

ALBA

A Fortran 90 Program to Determine 3D Patterson Functions from X-Ray and Neutron Diffraction Data by the Maximum-Entropy Patterson Method

Ruben A. Dilanian and Fujio Izumi*

*Quantum Beam Unit, National Institute for Materials Science,
1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*

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* To whom correspondence should be addressed.

E-mail: fujioizumi@me.com

Web: <http://fujioizumi.verse.jp/>

1. Introduction

ALBA is a Fortran program for the **Maximum-Entropy Patterson** (MEP) analysis of observed integrated intensities [1, 2] (1) estimated by the Le Bail method [3] from powder diffraction data and (2) determined from single-crystal diffraction data.

Integrated intensities of overlapped reflections in powder diffraction data are, more or less, improved by the sophisticated MEP method, which is favorable for *ab initio* structure analysis from powder diffraction data. The name of the program originates from its most significant feature; that is, MEP analysis is carried out **After Le Bail Analysis**. Only a program for MEP analysis from integrated intensities obtained by the Pawley method has hitherto been developed by David [1, 2].

ALBA is used in combination with a multi-purpose pattern-fitting system RIETAN-2000 [4] or EXPO for *ab initio* structure analysis from powder diffraction data by a direct method [5–7]. In addition, Patterson functions resulting from MEP analysis with ALBA can be visualized in three dimensions with VEND contained in the VENUS package [8].

VENUS also includes a Fortran program, PRIMA, for determination of electron and nuclear densities by the maximum-entropy method (MEM). We built a powerful MEM engine into ALBA, making alterations to that of PRIMA. Thus, ultra-fast MEP analysis is possible with ALBA.

Most Rietveld-analysis programs incorporate the feature of Le Bail analysis because of the ease with which it can be implemented in this type of software. Therefore, ALBA makes it possible to use them to improve integrated intensities for overlapped reflections by minor modifications, adding value to them.

Ruben A. Dilanian
Fujio Izumi

2. Installation.

The installation of the Windows version of ALBA will be described here.

The following files are contained in folder RIETAN_VENUS:

ALBA.exe: an executable binary file.

spgra.dat: A file storing information about 230 space groups.

asfdc.dat: A file storing atomic scattering factors and coherent-scattering lengths.

Folder RIETAN_VENUS must be located in C:\Program Files\.

An environment variable, ALBA, has to be set on execution of ALBA.exe. It is usually set in a batch file, *.bat, in the following way:

```
SET ALBA=C:\Program Files\RIETAN_VENUS\
```

Never forget to put ‘\’ as the last character. For example, refer to the following batch file included in the distributed package:

```
C:\Program Files\RIETAN_VENUS\Batch_files\ALBA.bat
```

3. Input and Output files

Table 1 lists all the files input and output by ALBA. In this table, <INPFILE> is absolute path + file name (= basename + extension), and <INTFILE> is absolute path + basename. Needless to say, the absolute path may be unnecessary on the use of a batch file (templates are included in the distribution file) if both <INPFILE> and <INTFILE> are located in the current directory.

Table 1. Input and output files for ALBA

Input files		
ALBA input file	<INPFILE>	Various settings and parameters for ALBA
Intensity data file	<INTFILE>.ffo	Integrated intensities resulting from Le Bail analysis with RIETAN-2000
	<INTFILE>.hkl	Integrated intensities resulting from Le Bail analysis with EXTRA (EXPO)
	<INTFILE>.raw	Integrated intensities resulting from single-crystal diffraction experiments
Output files		
Standard output file	<INTFILE>.out	The result of MEP analysis
Wilson statistics file	<INTFILE>.wil	Data for a Wilson plot
Integrated intensities file	<INTFILE>.ffi	*.ffo format (RIETAN-2000)
	<INTFILE>.hki	*.hkl format (EXPO)
	<INTFILE>.rai	*.raw format
Overlapped reflections file	<INTFILE>.ovr	Calculated and observed integrated intensities for overlapped reflections
Three-dimensional data file	<INTFILE>.pri	Patterson functions with the *.pri format of VEND.

In *.raw, h , k , l , $|F_o(\mathbf{h}_j)|$, and σ_j are input in each line with at least one space between two data, where $hkl \equiv \mathbf{h}_j$ is the diffraction indices of the j th reflection, $|F_o(\mathbf{h}_j)|$ is the absolute value of the observed structure factor, and σ_j is the estimated standard deviation of $|F_o(\mathbf{h}_j)|$.

<INTFILE>.ffi, <INTFILE>.hki, and <INTFILE>.rai are output when <INTFILE>.ffo, <INTFILE>.hkl, and <INTFILE>.raw have been input by ALBA, respectively.

4. How to run ALBA

4.1 Interactive mode

Run ALBA by double-clicking its icon. Then, the program asks several questions that have to be answered by the user. In what follows, these questions are represented by *italic characters*.

*Various settings for ALBA can be typed on the computer or read from an input file.
Which will you choose (0: manual input, 1: from a file)?*

If you have chosen '1', the name of an ALBA input file must be input:
The name of an ALBA input file.

If you have chosen '0', the following questions must be answered:
*Title (CHARACTER*80).*

Lattice parameters (a, b, c, alpha, beta, and gamma).

Space-group number and setting.

The number of pixels along a, b, and c directions.

*Integrated intensities were determined from
0: X-ray diffraction data.
1: Neutron diffraction data of a compound containing no element
with a negative coherent-scattering length.*

The number of chemical species.

Real chemical species and numbers of atoms in the unit cell.

For example, in the case of BaSO₄,

Ba	4
S	4
O	16

The name of an intensity data file.

*(*ffo created by RIETAN-2000, *.hkl created by EXPO, or *.raw)*

The following question appears only for a *.hkl file created by EXPO (see Sect. 3).

Wavelength.

Which integrated intensities will you use?

0: The integrated intensity is defined as $|F|^2$.

1: The integrated intensity is defined as multiplicity $\times |F|^2$.

The initial Lagrangian multiplier.

The coefficient, t , to adjust the Lagrangian multiplier.

The next question appears only for a *.ffo file created by RIETAN-2000 (see Sect. 3).

The coefficient, SCIO, to adjust estimated standard deviations.

Will you group overlapped reflections? (NGSW)

0: Yes (reflections overlapped heavily are grouped).

1: No (all the reflections are independently input).

Needless to say, NGSW = 1 when *.raw in input.

The next question appears if NGSW = 0.

Maximum difference in d /Angstrom in the grouped reflections.

The next question appears only for a *.hkl file created by EXPO (see Sect. 3).

Parameters (v , p , and b) to estimate standard deviations, s .

$$s = v * \sqrt{p * |F|^2 + (b + |F|^2) / |F|^2}$$

After answering all the above questions, the conditions of MEP analysis are displayed in the screen. Before MEP iterations start, two questions must be answered.

The maximum number of MEP iterations.

Will you save a settings file? (SAVE)

0: No.

1: Yes.

The next question appears if $\text{SAVE} = 1$.

Input the name of an ALBA input file including its absolute path.

When $\Delta C = C^{(n)} - C^{(n-1)} > 0$, where $C^{(n)}$ and $C^{(n-1)}$ are respectively constraint functions for n and $n-1$ iterations (see Sect. 9), ALBA automatically changes the current value of the Lagrangian multiplier, λ , with the following message displayed in the screen:

A new value of lambda has been determined.

When the convergence is reached, *i.e.*, $C < 1$ or $R_{\text{wp}} < R_{\text{exp}}$ (for these two R factors, refer to Sect. 6), ALBA terminates after outputting CPU times.

4.2 Automatic mode.

You can also set all the flags and parameters (refer to Sect. 7) at those recorded in the ALBA input file, <INPFILE>. In this case, drag and drop <INPFILE> onto the icon of the executable binary file, ALBA.exe.

4.3 Running ALBA in the command prompt window

ALBA is launched not only by double clicking its icon but by entering the following command in the command prompt window:

ALBA <INPFILE>

C:\Program Files\RIETAN_VENUS\ALBA.bat will also serve us as a template of a batch file to launch ALBA.exe.

5. Estimated standard deviations

The standard deviation, σ_j , of the absolute value of the observed structure factor, $|F_o(\mathbf{h}_j)|$, for reflection \mathbf{h}_j is estimated in conventional ways described in Table 2.

Table 2. How to estimate standard deviations of $|F_o(\mathbf{h}_j)|$ from observed integrated intensities

Intensity data files	Equations
*.ffo (RIETAN)	$\sigma_j = \frac{ F_o(\mathbf{h}_j) }{2} \sqrt{\frac{1}{EI_o(\mathbf{h}_j)}},$ <p>where E is a parameter to adjust σ_j, and $I_o(\mathbf{h}_j)$ is the observed integrated intensity [8].</p>
*.hkl (EXPO)	$\sigma_j = v \sqrt{p F_o(\mathbf{h}_j) ^2 + \frac{\beta + F_o(\mathbf{h}_j) ^2}{ F_o(\mathbf{h}_j) ^2}},$ <p>where v is the noise level, p is the instability factor, and β is the influence of the non-zero background [9].</p>

In general, E (*SCIO* in <SETFILE>) should be decreased when analyzing diffraction data of poor statistics. E is usually determined so as to give the minimum number of cycles in a series of MEP analyses where the initial Lagrangian multiplier, λ_0 , is set at a small value. After the estimation of the appropriate E value, various parameters and settings in ALBA may be changed.

Takahashi [10] proposed an empirical method of estimating σ_j 's to be recorded in *.raw (Table 1) for single-crystal diffraction data from the multiplicity m_j , the Bragg angle θ_j , and the wavelength λ :

$$\sigma_j = \frac{E}{\sqrt{m_j}} \cdot \frac{\sin \theta_j}{\lambda}.$$

6. *R* factors

Two *R* factors are output in <INPFILE>.out:

$$R_{\text{wp}} = \sqrt{\sum_{j=1}^M w_j \left[|F_{\text{c}}(\mathbf{h}_j)| - |F_{\text{o}}(\mathbf{h}_j)| \right]^2 \bigg/ \sum_{j=1}^M w_j |F_{\text{o}}(\mathbf{h}_j)|^2},$$

$$R_{\text{exp}} = \sqrt{M \bigg/ \sum_{j=1}^M w_j |F_{\text{o}}(\mathbf{h}_j)|^2},$$

where M is the total number of reflections, $w_j = 1/\sigma_j^2$, and $F_{\text{c}}(\mathbf{h}_j)$ is the calculated structure factor for reflection \mathbf{h}_j .

7. ALBA input file

All the information that is necessary for MEP analysis is stored in the ALBA input file. Using this file you can run ALBA in automatic or manual modes. Lines which started with '#' is regarded as comments.

Title. (CHARACTER*80)

BaSO4

Lattice parameters.

8.87590 5.45213 7.15271 90.00000 90.00000 90.00000

Space group number, setting, and number of pixels.

62 1 64 64 64

Integrated intensities were determined from

0: X-ray diffraction data.

1: Neutron diffraction data of a compound containing no element

with a negative coherent-scattering length.

0

The number of chemical species

3

Real chemical species and amounts of substances

Ba 4

S 4

O 16

The name of a intensity data file.

(*.ffo created by RIETAN-2000, *.hkl created by EXP0, or *.raw)

BaSO4.ffo

Wavelength (dummy for *.ffo and *.raw)

1.54051

Which integrated intensities will you use?

0: The integrated intensity is defined as $|F|^2$.

```

# 1: The integrated intensity is regarded as multiplicity X |F|^2.
0

# The initial Lagrangian multiplier.
0.01

# The coefficient, t, to adjust the Lagrangian multiplier.
0.02

# The coefficient, SCIO, to adjust estimated standard deviations.
# (dummy for *.hkl and *.raw)
1000

# Will you group overlapped reflections?(NGSW)
# 0: Yes (reflections overlapped heavily are grouped).
# 1: No (all the reflections are independently input).
0

# Maximum difference in d/Angstrom in grouped reflections.
# (dummy if NGSW = 1)
0.0005

# Parameters (v, p, and b) to estimate standard deviations, s.
#  $s = v * \sqrt{p * |F|^2 + (b + |F|^2) / |F|^2}$ .
# (dummy for *.ffo created by RIETAN-2000)
1.000 0.0005 0.000

# The maximum number of MEP iterations.
888888

```

8. Symmetry of the Patterson map

The Patterson function, $P(\mathbf{u})$, is defined as the self-convolution of the electron density $\rho(\mathbf{r})$ at the position \mathbf{r} in the three-dimensional gridded space:

$$P(\mathbf{u}) = \rho(\mathbf{r}) * \rho(-\mathbf{r}).$$

This equation is alternatively represented as

$$P(\mathbf{u}) = \frac{1}{V} \sum_j |F_c(\mathbf{h}_j)|^2 \cos(2\pi \mathbf{h}_j \mathbf{u}),$$

where V is the unit cell volume, and \mathbf{u} is the interatomic vector, $\mathbf{u} = \mathbf{r}(\text{A}) - \mathbf{r}(\text{B})$, for atoms A and B. Because all the interatomic vectors can be translated to a common origin, the symmetry elements lose their translation components. Table 3 lists 24 Patterson symmetries for three dimensions [11].

Table 3. Patterson symmetry

Crystal symmetry	Patterson symmetry (Bravais lattice)	Space-group numbers
Triclinic	$P\bar{1}$	1–2
Monoclinic	$P2/m$, $C2/m$	3–15
Orthorhombic	$Pmmm$, $Cmmm$, $Immm$, $Fmmm$	16–73
Tetragonal	$P4/m$, $I4/m$	74–88
	$P4/mmm$, $I4/mmm$	89–142
Trigonal	$P\bar{3}$, $R\bar{3}$	143–148
	$P\bar{3}1m$, $R\bar{3}m$, $P\bar{3}m1$	149–167
Hexagonal	$P6/m$	168–176
	$P6/mmm$	177–194
Cubic	$Pm\bar{3}$, $Im\bar{3}$, $Fm\bar{3}$	195–206
	$Pm\bar{3}m$, $Im\bar{3}m$, $Fm\bar{3}m$	207–230

9. Heavy-atom method

Three-dimensional distribution of Patterson functions can be interpreted rather easily when heavy atoms are contained [12]. Peaks due to vectors between heavy atoms generally dominate in Patterson maps. Let Z_h and Z_l be atomic numbers of heavy and light elements, respectively. Then, the most popular criterion to judge the effectiveness of the heavy-atom method is

$$\frac{\sum Z_h^2}{\sum Z_l^2} \approx 1.$$

In the Patterson map, symmetry elements in the space group leave traces consisting of particular clustering of interatomic vectors on specific lines and planes, which are called Harker lines and sections, respectively. For example, space group $P2_1/n$ with equivalent positions:

$$x, y, z; \bar{x} + 1/2, y + 1/2, \bar{z} + 1/2; \bar{x}, \bar{y}, \bar{z}; x + 1/2, \bar{y} + 1/2, z + 1/2$$

has Patterson peaks located on a Harker section (uvw):

$$(2x + 1/2, 1/2, 2z + 1/2)$$

$$u = x - \bar{x} - 1/2 = 2x + 1/2$$

$$v = y - \bar{y} - 1/2 = 1/2$$

$$w = z - \bar{z} - 1/2 = 2z + 1/2$$

and on a Harker line [uvw]:

$$[1/2, 2y + 1/2, 1/2]$$

$$u = x - x - 1/2 = 1/2$$

$$v = y - \bar{y} - 1/2 = 2y + 1/2$$

$$w = z - z - 1/2 = 1/2$$

From these peak positions in the Patterson maps, we can easily obtain x , y , and z coordinates of heavy atoms.

10. The algorithm of the MEP method

ALBA basically uses the algorithm of the MEP method reported by David [1, 2].

In the MEP method, the maximum-entropy probability density can be obtained by maximizing the information entropy, S :

$$S = - \sum_{k=1}^N P_k \log(P_k / Q_k),$$

where $N (= N_a \times N_b \times N_c)$ is the total number of pixels in the unit cell, P_k is the normalized Patterson density, and Q_k is the normalized Patterson density based on the prior information. The initial value of the Patterson function is calculated from the total number of electrons (X-ray diffraction) or total coherent-scattering lengths, b_c , (neutron diffraction) in the unit cell, T , and the unit-cell volume, V .

Let M_F be the number of isolated reflections, and M_G the number of groups for overlapping reflections. During MEP iterations, S is maximized under the following four constraints:

$$P_k > 0,$$

$$C_F = \frac{1}{M_F} \sum_{j=1}^{M_F} \frac{[|F_c(\mathbf{h}_j)| - |F_o(\mathbf{h}_j)|]^2}{\sigma_j^2} = 1, \quad \text{F-constraint for isolated reflections}$$

$$C_G = \frac{1}{M_G} \sum_{j=1}^{M_G} \frac{(G_{cj} - G_{oj})^2}{\sigma_j^2} = 1, \quad \text{G-constraint for overlapping reflections}$$

$$D = \sum_{k=1}^N P_k = 1. \quad \text{Normalization constraint}$$

G_{cj} and G_{oj} in the G-constraint are calculated from the total number of reflections, L_j , and the multiplicity, m_i , of the i th reflection in the j th group:

$$G_{cj}^2 = \frac{\sum_{i=1}^{L_j} m_i |F_c(\mathbf{h}_i)|^2}{\sum_{i=1}^{L_j} m_i},$$

$$G_{0j}^2 = \frac{\sum_{i=1}^{L_j} m_i |F_0(\mathbf{h}_i)|^2}{\sum_{i=1}^{L_j} m_i}.$$

To maximize S under the above equality constraints, we derive another function containing two Lagrangian multipliers, λ and μ :

$$Q = S - \lambda(C - 1) - \mu(D - 1)$$

with

$$C = C_F + C_G.$$

Q is maximized by setting its partial derivatives with respect to P_k and the Lagrangian multipliers, λ and μ , at zero:

$$\partial Q / \partial P_k = 0,$$

$$\partial Q / \partial \lambda = 0,$$

$$\partial Q / \partial \mu = 0.$$

The maximum-entropy distribution of Patterson functions in the unit cell is reached through MEP iterations $n = 1, 2, 3, \dots$

$$P_k^{(n+1)} = \frac{P_k^{(n)}}{Z} \exp\left(-\lambda \frac{\partial C}{\partial P_k^{(n)}}\right)$$

with

$$Z = \sum_{k=1}^N P_k^{(n)} \exp\left(-\lambda \frac{\partial C}{\partial P_k^{(n)}}\right).$$

$|F_c(\mathbf{h}_j)|^2$ contained in $C (= C_F + C_G)$ is given by

$$|F_c(\mathbf{h}_j)|^2 = \frac{1}{K} \cdot \frac{V}{2} \sum_{k=1}^{N_a} P_k^{(n+1)} W_{jk}$$

with

$$W_{jk} = \sum_{l=1}^{N_p} \cos(2\pi \mathbf{h}_j \mathbf{R}_l \mathbf{r}_k),$$

where K is the scale factor (see Sect. 10), N_a is the number of pixels in the asymmetric unit, \mathbf{R}_l is the rotation matrix, and N_p is the number of symmetry operations for Patterson symmetry (Table 3).

PRIMA has an another feature of adjusting λ automatically during MEP iterations. In this technique, λ in the $(n+1)$ 'th iteration ($n = 1, 2, 3, \dots$), $\lambda^{(n+1)}$, is automatically adjusted with a coefficient, t :

$$\lambda^{(n+1)} = \lambda^{(n)} + t\lambda_0$$

with

$$\lambda^{(1)} = \lambda_0.$$

If $t = 0$ (default value), λ remains unchanged. When the MEP iterations tend toward divergence, $\lambda^{(n+1)}$ is decreased to $\lambda^{(n)}/2$.

11. Wilson plot

Whereas only relative values are determined for $|F_o(\mathbf{h}_j)|$'s, $|F_c(\mathbf{h}_j)|$'s must absolutely be evaluated for *ab initio* structure analysis. On the assumption of isotropic thermal motion for all the sites in the unit cell, $|F_o(\mathbf{h}_j)|$ is represented as

$$|F_o(\mathbf{h}_j)|^2 = K |F_{\text{abs}}(\mathbf{h}_j)|^2 \exp \left[-2B \left(\frac{\sin \theta_j}{\lambda} \right) \right],$$

where K is the scale factor, $|F_{\text{abs}}(\mathbf{h}_j)|$ is the structure factor in the absolute scale, B is the overall isotropic atomic displacement parameters, θ_j is the Bragg angle, and λ is the wavelength. In the case of X-ray diffraction data, we can calculate K and B by Wilson's statistical analysis of integrated intensities [13, 14]:

$$y = \ln(K) - 2B \cdot x$$

with

$$y = \ln \left(\frac{\langle |F_o(\mathbf{h}_j)|^2 \rangle}{\sum_{j=1}^N f_j^2} \right),$$

$$x = \langle s^2 \rangle,$$

where N is the total number of atoms in the unit cell, f_j is the atomic scattering factor, and $\langle s^2 \rangle$ is the mean of s^2 . A straight line is fit to a set of (x, y) data by a method of least squares. The intercept of the line on the y axis gives $\ln(K)$, and its slope $2B$. If a negative B values is obtained, K is set at 1, for convenience.

Finally, the following equation is used to obtain $|F'_{\text{abs}}(\mathbf{h}_j)|$:

$$|F'_{\text{abs}}(\mathbf{h}_j)|^2 = K' |F_o(\mathbf{h}_j)|^2$$

with

$$K' = 1/K,$$

$$|F'_{\text{abs}}(\mathbf{h}_j)|^2 = |F_{\text{abs}}(\mathbf{h}_j)|^2 \exp \left[-2B \left(\frac{\sin \theta_j}{\lambda} \right) \right].$$

Note that only relative values of $|F_c(\mathbf{h}_j)|$ result from the MEP analysis of neutron powder diffraction data with the current version of ALBA. Integrated intensities determined by single-crystal diffraction are assumed to have been adjusted with a scale factor.

12. License agreement

ALBA is copyrighted but distributed free of charge for personal noncommercial use under the following conditions.

Whenever original results acquired with ALBA are published in journals, proceedings, facility reports, *etc.* or reported in meetings with abstracts, the program name ALBA should explicitly be credited. Furthermore, cite the following reference:

F. Izumi, "Spectroscopy and Diffraction III," 5th Series of Experimental Chemistry, Vol. 11, ed. by Chem. Soc. Jpn., Maruzen, Tokyo (2006), pp. 220–223.

ALBA is distributed in the hope that it will be useful, but without any warranty or support; without even the implied warranty of merchantability or fitness for a particular purpose.

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