Magnetic Diffraction: Tutorial

Roger Johnson

Neutron powder diffraction: REFeO$_3$

Pbnm   Fe1: $\left(\frac{1}{2},0,0\right)$, Fe2: $\left(0,\frac{1}{2},0\right)$, Fe3: $\left(\frac{1}{2},0,\frac{1}{2}\right)$, Fe4: $\left(0,\frac{1}{2},\frac{1}{2}\right)$
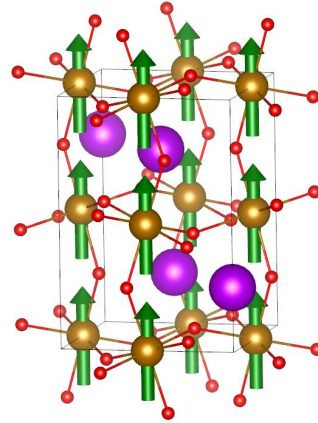
(1) 1   (2) 2(0.5,0,0) x,0.25,0   (3) 2(0,0,0.5) 0,0,z (4) 2(0,0.5,0) 0.25,y,0.25
(5) -1   0,0,0   (6) b 0.25,y,z (7) m x,y,0.25   (8) n(0.5,0,0.5) x,0.25,z

a) Identify reflection conditions of the space group

b) Identify any additional reflection conditions of the Fe sublattice

c) Identify symmetry relations between Fe sites

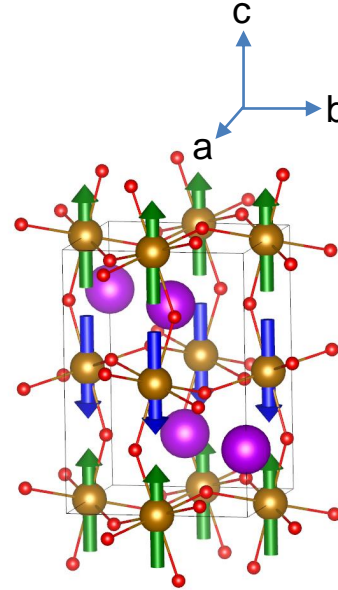d) Calculate the structure factor of the 4 magnetic structures

$$\boldsymbol{M}_{uc}(\boldsymbol{Q}) \propto \sum_{d} \boldsymbol{\mu}_d \exp(i\boldsymbol{Q}.\boldsymbol{d})$$

e) Identify magnetic reflection conditions of the 4 magnetic structures
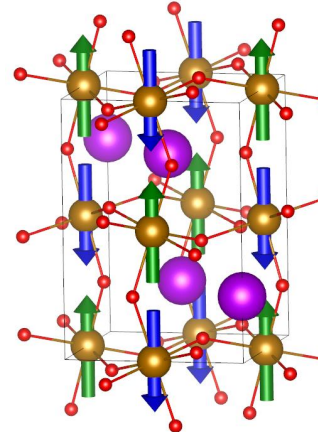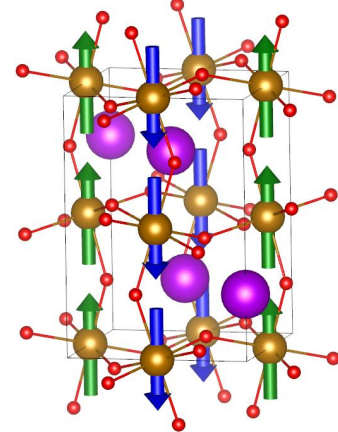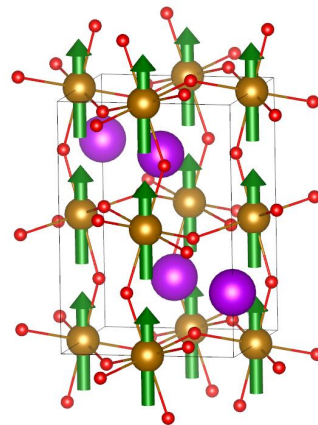
f) Relate answer (e) to the answers (a-c)

Neutron powder diffraction: REFeO$_3$

Pbnm   Fe1: $\left(\frac{1}{2},0,0\right)$, Fe2: $\left(0,\frac{1}{2},0\right)$, Fe3: $\left(\frac{1}{2},0,\frac{1}{2}\right)$, Fe4: $\left(0,\frac{1}{2},\frac{1}{2}\right)$

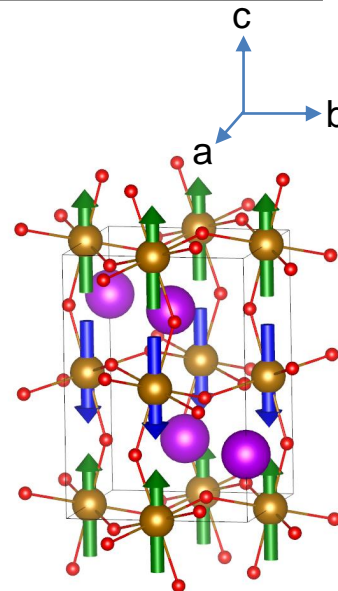(1) 1   (2) 2(0.5,0,0) x,0.25,0   (3) 2(0,0,0.5) 0,0,z (4) 2(0,0.5,0) 0.25,y,0.25
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a)   Identify reflection conditions of the space group

b)   Identify any additional reflection conditions of the Fe sublattice

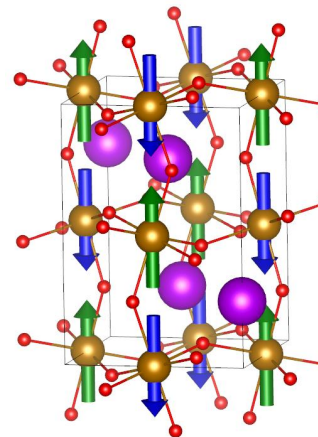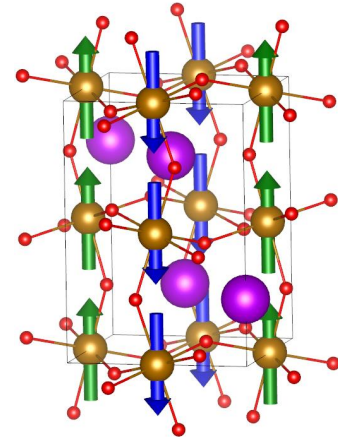c)   Identify symmetry relations between Fe sites

F: A:

G: C:

Neutron powder diffraction: $REFeO_3$

a) Identify reflection conditions of the space group ($Pbnm$)

b-glide: $0kl$: $k = 2n$ n-glide: $h0l$: $h+l = 2n$

$2_1^{(x)}$: $h00$: $h = 2n$ $2_1^{(y)}$: $0k0$: $k = 2n$ $2_1^{(z)}$: $00l$: $l = 2n$

b) Identify any additional reflection conditions of the Fe sublattice

hkl: $h+k = 2n$ hkl: $l = 2n$

c) Identify symmetry relations between Fe sites

Fe1 <-> Fe2: b, $2_1^{(x)}$ Fe1 <-> Fe3: m, $2_1^{(z)}$ Fe1 <-> Fe4: n, $2_1^{(y)}$

Fe2 <-> Fe3: n, $2_1^{(y)}$ Fe2 <-> Fe3: m, $2_1^{(z)}$

Fe3 <-> Fe4: b, $2_1^{(x)}$

Neutron powder diffraction: $REFeO_3$

d) Calculate the structure factor of the 4 magnetic structures

e) Identify magnetic reflection conditions of the 4 magnetic structures
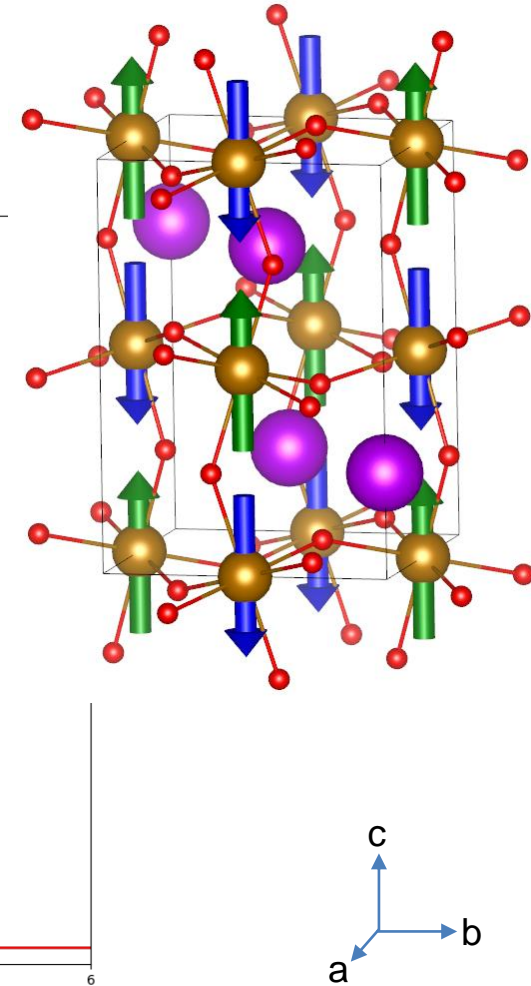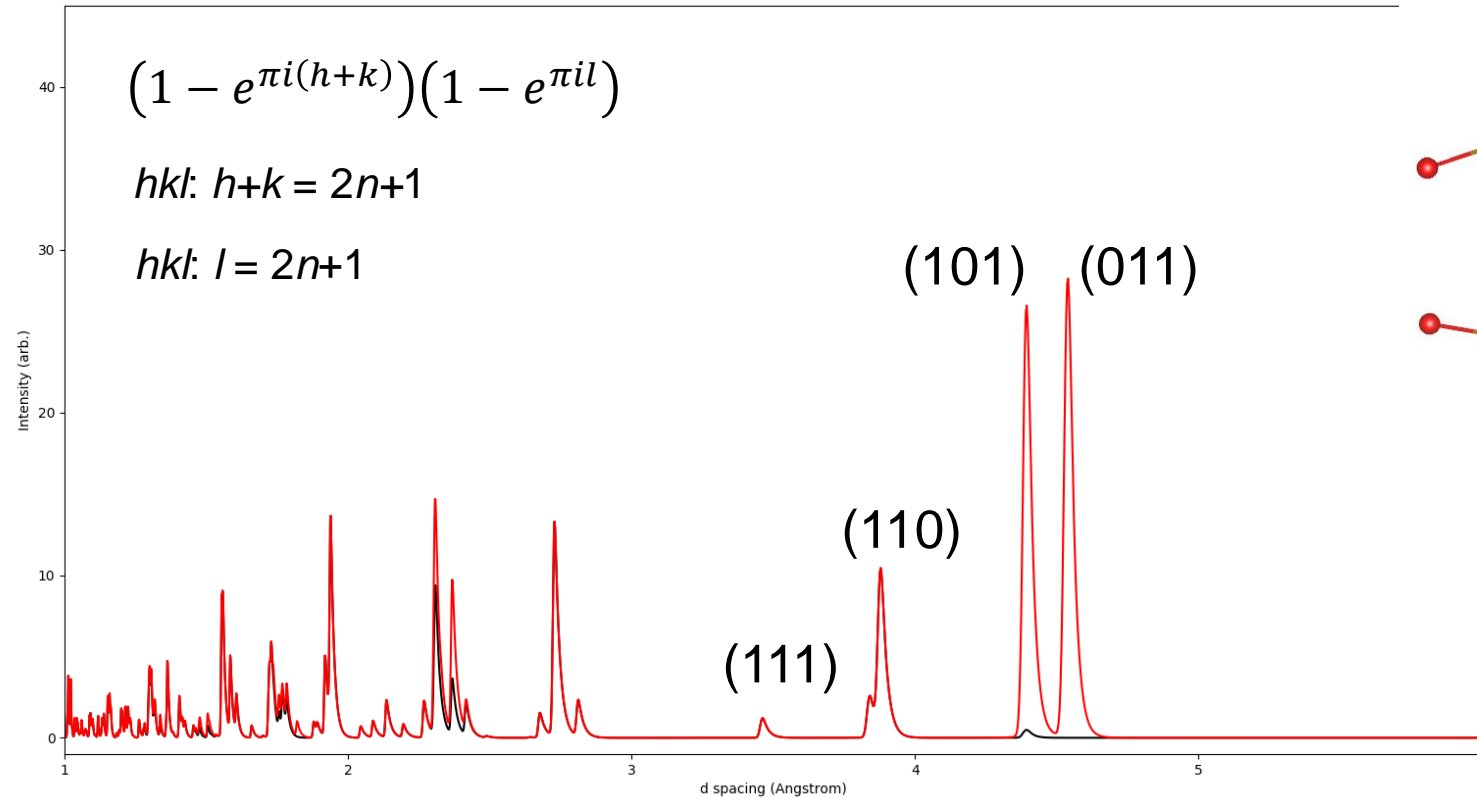
Neutron powder diffraction: F
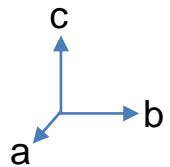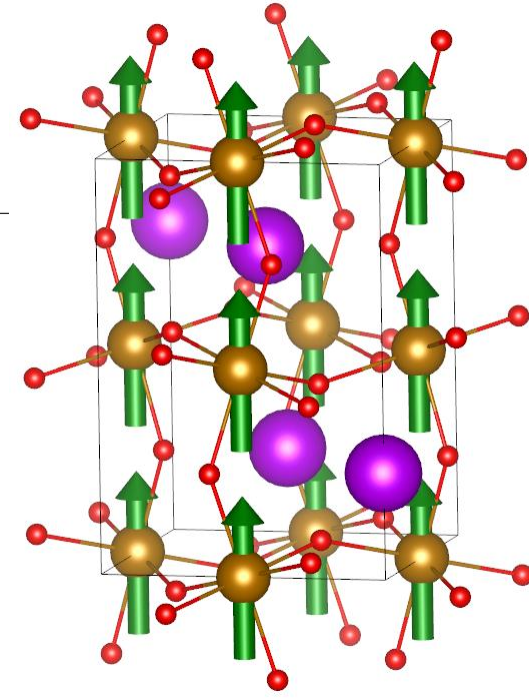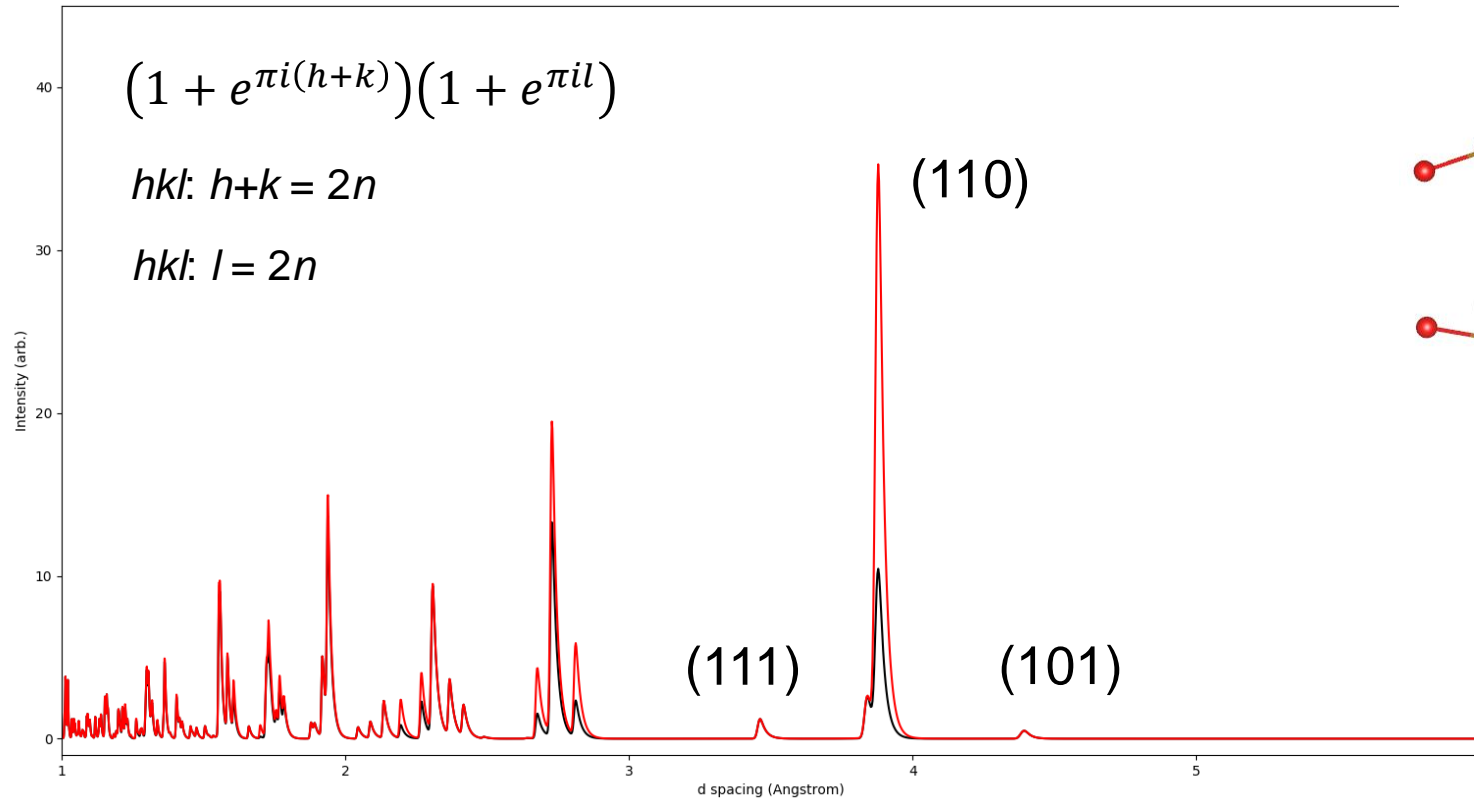
$$\left(1 + e^{\pi i(h+k)}\right)\left(1 + e^{\pi i l}\right)$$

hkl: *h+k = 2n*

hkl: *l = 2n*

(110)

(111)

(101)

Neutron powder diffraction: G

$$\left(1 - e^{\pi i(h+k)}\right)\left(1 - e^{\pi i l}\right)$$

hkl: $h+k = 2n+1$

hkl: $l = 2n+1$

(101)   (011)

(110)

(111)

Intensity (arb.)

d spacing (Angstrom)

c

b

a

Neutron powder diffraction: A

$$\left(1 + e^{\pi i(h+k)}\right)\left(1 - e^{\pi i l}\right)$$

hkl: *h+k* = 2*n*

hkl: *l* = 2*n*+1

(111)

(201)

(110)

(101)

Intensity (arb.)

d spacing (Angstrom)

c

b

a

Neutron powder diffraction: C

$$\left(1 - e^{\pi i(h+k)}\right)\left(1 + e^{\pi il}\right)$$

hkl: *h+k = 2n+1*

hkl: *l = 2n*
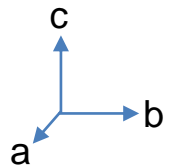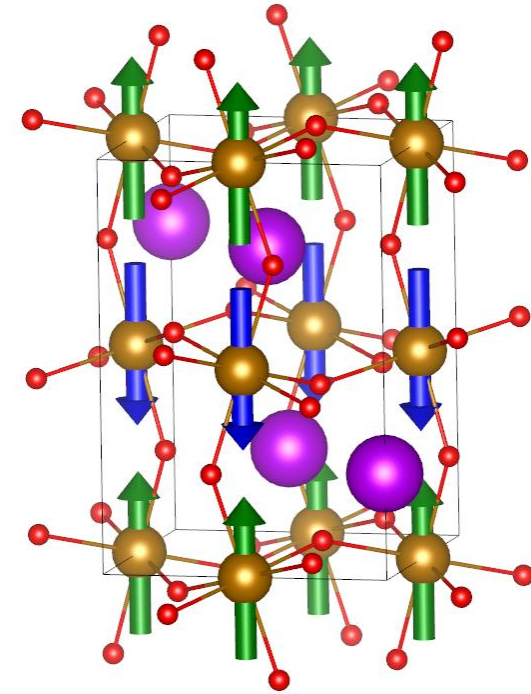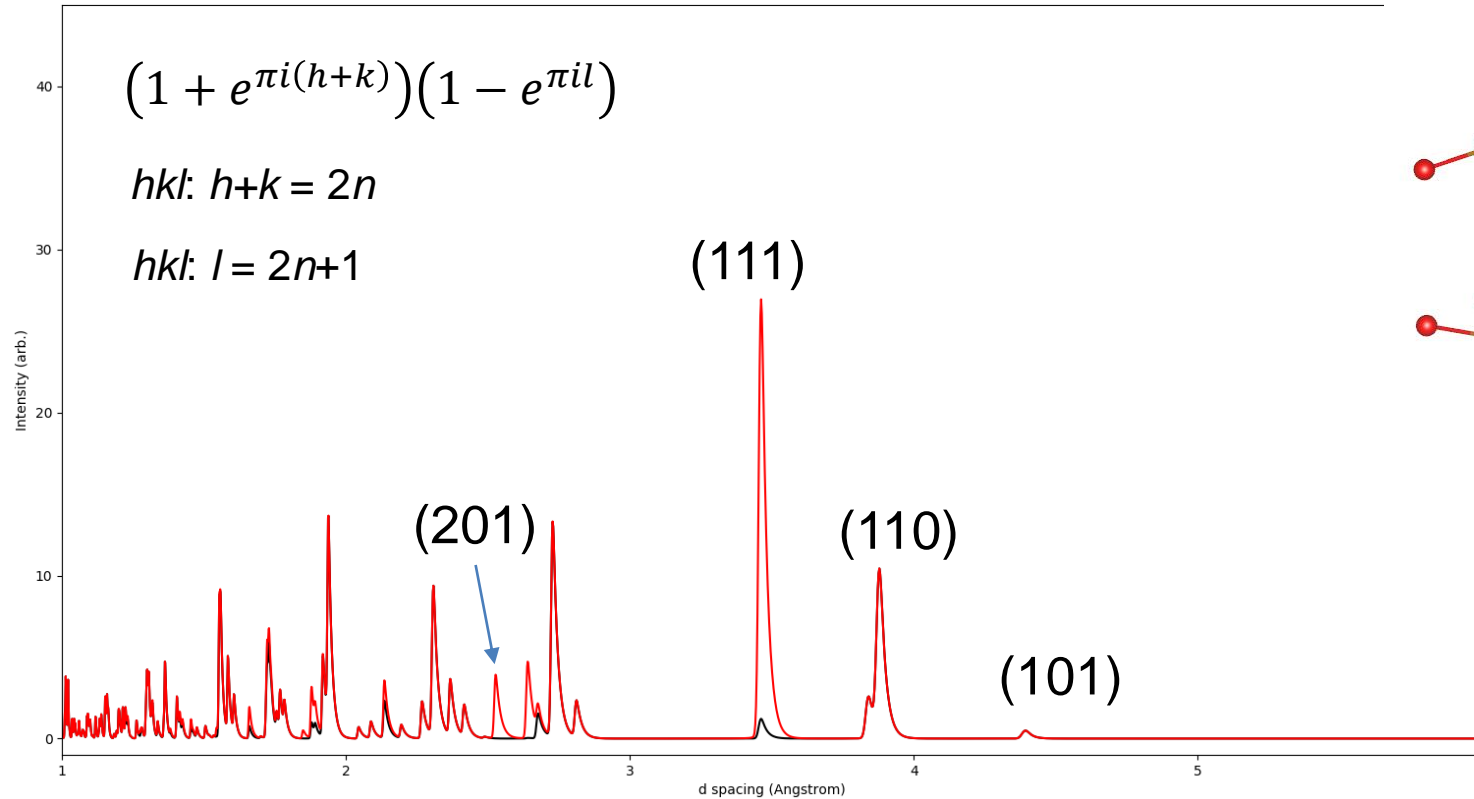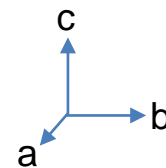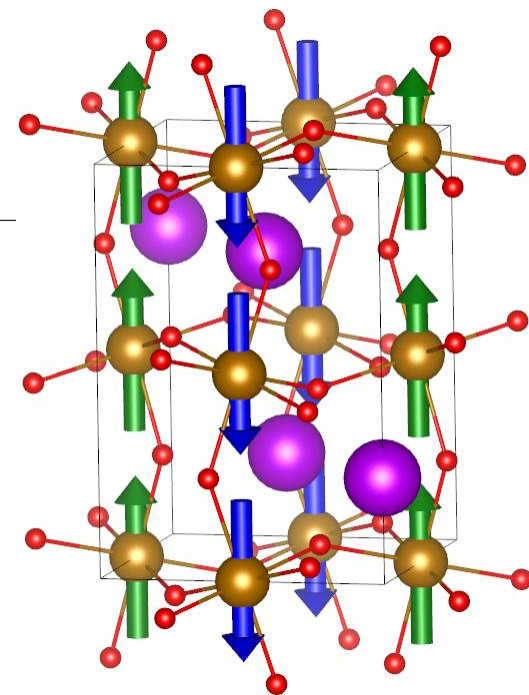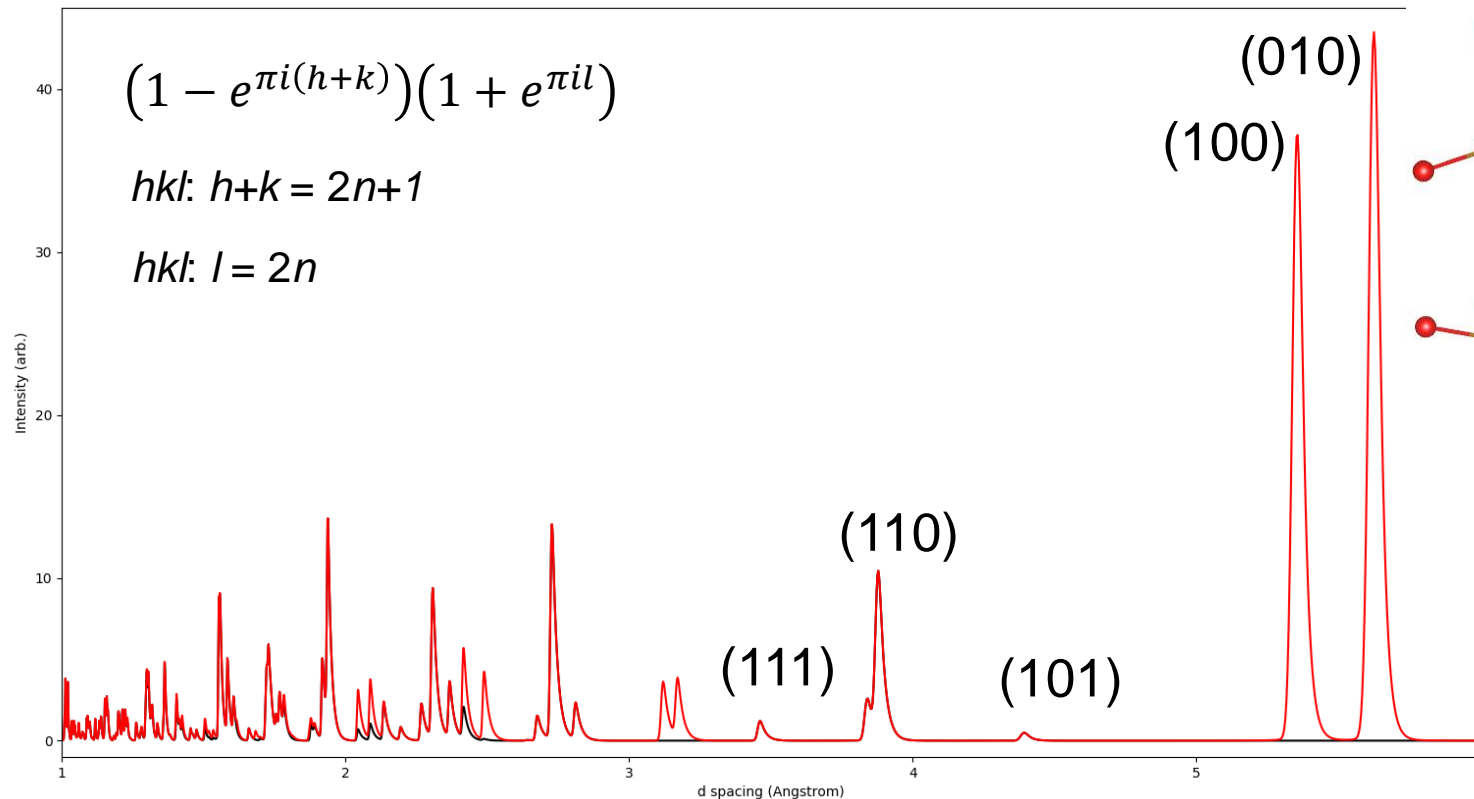
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b) Identify any additional reflection conditions of the Fe sublattice

hkl: $h+k = 2n$ hkl: $l = 2n$

c) Identify symmetry relations between Fe sites

Fe1 <-> Fe2: b, $2_1^{(x)}$ Fe1 <-> Fe3: m, $2_1^{(z)}$ Fe1 <-> Fe4: n, $2_1^{(y)}$

Fe2 <-> Fe3: n, $2_1^{(y)}$ Fe2 <-> Fe3: m, $2_1^{(z)}$

Fe3 <-> Fe4: b, $2_1^{(x)}$

$$\left(1 + e^{\pi i(h+k)}\right)\left(1 + e^{\pi i l}\right)$$

hkl: $h+k = 2n$

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Fe3 <-> Fe4: b, $2_1^{(x)}$

$$\left(1 - e^{\pi i(h+k)}\right)\left(1 - e^{\pi i l}\right)$$

hkl: $h+k = 2n+1$

hkl: $l = 2n+1$