
$$

Assumption: magnetic order does not enlarge the unit cell

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^{+}(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(5) 2 $\frac{1}{4},y,0$	(6) 2 $x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(8) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}$ $0,0,0$	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^{+}$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^{-}$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(13) a $x,0,z$	(14) c $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

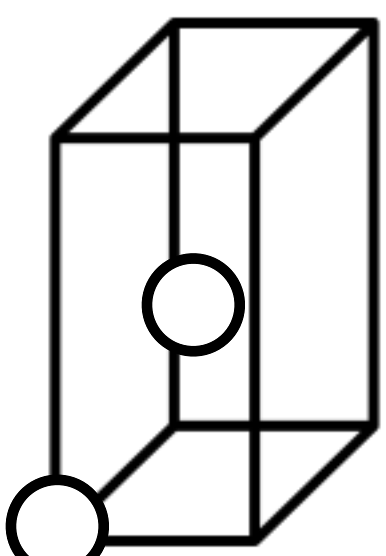
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$	(8) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^{+}$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-}$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(13) c $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z

Assumption: magnetic order does not enlarge the unit cell

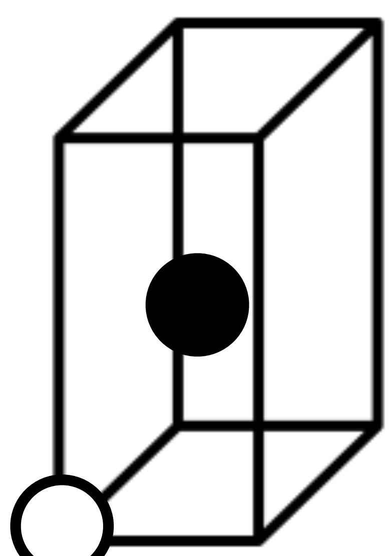
	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

- magnetic moments are rotated under symmetry operations (M_x,M_y,M_z) -> $(-M_y,M_x,M_z)$
- combining site shuffling and moment rotation
- propagation vector k=(0,0,0) or k=(1,0,0)

k=(0,0,0)



k=(1,0,0)



Representation Analysis

Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2};\ -\frac{1}{4} \le y \le \frac{1}{4};\ 0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})\ \frac{1}{4},0,z$	(3) $4^{+}(0,0,\frac{1}{4})\ -\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4})\ \frac{1}{4},0,z$
(5) $2\ \frac{1}{4},y,0$	(6) $2\ x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ x,x+\frac{1}{4},\frac{3}{8}$	(8) $2\ x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}\ 0,0,0$	(10) $a\ x,y,\frac{1}{4}$	(11) $\bar{4}^{+}\ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^{-}\ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{1}{8}$
(13) $a\ x,0,z$	(14) $c\ 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\ 0,\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{3}{4})\ \frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4})\ \frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)\ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ x,x-\frac{1}{4},\frac{1}{8}$	(8) $2\ x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b\ x,y,0$	(11) $\bar{4}^{+}\ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-}\ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$
(13) $c\ x,\frac{1}{4},z$	(14) $b\ \frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ x,x,z$

Assumption: magnetic order does not enlarge the unit cell

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

- magnetic moments are rotated under symmetry operations $(M_x,M_y,M_z) \rightarrow (-M_y,M_x,M_z)$
- combining site shuffling and moment rotation

$$\begin{pmatrix}
0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&-1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0
\end{pmatrix}$$

- Find a basis that brings all 32 24x24 matrices to a smallest block-diagonal form
- A second order phase transition involves an order parameter belonging to a single irreducible representation

Representation Analysis

- 24x24 matrices split into:

  4 x 2D
  4 x 4D

- In general, any physical quantity can be expressed in terms of

  8 x 1D
  6 x 2D

for the factor group G(k)/T(k) under consideration (32 symmetry operations, 14 classes)

Representation Analysis

- 24x24 matrices split into:

  4 x 2D
  4 x 4D

- In general, any physical quantities can be expressed in terms of

  8 x 1D
  6 x 2D (Gamma1-Gamma6)

for the factor group G(k)/T(k) under consideration (32 symmetry operations, 14 classes)

Representation Analysis

Gamma2

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	-1	0	0	-1	0	0	-1	0	0	0	1	0	0	1	0	0	1	0	0	1	0
2	0	-1	0	0	-1	0	0	-1	0	0	-1	0	1	0	0	1	0	0	1	0	0	1	0	0
3	0	1	0	0	1	0	0	1	0	0	1	0	1	0	0	1	0	0	1	0	0	1	0	0
4	1	0	0	1	0	0	1	0	0	1	0	0	0	1	0	0	1	0	0	1	0	0	1	0

Gamma3

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	0	0	0	0	0	-1	0	0	1	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0	0	-1	0	0	1	0
3	0	-1	0	0	1	0	0	0	0	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0
4	0	0	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0	0	1	0	0	-1	0	0

Gamma4

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	-1	0	0	1	0	1	0	0	-1	0	0	0	-1	0	0	1	0
2	-1	0	0	1	0	0	0	1	0	0	-1	0	1	0	0	-1	0	0	0	1	0	0	-1	0
3	0	-1	0	0	1	0	-1	0	0	1	0	0	0	-1	0	0	1	0	1	0	0	-1	0	0
4	0	-1	0	0	1	0	1	0	0	-1	0	0	0	-1	0	0	1	0	-1	0	0	1	0	0

Gamma5

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	-1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	-1	0	0	-1	0
3	0	-1	0	0	-1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	-1	0	0	-1	0	0

Representation Analysis

Gamma2

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	-1	0	0	-1	0	0	-1	0	0	0	1	0	0	1	0	0	1	0	0	1	0
2	0	-1	0	0	-1	0	0	-1	0	0	-1	0	1	0	0	1	0	0	1	0	0	1	0	0
3	0	1	0	0	1	0	0	1	0	0	1	0	1	0	0	1	0	0	1	0	0	1	0	0
4	1	0	0	1	0	0	1	0	0	1	0	0	0	1	0	0	1	0	0	1	0	0	1	0

Inconsistent with x-ray data

Gamma3

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	0	0	0	0	0	-1	0	0	1	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0	0	-1	0	0	1	0
3	0	-1	0	0	1	0	0	0	0	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0
4	0	0	0	0	0	0	1	0	0	-1	0	0	0	0	0	0	0	0	1	0	0	-1	0	0

Gamma4

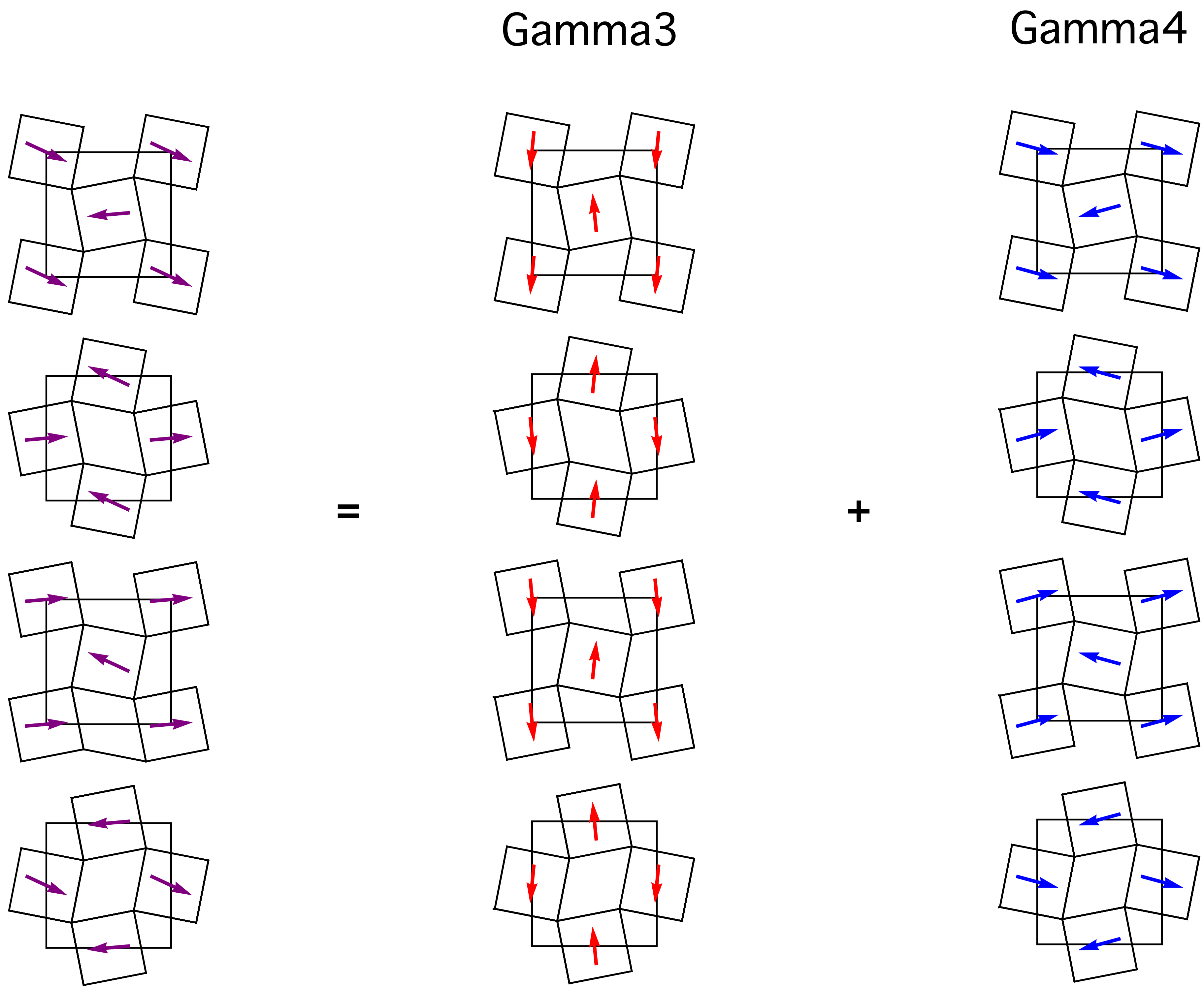
	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	-1	0	0	1	0	1	0	0	-1	0	0	0	-1	0	0	1	0
2	-1	0	0	1	0	0	0	1	0	0	-1	0	1	0	0	-1	0	0	0	1	0	0	-1	0
3	0	-1	0	0	1	0	-1	0	0	1	0	0	0	-1	0	0	1	0	1	0	0	-1	0	0
4	0	-1	0	0	1	0	1	0	0	-1	0	0	0	-1	0	0	1	0	-1	0	0	1	0	0

Gamma5

	1x	1y	1z	2x	2y	2z	3x	3y	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	-1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	-1	0	0	-1	0
3	0	-1	0	0	-1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	-1	0	0	-1	0	0

Inconsistent with x-ray data

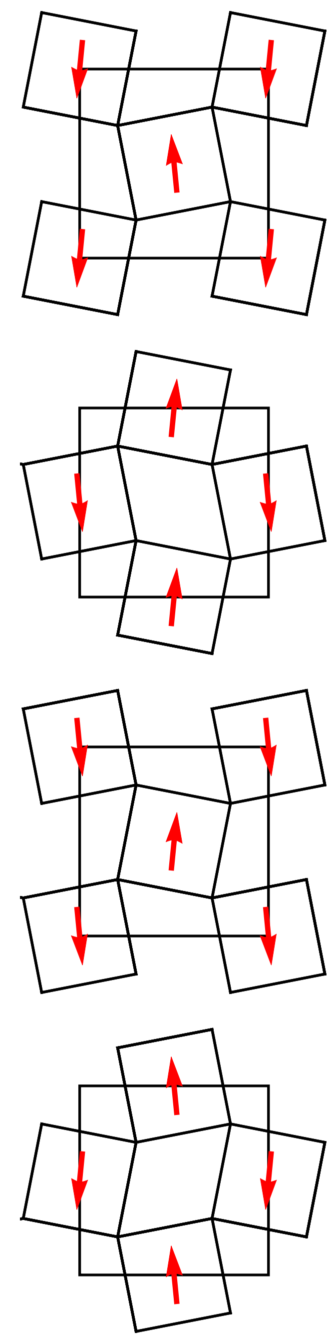
New magnetic solution



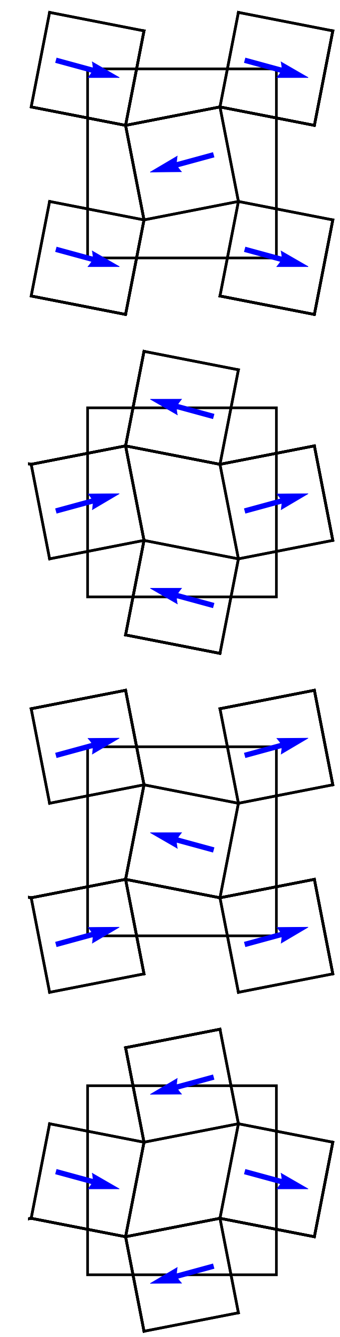
Requires two order parameters of different symmetries in 141/acd

Symmetry of the magnetic order

Gamma3



Gamma4



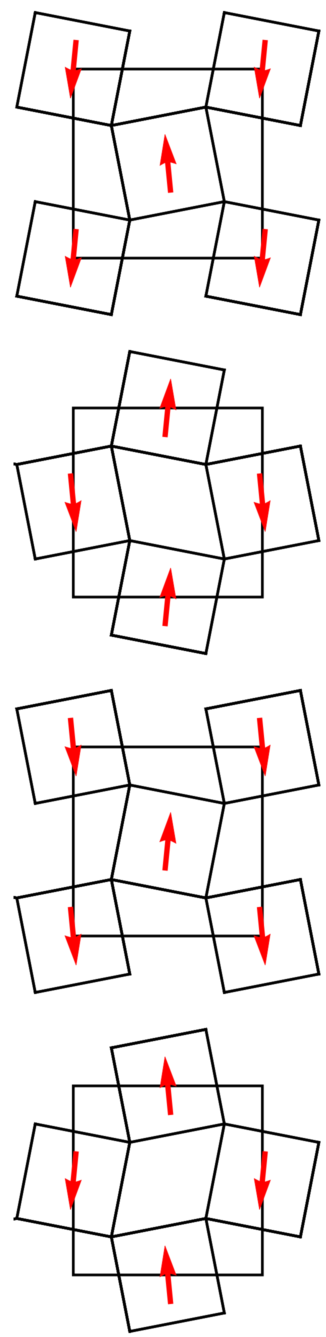
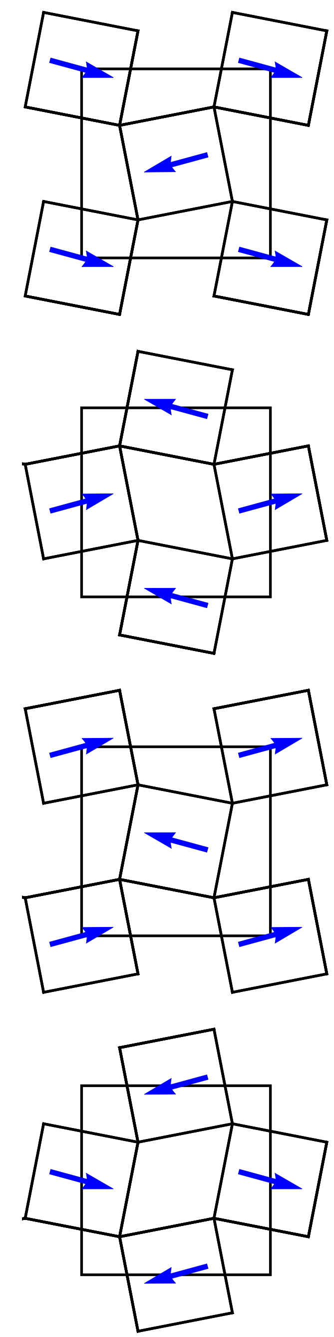
invariant under

Gamma3: 1,2,9,10,21,22,29,30

Gamma4: 1,2,5,6,9,10,13,14

Symmetry of the lattice

Separately, Gamma3 and Gamma4 both leads to lattice symmetry of Ibca, but...

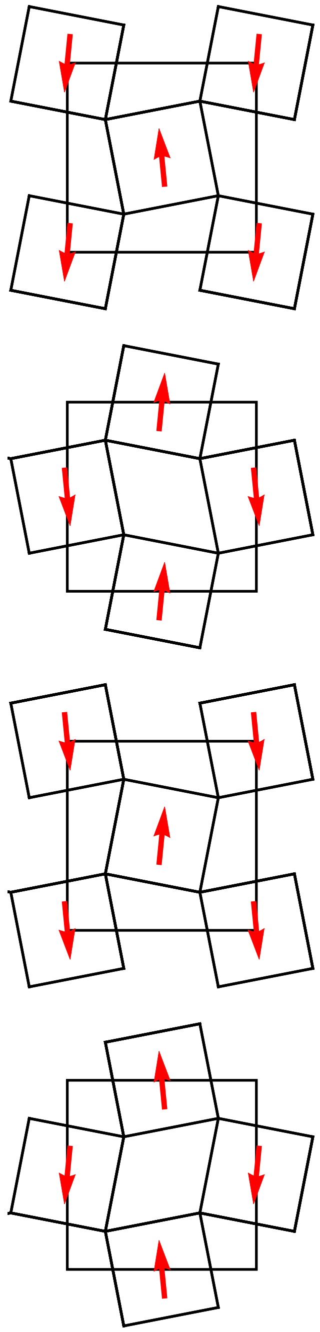
	Gamma3	Gamma4
	 Ibca	 Ibca
invariant under	1,2,9,10,21,22,29,30	1,2,5,6,9,10,13,14
invariant under with timer reversal	5,6,13,14,17,18,25,26	17,18,21,22,25,26,29,30

Symmetry of the lattice

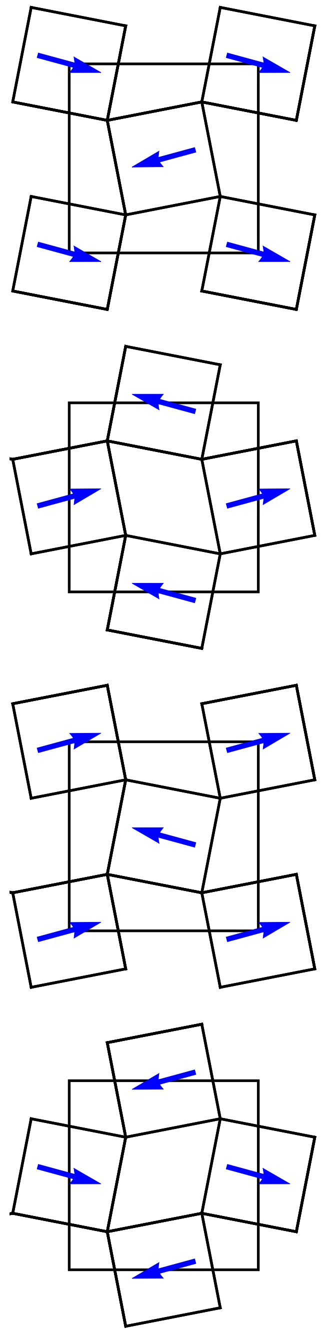
Separately, Gamma3 and Gamma4 both leads to lattice symmetry of Ibca, but...

when simultaneously present, the lattice will be I2/a (C2/c)

Gamma3



Gamma4



invariant under 1,2,9,10

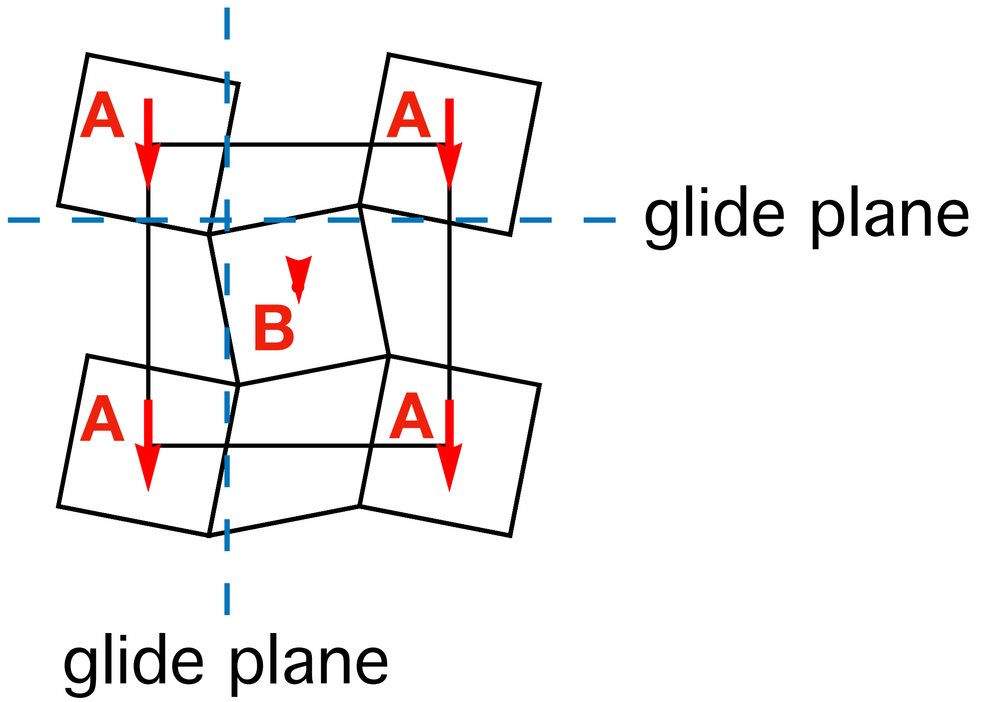
invariant under with timer reversal 17,18,25,26

Summary

DFT results from I41/acd
(Sublattice A and B symmetrywise equivalent)

Spontanesous disproportionation!

Actual space group 141/a
(glide planes c &d removed)



Magnetism drives lattice symmetry lowering!

Modulation of moment size, a new type of instability from pseudospins!