

# Manual for Powder Indexing Software

## Conograph

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## Contents

1. Overall configuration .....	1-1
2. Creating new project/opening existing project.....	2-1
2.1. Creating a new project .....	2-1
2.2. Opening a project.....	2-4
2.3. Opening a sample project .....	2-6
3. Peak search .....	3-1
3.1. Peak search execution .....	3-1
3.2. Checking peak search results.....	3-3
3.3. Removing and adding peaks manually .....	3-4
4. Parameters used for indexing .....	4-1
4.1. Search parameters and diffractometer parameters .....	4-2
4.2. Advanced indexing parameters.....	4-5
5. Indexing.....	5-1
5.1. Indexing execution.....	5-1
5.2. When indexing is complete .....	5-2
5.3. Sorting /filtering lattice parameters .....	5-3
5.4. Find plausible indexing solutions .....	5-6
5.5. Decide the correct lattice parameters .....	5-10
6. Refining lattice parameters and zero point shift .....	6-1
6.1. Method for refinement execution .....	6-1
6.1.1. Refinement of lattice parameters selected from the list.....	6-1
6.1.2. Refining lattice constants entered by user.....	6-3
6.2. <b>Undo</b> button.....	6-5
7. Result output.....	7-1
7.1. *.index.xml .....	7-1
7.2. Igor text file and *.index2.xml file .....	7-1
7.3. Backup file.....	7-2
8. Space group determination.....	8-1
9. Other GUI operations .....	9-1
9.1. Configuration parameters .....	9-1
9.2. Help menu .....	9-1
10. Parameters that can be changed to obtain better results .....	10-1
10.1. Peak search .....	10-1
10.2. Powder indexing .....	10-3

10.2.1.	Conduct a more exhaustive search .....	10-3
10.2.2.	Enhance computing speed.....	10-3
10.2.3.	Improve the efficacy of figures of merit .....	10-4
11.	Input/output text file formats.....	11-1
12.	Addendum.....	12-1
12.1.	Request for citation .....	12-1
12.2.	Bug report.....	12-1

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## 1. Overall configuration

Conograph was developed by the High Energy Accelerator Research Organization for running two command-user-interface (CUI) programs for powder indexing and peak searching through operations on a graphical user interface.

This software is provided with an installer (setup.exe) that allows installation of the required runtime.

Fig. 1-1 shows a screenshot of the Conograph user interface.

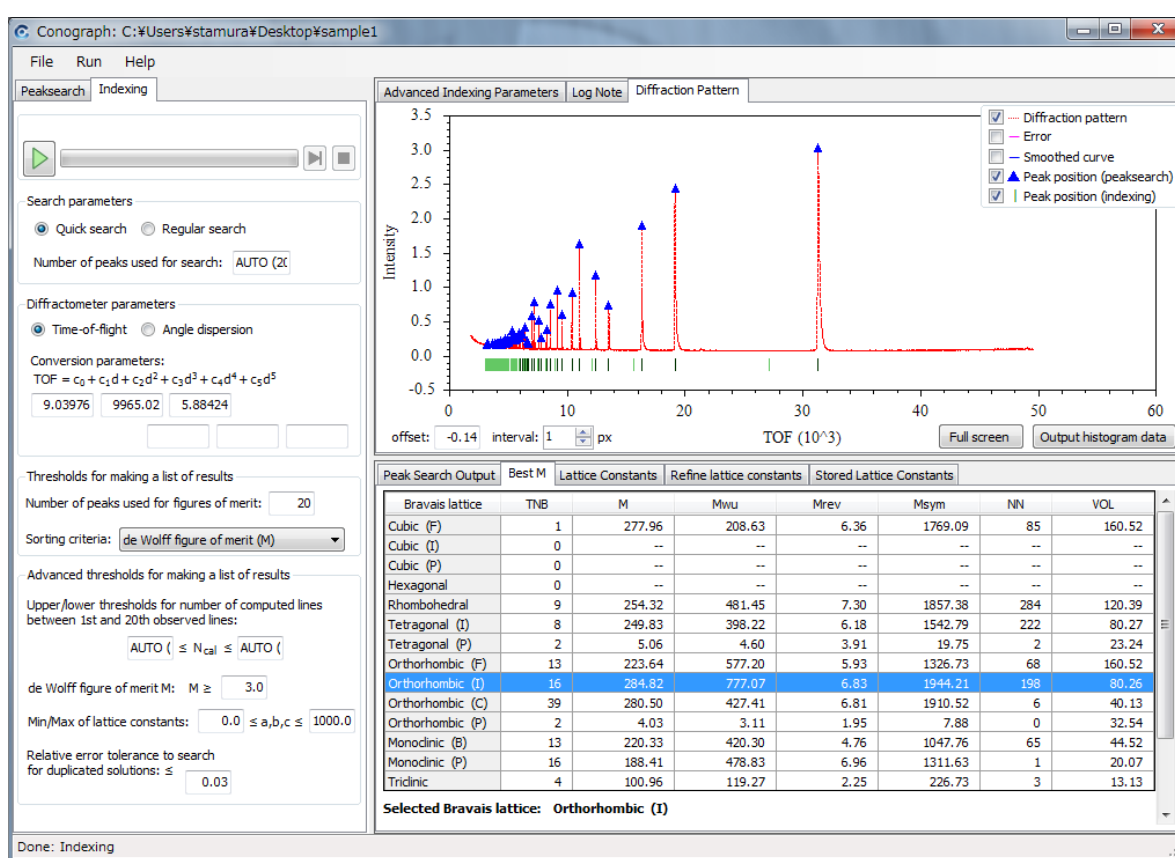
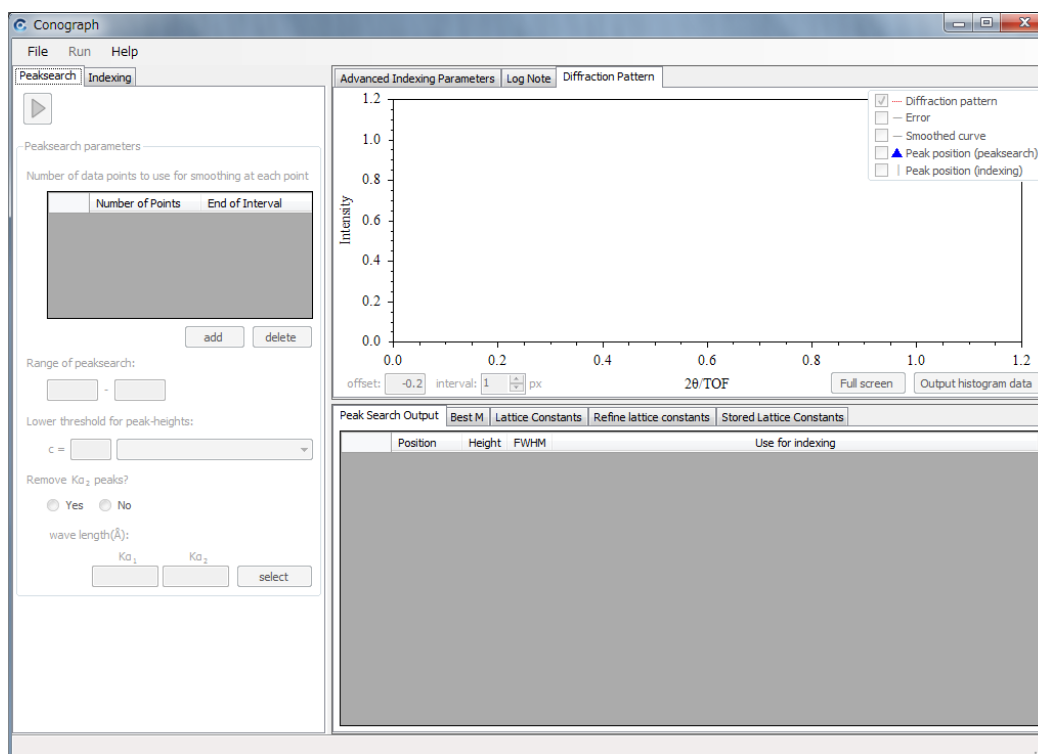


Fig. 1-1 Conograph user interface

## 2. Creating new project/opening existing project

Fig. 1-1 shows a screenshot of the Conograph UI immediately after the application is started. To conduct peak searches or indexing, it is necessary to create a new project or open an existing project.

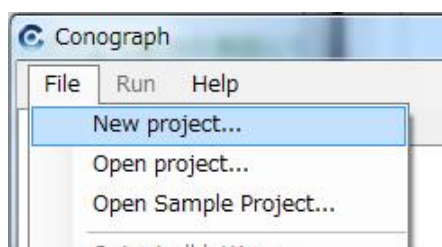
This chapter explains the procedures for both operations.



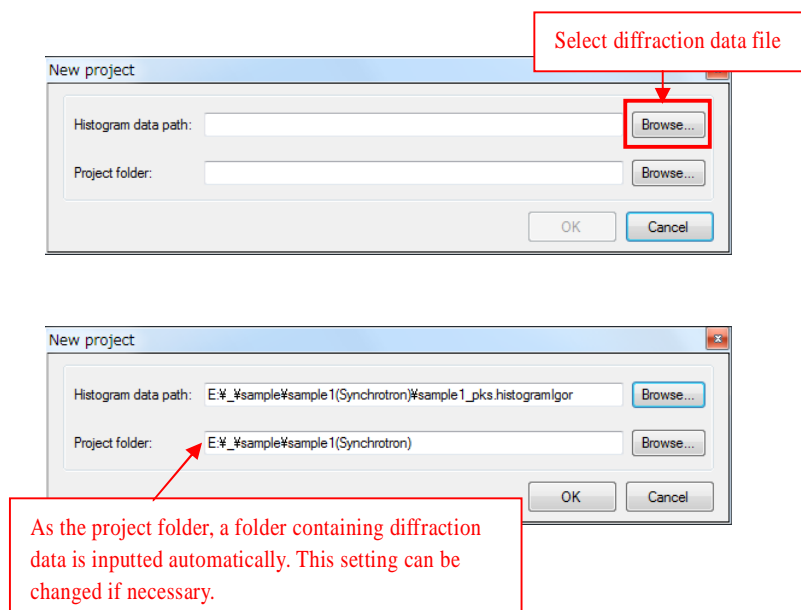
**Fig. 2-1 Screenshot immediately after opening Conograph**

### 2.1. Creating a new project

To create a new project, first select **File > New project** as shown below.



In the dialog box for creating projects, you can specify the diffraction data file and project folder, as shown in Fig. 2-2.

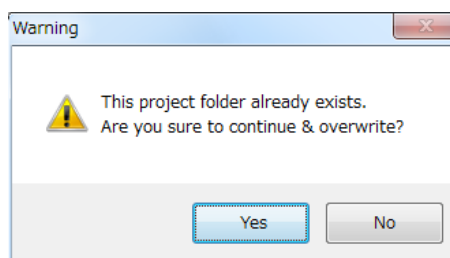


**Fig. 2-2 Dialog box for creating new project**

The diffraction data file can be formatted in three types of format: XY (Fig. 2-3), IGOR (Fig. 2-4), and Rietan (Fig. 2-5). For the XY and IGOR formats, the observation errors of y-values (in the second column) can be input in the third data column. If the third column is empty, the roots of the y-values are used as the observation errors. In the file, LF, CR+LF, and CR can be used as a line feed code, and spaces and tabs as a delimiter.

The project is created by clicking the OK button after providing the project information. A folder named **auto\_generated\_files** is created in the project folder, and used to store all the automatically outputted files. This folder contains all the files necessary for using Conograph. Thus, it contains a copy of the diffraction data file specified in Fig. 2-2 and parameter set up files (Fig. 11-16).

When the specified project folder already exists and contains the **auto\_generated\_files** folder as a subfolder, the following dialog box appears:



If you select **Yes**, all the files originally present in the **auto\_generated\_files** folder are deleted and cannot be retrieved.

tof	yint	yerr
7.00000	4942	70.29935988
7.01697	4956	70.39886363
7.03395	5084	71.30217388
~omitted~		
89.66605	818	28.60069929
89.68303	818	28.60069929
89.70000	818	28.60069929

**Fig. 2-3 Example of XY format**

```

IGOR
WAVES/0 tof, yint, yerr
BEGIN
  8792.00000      0.85962      0.05899
  8808.00000      0.79276      0.05643
  8824.00000      0.75064      0.05470
~omitted~
199536.00000     0.40015      0.01698
199664.00000     0.36920      0.01634
199792.00000     0.39202      0.01686
END

```

**Fig. 2-4 Example of IGOR format**

```

3500    10.0000 0.0200
15, 16, 26, 19
30, 15, 23, 22
26, 25, 20, 17
~omitted~
8, 12, 4, 9
13, 12, 8, 6
7, 6, 11, 1

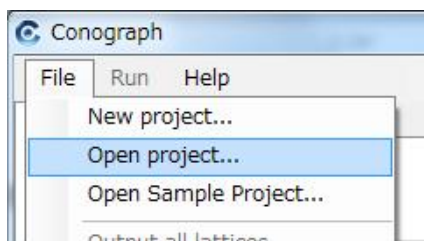
```

**Fig. 2-5 Example of Rietan format**



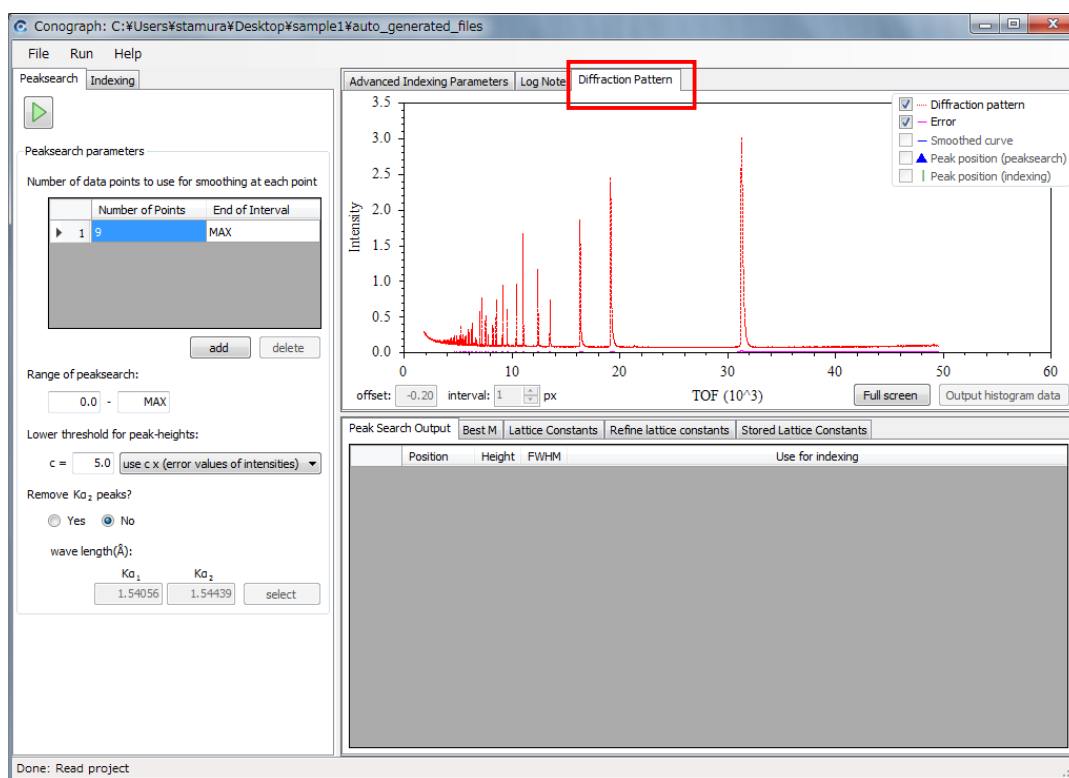
## 2.2. Opening a project

To open an existing project, select **File > Open project** as shown below.






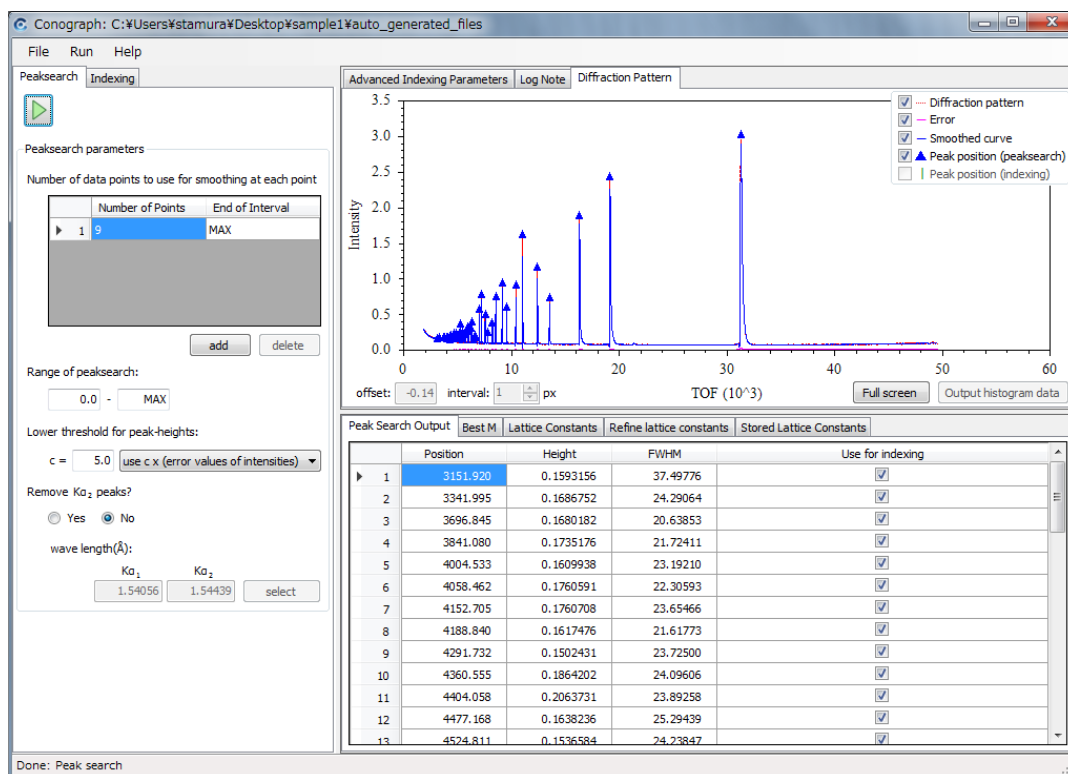
Then, the file folder selection dialog box is displayed. You can specify a project folder in the dialog box.

Fig. 2-3 shows the status of the software immediately after a project is opened and the diffraction pattern file and parameter setup file (\*.inp.xml) are loaded. In the **Diffraction pattern** frame (red square in the figure), the measured diffraction pattern (í) and errors ( , only when there is an error in the diffraction pattern file) are displayed.



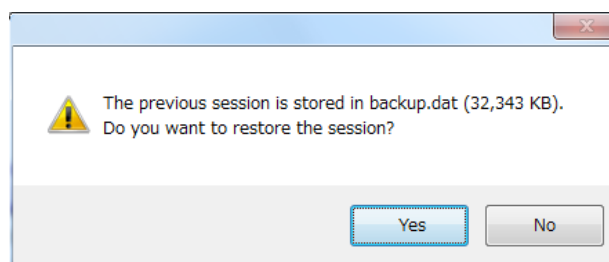
**Fig. 2-6 Screenshot immediately after opening a project (prior to peak search)**

If a peak search has been performed in the opened project and the file **\*\_pks.histogramlgor** exists, the indexing frame is displayed, as shown in Fig. 2-7. In addition to the diffraction pattern (  ), the peak positions (  ) and a smoothed diffraction pattern (  ) are displayed.



**Fig. 2-7 Screenshot immediately after opening a project (after peak search)**

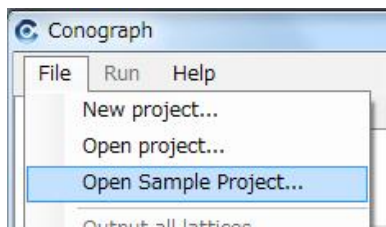
Further, when a backup file exists, the following dialog box appears:



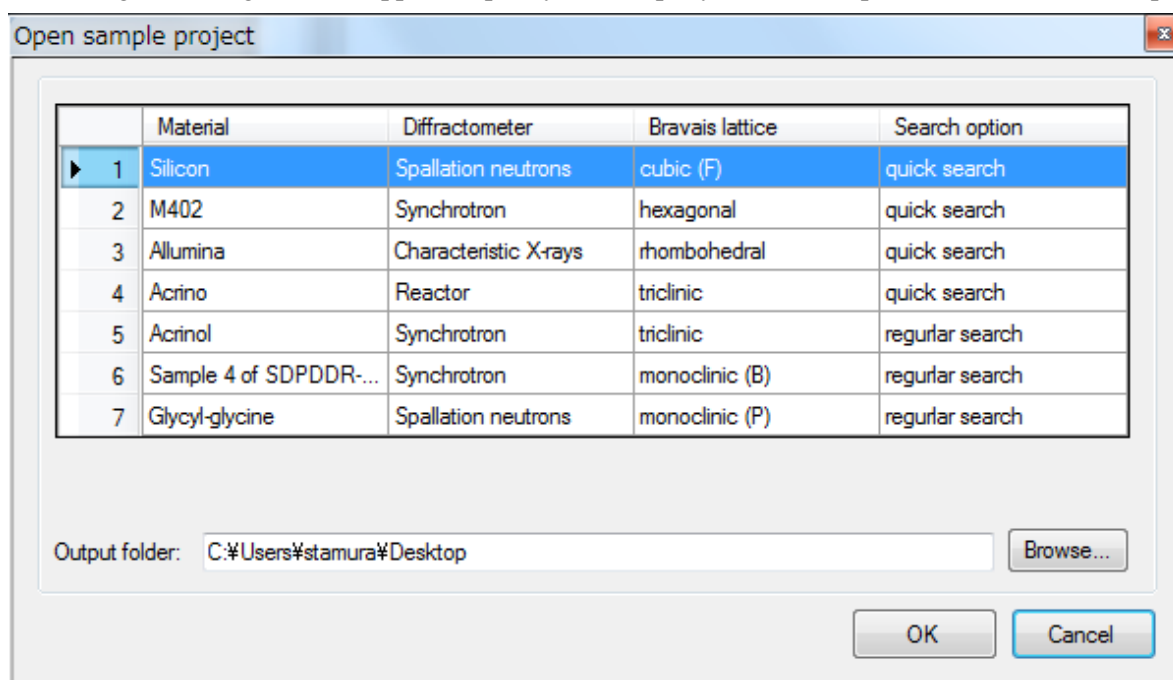
When you select **Yes**, the project is opened, loading indexing results saved in the backup file. If you select **No**, the opened project retains the status prior to indexing.

### 2.3. Opening a sample project

To open a prepared sample project, select **File > Open Sample Project**:



Then, using the dialog box that appears, specify the sample you want to open and the folder to output.



Subsequently, the selected sample project is created in the specified **Output folder**, and the project is opened.

### 3. Peak search

#### 3.1. Peak search execution

After opening the project, first, a peak search must be performed in order to obtain peak positions for indexing. A peak search is performed using the **Peak search** frame:

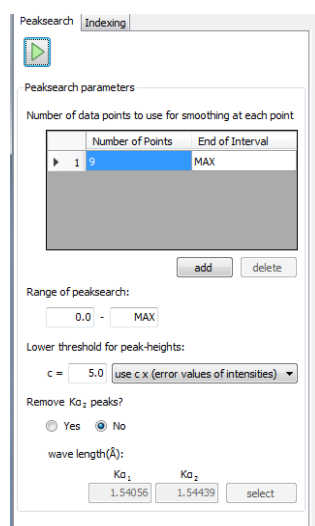
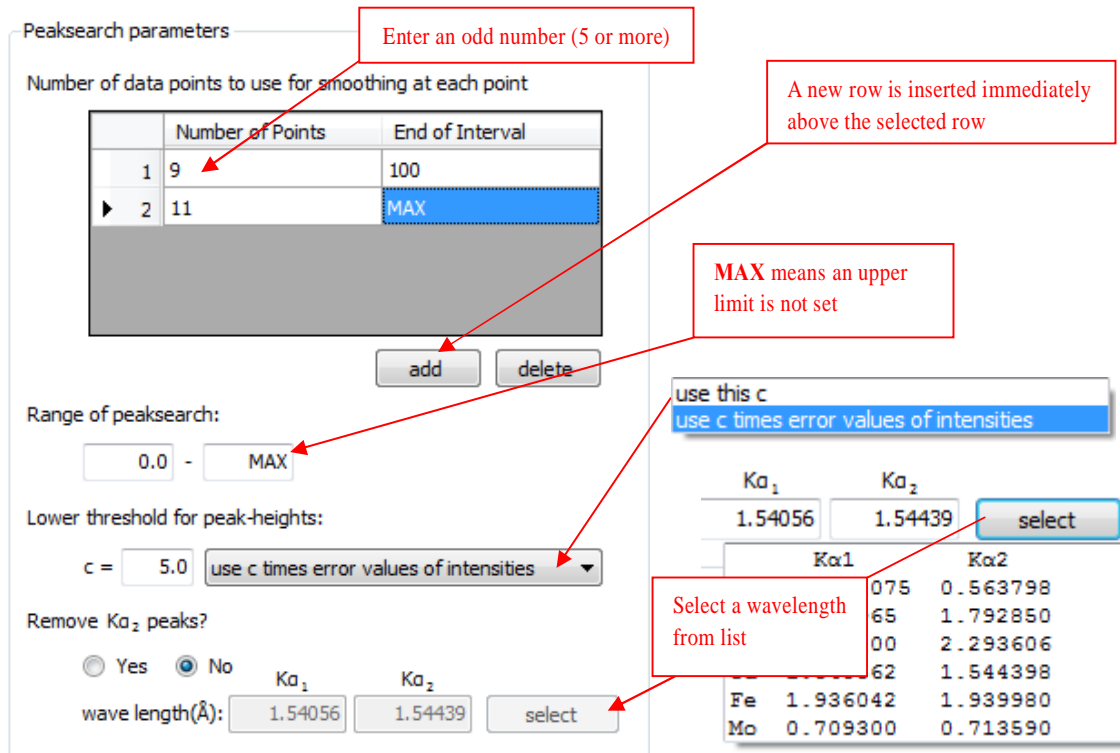
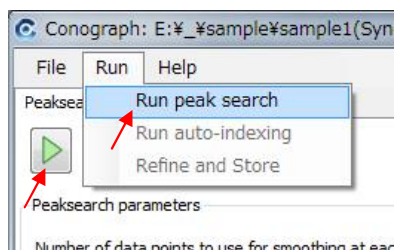


Fig. 3-1 explains the operations available in the **Peak search** frame.

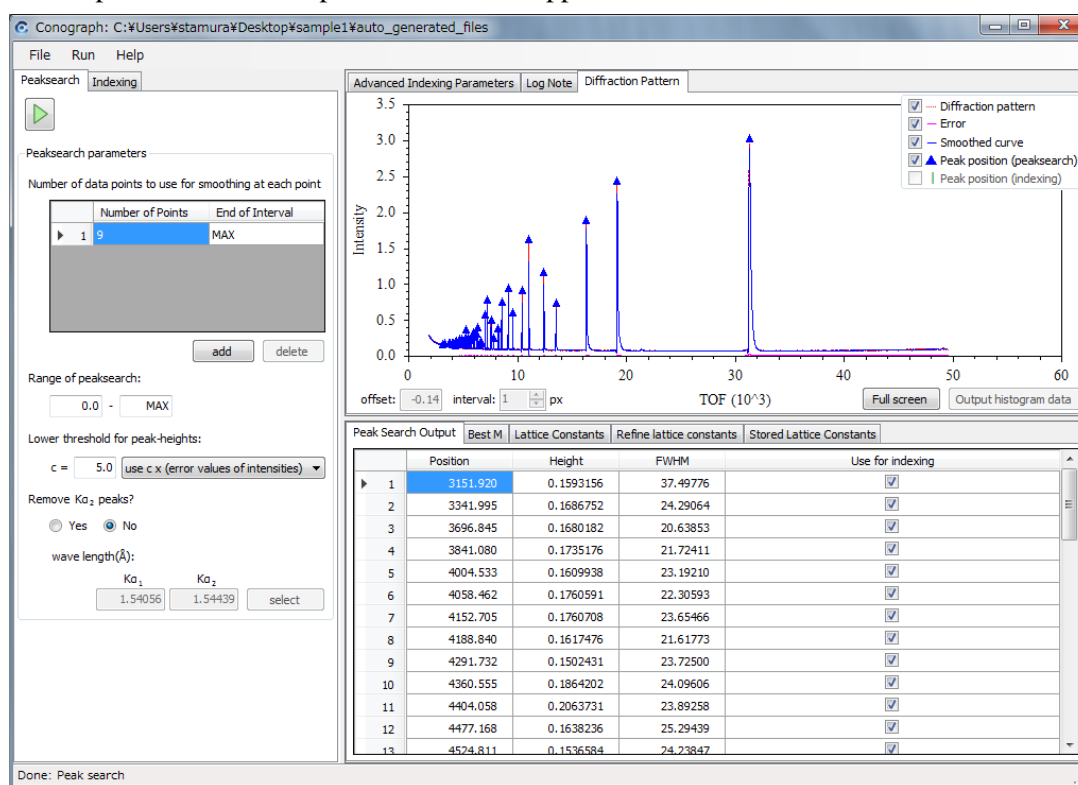


**Fig. 3-1 Setting peak search parameters**

To conduct a peak search, click the Run button  or select **Menu > Run > Run peak search**:



When the peak search is completed, the screen appears as follows.



In the **Diffraction Pattern** frame, a smoothed diffraction pattern ( ) and peak positions ( ) are displayed. Simultaneously, they are stored in the file **auto\_generated\_files folder/\*\_pks.histogramIgor<sup>1</sup>**.

<sup>1</sup>If the peak search results found at the end of the \*\_pks.histogramIgor file (Fig. 11-4) are modified using a text editor, the results are loaded on the application when the same project is reopened.

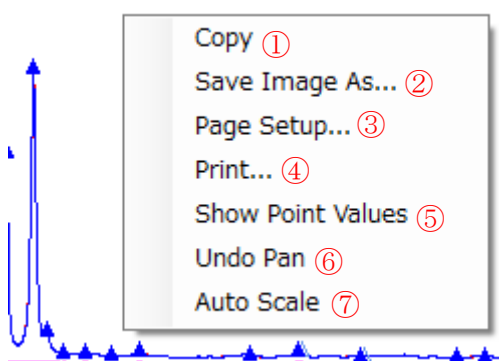
### 3.2. Checking peak search results

To obtain appropriate peak search results for indexing, you should check whether the following problems occur, in particular, for the low-angle peaks, by magnifying the graphical display of the diffraction pattern:

- Are there many diffraction peaks that have not been detected?
- Has noise (including small peaks that may not be diffraction peaks) been detected as a peak?

The aforementioned problems during peak search can be resolved by adjusting some of the peak search parameters and re-executing peak search (for parameter adjustment, refer to Section 10.1).

The graph magnification in the **Diffraction Pattern** frame is changed by using the mouse wheel or rubber band (= rectangular range) selection using left drag. A parallel shift of the display area is achieved by using **Ctrl + left drag** or **center drag**. The shortcut menu that appears when you right-click on the graph is shown in Fig. 3-2. Its components and their descriptions are listed in Table 3-1.



**Fig. 3-2 Shortcut menu**

**Table 3-1 Shortcut menu**

①	Copies graph contents onto the clipboard
②	Saves graph contents in an image file
③	Sets up for printing
④	Prints graph contents
⑤	Switches between ON/OFF for displaying point coordinates on graph
⑥	Returns to the previous display status
⑦	Adjusts scale to fit entire graph

### 3.3. Removing and adding peaks manually

This section introduces a method for modifying peak search results using the GUI operations. However, even if the results are not satisfactory, you should attempt to adjust the peak search parameters first, before proceeding to the following operations.

Peaks used in indexing can be selected using the check boxes that appear in the **Use for indexing** column in the **Peak Search Output** frame (Fig. 3-3). Whether or not peaks are used is represented visually in the **Diffraction Pattern** frame, as shown in Fig. 3-4.

	Position	Height	FWHM	Use for indexing
1	3151.1			<input checked="" type="checkbox"/>
2	3341.1			<input checked="" type="checkbox"/>
3	3696.845	0.1680182	20.63853	<input checked="" type="checkbox"/>
4	3841.080	0.1735176	21.72411	<input checked="" type="checkbox"/>
5	4004.533	0.1609938	23.19210	<input checked="" type="checkbox"/>
6	4058.462	0.1760591		<input checked="" type="checkbox"/>
7	4152.705	0.1760708		<input checked="" type="checkbox"/>
8	4188.840	0.1617476	21.81773	<input checked="" type="checkbox"/>
9	4291.732	0.1502431	23.72500	<input checked="" type="checkbox"/>

Fig. 3-3 Input peak positions

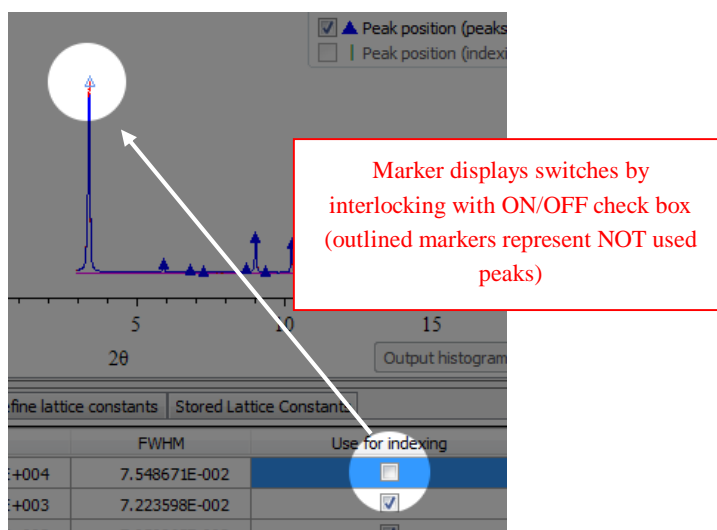
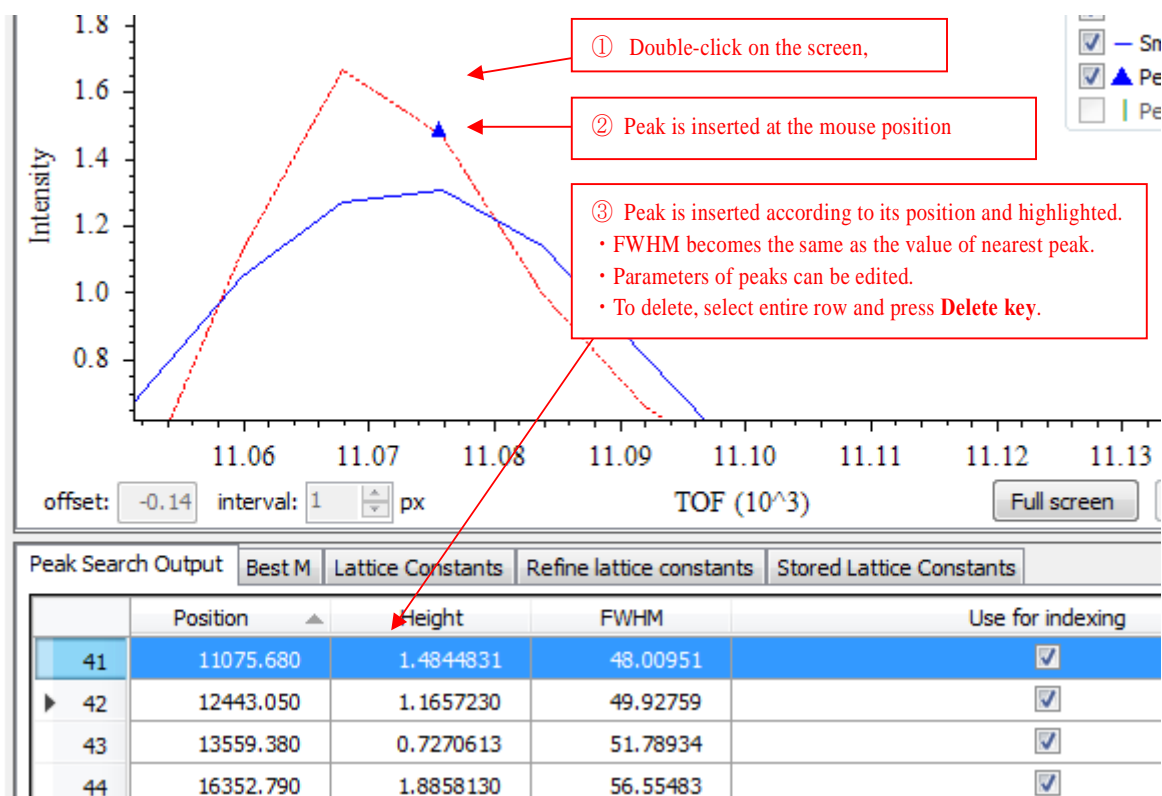


Fig. 3-4 Representation of NOT used peaks in the Diffraction Pattern frame

A peak can be inserted manually at the mouse pointer position by double-clicking on the diffraction pattern. Its height is automatically decided by interpolation. The specific values of the peak position and the full width at half maximum (FWHM) can be edited in the **Peak Search Output** frame (Fig. 3-5).



**Fig. 3-5 Manual insertion of a peak**



## 4. Parameters used for indexing

The parameters used in indexing are located in three frames (Fig. 4-1):

1. **Indexing** frame
  - a. Search parameters and diffractometer parameters
  - b. Sorting criteria and thresholds for lattice parameters displayed in the list (can be changed after indexing)
2. **Advanced indexing parameters** frame
3. **Peak Search Output** frame

Immediately after a new project is created, the values recommended for the respective parameters are set. Basically, it is not necessary to change the values, except for the diffractometer parameters.

The parameter in item 3 above is introduced in Section 3.3. The criteria and thresholds in item 1b are introduced in Section 5.3, because they can be changed even after indexing. In the current section, the remaining two types of parameters are explained.

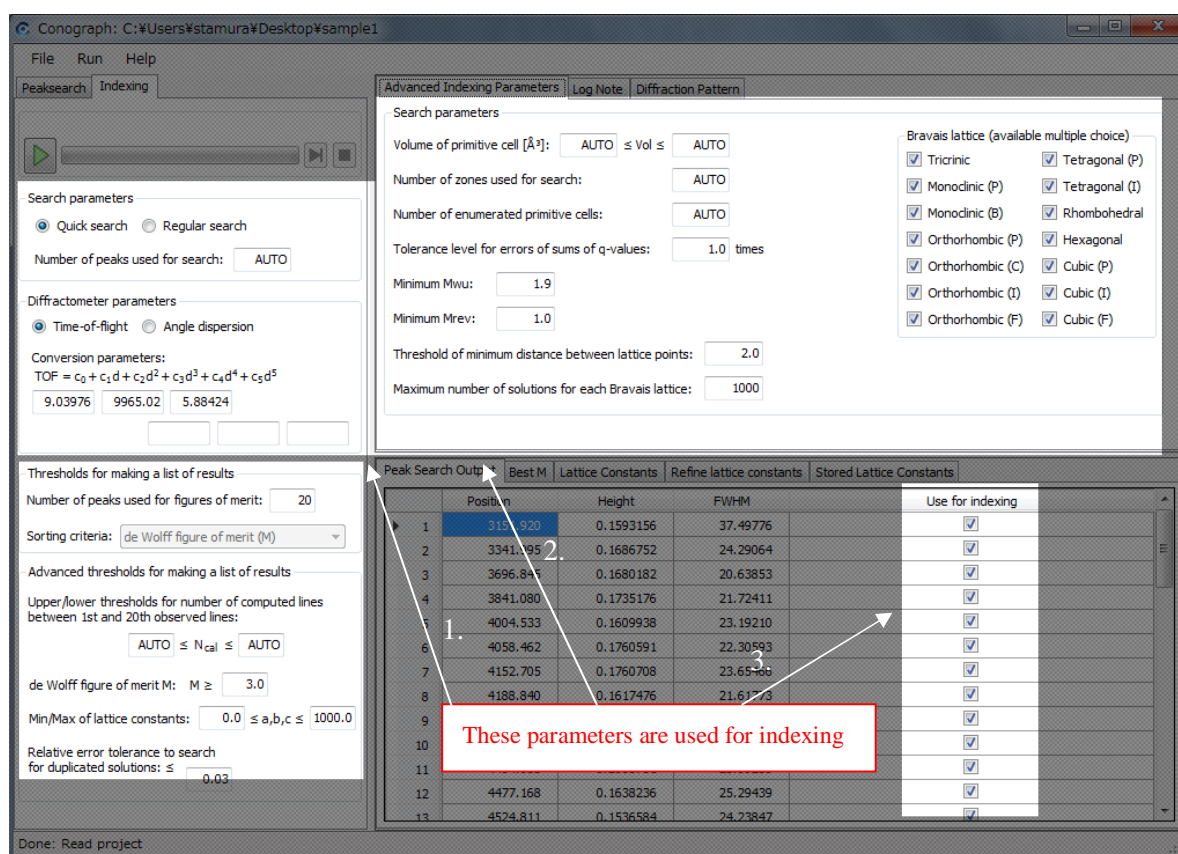
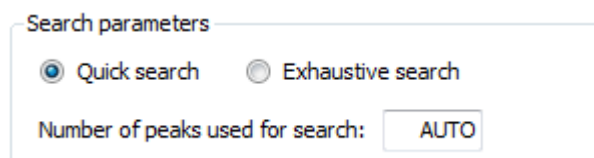


Fig. 4-1 Input parameters of powder indexing

#### 4.1. Search parameters and diffractometer parameters

In the **Search parameters** area, the search method and number of peaks used for powder indexing can be specified. There are two search method options:

- Quick search (when the size of the unit cell is small or for cases with high symmetry),
- Exhaustive search (for all cases)



**Fig. 4-2 Search parameters**

Since the basic algorithms of the two search methods are the same, the two methods can return the same result, if you adjust the parameters used for the quick search.

Powder indexing with **Quick search** is successful in many cases. However, **Memory-efficient search** should be used in more difficult cases. Powder indexing with **Memory-efficient search** occasionally takes more than 10 minutes.

In the **Diffractometer parameters** area, the time-of-flight or angle dispersion method can be selected. Except for the zero point shift, the parameter values are unique to the respective diffractometer (Fig. 4-3, Fig. 4-4, and Table 4-1). Entering 0 deg. for the zero point shift is normally effective. More precise values can be estimated by executing refinement after indexing.

**Diffractometer parameters**

① ☒ Time-of-flight ☐ Angle dispersion

Conversion parameters:  
 $TOF = c_0 + c_1 d + c_2 d^2 + c_3 d^3 + c_4 d^4 + c_5 d^5$

9.03976 9965.02 5.88424

②

---

**Diffractometer parameters**

① ☐ Time-of-flight ☒ Angle dispersion

Wavelength: 1.54056 Å ③

Zero point shift:  $\Delta 2\theta =$  0.0 deg. ④

⑤

Estimate zero point shift

**Fig. 4-3 Diffractometer parameters**

(Top: Time-of-flight method; Bottom: Angle dispersion method)

**Table 4-1 Diffractometer parameters**

①	Selects "Time-of-flight" or "Angle dispersion"
②	Conversion parameters represented as polynomial coefficients from zero to fifth order
③	Wavelength [Å]
④	Peak shift parameter $\Delta 2\theta$ [degrees]
⑤	Estimates zero point shift by using the reflection pair method

The zero point shift can be estimated by conducting the reflection pair method [1] (Fig. 4-3). In the reflection point method, the zero point shift is estimated by using two peak positions that have a ratio of d-values equal to two-fold. As shown in Fig. 4-3, the one that appears to be correct can be selected from various candidates.

**Diffractometer parameters**

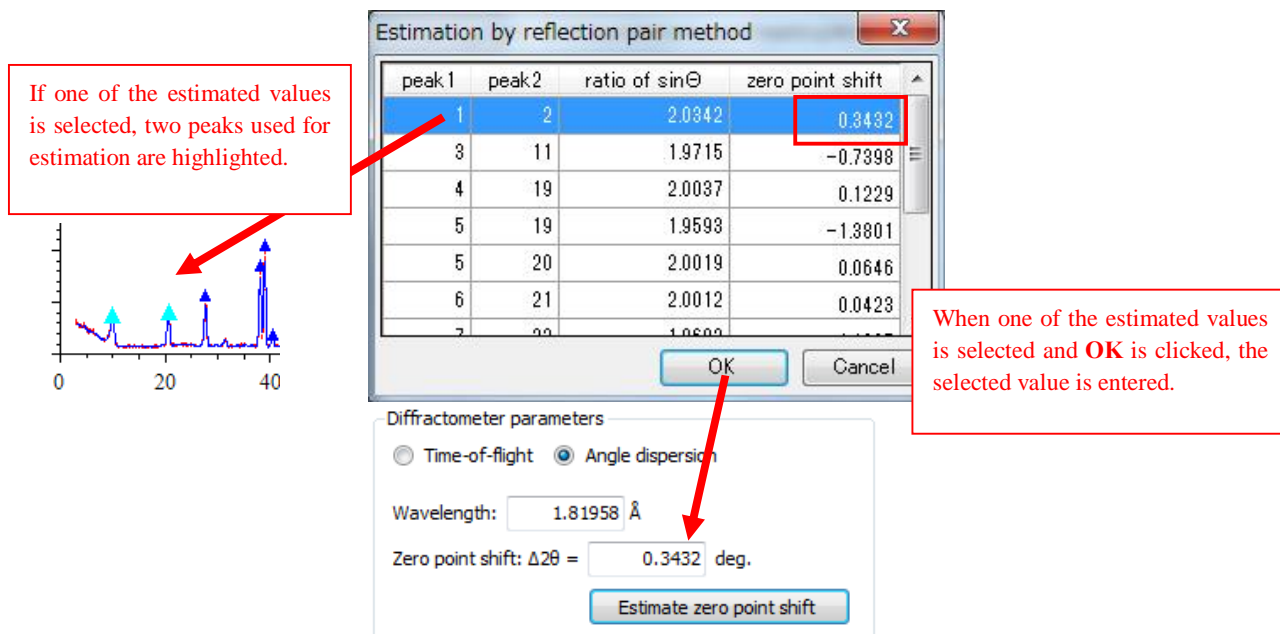
☐ Time-of-flight ☒ Angle dispersion

Wavelength: 1.81958 Å

Zero point shift:  $\Delta 2\theta =$  0.0 deg.

Estimate zero point shift

When button is clicked, the zero point shift is estimated and a list of candidates appears.



**Fig. 4-4 Estimation of zero point shift**

## 4.2. Advanced indexing parameters

The recommended values for the parameters in this frame are set automatically when a project is created. Although in general the values need not be changed, it should be noted that when they were determined the most difficult cases of powder indexing were considered. Hence, improvement, particularly in computation time, may be obtained by changing these parameters, as described in Section 10.2.

Search parameters

Volume of primitive cell [ $\text{\AA}^3$ ]:   $\leq \text{Vol} \leq$   ①

Number of zones used for search:  ②

Number of enumerated primitive cells:  ③

Tolerance level for errors of sums of q-values:  times ④

Minimum Mwu:  ⑤

Minimum Mrev:  ⑥

Threshold of minimum distance between lattice points:  ⑦

Maximum number of solutions for each Bravais lattice:  ⑧

Bravais lattice (available multiple choice)

☒ Triclinic ☒ Tetragonal (P)

☒ Monoclinic (P) ☒ Tetragonal (I)

☒ Monoclinic (B) ☒ Rhombohedral

☒ Orthorhombic (P) ☒ Hexagonal

☒ Orthorhombic (C) ☒ Cubic (P)

☒ Orthorhombic (I) ☒ Cubic (I) ⑨

☒ Orthorhombic (F) ☒ Cubic (F)

**Fig. 4-5 Advanced indexing parameters**

A description of the parameters and their recommended values are listed in Table 4-2.


**Table 4-2 Advanced indexing parameters**

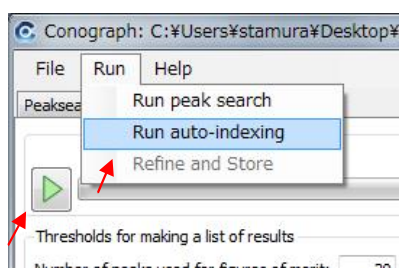
	Contents	Recommended value
①	Lower and upper limit of primitive cell volume	AUTO
②	Maximum value from four q values ( $= 1/d^2$ ) ( $q_1, q_2, q_3, q_4$ ) acquired from selected topography that satisfies Ito equation	AUTO
③	Maximum number of powder indexing solutions to be enumerated (before Bravais lattice determination)	AUTO
④	Reference value to determine whether linear sum of q ( $= 1/d^2$ ) value is equal to zero, including Ito formula	1.0
⑤	Lower thresholds for the Wu FOM ( $M^{\text{Wu}}$ ), the reversed FOM ( $M^{\text{Rev}}$ ), and the distance between two closest points in the crystal lattice. If a solution has values below these thresholds, it is deleted, and cannot be retrieved after indexing is executed.	1.9
⑥		1.0
⑦		2.0
⑧	If a solution has a rank below this number when all the solutions with the same Bravais types are sorted in the order of the de Wolff FOM (M), it is deleted, and cannot be retrieved after indexing is executed.	1000
⑨	Untick the checkbox, if lattice parameter candidates of the Bravais type are NOT necessary.	<input checked="" type="checkbox"/> (Yes)



## 5. Indexing

After executing a peak search and setting diffractometer parameters, indexing can be started.

### 5.1. Indexing execution

To start indexing and obtain a list of lattice parameter candidates, click the **Run indexing** button , or select **Menu > Run > Run auto-indexing** (the values of the input parameter are stored in the \*\_pks.histogramIgor and \*.inp.xml files from the auto\_generated\_files folder):



While the indexing is being executed, the progress is outputted in the **Log Note** frame (Fig. 5-1). The Skip button  can be used only when searching a solution, and when it is clicked, the solution search is aborted and the program shifts to subsequent processing. On the other hand, the Cancel button  can be used at any time, and when it is clicked, the indexing is discontinued.

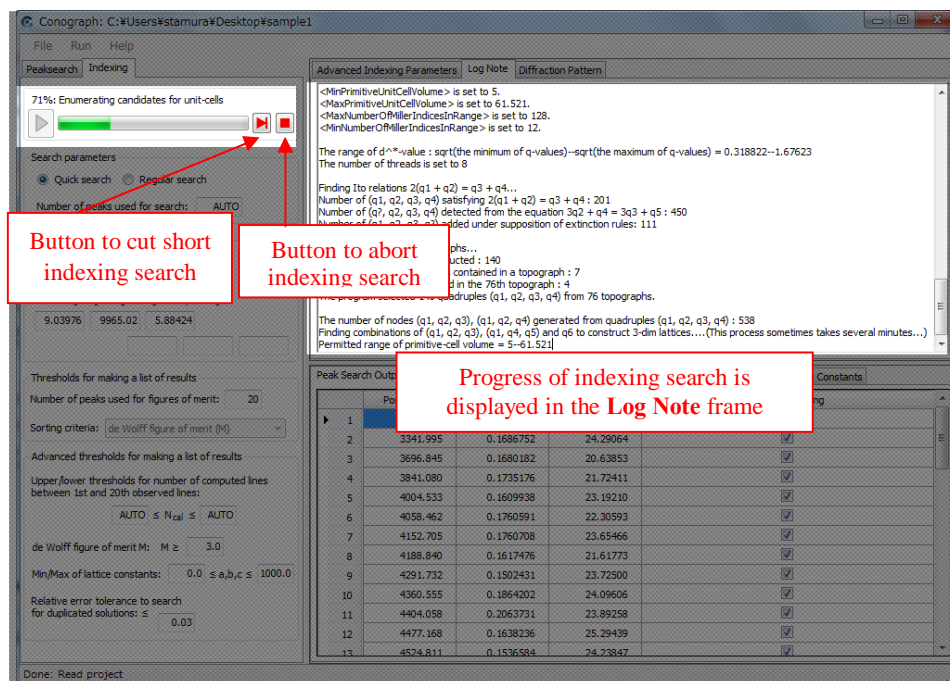


Fig. 5-1 Screenshot during indexing execution

## 5.2. When indexing is complete

When indexing is complete, the screen shown in Fig. 5-2 appears.

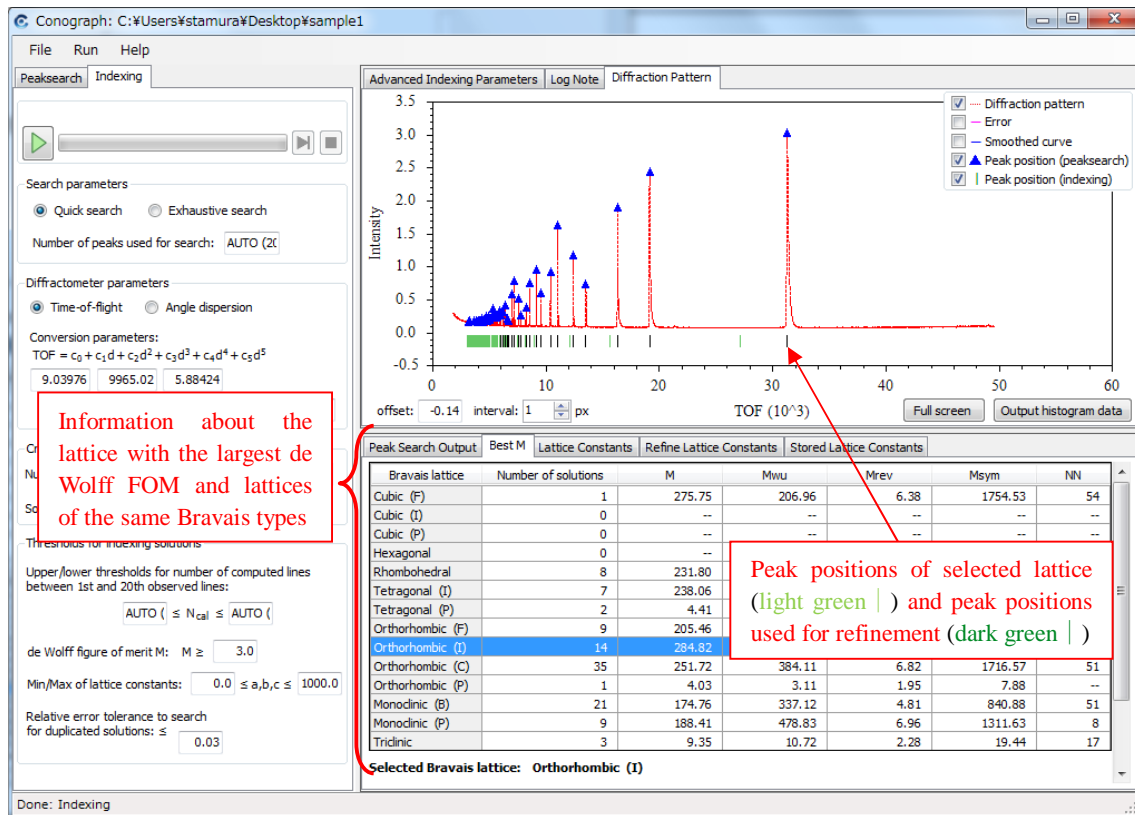


Fig. 5-2 Screenshot immediately after indexing execution

The lattice with the largest de Wolff FOM (Section 5.3) is automatically selected, and its information is displayed in the Selected Lattice Constants frame. In the **Diffraction Pattern** frame, the peak positions of the selected lattice are displayed with a light green tick mark (|). From these, the peak positions used for refinement (Chapter 6) are selected and displayed with a dark green tick mark (|).

### 5.3. Sorting /filtering lattice parameters

The lattice parameter candidates obtained by indexing can be sorted and filtered using parameters in the **Criteria for lattice parameters in candidate list** and **Advanced thresholds for lattice parameters in candidate list** areas of the **Indexing** frame.

The lattice parameters listed in the drop-down menu of the **Lattice Constants** frame are sorted and filtered using the parameters in the areas of Fig. 5-3. After indexing, sorting and filtering can be redone at any time, by changing the values of these parameters.

Thresholds for making a list of results

Number of peaks used for figures of merit: 20 ①

Sorting criteria: de Wolff figure of merit (M) ②

Advanced thresholds for making a list of results

Upper/lower thresholds for number of computed lines between 1st and 20th observed lines: AUTO ( ≤ N<sub>cal</sub> ≤ AUTO ( ③

de Wolff figure of merit M: M ≥ 3.0 ④

Min/Max of lattice constants: 0.0 ≤ a,b,c ≤ 1000.0 ⑤

Relative error tolerance to search for duplicated solutions: ≤ 0.03 ⑥

**Sorting criteria**

Sorting criteria for lattice parameters. For details, refer to Table 5-1 and Table 5-2.

**Criteria for lattice constants displayed in list**

Thresholds that limit lattice parameters to be displayed. For details, refer to Table 5-1. The lattice parameters are re-filtered whenever the Enter key is pressed or the mouse cursor is moved to another text box.

Peak Search Output	Lattice Constants	Selected Lattice Constants	Refine lattice constants	Stored L
Bravais lattice	M, Mwu, Mrev, Msym, NN; a, b, c, α, β, γ			
Cubic (F)	277.96, 208.63, 6.36, 1769.09, 85; 5.43, 5.43, 5.43, 90.0, 90.0, 90.0			
Cubic (I)	--			
Cubic (P)	--			
Hexagonal	--			
Rhombohedral	254.32, 481.45, 7.30, 1857.38, 284; 3.84, 3.84, 9.41, 90.0, 90.0, 120.0			
Tetragonal (I)	249.83, 398.22, 6.18, 1542.79, 222; 3.84, 3.84, 5.44, 90.0, 90.0, 90.0			
Tetragonal (P)	5.06, 4.60, 3.91, 19.75, 2; 2.72, 2.72, 3.14, 90.0, 90.0, 90.0			
Orthorhombic (F)	223.64, 577.20, 5.93, 1326.73, 68; 5.43, 5.43, 5.44, 90.0, 90.0, 90.0			
Orthorhombic (I)	284.82, 777.07, 6.83, 1944.21, 198; 3.84, 3.84, 5.43, 90.0, 90.0, 90.0			
Orthorhombic (C)	280.50, 427.41, 6.81, 1910.52, 6; 3.84, 5.43, 1.92, 90.0, 90.0, 90.0			
Orthorhombic (P)	4.03, 3.11, 1.95, 7.88, 0; 2.70, 3.14, 3.84, 90.0, 90.0, 90.0			
Monoclinic (B)	220.33, 420.30, 4.76, 1047.76, 65; 3.99, 5.43, 2.13, 90.0, 105.5, 90.0			
Monoclinic (P)	188.41, 478.83, 6.96, 1311.63, 1; 3.33, 1.92, 3.33, 90.0, 109.5, 90.0			
Triclinic	100.96, 119.27, 2.25, 226.73, 3; 2.07, 2.10, 3.30, 106.8, 91.0, 105.8			

**List of powder indexing solutions**

Lattice parameters that satisfy Criteria for lattice constants displayed in list are classified according to the Bravais type, and sorted according to the specified sorting criteria.

**Fig. 5-3 Sorting criteria and thresholds for lattice parameters in candidate list**

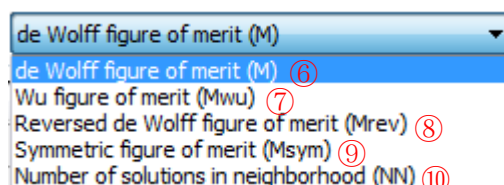


An explanation of the parameters and their recommended values are listed in Table 5-1. The recommended values are set up automatically in the text box when a project is created.

**Table 5-1 Thresholds for lattice parameters displayed in candidate list**

	Contents	Recommended value
①	Number of n peaks used for calculation of figures of merit (FOM). (The first n smallest q-values are used. This parameter can be larger than the number of peaks contained in the diffraction pattern, because it is automatically reduced.)	20
②	If the lattice parameters are specified, it is possible to calculate the number of peaks that exist in the range from the first to the n <sup>th</sup> observed peaks. Lower and upper thresholds of the number.	AUTO
③	Only lattice candidates with a de Wolff FOM ( $M_n$ ) greater than this value are displayed.	3
④	Lower and upper thresholds of lattice parameters a, b, c (Å).	
⑤	Relative resolution of $d^*$ (= $1/d$ ) value. (Used for deciding whether two lattices are identical.)	0.03

Immediately after indexing is executed, lattice parameters in the list are sorted according to the de Wolff FOM ( $M_n$ ). By using the **Sorting criteria** drop-down menu (Fig. 5-4), it is possible to change the sorting criteria for the lattice parameters (refer to Table 5-2).



**Fig. 5-4 Sorting criteria for lattice parameters**

Among the aforementioned five FOM, the de Wolff FOM gives preference to the lattice parameters with high symmetry, and has the best efficiency. However, another FOM occasionally might be more effective than the de Wolff FOM, particularly if the powder diffraction pattern contains impurity peaks [5].

The first four FOM (⑥--⑨ in Table 5-2) are defined in such a way that the values become close to 1 if there is no correlation between the observed and computed lines. A lattice satisfying  $M_n > 10$ ,  $M_n^{Wu} > 10$ ,  $M_n^{Rev} > 3$ , or  $M_n^{Sym} > 30$  is in general likely to be the correct solution. However, sometimes several distinct lattices may obtain large FOM values simultaneously. To select the most appropriate lattice parameters, all the plausible solutions should be checked using the methods described in Sections 5.4 and 5.5.

**Table 5-2 Sorting criteria for lattice constants displayed in list**

⑥	Sort in descending order by the de Wolff FOM (M) [6] (computed by using the method described in [5] to increase the numerical stability). The de Wolff FOM possesses these properties:  a) Insensitive to existence of unobserved computed lines (according to extinction rule) b) Sensitive to existence of un-indexed observed lines (such as impurity peaks) c) When almost identical lattices belong to different Bravais types, the lattice with higher symmetry normally obtains a higher value.
⑦	Sort in descending order by Wu FOM ( $M^{Wu}$ ) [7]. In terms of a) and b), it is similar to the de Wolff FOM; in terms of c), it is opposite, that is, a lattice with a lower symmetry is more likely to obtain a high value.
⑧	Sort in descending order by Reversed FOM ( $M^{Rev}$ ) [5]. $M^{Rev}$ is computed by exchanging the roles of observed peak positions and calculated peak positions in the definition of the de Wolff FOM. Because of this, it has properties that are opposite to those of the de Wolff FOM: a) Sensitive to existence of unobserved computed lines b) Insensitive to existence of un-indexed observed lines c) Tends to select a lattice with lower symmetry As in the case of the de Wolff FOM, if there is no correlation between observed lines and computed lines, the value becomes close to one.
⑨	Sort in descending order by Symmetric FOM ( $M^{Sym} = M \cdot M^{Rev}$ ) [5]. According to its definition, it has properties between ⑥M and ⑧ $M^{Rev}$ . As in a number of statistical quantities, such as chi-squares or R factors, the value remains the same after observed lines and computed lines are exchanged
⑩	Sort in descending order by NN (=number of lattices (NN) judged to be almost identical among the indexing solutions, by using the relative resolution in ⑤).

## 5.4. Find plausible indexing solutions

Several of the FOM introduced in Section 5.3 can extract a small number of candidates with high compatibility with inputted peak positions from multiple powder indexing solutions. However, none of the FOM is sufficiently effective when two lattices that belong to different Bravais types are compared. In order not to miss plausible solutions, in addition to their values of FOM, their Bravais types should be checked.

By using **Best M Frame** (Fig. 5-5) , it is possible to compare the best FOM values of the solutions in each Bravais type. By clicking the name of a Bravais type, the solutions with the largest FOM are displayed.

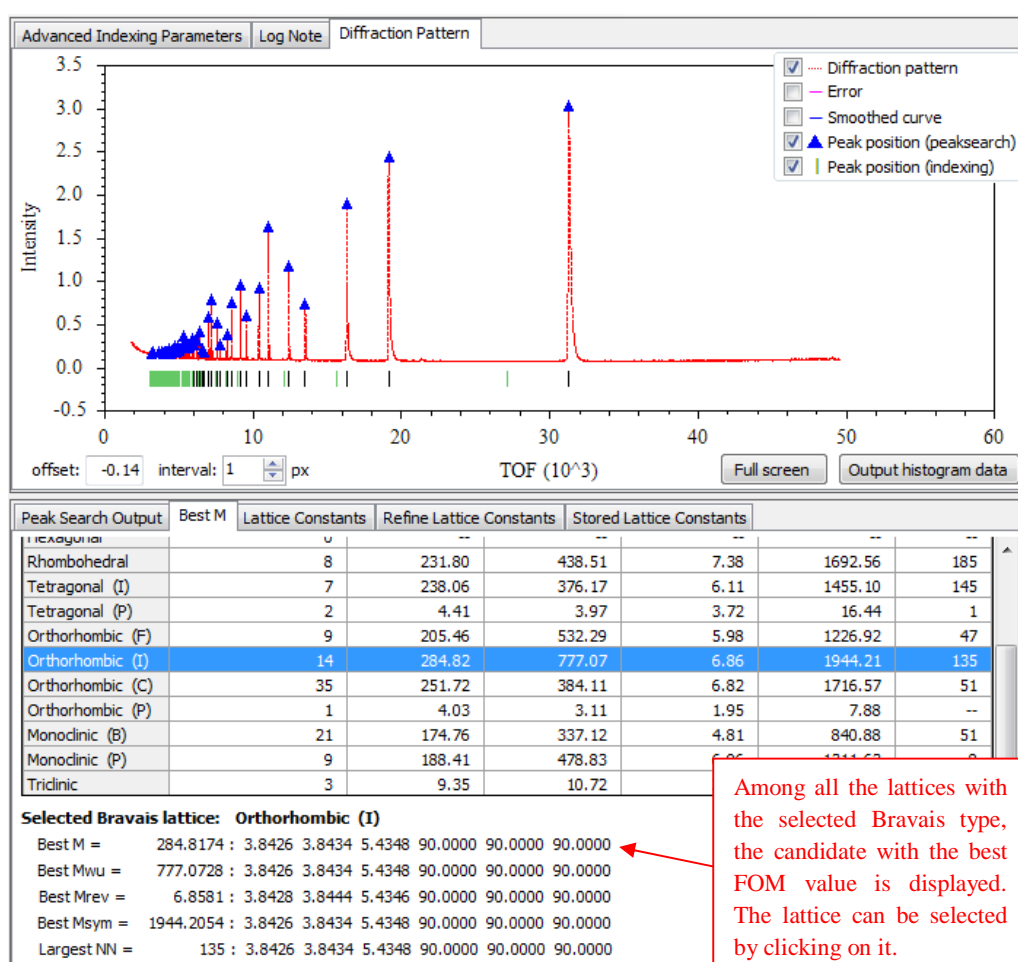
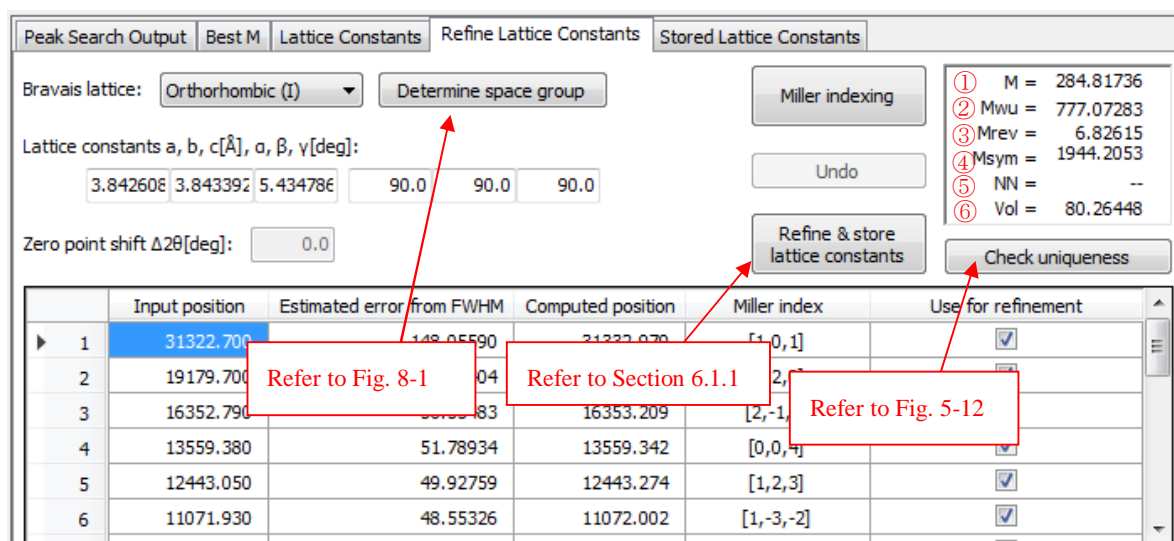


Fig. 5-5 Best M frame

In order not to spend much time searching for plausible solutions, you should check the information displayed in Best M frame in terms of the following two points:

- (i) Which Bravais types include a solution with a fairly large de Wolff FOM ( $M_n$ ) lattice (for example,  $M_n > 10$ )?
- (ii) Among all the lattices of such a Bravais type, does the same lattice obtain the maximum value in almost all FOM, including the de Wolff FOM? This is because different FOM have complementary properties (refer to Table 5-2), and therefore, a lattice that has obtained the maximum values for  $M_n$ ,  $M_n^{\text{Rev}}$ , and  $M_n^{\text{Sym}}$  has a high possibility of being the true solution.

By clicking on a set of lattice parameters in **Best M Frame** (Fig. 5-5), the tick marks in the **Diffraction Pattern frame** are automatically updated, and information about the parameters is displayed in the **Selected Lattice Constants frame** (Fig. 5-6, Table 5-3).



**Fig. 5-6 Selected Lattice Constants frame**

**Table 5-3 Information displayed in Selected Lattice Constants frame**

①	Value of the de Wolff FOM ( $M$ ) of the selected lattice
②	Value of Wu FOM ( $M^{\text{Wu}}$ ) of the selected lattice
③	Value of Reversed FOM ( $M^{\text{Rev}}$ ) of the selected lattice
④	Value of Symmetric FOM ( $M^{\text{Sym}}$ ) of the selected lattice
⑤	Value of NN of the selected lattice, <i>i.e.</i> , the number of lattices that are found during indexing execution and judged to be identical with ⑦
⑥	Unit-cell volume ( $\text{\AA}^3$ )

All the lattice parameters saved during the execution of powder indexing are displayed in **Lattice Constant Frame** (Fig. 5-7). It is possible to check peak positions of all the solutions in **Lattice Constant Frame** by scrolling them, using the up and down arrow keys or the mouse wheel. By clicking the name of a Bravais type in **Lattice Constant Frame**, the solution with the largest FOM

(specified in **Indexing Frame**) is selected:

Bravais lattice	M, Mwu
Cubic (F)	--
Cubic (I)	--
Cubic (P)	--
Hexagonal	30.17, 21.05, 4.85, 146.33, 78; 29.80, 29.80...
Rhombohedral	20.69, 15.47, 2.62, 54.23, 63; 51.61, 51.61, ...
Tetragonal (I)	4.07, 3.20, 1.92, 7.84, 1; 36.48, 36.48, 32.6...
Tetragonal (P)	7.78, 7.17, 2.04, 15.90, 8; 36.48, 36.48, 16....
Orthorhombic (F)	15.69, 14.54, 2.45, 38.47, 18; 27.47, 29.83, ...
Orthorhombic (I)	7.82, 7.96, 2.16, 16.87, 28; 22.49, 29.97, 51...
Orthorhombic (C)	17.09, 24.62, 7.42, 126.69, 279; 29.77, 51.6...
Orthorhombic (P)	24.80, 22.72, 5.09, 126.15, 33; 13.75, 14.90...
Monoclinic (B)	22.29, 39.86, 5.83, 130.01, 135; 29.80, 51.6...
Monoclinic (P)	26.15, 31.77, 5.39, 140.88, 18; 13.76, 14.90...
Tridinic	20.79, 37.70, 5.44, 113.01, 12; 13.76, 14.90...

By clicking here, the solution with the largest FOM among solutions with the same Bravais type is selected

Scrolling using arrow keys or mouse wheel

**Fig. 5-7 List of lattice parameter candidates obtained by indexing**

It should be also noted that the values of the FOM are occasionally improved greatly by refinement (Fig. 5-8). The operations necessary for refinement are explained in Section 6.1.1.

Advanced Indexing Parameters

Log Note

Diffraction Pattern

```

[!] Outputting lattice candidates shown:
C:\Users\rtomi\Desktop\sample2\auto_generated_files\allumina.index.xml
-----
---- optimize ----
Initial unit-cell parameters : 4.7521 4.7521 12.9704 90 90 120
Wave-length: 1.54056
Initial zero point shift: 0
Reduced unit-cell parameters : 4.7521 4.7521 12.9704 90 90 120
Optimizing lattice parameters by linear least squares...

1) Initial M20 = 27.6254
M20 of optimized solution = 266.635

2) Initial M20 = 266.635
M20 was not improved.

Optimized unit-cell parameters : 4.76098 4.76098 12.9954 90 90 120
Optimized zero point shift : -0.147583
Reduced unit-cell parameters : 4.76098 4.76098 12.9954 90 90 120
-----

```

Select a lattice

Initial value of lattice parameters

Initial de Wolff FOM

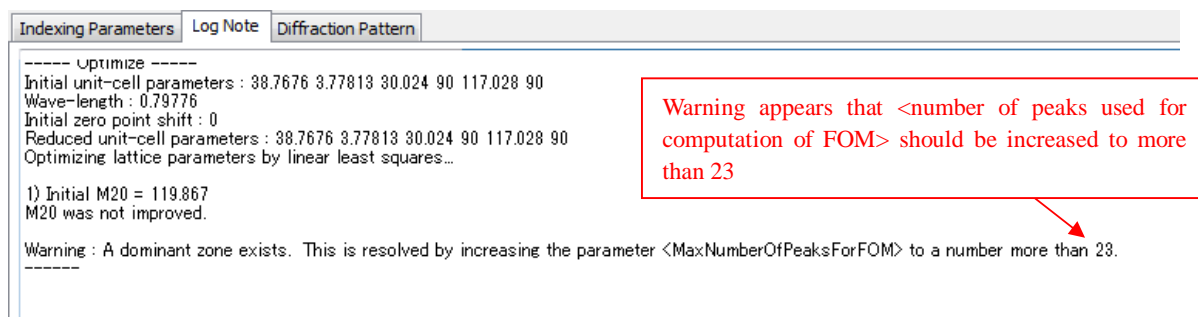
The de Wolff FOM was improved. Refinement is stopped if there is no further improvement

Refined lattice parameters and zero point shift

Niggli-reduced parameters

**Fig. 5-8 Message outputted in Log Note frame during refinement execution**

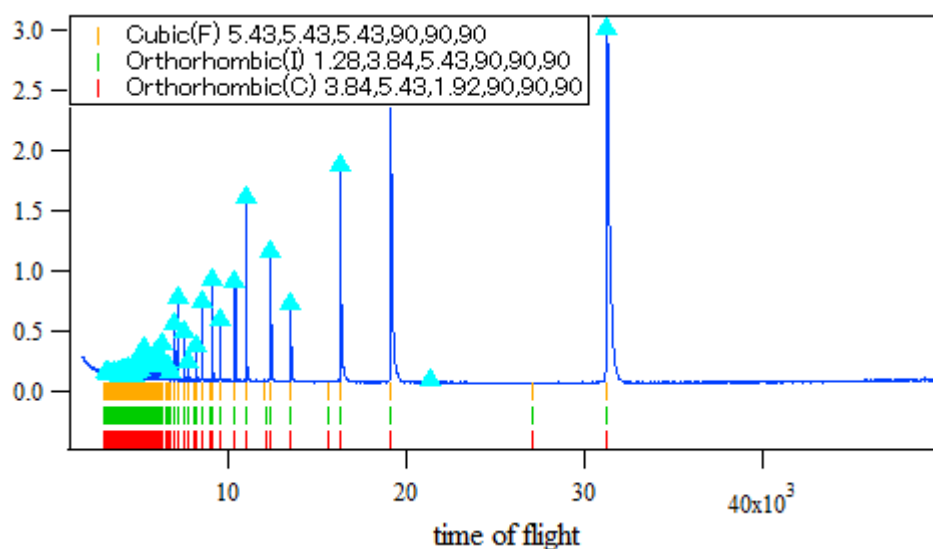
While the refinement is being executed, a warning concerning dominant zones may appear in the **Log Note** frame (Fig. 5-9). When this warning appears, it may be considered that the FOM did not work efficiently. Therefore, it is advisable to increase the <Number of peaks used for computation of FOM> in the **Criteria for lattice constants in the list** area (Fig. 5-3), according to the warning. Next verify that there is no warning when refinement is executed again.



**Fig. 5-9 Log message reporting that a dominant zone is found**

## 5.5. Decide the correct lattice parameters

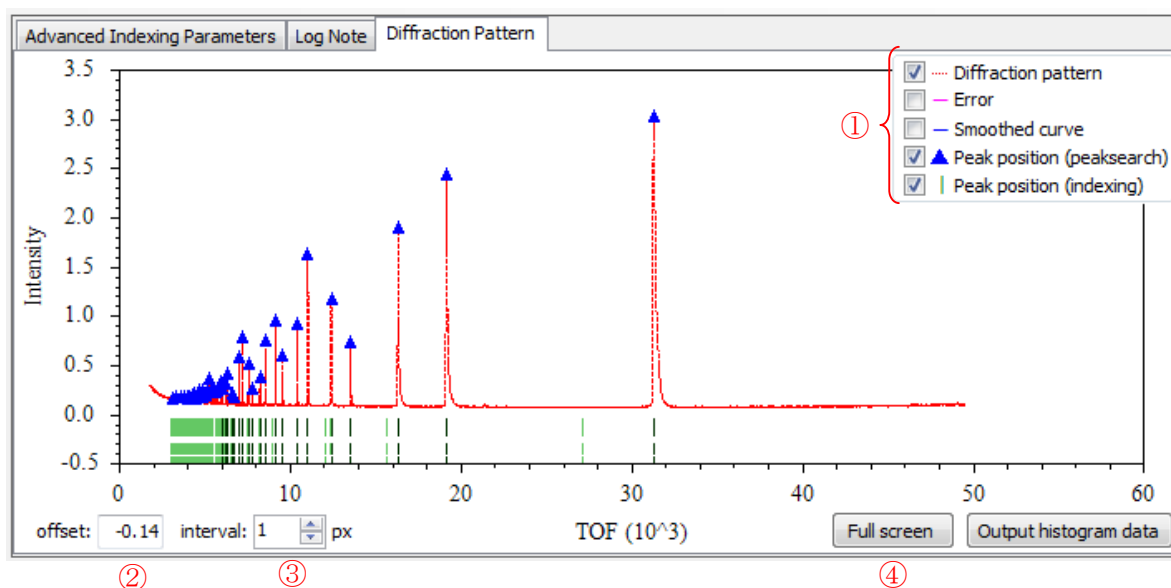
Before drawing a conclusion as to which solution for the lattice constants is correct, the computed lines ( | ) and the observed lines ( ) should be compared. In addition, the lattice parameters may not be determined uniquely from the peak positions (Fig. 5-10). This phenomenon occurs infrequently in low-symmetry cases and consistently in high-symmetry cases, and is known as *geometrical ambiguity* [2]. Therefore, it should be checked in respective cases whether or not the uniqueness of solutions holds by using Conograph's **Check Uniqueness** button (Fig. 5-12).



**Fig. 5-10 Example of distinct lattice parameters with identical peak positions**

The peak positions of all the lattices that have been refined can be displayed as tick marks on the **Diffraction Pattern** frame. This allows the peak positions ( | ) of several lattice parameters to be compared simultaneously. In order to hide tick marks of some of the lattices, untick the corresponding check boxes labeled **Plot** (or the corresponding lattice can be deleted) in the **Stored Lattice Parameters** frame.

The methods for changing the display of tick marks are shown in Fig. 5-11 and Table 5-4.



**Fig. 5-11 Diffraction Pattern frame**

**Table 5-4 Diffraction Pattern frame**

①	Displays/hides switch
②	Height (y-coordinate) of the position of tick marks displayed at the top. Press Enter key to reflect the change. This height can be increased or decreased by locating the cursor in the text box and rotating the mouse wheel.
③	Space between tick marks and tick marks immediately below
④	Enlarges the <b>Diffraction Pattern</b> frame to full screen.



If the peak positions of a solution accord well with the observed lines in the diffraction patterns, select the solution and click the **Check Uniqueness** button. Then, all the lattices with almost the same peak positions as the currently selected lattice are generated [3].

If such lattices exist, a window appears as shown in Fig. 5-12. The available operations in the window are the same as in the **Diffraction Pattern** frame. By clicking the **Output histogram data** button, a histogram file that contains the peak positions of all the lattice parameters displayed is outputted.

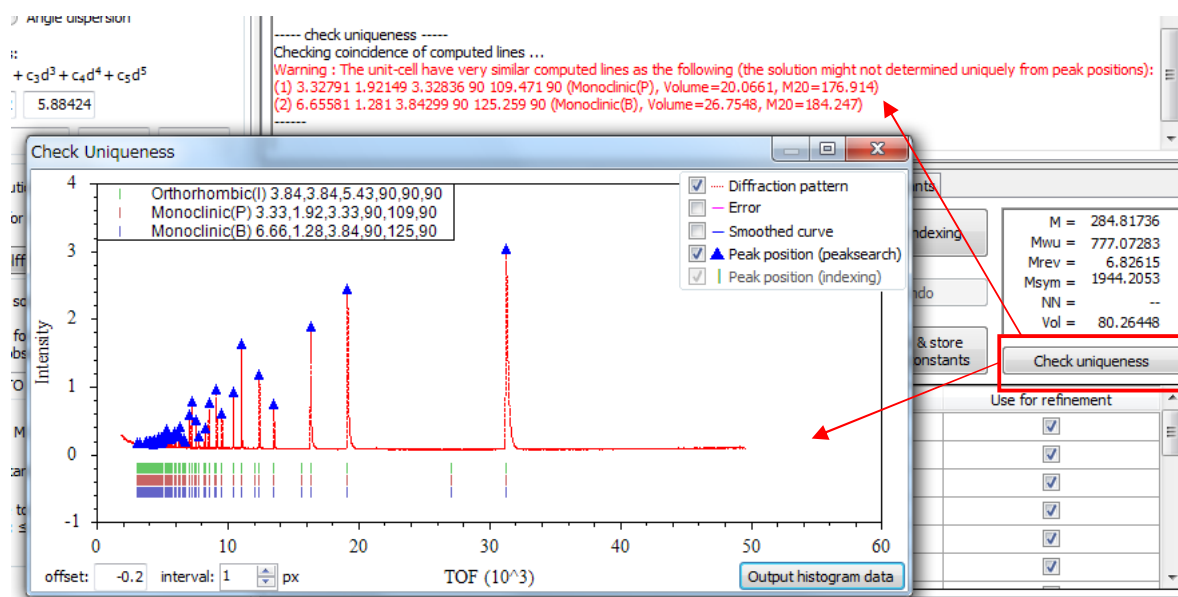


Fig. 5-12 Check uniqueness of solutions

## 6. Refining lattice parameters and zero point shift

The method for refining lattice parameter candidates obtained by indexing (and zero point shift for angle dispersion methods) is explained in the following sections. The refinement is conducted using linear/non-linear least squares methods.

### 6.1. Method for refinement execution

#### 6.1.1. Refinement of lattice parameters selected from the list

To refine the lattice parameters and zero point shift, select the lattice parameters and then click the **Refine & store lattice constants** button in the **Refine Lattice Constants** frame (or by selecting **Menu > Run > Refine & store lattice constants**):

Bravais lattice: Orthorhombic (1) Determine space group Miller indexing

Lattice constants a, b, c[Å], α, β, γ[deg]: 3.842608 3.843392 5.434786 90.0 90.0 90.0

Zero point shift Δ2θ[deg]: 0.0 Undo

Refine & store lattice constants Check uniqueness

	Input position	Estimated error from FWHM	Computed position	Miller index	Use for refinement
1	31322.700	148.05590	31332.979	[1,0,1]	<input checked="" type="checkbox"/>
2	19179.700	80.59404	19180.509	[0,2,0]	<input checked="" type="checkbox"/>
3	16352.790	56.55483	16353.209	[2,-1,1]	<input checked="" type="checkbox"/>
4	13559.380	51.78934	13559.342	[0,0,4]	<input checked="" type="checkbox"/>
5	12443.050	49.92759	12443.274	[1,2,3]	<input checked="" type="checkbox"/>
6	11071.930	48.55326	11072.002	[1,-3,-2]	<input checked="" type="checkbox"/>

M = 284.81736  
Mwu = 777.07283  
Mrev = 6.82615  
Msym = 1944.2053  
NN = --  
Vol = 80.26448

Fig. 6-1 shows a screenshot when the refinement is being executed. The refined lattice parameters are saved and displayed in the **Stored Lattice Constants** frame.

Advanced Indexing Parameters
Log Note
Diffraction Pattern

<MinNumberOfMillerIndicesInRange> is set to 12.

The range of d<sup>h\*</sup>-value : sqrt(the minimum of q-values)--sqrt(the maximum of q-values) = 0.318822--1.67623

----- check uniqueness -----

Checking coincidence of computed lines ...

Warning : The unit-cell have very similar computed lines as the following (the solution might not determined uniquely from peak positions):

(1) 3.32791 1.92149 3.32836 90 109.471 90 (Monoclinic(P), Volume=20.0661, M20=176.914)

(2) 6.65581 1.281 3.84299 90 125.259 90 (Monoclinic(B), Volume=26.7548, M20=184.247)

----- Refine -----

Initial unit-cell parameters : 3.84261 3.84339 5.43479 90 90 90

Reduced unit-cell parameters : 3.84261 3.84339 5.43479 90 90 90

Optimizing lattice parameters by linear least squares...

1) Initial M20 = 284.817

M20 was not improved.

Peak Search Output
Best M
Lattice Constants
Refine Lattice Constants
Stored Lattice Constants

Bravais lattice: Orthorhombic (I) Determine space group

Lattice constants a, b, c[Å], α, β, γ[deg]:

3.842608
3.843392
5.434786
90.0
90.0
90.0

Zero point shift Δ2θ[deg]: 0.0

Miller indexing

Undo (Ref.)

Refine & store lattice constants

Check uniqueness

M = 284.81736

Mwu = 777.07283

Mrev = 6.82615

Msym = 1944.2053

NN = --

Vol = 80.26448

	Input position	Estimated error from FWHM	Computed position	Miller index	Use for refinement
▶ 1	31322.700	148.05590	31332.979	[1,0,-1]	<input checked="" type="checkbox"/>
2	19179.700	80.59404	19180.509	[0,2,0]	<input checked="" type="checkbox"/>
3	16352.790	56.55483			
4	13559.380	51.78934			
5	12443.050	49.92759			
6	11071.930	48.55326			

After refinement, these values are automatically updated using the obtained lattice parameters.

Log reporting the results of refinement

Information here can be copied by specifying a range by dragging and then pressing **Ctrl + C**

**Fig. 6-1 Screenshot during refinement execution**

The peak positions to be used for refinement can be selected manually from the **Use for refinement** column in the **Refine lattice constants** frame. The color of a tick mark changes from dark green (I) to light green (I), according to a change in the corresponding flag.

Peak Search Output
Best M
Lattice Constants
Refine Lattice Constants
Stored Lattice Constants

Bravais lattice: Orthorhombic (I) Determine space group

Lattice constants a, b, c[Å], α, β, γ[deg]:

3.842608
3.843392
5.434786
90.0
90.0
90.0

Zero point shift Δ2θ[deg]: 0.0

Miller indexing

Undo (Ref.)

Refine & store lattice constants

Check uniqueness

M = 284.81736

Mwu = 777.07283

Mrev = 6.82615

Msym = 1944.2053

NN = --

Vol = 80.26448

	Input position	Estimated error from FWHM	Computed position	Miller index	Use for refinement
▶ 1	31322.700	148.05590	31332.979	[1,0,-1]	<input checked="" type="checkbox"/>
2	19179.700	80.59404	19180.509	[0,2,0]	<input checked="" type="checkbox"/>
3	16352.790	56.55483	16353.209	[2,1,-1]	<input checked="" type="checkbox"/>
4	13559.380	51.78934	13559.342	[0,0,4]	<input checked="" type="checkbox"/>
5	12443.050	49.92759	12443.274	[1,2,-3]	<input checked="" type="checkbox"/>
6	11071.930				<input checked="" type="checkbox"/>

Peaks to be used for refinement are checked

### 6.1.2. Refining lattice constants entered by user

This section explains the method for refining lattice parameters specified manually by the user. In this case, although indexing execution is not required for refinement, a peak search is required for obtaining peak positions.

The diffractometer parameter **Wavelength of diffractometer** (or **Conversion Parameters**) can be inputted from the **Indexing** frame. When the angle dispersion is selected, it is also possible to enter an initial value of the zero point shift from the **Refine lattice constants** frame (normally, it is not necessary to set the initial value to a value other than 0):

	Input position	Estimated error from FWHM	Computed position	Miller index	Use for refinement
1	31322.700	148.05590	31332.979	[1,0,-1]	<input checked="" type="checkbox"/>
2	19179.700	80.59404	19180.509	[0,2,0]	<input checked="" type="checkbox"/>

If the **Miller indexing** button is clicked, the Miller indexing of peaks is performed using the Bravais lattice and lattice parameters entered. Subsequently, the Miller indices assigned to peaks are displayed:

	Input position	Estimated error from FWHM	Computed position	Miller index	Use for refinement
1	31322.700	148.05590	31332.979	[1,0,-1]	<input checked="" type="checkbox"/>
2	19179.700	80.59404	19180.509	[0,2,0]	<input checked="" type="checkbox"/>
3	16352.790	56.55483	16353.209	[2,1,-1]	<input checked="" type="checkbox"/>
4	13559.380	51.78934	13559.342	[0,0,4]	<input checked="" type="checkbox"/>
5	12443.050	49.92759	12443.274	[1,2,-3]	<input checked="" type="checkbox"/>
6	11071.930	48.55326	11072.002	[1,3,-2]	<input checked="" type="checkbox"/>

The refinement of the lattice parameters is performed using the assigned Miller indices. If required, it is possible to manually specify which peak positions are to be used for refinement, by using the flags in the rightmost column (refer to Table 6-1 for the meaning of the other columns). When the **Refine & store lattice constants** button is clicked, lattice parameters are refined, and appended in the **Stored Lattice Constants** frame.

**Table 6-1 Information about peaks in Refine lattice constants frame**

Column	Contents
1	Peak positions of the considered diffraction pattern
2	These values (calculated from the full widths at half maximum of peaks) are used as weights for least squares method
3	Peak positions of the selected lattice constants computed by using the Miller indices in column 4 and diffractometer parameters
4	Miller indices used for refining lattice parameters
5	Checked, if the peak position is used for refining lattice parameters

## 6.2. Undo button

By clicking the **Undo** button, it is possible to restore the lattice parameters and the zero point shift to the values that existed before you keyed in the numbers in the text boxes or executed refinement (Fig. 6-2). This **Undo** cannot be applied successively, and therefore, only the last values of the parameters can be retrieved.

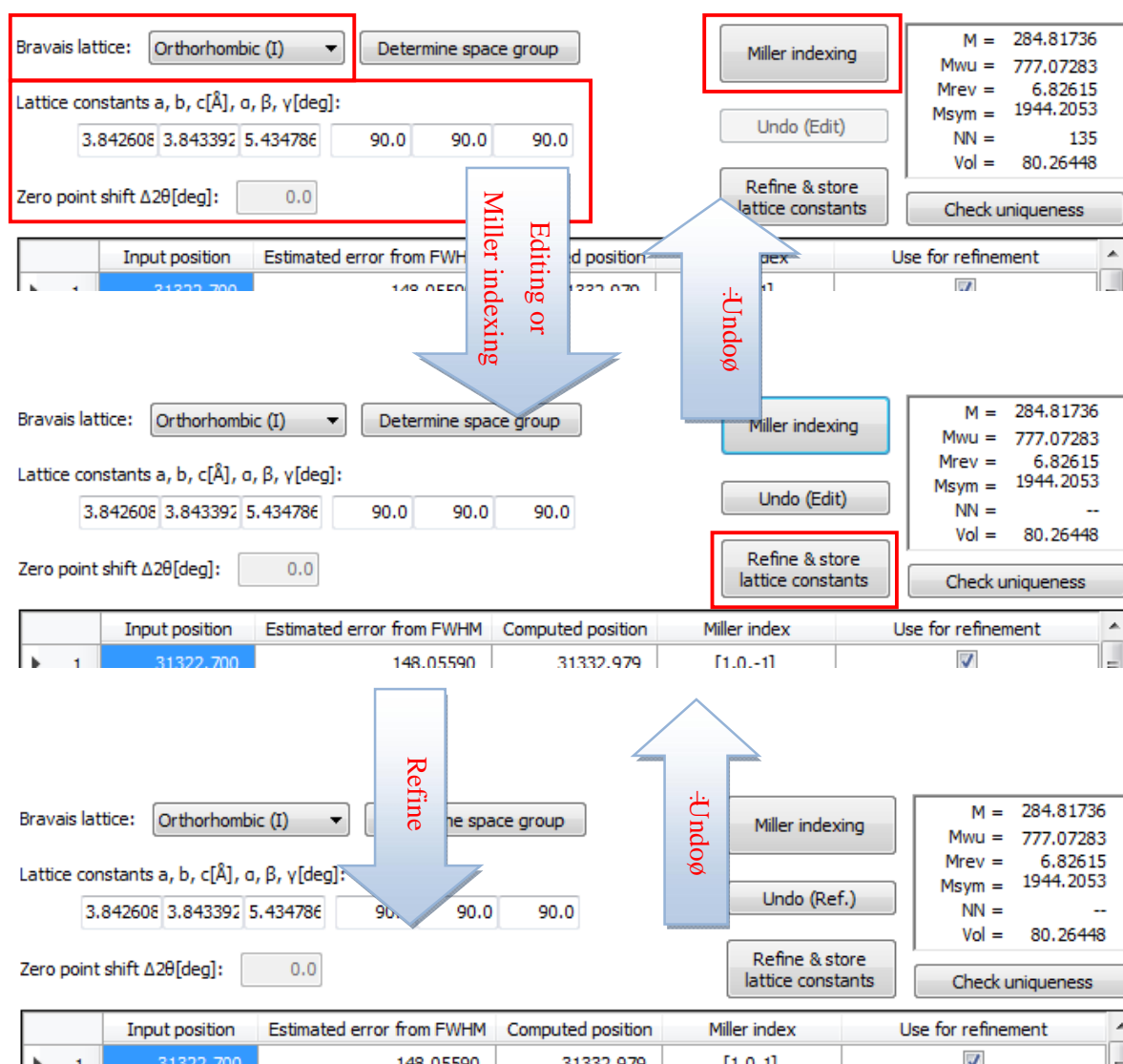


Fig. 6-2 Undo button

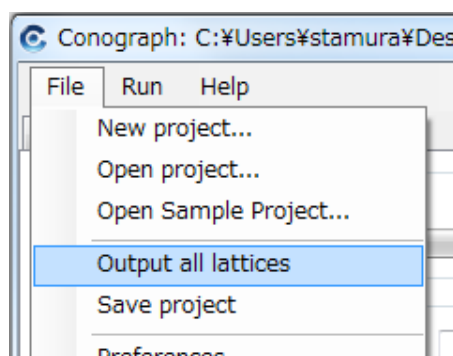
## 7. Result output

There are three types of output files, **\*.index.xml** (**\*.index2.xml**), **\*.histogramIgor**, and a backup file (all are text files, except for the backup file). The respective output files are explained in the following sections.

### 7.1. \*.index.xml

The **auto\_generated\_files/\*.index.xml** file is outputted in the project folder, if either of the following events occurs:

- Indexing execution is completed
- The application is closed or another project is started
- **File > Output all lattices** (Fig.7-1) is selected.

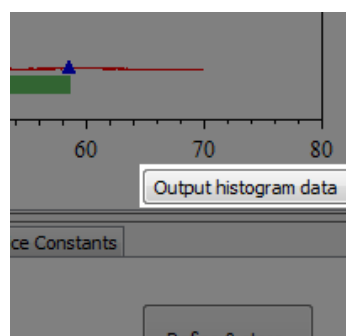


**Fig.7-1 Output all lattices**

From the lattice parameter candidates obtained by indexing, the lattice constant information displayed on the GUI is indicated in the **\*.index.xml** file (for the format, refer to Fig. 11-5 and 10-7). If the name of the diffraction data file is **\*.histogramIgor**, the name of the output file becomes **\*.index.xml**. The same file is always overwritten at the time of the above events.

### 7.2. Igor text file and \*.index2.xml file

When the **Output histogram data** button (Fig.7-2) is clicked, the **\*.histogramIgor** file is outputted in the project folder. In this file, in addition to the contents of the input diffraction data file, the Miller indices and the peak positions of the lattice parameters that show tick marks in the **Diffraction Pattern** frame are saved.



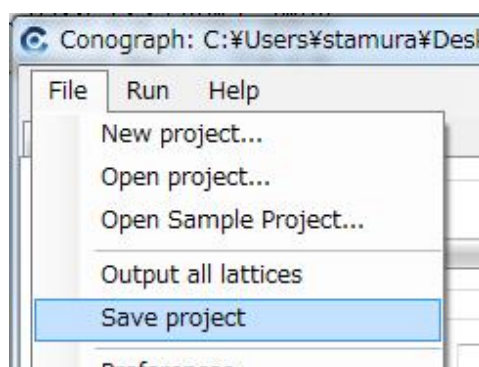
Output **\*.histogramIgor** file containing Miller indices and their corresponding peak positions (tick marks)

**Fig.7-2 Output of Igor file**

At the same time, information about the lattice parameters outputted in the **\*.histogramIgor** file is outputted as the **\*.index2.xml** file.

### 7.3. Backup file

When **File > Save project** (Fig. 7-3) is selected, a backup file is created in the folder as the **auto\_generated\_files/backup.dat** file, which stores all the lattice parameter candidates that were obtained by indexing or exist in the **Stored Lattice Constants** frame.



**Fig. 7-3 Saving a project**

This file is also outputted when a project containing a data set of lattice parameters is closed (this occurs when the application is closed or another project is opened).

By using the backup file, the condition at the time of saving **backup.dat** can be reproduced when Conograph is started in the next session. When the project is opened in the next session, the user is asked whether s/he wishes to open the backup file, if it exists in the project folder. The existing backup file is overwritten whenever either of the above events occurs in the opened project.



## 8. Space group determination

In the stages described thus far, only the systematic absences caused by the Bravais lattice type were considered during computation of the figures of merit. However, additional extinction derived from the space group may have happened. If the **Determine Space Group** button in the **Refine Lattice Constants** frame is clicked, the value of the de Wolff figure of merit  $M$  is recomputed by using the reflection conditions of each space group with the Bravais lattice type selected in the frame, and a window as in Fig. 8-1 appears. The  $M$  values of all the space groups are listed up in the window, and it is possible to check which space group fits well to the observed peaks.

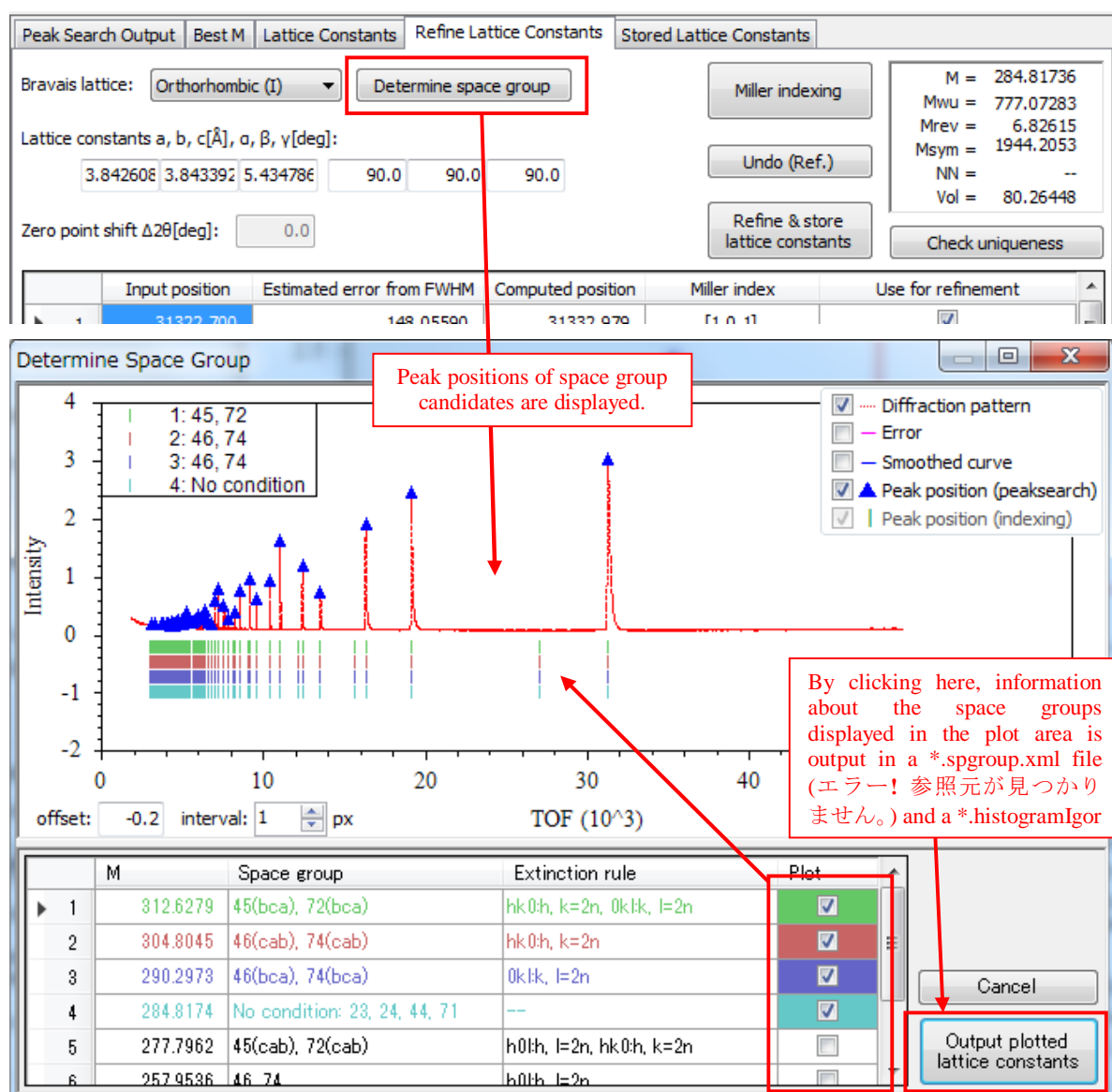
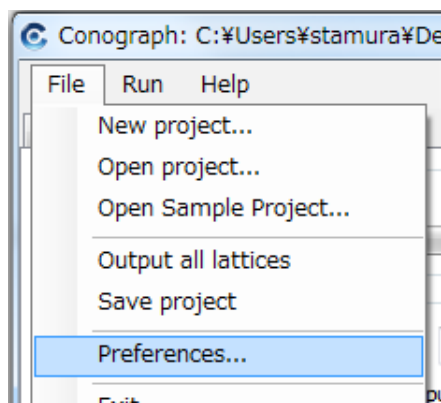


Fig. 8-1 空間群の決定

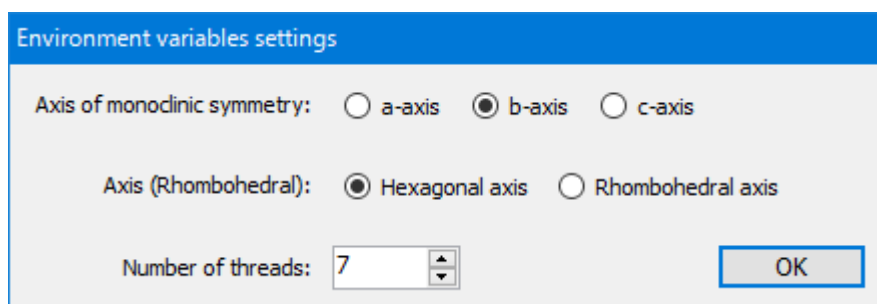
## 9. Other GUI operations

### 9.1. Configuration parameters

Select the **Menu > File > Preferences** as follows:



Then, the following **Environment variables settings** dialog box is displayed.

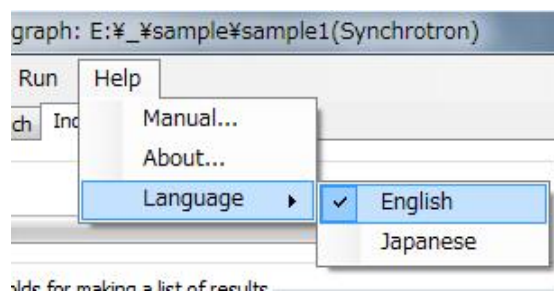


The <Number of threads> is used when running parallel computing. The number to which this parameter can be set depends on the computer. The initial value is set to (the number of threads the computer has) - 1. The higher the value, the greater is the speed; however, the computational cost also becomes high. It is advisable to set a small value if you want to run another application simultaneously.

The used configuration parameters are stored in the **auto\_generated\_files/\*.inp.xml** file. The values of the configuration parameters when the application is closed are stored in the software setup file and are reset when the next session starts.

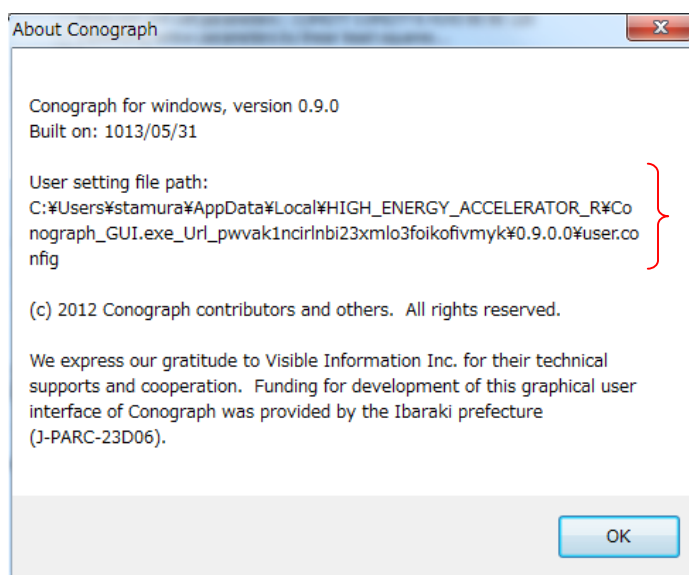
### 9.2. Help menu

From the **Help** menu, you can select three commands, **Manual**, **About**, and **Language**:



When **Manual** is selected, the user manual (*i.e.*, this manual) appears.

When **About** is selected, the following dialog box appears:



In this user setting file, the language, previously opened project path, and configuration parameters are stored.

In **Language**, English or Japanese can be selected as the language of the application. The application has to be restarted in order to activate a change in this setting.

## 10. Parameters that can be changed to obtain better results

### 10.1. Peak search

In peak search, it is recommended that diffraction peaks are collected as uniformly as possible on the basis of peak height. Filtering diffraction peaks manually (including removal of overlapped peaks) is unnecessary and not desirable, unless there is valid prior information.

In order to obtain such a peak search result, only the following parameters need to be adjusted:

- (1) <Threshold for peak height>
- (2) <Number of data points used for smoothing histogram>.

In addition, in cases of characteristic X-ray data that contain  $\alpha_2$  peaks, the  $\alpha_2$  peaks must be removed prior to powder indexing (Fig. 3-1).

The following are notes related to the adjustment of the parameters (1) and (2).

#### (1) <Threshold for peak height>

This parameter is used as a lower threshold for magnitudes of intensities to be detected in a peak search. If  $c \times (\text{error value of intensity})$  is used, as in the default setting, a peak at peak-position  $x$  is detected, if and only if it has a peak height greater than  $(\text{the threshold}) \times \text{Err}[y]$ , where  $\text{Err}[y]$  is the value of the error in intensity at  $x$ . The peak height used here is obtained by subtracting the estimated background value from  $y$ . Our recommended threshold value is within the range of  $3\hat{\sigma} - 10$ .

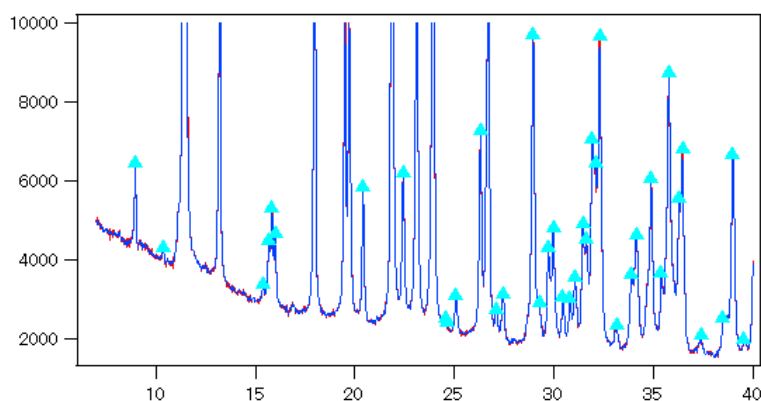
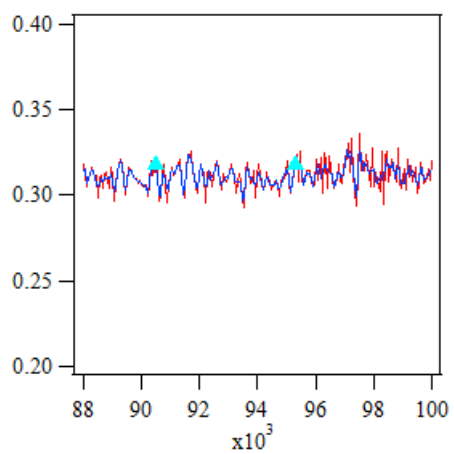


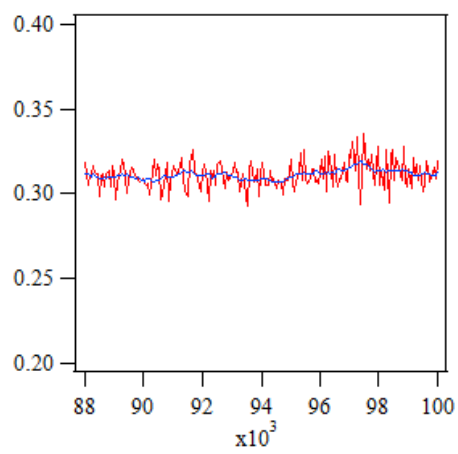
Fig. 10-1 Example of peak search results in radiation beam data

#### (2) <Number of data points used for differential calculation>

This parameter can be used to avoid background noise being picked up as peaks. If it has a small value, the smoothing curve is fit more finely to local irregularity, because the number of data points for computing each  $y$ -value of the smoothing curve is set to this value. Fig. 10-2 shows an example.



**Fig. 10-2**  $\langle \text{Number of data points} \rangle = 5$



**Fig. 10-3**  $\langle \text{Number of data points} \rangle = 25$

## 10.2. Powder indexing

It has been confirmed that a search using the recommended parameter values provides correct solutions in an extremely wide range of cases, in particular, in memory-efficient search [4]. Nevertheless, if good results are not obtained, they may be improved by changing some of the parameters. In the following, the parameters to be changed in order to conduct a more exhaustive search (Section 10.2.1), enhance computing speed (Section 10.2.2), and improve the efficacy of the figures of merit (Section 10.2.3) are explained.

### 10.2.1. Conduct a more exhaustive search

(1) <Searching method> in **Indexing** frame: **Quick search**  $\Rightarrow$  **Memory-efficient search**.

(2) <Number of peaks used in the search> (**Indexing** frame): **AUTO**  $\Rightarrow$  a number greater than 48

When **AUTO** is entered, 48 peaks are used for powder indexing, unless the diffraction pattern contains only a smaller number of peaks. However, even this number of peaks may be insufficient if a dominant zone exists. In such cases, increasing the number is effective.

(3) <Tolerance level for errors of sums of q values> (**Advanced Indexing parameter** frame): 1  $\Rightarrow$  1.5

In cases of characteristic X-rays or reactor sources, better results may be yielded if a large value is used.

### 10.2.2. Enhance computing speed

(1) Increase <Number of threads> (**File > Preferences**)

The simplest method is to increase the number of threads used.

(2) <Search parameters> (**Indexing parameters** frame): **Memory-efficient search**  $\Rightarrow$  **Quick search**.

(3) <Bravais lattice> (**Advanced Indexing Parameters** frame): untick

If you have prior information about the Bravais type, the information can be used to reduce the time required in the stage after Bravais lattice determination.

(4) Increase values of <Volume of primitive cell> or <Thresholds of minimum distance between lattice points> (**Advanced Indexing Parameter** frame)

If you have prior information about these parameters, the information can be used to reduce

the time required for powder auto-indexing.

### 10.2.3. Improve the efficacy of figures of merit

- (1) <Zero point shift> (**Indexing** frame): 0 deg.  $\Rightarrow$  more accurately estimated value

For diffraction patterns with a large zero point shift ( $2\theta > \text{approximately } 0.1^\circ$ ), the FOM values sometimes become small. The results may be improved by conducting powder indexing using the estimated value of the zero point shift. The zero point shift can be estimated by using one of the following methods.

- (a) The reflection pair method [1],
- (b) After conducting powder indexing once, refine the zero point shift and lattice parameters with relatively larger  $M_n^{\text{Rev}}$  and  $M_n^{\text{Sym}}$  (for instance,  $M_n^{\text{Rev}} > 3$  or  $M_n^{\text{Sym}} > 10$  approximately), and re-execute indexing, using the obtained zero point shift.

In both methods, it is necessary to test several candidate values.

- (2) <Number of peaks used for computation of FOM> (**Indexing** frame): 20  $\Rightarrow$  a number greater than 20

The value 20 frequently used for this parameter might be insufficient if a problem called dominant zone occurs. If a dominant zone is found when refining the lattice constants and zero point shift, a warning message and the number of peaks required appear in the **Log Note** frame. In that case, set this parameter to a value greater than the number displayed.

- (3) Improve results of peak search (or change the <Use for Indexing> flags in **Peak search output** frame)

Impurity peaks greatly affect the sorting results. Because of this, it is desirable to reduce the number of impurity peaks as far as possible, at least in the range of the first to n-th peaks, when the parameter <Number of peaks used for computation of FOM> is set to n.

## 11. Input/output text file formats

The formats for the input/output text files, cntl.inp.xml, \*.inp, \*.histogramIgor, and \*.index files, are shown in this section.

```
<ZCodeParameters>
  <ConographInputFile>
    <!-- Control parameters for calculation.-->
    <ControlParamFile> HRP000675.BS.bin04f.inp.xml </ControlParamFile>
    <!-- Peak-position data.-->
    <PeakDataFile> HRP000675.BS.bin04f_pks.histogramIgor </PeakDataFile>
    <!-- Output file -->
    <OutputFile> hrp000675.bs.bin04f.index </OutputFile>
  </ConographInputFile>

  <PeakSearchInputFile>
    <ControlParamFile> HRP000675.BS.bin04f.inp.xml </ControlParamFile>
    <HistogramDataFile>
      <FileName> HRP000675.BS.bin04f.histogramIgor </FileName>
      <!-- "XY": general, "IGOR":IGOR; "Rietan":Rietan.-->
      <Format> IGOR </Format>
      <!-- When "IsErrorContained" equals 1, input errors in the 3rd column of the histogram.-->
      <IsErrorContained> 1 </IsErrorContained>
    </HistogramDataFile>
    <Outfile> HRP000675.BS.bin04f_pks.histogramIgor </Outfile>
  </PeakSearchInputFile>
</ZCodeParameters>
```

**Fig. 11-1 Example of cntl.inp.xml**



```

<?xml version="1.0" encoding="UTF-8" ?>

<ZCodeParameters>
  <ConographParameters>
    <!-- Parameters for the histogram.-->
    <!-- 0:tof, 1:angle dispersion-->
    <IsAngleDispersion> 0 </IsAngleDispersion>

    <!-- Conversion parameters for tof : a polynomial of any degree -->
    <ConversionParameters> 0 1 0 </ConversionParameters>

    <!-- Peak shift parameters for angle dispersion : Z(deg.), Ds(deg.), Ts(deg.).
          2*d*sin(theta0) = Wlength, 2*theta = 2*theta0 + Z + Ds*cos(theta0) + Ts*sin(2*theta0). -->
    <PeakShiftParameters> 0 </PeakShiftParameters>

    <!-- Wave length(angstrom) for angle dispersion. -->
    <WaveLength> 1.54056 </WaveLength>

    <!-- Parameters for search.-->
    <SearchLevel>
      <!-- 0:quick search (suitable for lattices with higher symmetries.),
            1:exhaustive search (suitable for lattices with lower symmetries.)-->
            0
    </SearchLevel>

    <!-- Number of reflections for calculation.-->
    <MaxNumberOfPeaks> AUTO </MaxNumberOfPeaks>

    <!-- The critical value c to judge if linear sums of Q equal zero. ( abs(¥sigma_i Q_i) <= c * Err<¥sigma_i Q_i> ) -->
    <CriticalValueForLinearSum> 1 </CriticalValueForLinearSum>

    <!-- Minimum of the volume of primitive unit-cell (>=0) -->
    <MinPrimitiveUnitCellVolume> AUTO </MinPrimitiveUnitCellVolume>

    <!-- Maximum of the volume of primitive unit-cell (>0) -->
    <MaxPrimitiveUnitCellVolume> AUTO </MaxPrimitiveUnitCellVolume>

    <!-- Maximum number of quadruples (q1,q2,q3,q4) taken from selected topographs.-->
    <MaxNumberOfTwoDimTopographs> AUTO </MaxNumberOfTwoDimTopographs>

    <!-- Maximum number of seeds of 3-dimensional topographs -->
    <MaxNumberOfLatticeCandidates> AUTO </MaxNumberOfLatticeCandidates>

    <!--Output for each crystal system? (0:No, 1:Yes)-->
    <OutputTriclinic> 1 </OutputTriclinic>
    <OutputMonoclinicP> 1 </OutputMonoclinicP>
    <OutputMonoclinicB> 1 </OutputMonoclinicB>
    <OutputOrthorhombicP> 1 </OutputOrthorhombicP>
    <OutputOrthorhombicB> 1 </OutputOrthorhombicB>
    <OutputOrthorhombicI> 1 </OutputOrthorhombicI>
    <OutputOrthorhombicF> 1 </OutputOrthorhombicF>
    <OutputTetragonalP> 1 </OutputTetragonalP>
    <OutputTetragonalI> 1 </OutputTetragonalI>
    <OutputRhombohedral> 1 </OutputRhombohedral>
    <OutputHexagonal> 1 </OutputHexagonal>
    <OutputCubicP> 1 </OutputCubicP>
    <OutputCubicI> 1 </OutputCubicI>
    <OutputCubicF> 1 </OutputCubicF>

```

**Fig.11-2 Example of \*.inp.xml (1/2)**

```

<!-- Parameters for output.-->
<!-- Relative resolution to judge whether two lattices are equivalent or not.
      If the relative difference of two lattice parameters is within this value,
      only that with a better figure of merit is output.-->
<Resolution> 0.05 </Resolution>

<!-- Maximum number of false (unindexed) peaks.-->
<MaxNumberOfUnindexedPeaks> 20 </MaxNumberOfUnindexedPeaks>

<!-- Number of reflections to calculate figure of merit.-->
<MaxNumberOfPeaksForFOM> 20 </MaxNumberOfPeaksForFOM>

<!-- Output the candidates with better FOM than the following value.-->
<MinFOM> 3 </MinFOM>

<!-- Number of hkl among input reflections.-->
<MaxNumberOfMillerIndicesInRange> AUTO </MaxNumberOfMillerIndicesInRange>
<MinNumberOfMillerIndicesInRange> AUTO </MinNumberOfMillerIndicesInRange>
<!-- Minimum and maximum of the unit cell edges a, b, c (angstrom).-->
<MaxUnitCellEdgeABC> 1000 </MaxUnitCellEdgeABC>
<MinUnitCellEdgeABC> 0 </MinUnitCellEdgeABC>

</ConographParameters>

<PeakSearchPSPParameters>
  <ParametersForSmoothingDevison>
    <!--NumberOfPointsForSGMethod : odd number.-->
    <NumberOfPointsForSGMethod> 9 </NumberOfPointsForSGMethod>

    <EndOfRegion>
      <!-- The maximum point of smoothing range. -->
      MAX
    </EndOfRegion>
  </ParametersForSmoothingDevison>

  <PeakSearchRange>
    <Begin> 0.0 </Begin>
    <End> MAX </End>
  </PeakSearchRange>

  <!--0 : Use the threshold, 1 : Use a constant times the error of y-value as a threshold.-->
  <UseErrorData> 1 </UseErrorData>

  <!--When "UseErrorData" is 0, it is used as the threshold for peak search.
        Otherwise, "Threshold" times the error of y-value is used as a threshold.-->
  <Threshold> 5.0 </Threshold>

  <!-- 0 : "Threshold" is applied to estimated y-values of peak-tops when the background of the histogram is removed,
        1 : "Threshold" is applied to actual y-values of peak-tops.-->
  <UseBGRemoved> 0 </UseBGRemoved>

  <!-- 0 : deconvolution is not applied.
        1 : deconvolution is applied.-->
  <Alpha2Correction> 0 </Alpha2Correction>
  <Waves>
    <Kalpha1WaveLength> 1.54056 </Kalpha1WaveLength>
    <Kalpha2WaveLength> 1.54439 </Kalpha2WaveLength>
  </Waves>
</PeakSearchPSPParameters>
</ZCodeParameters>

```

**Fig. 11-3 Example of \*.inp.xml (2/2)**

```

IGOR
WAVES/O tof, yint, yerr
BEGIN
  1850.00  2.871904E-001  3.359009E-003
  1854.00  2.834581E-001  3.337111E-003
  1858.00  2.848073E-001  3.351369E-003
  ~Omitted~
  49564.0  9.989611E-002  1.378697E-002
  49588.0  1.010892E-001  1.386346E-002
END
WAVES/O peak, peakpos, height, FWHM, Flag
BEGIN
  1  3.148311E+003  1.535192E-001  3.749774E+001  1
  2  3.340909E+003  1.676432E-001  2.429063E+001  1
  3  3.697289E+003  1.661457E-001  2.063853E+001  1
  ~Omitted~
  49  3.133224E+004  2.968128E+000  1.480559E+002  1
  50  4.906641E+004  1.092195E-001  1.791403E+002  1
END
WAVES/O dphase_1, xphase_1, yphase_1, h_1, k_1, l_1
BEGIN
  3.138130E+000  3.133851E+004  0.000000E+000  1  -1  1
  2.717700E+000  2.713443E+004  0.000000E+000  0
  1.921704E+000  1.918059E+004  0.000000E+000  0
  ~omitted~
  6.405680E-001  6.394727E+003  0.000000E+000  2  2  -8
  6.405680E-001  6.394727E+003  0.000000E+000  0  6  -6
END
X Display yint vs tof
X AppendToGraph yphase_1 vs xphase_1
X ModifyGraph mirror(left)=2
X ModifyGraph mirror(bottom)=2
X ModifyGraph rgb(yint)=(0,65535,65535)
X ModifyGraph
offset(yphase_1)={0,0},mode(yphase_1)=3,marker(yphase_1)=10,msize(yphase_1)=3,mrkThick(ypha
se_1)=0.6,rgb(yphase_1)=(3,52428,1)

```

Only output

**Fig. 11-4 Example of \*.histogramIgor**

```

<ConographOutput>
  <!-- Information on the best M solution for each Bravais type.
    TNB : total number of solutions of the Bravais types,
    M : de Wolff figure of merit,
    Mwu : Wu figure of merit,
    Mrev : reversed de Wolff figure of merit,
    Msym : symmetric de Wolff figure of merit,
    NN : number of lattices in the neighborhood,
    VOL : unit-cell volume.
  Bravais Lattice : TNB, M, Mwu, Mrev, Msym, NN, VOL
    Cubic(F) :      25      7.6120e+000  213      1.5861e+002
    Cubic(I) :      17      2.1801e+000  246      2.0063e+001
    Cubic(P) :       0
    Hexagonal :     4      2.1261e+000   43      1.3385e+001
    Rhombohedral :  20      4.6341e+000  149      1.0755e+002
    Tetragonal(I) :  14      3.3966e+000  633      8.0329e+001
    Tetragonal(P) :   0
    Orthorhombic(F) : 0
    Orthorhombic(I) : 0
    Orthorhombic(B) : 1      2.6029e+000    8      5.7058e+001
    Orthorhombic(P) : 0
    Monoclinic(B) :   0
    Monoclinic(P) :   0
    Triclinic :      0
  -->

  <!-- Information on the selected candidates.-->
  <SelectedLatticeCandidate number="140153">
    <CrystalSystem>      Cubic(F) </CrystalSystem>

    <!-- a, b, c(angstrom), alpha, beta, gamma(deg).-->
    <LatticeParameters>  5.4354e+000  5.4354e+000  5.4354e+000  9.0000e+001  9.0000e+001  9.0000e+001
  </LatticeParameters>

    <!-- A*, B*, C*, D*, E*, F*(angstrom^(-2)).-->
    <ReciprocalLatticeParamters>  3.3848e-002  3.3848e-002  3.3848e-002  0.0000e+000  0.0000e+000
  0.0000e+000 </ReciprocalLatticeParamters>
    <!-- A*, B*, C*, D*, E*, F*(angstrom^(-2)) first given by peak-positions.-->
    <InitialReciprocalLatticeParamters>  3.4129e-002  3.4129e-002  3.4129e-002  0.0000e+000  0.0000e+000
  0.0000e+000 </InitialReciprocalLatticeParamters>
    <VolumeOfUnitCell>  1.5861e+002 </VolumeOfUnitCell>
    <FigureOfMeritWolff name="Fw20">  7.6120e+000 </FigureOfMeritWolff>
    <NumberOfLatticesInNeighborhood>  213 </NumberOfLatticesInNeighborhood>

    <!-- Number of pairs of hkl and -h-k-l up to the 20th reflection.-->
    <NumberOfMillerIndicesInRange>  2.7750e+001 </NumberOfMillerIndicesInRange>

    <EquivalentLatticeCandidates>
      <LatticeCandidate number="13034">
        <CrystalSystem>      Cubic(I) </CrystalSystem>
        <LatticeParameters>  4.1917e+000  4.1917e+000  4.1917e+000  9.0000e+001  9.0000e+001
      9.0000e+001 </LatticeParameters>
        <ReciprocalLatticeParamters>  2.8457e-002  2.8457e-002  5.6913e-002  0.0000e+000  0.0000e+000
      0.0000e+000 </ReciprocalLatticeParamters>
        <FigureOfMeritWolff name="Fw20">  1.3537e+000 </FigureOfMeritWolff>
        <NumberOfLatticesInNeighborhood>  213 </NumberOfLatticesInNeighborhood>
      </LatticeCandidate>
    ~Omitted~
  </EquivalentLatticeCandidates>

```

**Fig. 11-5 Example of \*.index.xml (1/2)**

```

<IndexingResults>
  <!--      q_obs,      q_cal,      peak_pos,      pos_cal,      closest_hkl,
is_the_difference_between_q_obs_and_q_cal_small_compared_to_q_err?.-->
    4.1501e-002      1.0154e-001      4.9066e+004      3.1339e+004      [-1,1,1]      0
    1.0159e-001      1.0154e-001      3.1332e+004      3.1339e+004      [-1,-1,-1]      1
    2.1784e-001      2.7079e-001      2.1387e+004      1.9181e+004      [0,-2,-2]      0
  ~Omitted~
    2.2680e+000      2.2678e+000      6.6286e+003      6.6288e+003      [7,3,-3]      1
    2.4367e+000      2.4371e+000      6.3952e+003      6.3947e+003      [-6,6,0]      1
</IndexingResults>

<FittingResults>
  <!-- q_obs, q_err, q_cal, peak_pos, peak_width, pos_cal, hkl, fix_or_fit.-->
    4.1501e-002      1.2834e-004      1.0154e-001      4.9066e+004      1.7914e+002
3.1339e+004      [-1,1,1]      0
    1.0159e-001      4.0706e-004      1.0154e-001      3.1332e+004      1.4806e+002
3.1339e+004      [-1,-1,-1]      1
    2.1784e-001      8.7727e-004      2.7079e-001      2.1387e+004      1.0149e+002
1.9181e+004      [0,-2,-2]      0
  ~omitted~
    2.2680e+000      7.2533e-003      2.2678e+000      6.6286e+003      2.4936e+001
6.6288e+003      [7,3,-3]      1
    2.4367e+000      8.1458e-003      2.4371e+000      6.3952e+003      2.5146e+001
6.3947e+003      [-6,6,0]      1
</FittingResults>

</SelectedLatticeCandidate>

<!-- Candidates for Cubic(F) -->
  ~omitted~
</ConographOutput>

```

**Fig.11-6 Example of \*.index.xml (2/2)**

```

<ZCodeParameters>
  <ConographOutput>
    <TypeOfReflectionConditions>
      <Candidates>
        <SpaceGroups> 45(bca),72(bca) </SpaceGroups>
        <ReflectionConditions> hk0:h,k=2n,0kl:k,l=2n </ReflectionConditions>
        <FigureOfMeritWolff name="M20"> 3.126279e+002 </FigureOfMeritWolff>
        <IndexingResults>
          <!-- q_obs, q_err, q_cal, peak_pos, peak_width, pos_cal, hkl, fix_or_fit.-->
            1.016473e-001  9.594352e-004  1.015807e-001  3.132270e+004  1.480559e+002
            3.133298e+004      [1,0,-1]      1
            2.708116e-001  2.274422e-003  2.707887e-001  1.917970e+004  8.059404e+001
            1.918051e+004      [0,2,0]      1
            3.724714e-001  2.575261e-003  3.724523e-001  1.635279e+004  5.655483e+001
            1.635321e+004      [2,1,1]      1
            ~Omitted~
            2.539049e+000  2.019023e-002  2.539077e+000  6.265138e+003  2.488311e+001
            6.265104e+003      [3,4,-5]      1
            2.707958e+000  2.205347e-002  2.707998e+000  6.066813e+003  2.467594e+001
            6.066769e+003      [2,6,0]      1
          </IndexingResults>
        </Candidates>

        ~Omitted~
      </TypeOfReflectionConditions>
    </ConographOutput>
  </ZCodeParameters>

```

Fig. 11-7 Example of \*.out.xml

## 12. Addendum

### 12.1. Request for citation

Please cite the following when research findings obtained using Conograph are mentioned in academic manuscripts:

R. Oishi-Tomiyasu, "Robust powder auto-indexing using many peaks", *J. Appl. Cryst.*, 47 (2014), pp. 5936598.

The methods and figures of merit of Conograph are also introduced in the following papers:

- R. Oishi-Tomiyasu, "A method to enumerate all geometrical ambiguities in powder indexing and its application", submitted.
- R. Oishi-Tomiyasu, "Distribution rules of systematic absences on the Conway topograph and their application to powder auto-indexing", *Acta Cryst. A* 69 (2013), pp. 6036610.
- R. Oishi-Tomiyasu, "Reversed de Wolff figure of merit and its application to powder indexing solutions", *J. Appl. Cryst.*, 46 (2013), pp. 127761282.
- R. Oishi-Tomiyasu, "Rapid Bravais-lattice determination algorithm for lattice parameters containing large observation errors", *Acta Cryst. A* 68 (2012), pp. 5256535.
- R. Oishi, M. Yonemura, T. Ishigaki, A. Hoshikawa, K. Mori, T. Morishima, S. Torii, T. Kamiyama, "New approach to indexing method of powder diffraction patterns using topographs", *Zeitschrift für Kristallographie Supplements* 30 (2009), pp. 15620.

### 12.2. Bug report

Please send the following information to the e-mail address [conograph-bug@lists.osdn.me](mailto:conograph-bug@lists.osdn.me). All comments will be considered and reflected at the time of Conograph version upgrading.

- (i) OS used (including 32-bit and 64-bit)
- (ii) Conograph version used (indicated in the GUI Help menu)
- (iii) Particulars of problem
- (iv) Details of conditions when problem occurred
- (v) Possibility of recurrence (does it occur always or sometimes?)
- (vi) Name, affiliation, e-mail address (to allow us to contact you)

Depending on the contents of the problem, we may request the input/output files and other information. We seek your cooperation in this regard.

## References

- [1] C. Dong, F. Wu, H. Chen, *Correction of zero shift in powder diffraction patterns using the reflection-pair method*, J. Appl. Cryst., 32, pp. 8506853 (1999).
- [2] A. D. Mighell, A. Santoro, *Geometrical Ambiguities in the Indexing of Powder Patterns*, J. Appl. Cryst., 8, pp. 3726374 (1975).
- [3] R. Oishi-Tomiyasu, *A method to enumerate all geometrical ambiguities in powder indexing and its application*, submitted.
- [4] R. Oishi-Tomiyasu, *Robust powder auto-indexing using many peaks*, J. Appl. Cryst., 47 (2014), pp. 5936598.
- [5] R. Oishi-Tomiyasu, *Reversed de Wolff figure of merit and its application to powder indexing solutions*, J. Appl. Cryst., 46 (2013), pp. 127761282.
- [6] P. M. de Wolff, *A simplified criterion for the reliability of a powder pattern indexing*, J. Appl. Cryst., 1, pp. 1086113 (1968).
- [7] E. Wu, *A modification of the de Wolff figure of merit for reliability of powder pattern indexing*, J. Appl. Cryst., 21, pp. 5306535 (1988).