Jana2006

Program for structure analysis of crystals periodic in three or more dimensions from diffraction data

after four years of development

Václav Petříček, Michal Dušek & Lukáš Palatinus
Institute of Physics, Prague, Czech Republic
Institute of Physics, Prague 6, Cukrovarnická street
History

1980 SDS
*Program for solution and refinement of 3d structures*

1984 Jana
*Refinement program for modulated structures*

1994 SDS94 and Jana94
*Set of programs for 3d (SDS) and modulated (Jana) structures running in text mode.*

1996 Jana96
*Modulated and 3d structures in one program. Graphical interface for DOS and UNIX X11.*

1998 Jana98
*Improved Jana96. First widely used version. Graphical interface for DOS, DOS emulation and UNIX X11*

2000 Jana2000
*Support for powder data and multiphase refinement. Graphical interface for Win32 and UNIX X11.*

2006 Jana2006
*Combination of data sources, magnetic structures, TOF data. Dynamical allocation of memory. Only for Windows.*
Where to start?

Specify type of the file to be imported:
- known diffractometer formats
- reflection file corrected for LP and absorption

Data reduction file from:
- smazat.hkl
- _CAD4
- _Monius-CCD
- _Siemens P4
- _Bruker-CCD
- _Oxford Diffraction-CCD
- _Oxford Diffraction-PD
- _Rigaku-CCD
- _Sutter format
- PSI format
- Free format of $hkl, F(hkl)$
- Debye-Scherrer method
- Bragg-Brentano method - Fixed Divergence Slit
- Bragg-Brentano method - Variable Divergence Slit
- Another/unknown method
Data input

X-rays OR neutrons OR electrons

OR

Powder data of one or more phases

OR

Single crystal data of one or more domains

Import Wizard

Format conversion, cell transformation, sorting reflections to twin domains

Data Repository

Data repository

<table>
<thead>
<tr>
<th>File</th>
<th>Type</th>
<th>Radiation</th>
</tr>
</thead>
<tbody>
<tr>
<td>ba5co6_neutrons.m92</td>
<td>Powder CW</td>
<td>Neutrons 1.594</td>
</tr>
<tr>
<td>be6co6co16.xy</td>
<td>Powder CW</td>
<td>X-rays 1.54051</td>
</tr>
<tr>
<td>D:\PASCAL\sadceninject.hkl</td>
<td>(hkl) imported</td>
<td>X-rays Mo K(\alpha)</td>
</tr>
</tbody>
</table>

[Buttons: Info, Reimport, Modify, Delete, Undelete, Import new]
**Program Scheme**

- **Reading of one or more data sets**
  - M95 + M50
    - Determining symmetry, merging symmetry equivalent reflections, absorption correction
    - Refinement of powder profile parameters
  - M90, M41
    - Solution (by calling external programs)
  - M40
    - Refinement
    - Transformation
    - Introduction of twinning
    - Change of symmetry

- Plotting, geometry parameters, Fourier maps ….
Topics

- Basic crystallography
- Advanced tools
- Incommensurate structures
- Commensurate structures
- Composite structures
- Magnetic structures

Jana2006 is still old fashioned: written in Fortran; not using external libraries (except basic graphics); not written by a team of programmers → flexibility

**NOT included in Jana2006:**

**Phase problem solution:** calls SIR97,2000,2004; EXPO, EXPO2004, Superflip

**Plotting:** calls Diamond, Vesta, MC (marching cube) and other plotting software

**Validations and geometry analysis:** relies on Platon
Basic crystallography

Wizards for symmetry determination
External calls to Charge flipping and Direct methods
Tools for editing structure parameters
Tools for adding hydrogen atoms
Constrains, Restains
Fourier calculation
Plotting (by an external program)
CIF output

Under development: graphical tools for atomic parameters, CIF editor
Advanced tools
common for 3d and modulated structures

Fourier methods

Transformation tools, group-subgroup relations
Twinning (merohedric or general), treating of overlapped reflections

User equations and restrictions

Disorder and “Rigid body” approach
Anharmonic ADP

Multiphases for both powder and single crystal data

Multipole refinement

Powder data:
Anisotropic strain broadening (generalized to satellites)
Fundamental approach
TOF data

Local symmetry
**Twinning** (pseudo-merohedric three-fold twin)

Twinning matrices for data indexed in hexagonal cell:

\[
\begin{pmatrix}
-1 & 0 & 0 \\
0 & -\frac{1}{2} & \frac{1}{2} \\
0 & \frac{3}{2} & \frac{1}{2}
\end{pmatrix}
\]

\[
\begin{pmatrix}
-1 & 0 & 0 \\
0 & -\frac{1}{2} & -\frac{1}{2} \\
0 & -\frac{3}{2} & \frac{1}{2}
\end{pmatrix}
\]
Disorder of tert-butyl groups in N-(3-nitrobenzoyl)-N', N''-bis (tert-butyl) phosphoric triamide. The groups were described like split “rigid” bodies. One of rigid body rotation axis was selected along C-N bond in order to estimate importance of rotation along C-N for description of disorder.
Anharmonic description of ADP (ionic conductor $\text{Ag}_8\text{TiSe}_6$)

Plot: Jana calculates electron density map and calls Marching Cube.
Local icosahedral symmetry for atom C of C₆₀
Single crystal multiphase systems

View along \(\mathbf{a}\)

\(\blacktriangleright\) Lindströmite

View along \(\mathbf{a}\)

Krupkaite \(\blacktriangleright\)
Incommensurate structures

Modulation of occupation, position and ADP
Traditional way of solving from arbitrary displacements
Solving by charge flipping

Modulation of anharmonic ADP
Modulation of Rigid bodies including TLS parameters

Special functions
Fourier sections

Plotting of modulated parameters as a function of t
Plotting of modulated structures
Calculation of geometric parameters
Charge Flipping (Superflip of Lukas Palatinus)
Twinning of modulated structures


Average structure: 4.89 4.89 4.34 90 90 120, P6$_3$/mmc
Modulated structure: modulated composite structure, C2/m($\alpha 0\beta$), 6-fold twinning around the hexagonal c

Reconstruction of (h,k,1.835) from CCD measurement.
Disorder in modulated structures

$\text{Cr}_2\text{P}_2\text{O}_7$, incommensurately modulated phase at room temperature

$\text{Cr}_1 (0.500000, -0.187875, 0.000000)$
$\Delta[\text{Cr}_1] = 1$
New atom: $\text{Cr}_{1a} (0.47, -0.187875, 0.03)$
$t_{40}[\text{Cr}_{1a}] = t_{40}[\text{Cr}] + 0.5 \times \Delta[\text{Cr}_1]$
$\Delta'[\text{Cr}_1] = \Delta[\text{Cr}_1] - x$
$\Delta[\text{Cr}_{1a}] = x$
New parameters for refinement:
x and position of $\text{Cr}_{1a}$
Temperature parameters of $\text{Cr}_{1a}$ can be put equal to $\text{Cr}_1$. No modulation can be refined for $\text{Cr}_{1a}$.
Analogically one can split positions of $\text{P}_1$, $\text{O}_2$ and $\text{O}_3$. Refinement is very difficult, the changes should be done simultaneously.
Commensurate structures

Example of six-fold commensurate structure

**Superspace description**: 4d cell, atomic position + modulation function, superspace symmetry

**Supercell description**: 3d six-fold supercell, atomic positions in six cells, 3d symmetry

Both description are equivalent. Jana2006 can automatically transform commensurate structure to 3d structure in a supercell

Origin of R3 section may influence symmetry in the supercell. Jana2006 can automatically find all possible supercell symmetries.
Commensurate families

In this example known $\text{M}_2\text{P}_2\text{O}_7$ diphosphates are derived from the same superspace symmetry.

Table 6. Survey of the symmetries of the low-temperature phases of diphosphates $M_2P_2O_7$ ($M^{2+} = \text{Mg, Cr, Co, Ni, Cu, Zn}$). The parent superspace group of the structures is $C2/m(\alpha, 0, \gamma)0s$. The symmetry of the supercell can be derived from this superspace group using the tabulated $q$-vector and $t_0$.

<table>
<thead>
<tr>
<th>metal(II)</th>
<th>q-vector</th>
<th>$t_0$</th>
<th>space group of the supercell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr, Zn</td>
<td>$(-\frac{1}{3}, 0, \frac{1}{2})$</td>
<td>0</td>
<td>$I2/c$</td>
</tr>
<tr>
<td>Co, Mg, Ni</td>
<td>$(\frac{1}{2}, 0, \frac{1}{2})$</td>
<td>$\frac{1}{8}$</td>
<td>$B2_1/c$</td>
</tr>
<tr>
<td>Cu</td>
<td>$(0, 0, \frac{1}{2})$</td>
<td>0</td>
<td>$C2/c$</td>
</tr>
</tbody>
</table>
Composite structures

Hexagonal perovskites
Two hexagonal subsystems with common $a, b$ but incommensurate $c$.

$q$ is closely related with composition

$$q = (0, 0, \gamma)$$

$$\gamma = \frac{c_2}{c_1}$$

$$W = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}, \quad H^1 = H^2W$$
Modulated structure of $\text{Sr}_{14/11}\text{CoO}_3$

$q = 0.63646(11) \approx 7/11$


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Fig. 4. Projection along the $c$ axis of the $\text{Sr}_{14/11}\text{CoO}_3$ structure [(3 + 1)-dimensional commensurate model].

Fig. 7. Projection perpendicular to the $c$ axis of one of the $[\text{CoO}_3]$ chains and the neighboring $\text{Sr}$ atoms for the $\text{Sr}_{14/11}\text{CoO}_3$ structure [(3 + 1)-dimensional commensurate model].
Magnetic structures

Magnetic structure factor:

$$\mathbf{F}_m(h) = p \sum_i f_i(h) T_i(h) \mathbf{S}_i \exp(2\pi i \mathbf{h} \cdot \mathbf{r}_i)$$

- $f_i$: magnetic form factor
- $T_i$: temperature factor
- $\mathbf{S}_i$: magnetic moment
- $\mathbf{r}_i$: atomic position

Intensity of magnetic diffraction:

$${I}_m(h) = \mathbf{F}_m^2(h) - \left[ h / h \cdot \mathbf{F}_m(h) \right]^2$$

Total intensity:

$$I(h) = I_\lambda(h) + I_m(h)$$

The distribution of the magnetic moments over the nuclear structure can be described by a modulation wave:

$$\mathbf{S}_i(x_4) = \mathbf{S}_{i0} + \sum_{n=1}^{N} [\mathbf{S}_{ins} \sin(2\pi nx_4) + \mathbf{S}_{ikc} \cos(2\pi nx_4)]$$
**Superspace approach**

The elementary cell of magnetic structure can be the same or different of the cell of the nuclear structure. For the same cell the magnetic reflections contribute to nuclear reflections. For a different cell part of magnetic reflections or all of them form a separate peaks.

The distribution of the magnetic moments over the nuclear structure can be described by a modulation wave:

\[
S_i(x_4) = S_{i0} + \sum_{n=1}^{N} [S_{ins} \sin(2\pi nx_4) + S_{ikc} \cos(2\pi nx_4)]
\]

The structure factor of modulated magnetic structures is similar to that for non-modulated magnetic structure. Each n-th term in the above equation will create magnetic satellites of the order n.

The magnetic cell is often a simple supercell, with q vector (wave vector) having a simple rational component and the structure can be treated like a commensurate one.
For magnetic wave the property is not position but the spin moment. This approach allows for very complicated magnetic structures and for combination of magnetic and nuclear modulation (using the same or more q vectors). Warning: this is a new tool tested with only a few magnetic structures.
**Future development (Jana2012)**

Electron diffraction
Interface
Documentation (hard to believe)

Input of data ➔ Solution

Editing of structure model ➔ Transformations ➔ Fourier calculation and interpretation

External plotting ➔ Calculation of geometry ➔ CIF output ➔ Plotting of modulated parameters

Refinement
User support

jana.fzu.cz

**Ad hoc workshops on Jana:** details here

**March 2011: 7th Workshop in Bayreuth**
Ad hoc workshops on Jana

Ad hoc workshops are small two days workshops organized in Praha by authors of Jana software. As soon as five people register for one or more topics listed below and some overlap in topics is found we shall create program of the workshop and discuss it with the participants. Then we shall fix the date of the workshop and arrange accommodation. Registration to a workshop with fixed program and/or date is possible for another five participants. Participants pay themselves all their expenses and they are expected to bring their own laptops with Windows. The registration fee is zero (in Czech Crowns). Workshop certificates are issued by our skilled artists on demand.

Topics
- (INT1) Introduction to Jana software, solution of simple 3d structures
- (INT2) Introduction to modulated structures, solution of simple 4d structures
- (PVD) Refinement of powder data
- (TV) Twins and multiphases of 3d and modulated structures
- (CHF) Application of charge flipping to 3d and modulated structures
- (DIS) Disorder, mixed sites, application of rigid body refinement for disordered structures
- (RIG) Rigid body refinement and application of local symmetry
- (CRENEL) Discontinuous modulation functions (crenel and sawtooth)
- (COMM) Commensurate structures
- (COMP) Composite structures
- (FIVE) Five dimensional structures
- (MAG) Magnetic structures
- (ELD) Electron diffraction
- any other topic (please specify)

Registration By e-mail to Michal Dusek (dusek@fzu.cz) with list of selected topics, rated by importance. Although the workshop can only have four topics (one topic takes 1/2 of day) the number of selected topics can be higher, it helps finding overlaps. Please indicate if you have already experience with Jana software. New users should select the topic "INT1". For new users of Jana it is also possible to do INT1 as a homework and participate in a more advanced workshop (INT1 cookbook will be sent by e-mail on request).

1st Jana2006 ad hoc workshop Status: Passed.
2nd Jana2006 ad hoc workshop Status: Passed.
3rd Jana2006 ad hoc workshop Status: Passed.
4th Jana2006 ad hoc workshop Status: Passed.
5th Jana2006 ad hoc workshop Two days in October 2010, registration is open.
6th Jana2006 ad hoc workshop Two days in December 2010, registration is open.
Special jana2006 workshop on electron diffraction Two days in 2011, registration is open.
Special jana2006 workshop on magnetic structures Two days in 2011, registration is open.
FUTURE Jana2006 ad hoc workshops This link serves for collecting requirements for future Jana2006 Ad Hoc workshops. As soon as an overlap in topics is found a new Ad Hoc Workshop is organized.
The Sixth Ad Hoc Workshop on Jana2006
Two days in December 2010
Inst. of Physics, Cukrovarnicka 10, Praha 6, Czech Republic
Library Lecture Room at the building A, 2nd floor.

Program
The program is composed of four halfdays. Each halfday starts with a lecture and continues with practical exercises. For practical exercises the users will be provided with a printed cookbook and with a flash disk containing the cookbook, installation files and necessary data. Lecturers for this workshop: Vladav Petricek, Michal Dusak and Lukas Palatinus.

- First halfday, 9h:
  (INT1) Introduction to Jana software, solution of simple 3d structures

- Second halfday:
  (CHF) Application of charge flipping to 3d and modulated structures
  (PVD) Refinement from powder data

- First halfday, 9h:
  (INT2) Introduction to modulated structures, solution of simple 4d structures from single crystal and powder data

- Second halfday:
  (TW) Twins and multiphases

Computers
Each participant should bring a laptop with operating system Windows2000/XP/Vista/Windows7, with Administration rights. Installation of all necessary software will be done at the beginning of the workshop. Wireless internet connection including Eduroam is available at the lecture room. Limited number of computers can be provided to people without laptop (please inform us before the workshop that it would be needed)

Workshop cookbook
Workshop cookbook cumulates examples from all Jana workshops. The latest version together with example files and installations files is available in jana page. cookbook.zip (>100MB). THE LINK IS UPDATED AFTER THE WORKSHOP, NOT BEFORE!

Participants

<table>
<thead>
<tr>
<th></th>
<th>Name</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Isa Doverbratt, Lund</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Carola Muller, Lund</td>
<td></td>
</tr>
</tbody>
</table>

Organizers
The workshop is organized by Department of structure analysis at the institute of Physics and Special interest group on aperiodic crystals at ECA. The date and programme are created in collaboration with participants.

Transportation from the Prague airport "Letiste Ruzynce"
Institute of Physics has two buildings 1.5 km apart. Make sure you are travelling to proper building at Cukrovarnicka street 10, Prague 6.
By taxi: AAA taxi - the yellow cars located in front of terminals - costs approximately 400 CZK, (15 Euro) to "Hotel u Sladku" as well as to the Institute.

CONNECTIONS WILL BE UPDATED!
By public transport: Take bus 179. For the institute change at the station "Vetřlik" to the tram 1, 2 or 18. For "Hotel U Sladku" change at the station "Vypich" to the tram 22 or 15.
Bus 179 at the airport
Bus, tram and metro timetables
Tickets for public transport
Airport - hotel - institute
Around the Institute
Accommodation
ACCOMMODATION WILL BE UPDATED!
Limited number of rooms is available for negotiated price at the three-star "Hotel u Sladku". This hotel has an excellent public-transport connection to the airport, to the main railway station, to the Prague city centre and to the Institute of Physics; free wireless connection at rooms and no cancellation fee. The prices per night negotiated for this workshop are 650 CZK (~25 Euro) for single bedroom, 900 CZK for double room.
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(the driving force are citations)

Jana2006 is continuously supported by Academy of Sciences of the Czech Republic and (occasionally) by (unpredictable) Grant agency of the CR