Argonne NATIONAL LABORATORY

Defining & Fitting Magnetic Models in GSAS

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GSAS Implementation of Magnetism

- GSAS allows 4 types of structural models (phases)
  1) Nuclear (no magnetism)
  2) Magnetic only (no nuclear scattering)
  3) Combined Nuclear & Magnetic
  4) Macromolecular (no magnetism, duh!)
- GSAS does not implement edge centering
  - Must use a doubled cell instead
  - This leads to challenges in coupling magnetic and nuclear symmetry
- Almost no magnetism implementation in EXPGUI
  - must use EXPEDT

Input of Magnetic Symmetry

- Define a [normal] Hermann-Mauguin space group
- Designate phase as magnetic
- In appropriate submenu, designate which of the unique operators will be red (antisymmetry). Default is black.
  - Note that not all combinations are allowed in GSAS because of group theory rules, but don't count on GSAS to prevent use of invalid input

Input Parameters for Magnetic Atoms

- Atoms in magnetic phases can be flagged as magnetic
- Magnetic atoms have three extra parameters: Mx, My, Mz
  - These are orthogonal spin components:
    - *Mx -- along* a *axis*
    - *My -- along b* axis (perpendicular to* a & c, e.g. *direction of* a x c*)*
    - *Mz -- in* a-c *plane and perpendicular to* a *(direction of* a *x* b**)*
  - For non-orthogonal systems, can use program GEOMETRY to see components computed in other directions
- GSAS will constrain components according to color symmetry
- Magnetic atoms will have an additional refinement flag, M
  - M varies Mx, My and (or) Mz as allowed by color symmetry

Other magnetism input for GSAS

- You must use the magnetic symmetry menu in GSAS even if you do not need to toggle any symmetry to red --- otherwise magnetic intensities are not computed
- Magnetic form factors: GSAS has a table with form factors from the "ILL Blue Book"
  - This does not include all possible magnetic ions
  - Make sure to enter the magnetic ions with the right valence (e.g. FE+3 not FE) or you will get the wrong form factor.
  - To see what is defined in GSAS, check for magnetic form factors in file c:\GSAS\DATA\ATMDATA.DAT
    - *Look for lines that begin "*XX+n M*" and "*XX+n N*"*

Strategies - 1

Since magnetic symmetry can be lower than that of the nuclear structure, how does one perform a fit?

1. Use two phases with different symmetry
   - *Constrain cell lengths between phases*
   - *Constrain magnetic atom positions to be the same between phases*
   - *Constrain magnetic atoms to special positions for the higher symmetry*
2. Use a single phase with the lower magnetic symmetry, but constrain crystallographically identical atoms to move together and stay on special sites

Strategies - 2

- GSAS does not implement all magnetic space groups directly (no edge centers)
  - Increase size of magnetic unit cell
  - Decrease phase fraction by $V_{nuclear}/V_{magnetic}$ (or refined moments will be incorrectly scaled)
  - Manually constrain moments of non-unique atoms

This is not automatic, it takes thought and sometimes some trial and error.

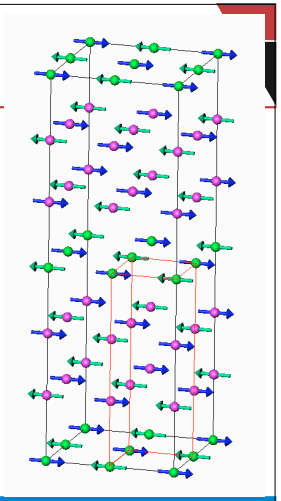
Strategies - 3

- Some people prefer to not deal with magnetic symmetry at all
  - Use magnetic cell with *P*1 symmetry (see 3rd example)
    - *Easy to build a model; hard to do refinements (lots of constraints)*
    - *OK for simpler structures, but use care to get it right*

Self-guided exercises

Same structure worked three ways

1. Use *Pmmm* for nuclear phase; use *Fmm'm'* (2x2x2) for magnetic phase (2 phases)
2. Use *Fmm'm'* for nuclear and magnetic scattering (single phase)
3. Use *Pmmm* for nuclear phase; use *P*1 (2x2x2) for magnetic phase (2 phases)



Other things to try

- List the generated magnetic spin directions with program GEOMETRY
- Visualize spin directions with VRSTPLOT and a VRML viewer
  - You will likely need to install VRweb from key (or other VRML 1.0 viewer like CosmoPlayer)
- Visualize spin directions with DRAWxtl (software on key)