X-ray diffraction – structure analysis

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Inorganic materials chemistry and functional materials

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Lectures at CUTN spring 2016
X-ray diffraction and structure analysis
Peak Intensities

- Many variables, some instrumental, some **sample dependent**
  - Instrument geometry and optics (transmission, reflection)
  - Radiation choice ($\lambda$ in the Bragg equation)
  - Lorentz polarisation

- **Sample (crystal structure & symmetry)**
  - Atom type and position in the structure (scattering and structure factors)
  - Occupation number - Site multiplicity (from space group)
  - Thermal displacement parameters
  - Absorption
  - Fluorescence (background; signal-to-noise)

- Sample preparation
  - Poor preparation gives poor data!
  - Preferred orientation
  - Particle size (nanopowders)
Systematic absences (systematic extinctions) arise when symmetry elements containing translational components are present

- **Lattice centering;** A, B, C, F, I Bravais lattices
- **Screw axes**
- **Glide planes**

The specific rules can be identified from the observed diffraction pattern and applied as to select the likely space group for the compound under study.

**Translations:** the same structure elements are repeated somewhere and this opens a possibility of destructive interference for certain diffraction planes (hkl)
Ray R1 hits the corner atom A of the unit cell.

Ray R3 reflects from atoms in positions within the unit cell.

\[
\delta_{R_1 R_3} = (R - B - S) = \frac{AB}{AC} \lambda = \frac{x}{a} \lambda
\]

\[
d_{h00} = \frac{a}{h}
\]

\[
\delta_{R_1 R_2} = (M - C - N) = 2d_{h00} \sin(\theta) = \lambda
\]

Phase \[\varphi_{R_1 R_3} = \frac{2\pi}{\lambda} \frac{x}{a} \lambda = 2\pi h \frac{x}{a} = 2\pi hx'\] for \(x'\) fractional coordinate

In 3-dimensions one will obtain \(\varphi = 2\pi (hx' + ky' + hz')\)
The sum of all waves scattered by all atoms in the unit cells has a resultant amplitude which depends on the scattering plane (hkl).

The resultant unit cell scattering factor is termed the **Structure Factor** \( F \).

When summarizing the scattering amplitudes for all atoms, these must be weighed by the respective atomic scattering factors \( f \), which strongly depends on nb of electrons in the X-ray scattering case.

\[
F_{n}^{hkl} = \sum_{j=1}^{n} f_{j} e^{i\varphi_{j}} = \sum_{j=1}^{n} f_{j} e^{i[2\pi(h x_{j}'+k y_{j}'+h z_{j}')]}
\]

\[
F = \text{Structure Factor} = \frac{\text{Amplitude of wave scattered by all atoms in unit cell}}{\text{Amplitude of wave scattered by an electron}}
\]

**Diffraction intensity** \( I \propto F^{2} \)

**Note:**

The structure factor depends on atomic coordinates \((x,y,z)\), type of atoms (atomic scattering factor), site occupancy, BUT independent of *shape* and *size* of unit cell \((a,b,c)\).
Using the **structure factor** to evaluate **systematic extinctions** for a body centered orthorhombic (I) structure

\[ F = f_j e^{i\varphi_j} = f_j e^{i[2\pi(h x'_j + k y'_j + h z'_j)]} \]

Bravais lattice \((0,0,0) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\); (plus any motif \((x_i, y_i, z_i)\))

\[ F_{hkl}^n = \sum_{j=1}^{n} f_j e^{i\varphi_j} = \sum_{j=1}^{n} f_j e^{i[2\pi(h x'_j + k y'_j + h z'_j)]} \]

Now summarizing over (just) the two atoms at \((0,0,0)\) and \((\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\):

\[ F = f e^{i[2\pi(h\cdot0 + k\cdot0 + h\cdot0)]} + f e^{i[2\pi(h\cdot\frac{1}{2} + k\cdot\frac{1}{2} + h\cdot\frac{1}{2})]} \]

\[ = f e^0 + f e^{i[2\pi(\frac{h+k+l}{2})]} = f[1 + e^{i\pi(h+k+l)}] \]

**Note:** \(e^{n\pi}\)

- = -1 for \(n\) odd
- = +1 for \(n\) even

For \((h+k+l)\) odd, \(F = 0\) and \(I = F^2 = 0\); e.g. \((100), (001), (111); (210), (032), (133) will be systematically absent (extinctions)\)

Whereas, for \((h+k+l)\) even, \(F = 2f\) and \(I = F^2 = 4f^2\), and Bragg reflections like \((110), (200), (211); (220), (022), (310)\) are allowed (have non-zero intensities)
X-ray diffraction; methods and analyses

Body-centered cubic (bcc)

Cubic lattice with vectors $a_x$, $a_y$, $a_z$.
Basis (atoms) at $r_0 = 0$ and $r_1 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

$$F_{hkl} = \begin{cases} 2f, & h + k + l \text{ even} \\ 0, & h + k + l \text{ odd} \end{cases}$$

A requirement for a reflection to appear in the diffraction pattern of a body-centered crystal, is that the sum of the Miller indices $(hkl)$ must be even. If the sum is an odd number, the intensity is zero due to destructive interference.

Systematic extinction
This rule applies to all I-centered structures!

Hence, the first diffraction peak to be observed in a powder diffraction pattern will be (110) followed by (200) and (211)
## Extinction Rules; lattices

<table>
<thead>
<tr>
<th>Bravais lattice</th>
<th>Reflections that <em>are allowed</em>, and maybe observed</th>
<th>Systematic absences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primitive (P)</td>
<td>all</td>
<td>None</td>
</tr>
<tr>
<td>Body centred (I)</td>
<td>((h + k + l)) even</td>
<td>((h + k + l)) odd</td>
</tr>
<tr>
<td>Face centred (F)</td>
<td>(h, k, l) all even / all odd</td>
<td>(h, k, l) mixed odd/even</td>
</tr>
<tr>
<td>Side centred (A,B,C)</td>
<td>(h + k) even (C) centred</td>
<td>(h + k) odd (C) centred</td>
</tr>
</tbody>
</table>

### Additional Extinction Rules;

Translations: screw axis / glide planes
X-ray diffraction; methods and analyses

For this symmetry operator certain intensities will cancel (become zero).
→ We consider the structure factor

\[ F = f \cos 2\pi (hx + ky + lz) + f \cos 2\pi (-hx - ky + l[(1/2) + z]) \]
Taking into account \( \cos a + \cos b = 2 \cos (a+b)/2 \cos (a-b)/2 \), we obtain
\[ F = 2f \cos \pi (2lz + l/2) \cos \pi (2hx + 2ky - l/2) \]

\[ F = 2f \cos \pi (2lz + l/2) \cos \pi (20x + 20y - l/2) \Rightarrow \cos \pi (-l/2) \]
This vanishes \( (F=0) \) for \( hkl \) reflections with \( h=0, k=0 \) and \( l=2n+1 \).
This defines the systematic absences owing to the given screw axis.

We may observe intensity for reflections of type \( 00l \) with \( l=2n \), but not for \( l=2n+1 \)

<table>
<thead>
<tr>
<th>2₁[100]</th>
<th>h00</th>
<th>h = 2n</th>
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<tbody>
<tr>
<td>2₁[010]</td>
<td>0k0</td>
<td>k = 2n</td>
</tr>
<tr>
<td>2₁[001]</td>
<td>00l</td>
<td>l = 2n</td>
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</table>
Space Group Determination

- Crystal symmetry is described by space groups
- Space groups describes the essential symmetry in terms of:
  - Bravais lattice centering
  - Mirror planes, inversion centres and rotation axes from molecular symmetry (crystallographic point groups)
  - Translational symmetry (periodic lattices only): Screw axes and glide planes

- Centring and translational symmetry elements lead to further interference phenomena in the diffraction pattern: **Systematic absences**

- Systematic absences are used to determine the space group based on the diffraction pattern:
  - Challenging, limited number of observations in powder data (single crystal is much easier)
  - Usually done with software
Systematic absences
(systematic extinctions) – space groups

**EXAMPLE:**
The following extinction rule is likely based on careful analysis of a diffraction pattern for an orthorhombic sample (powder XRD data):

\[
\begin{align*}
hkl: & \quad \text{none} \\
0kl: & \quad k+l=2n \\
hk0: & \quad h=2n \\
h00: & \quad h=2n \\
0k0: & \quad k=2n \\
00l: & \quad l=2n
\end{align*}
\]

i.e. we have fully indexed the diffraction pattern, we know \((hkl)\) for all observed diffraction peaks, and we believe to have identified a system for (some) peaks with zero intensity. There is NO observation of any peak that contradicts the proposed rules.

Which space groups could be possible?

What may we suggest based on the examples provided above?

**Any I, F, A, B, C centering?**

**Any screw axes?**
### “Our” likely extinctions:

- **hkl:** none
- **0kl:** $k+l=2n$
- **hk0:** $h=2n$
- **h00:** $h=2n$
- **0k0:** $k=2n$
- **00l:** $l=2n$

Using the International Tables of Crystallography to find the likely space group options.
Mn$_{0.63}$Cr$_{0.37}$As 10 K
Synchrotron radiation
Swiss Norwegian Beam Line
Grenoble 2001

X-ray diffraction; methods and analyses
Obtaining crystal structure information from powder diffraction data

**Step 1: Indexing of diffraction pattern** (TREOR, ITO, DICVOL, SIRPOW,..)
- Obtain suggestions for possible unit cell
- Evaluate thoroughly; figure of merit (size of cell relative to nb. peaks)

**Step 2: Profile fitting** (Le Bail fitting) (various Rietveld type codes)
- Are all peaks fitted?
- Evaluation of possible systematic extinctions
- Evaluation of likely space groups

**Step 3: Sample composition – chemical formula**
- Databasis: any isostructural compound already described (known structure)

**Step 4: Rietveld type analysis**: refining the crystal structure based on a model
Refinements according to the method described by H. Rietveld

Instrumental/sample dependent parameters
- Absorption
- Zero point or height error
- Peak width
- Background

Crystallographic parameters
- Unit cell dimensions
- Atomic coordinates
- Occupation numbers
- Displacement parameters

Step 1: Determine background – introduce corrections/models
Step 2: Optimize unit cell dimensions and zero point / height error
Step 3: Manually adjust peak width parameters to provide at least fair fit to the observed intensity profiles
Step 4: Refine atomic coordinates; heavy atoms first
Step 5: Refine peak width parameters
Step 6: Refine thermal displacement parameters (and occupation nb)
X-ray diffraction; methods and analyses

FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-ray and/or neutron data

Introduction • What’s new • Programs • Downloads • Examples & Tutorials • Support • References

The FullProf Suite (for Windows and Linux) is formed by a set of crystallographic programs (FullProf, WinPLOTR, EdPCR, GFourier, etc...) mainly developed for Rietveld analysis (structure profile refinement) or profile matching (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2\theta.

The programs can be run either in stand alone form (from a console window or clicking directly in a shortcut) or from the interfaces WinPLOTR and/or EdPCR.

The programs within the FullProf Suite are distributed in the hope that they will be useful, but WITHOUT ANY WARRANTY of being free of internal errors. In no event will the authors (or their employers) be liable to you for damages, including any general, special, incidental or consequential damages arising out of the use or inability to use the programs (including but not limited to loss of data being rendered inaccurate or losses sustained by you or third parties or a failure of the program to operate with any other programs). The authors are not responsible for erroneous results generated with the programs.

Welcome to the GSAS homepage here on CCP14

To install GSAS follow the links below which will take you to Brian Toby’s Trac website and to APS where the software can be downloaded with accompanying instructions.

The reference to use for GSAS in any resulting publications is:
Contact: Bob von Dreele - vondreele@anl.gov

The reference to use for EXPGUI in any resulting publications is:
Contact: Brian Toby - brian.toby@anl.gov
Mn\(_{0.63}\)Cr\(_{0.37}\)As at 10, 150, 200, 295 K

Synchrotron radiation
Swiss Norwegian Beam Line
Grenoble 2001
295 K: Paramagnetic

226 K: 2.Order para – antiferromagnetic transition (incommensurate $H_c$ spiral)

Around 160 K 1.Order magnetostructural phase transition (at LT: incommensurate $H_a$ spiral)

Large jumps in the unit cell dimensions $\Delta V \neq 0$
Practical exercise

Rietveld analysis of powder synchrotron data, for
(a) Orthorhombic MnP-type Mn$_{0.63}$Cr$_{0.37}$As solid solution (Pnma)
(b) LaCoO$_3$ rhombohedral perovskite in hexagonal setting (R-3cH)

Data files and input parameters:

**Mn$_{0.63}$Cr$_{0.37}$As at 230 K**: a/b/c approx: 5.645/3.561/6.239 Å
Atomic coordinates as given for MnP-type in the compendium
Raw data (format 10 in Fullprof): 230K.epf

**LaCoO$_3$ at 115 K**: a and c approximately 5.430 and 13.035 Å
La: 0,0,1/4
Co: 0,0,0
O: 0.554 0 ¼
Raw data (format 10 in Fullprof): LaCoO$_3$ _115K_nofield_1.dat
X-ray diffraction; methods and analyses

COMM Mn63Cr37As old SNBL data 2001 LOW-T cryostat capillary mode
! Current global Chi2 (Bragg contrib.) = 29.07
! Files => DAT-file: 230K, PCR-file: 230k

Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
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!

! Ipr Ppl loc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
  0 0 1 0 2 0 4 0 0 -3 10 0 0 0 0 0 0 0
!

! lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolarz -> Patt# 1
  0.499900 0.000000 0.00000 20.000 15.0000 0.9100 0.0000 0.00 0.0000
!

!NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
  20 0.05 0.20 0.20 0.20 0.20 9.0360 0.003000 36.4920 0.000 0.000
!

! 2Theta/TOF/E(Kev) Background for Pattern# 1 (Nba number of background points)
  9.0677 223.0543 0.00
!

! Excluded regions (Nex number of such intervals)
  0.00 9.00
  36.60 45.00
14  !Number of refined parameters
!  Zero    Code    SyCos    Code    SySin    Code  Lambda     Code MORE -&gt; Patt# 1
-0.00584  81.0  0.00000  0.0  0.00000  0.0  0.499700  0.00  0

! Data for PHASE number:  1  ==> Current R_Bragg for Pattern#  1:    25.68
!

**Mn0.63Cr0.37As 230K**
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
   2  0  0 0.0 0.0 1.0  0  0  0  0  0      15396.344  0  1  0
!

**P n m a**  

Space group symbol
!

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<th>2Th2/TOF2</th>
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</table>
Space group Pnma, Nb. 62

General 8-fold position \(x, y, z\); Wückoff symbol 8d

These are the eight points that we identified when analyzing the space group symmetry.

Special positions; lower multiplicity; here termed 4a, 4b, 4c

We can obtain these by inserting special values for one or more coordinates in the expressions for the general position.
X-ray diffraction; methods and analyses

COMM LaCoO3 SNBL 115K
! Current global Chi2 (Bragg contrib.) = 14.58
! Files => DAT-file: lacoo3_115k_nofield_1, PCR-file: lacoo3_115k_nofield_1
! Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut 0 7 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
! Ipr Ppl loc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana 0 0 1 0 1 0 4 0 0 -3 10 0 0 0 0 0 0
! lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolarz -> Patt# 1 0.499999 0.000000 0.00000 20.0000 8.00000 0.91000 0.00000 0.00 0.00000
!NCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0 10 0.10 1.00 1.00 1.00 1.00 3.0600 0.005001 40.4850 0.000 0.000
! Excluded regions (LowT HighT) for Pattern# 1
3.00 3.50
!
17 !Number of refined parameters
! Zero Code SyCos Code SySin Code Lambda Code MORE -> Patt# 1
-0.01114 51.0 0.00000 0.0 0.00000 0.0 0.499999 0.00 0
! Background coefficients/codes for Pattern# 1
108.36 10.992 31.198 -344.50 399.57 -72.637
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!-------------------------------------------------------------------------------
### X-ray diffraction; methods and analyses

**LaCoO₃**

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<th>Pr2</th>
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`R -3 c`  
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Profile Parameters for Pattern # 1

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</tr>
</tbody>
</table>

Profile Parameters for Pattern # 2

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<th>V</th>
<th>W</th>
<th>X</th>
<th>Y</th>
<th>GauSiz</th>
<th>LorSiz</th>
<th>Size-Model</th>
</tr>
</thead>
<tbody>
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<td>-0.001047</td>
<td>0.000270</td>
<td>0.018961</td>
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<tr>
<td>121.0000</td>
<td>131.0000</td>
<td>61.0000</td>
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</tbody>
</table>

Cell Info

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<th>b</th>
<th>c</th>
<th>alpha</th>
<th>beta</th>
<th>gamma</th>
<th>#Cell Info</th>
</tr>
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<td>90.000000</td>
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