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Current Version of Sindarin manual: 260519

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If you have a suggestion or want to report an issue, I would be glad to hear from you.

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1 THE SINDARIN

Sindarin is a program designed to perform various calculations for polycrystalline diffraction techniques, including but not limited to, Rietveld refinement, Fundamental Parameters Approach (FPA), and Whole Powder Pattern Modelling (WPPM). It is designed to be flexible and straightforward, utilizing a plain text file written in a proprietary grammar for calculations.

1.1 FEATURES

The main features of Sindarin include:

- Different structure details:
 - Rietveld (full structure information)
 - Pawley method (only cell information)
 - Without structure information.
- Background: Highly flexible
 - Combination of different background models
 - Several analytical functions
 - Read from file
 - Interpolation
 - Custom analytical function
- Profile: Comprehensive and flexible reflection profile calculation
 - Several analytical functions
 - Convolution of multiple profile functions
 - Profile asymmetry correction
 - Fundamental Parameters Approach (FPA)
 - Whole powder pattern modelling (WPPM)
 - Custom analytical function
- Reflection intensity corrections:
 - Monochromator correction
 - Absorptions
 - Preferred orientation
 - March-Dollase multi direction
 - Spherical harmonic symmetrized
 - Arbitrary and individual correction of reflection intensity
- Reflection position corrections:
 - Zero
 - Specimen Displacement
 - Shift: Arbitrary and individual correction of reflection position
- Different diffraction geometries:
 - Reflection
 - Transmission
 - Symmetric
 - Asymmetric
 - Flat specimen

- Thin film
- Capillary
- Variable divergence slit
- Radiation modeling
 - Possibility to model the radiation flexibly
 - Any wavelength
 - Any relative intensity of discrete lines
 - Any number of discrete lines
 - Profile modeling of each discrete line separately
 - Voigtian profiles described in wavelength with physical variation of the FWHM with the diffraction angle
 - Possibility to fit the incident beam polarization
- Multiple data files for the same experiment
- Multiple experiments fitted together
 - Possibility to simultaneously refine multiple experiment data under different conditions, for example, different radiations

1.2 WHY “SINDARIN GRAMMAR”?

Sindarin uses a plain text file to store the data for calculations. An internal interpreter reads this file and performs the calculations. To make the file readable, it has to use correct words that the interpreter recognizes and follow a specific pattern of writing. This is why Sindarin has its own vocabulary and grammar, like a written language — a set of words the Interpreter recognises and rules for how to combine them.

Don't worry if you think that Sindarin is like the old software that needed strict sequences of characters to work properly. I know that those software could be frustrating and time-consuming, especially when a small mistake like a space character could cause errors. Sindarin is different. It is flexible and user-friendly, and it doesn't have the rigid character sequence rules of the old software.

I chose this method because it is simple and flexible for creating theoretical models for diffraction. It lets you control the calculation and adjust the model to fit the needs of each experiment and data set.

You can edit the plain text file in any text editor you like. Nimloth is a good option because it is fully integrated with Sindarin. You can use it to edit texts, do calculations, and see results. It also has some tools that make your tasks easier. Another option is Visual Studio Code, which has a Sindarin extension that helps you use Sindarin with this editor. You can find more details in Section 2.

One last thing: when we say "idiom" in Sindarin, we mean the way of inputting data. We don't mean the same thing as in software development.

2 USER INTERFACE

To utilize Sindarin, users have several options available: a command line interface (CLI), integration with Visual Studio Code, and Nimloth, a dedicated user interface. All three options can be used on the three major operating systems (OS): Windows, macOS, and Linux. Nimloth will likely be the best choice for most users.

2.1 COMMAND LINE INTERFACE

The Command Line Interface (CLI) is Sindarin's basic interface and can be used in terminals of each OS. The structure of a Sindarin invocation is as follows

```
1| Sindarin [help] <sindarin file> [interpreter] [options]
```

Where [help], <sindarin file>, [interpreter] and [options] are the type of arguments. The [help] argument is used alone. To use a interpret invocation, the <sindarin file> is mandatory, and [interpreter] and [options] are optional.

If the terminal is not in Sindarin program folder, it will be necessary to write the full system path for executable program, not just “Sindarin” at the beginning of the invocation. The example below shows how to run the Sindarin when the program’s folder is a folder called “Sindarin” in the drive C: on Windows OS:

```
1| C:\Sindarin\Sindarin
```

It is highly recommended to add the Sindarin program folder to the OS environment variable. This way, you can omit the path for the program folder and just use “Sindarin” at the beginning of the invocation, even if the terminal is not in Sindarin folder.

Executing the help invocation or the Sindarin without an argument returns a list of possible arguments, like this:

```
1| Sindarin [help] <sindarin file> [interpreter] [options]
2|     [help]
3|         -h or --help: show these invocation information
4|         -t or --test: run test Sindarin inscription: \Test
5|                     est.sin
6|         -u or --update: run Sindarin program update from web
7|         -v or --version: show the version of Sindarin program
8|     <sindarin inscription> the system path of Sindarin inscription
9|     to be interpreted
10|    [interpreter]
11|        -I or --interpret: interpret the file (default)
12|        -S or --step: step in optimization calculation
13|        -W or --walk: walk in optimization calculation
14|        -M or --marathon: marathon in optimization calculation
15|    [options]
16|        -r or --results: get and write results to file
17|        -c or --charts: get and write charts to file
18|        -f or --format: format the Sindarin text before to
19|    interpret
20|        -n or --norewrite: Sindarin inscription will not change
```

18| -z or --all: enable all options, except --norewrite

Some arguments are explicated with more details bellow.

--update (-u)

If the message bellow is written in terminal after executing a Sindarin invocation, there is a new version of Sindarin available.

```
1| There is a new version of Sindarin
2| Current version: ###
3| New version: ###
4| Run the update invocation: Sindarin --update
```

If the computer is connected to the internet, run the invocation to update:

```
1| Sindarin -u
```

<sindarin file>

This argument is the full or relative system path to Sindarin inscription that will be interpreted. The path must be written according of operation system that is running, the “\” character is used on Windows and “/” on Linux and macOS. Below is an example of the file “test.sin” that is in folder “Test” inside the folder “Sindarin” in drive c: on Windows OS.

```
1| Sindarin C:\Sindarin\Test\Test.sin
```

[interpreter]

These arguments select the Interpreter invocation that will run with the Sindarin inscription. If this argument is omitted, the default is --interpret (-I). To read about the Interpreter Invocation, see the Sindarin Invocations section (page 33).

[options]

Some options when running an Interpreter invocation

--results(-r)

After executing the Interpreter invocation, the results will be written in a plain text file with the name “Sindarin inscription name - Results.txt” in the same folder as the Sindarin inscription.

--charts (-c)

After run Interpreter invocation, the experimental data, calculated diffraction, and background will be written in a plain text file named “Sindarin inscription name - Chart.txt” with a TSV (tab-separated values) format.

--format (-f)

Before running the Interpreter invocation, the text in the Sindarin inscription will be formatted. The nesting will be marked with the standard character (tab) and only one character per depth. Consecutive white spaces will be removed to leave only one character.

--norewrite (-n)

The default behavior of Sindarin is to rewrite the Sindarin inscription replacing the values of refinable variables with new values after an Interpreter invocation. If this argument is used, the original text will not be modified.

2.2 INTEGRATION WITH VISUAL STUDIO CODE

Visual Studio Code (VSCode) is a robust text editor that utilizes extension packages to modify behavior and add functionality. It specializes in editing code text and can run external programs when properly configured.

Sindarin for VS Code is an extension that integrates VSCode with Sindarin. This extension enables functionalities that simplify the use of Sindarin, eliminating the need to use the command line interface to run Sindarin. Instead, Sindarin can be executed directly from VSCode by clicking on Sindarin buttons enabled by the extension.

The use of VS Code with Sindarin is highly recommended over the command line interface to enhance user experience and productivity.

2.2.1 Text Highlighting

Sindarin text in VSCode is highlighted, with words appearing in different colors according to their type, such as class name, string, number, enumerator, operator, and others (see image below). This feature enhances the visibility of the text. The color scheme aligns with the one configured in VSCode and can be changed. For instructions on how to change the color scheme, refer to the official site:

<https://code.visualstudio.com/docs/getstarted/themes>

```

1 Computer
2   Convolution
3     ProfileMax 10
4 Experimental "teste.xye"
5   Radiation 1.54 1
6   Polynomial 100
7   CutOff 0.000001
8   //Polarization 0
9   IncidentAngle 4{0.03}
10  Phase
11    Scale @0.00099988725{±1.1E-07}
12    VoigtianSize 1000 1 0.5 0
13    Cell "230" 10
14      0 0.1 0.1 0.1 1 0.1
15 Simulation
16   Radiation 1.54 1
17   Polynomial 100
18   //Polarization 0
19   IncidentAngle 4{0.03}
20   Phase
21     Scale 0.001
22     VoigtianSize 1000 1 0.5 0
23     Cell "230" 10
24       0 0.1 0.1 0.1 1 0.1

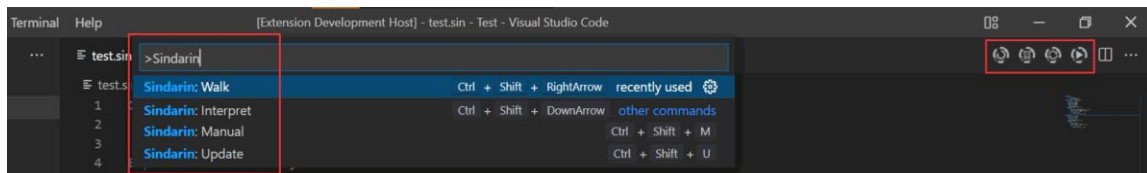
```

2.2.2 Sindarin Invocations

Several Sindarin invocations are enabled in VS Code:

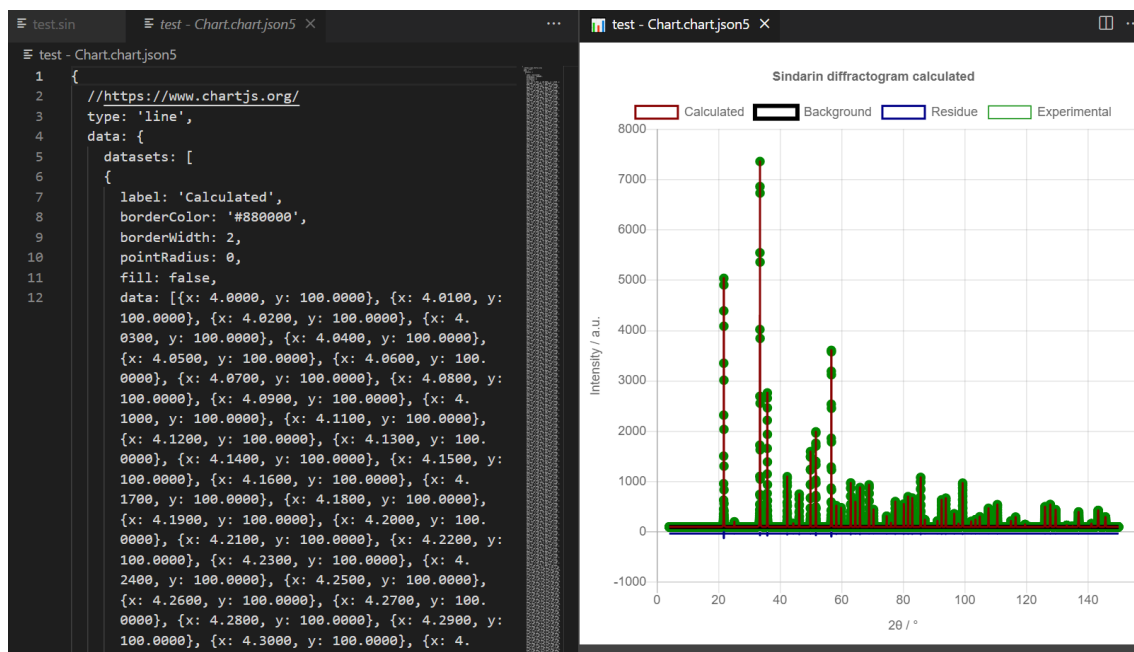
1. Interpret: Runs Sindarin to interpret for the current Sindarin inscription (Shortcut: Ctrl+Shift+Down Arrow)
2. Walk: Runs Sindarin to interpret and execute the optimization routine for the current sindarin file (Shortcut: Ctrl+Shift+Right Arrow)
3. Update: Runs Sindarin to update program from online repository, requires an internet connection (Shortcut: Ctrl+Shift+U)
4. Manual: Opens the Sindarin manual (Shortcut: Ctrl+Shift+M)

These invocations can be accessed by Command Palette (Ctrl+Shift+P), shortcut keys, or dedicated icons in the editor title (see image below).



2.2.3 See Diffractograms

The [Chart.js Preview](#) extension is installed alongside the Sindarin extension. This allows you to view diffractograms within VS Code (see image below) from the ".chart.json5" file generated after executing the interpret or walk invocations..



2.2.4 Using Sindarin with VS Code

To use Sindarin with VS Code, follow these steps:

1. Download and unzip the file to default folder.

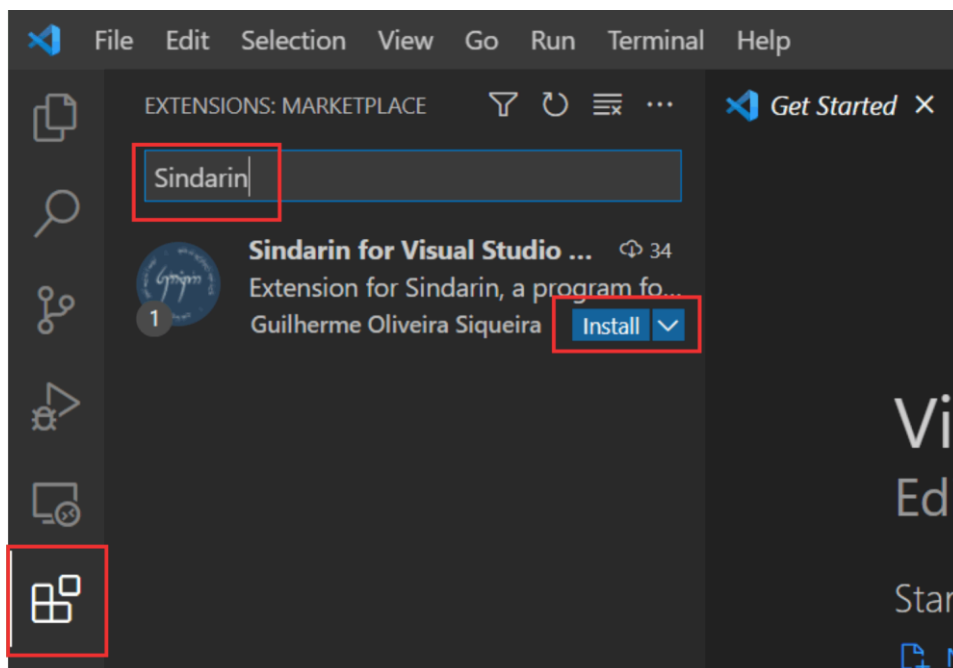
Default folders:

- Windows: C:\Sindarin
- Linux: ~/Sindarin
- macOS: ~/Sindarin

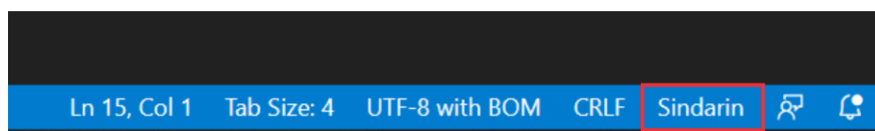
2. Download and install the VS Code from the official site:

<https://code.visualstudio.com/>

3. Go to Extensions in left side (Activity Bar of VS Code) (shortcut Ctrl+Shift+X), type 'Sindarin' to search the Sindarin for VS Code extension, and click on install bottom, as shown in the image bellow.

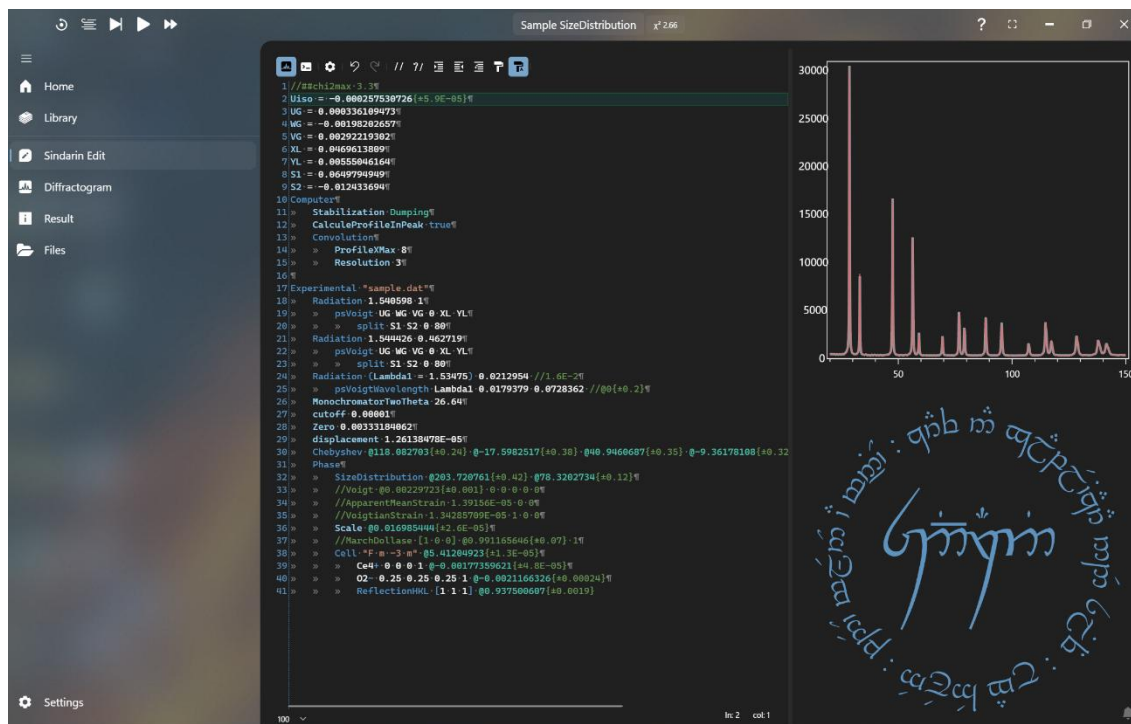


The extension will automatically activate when a text file with the “.sin” extension is opened, or if can be manually selected from the right side of the status bar (see image below)



2.3 NIMLOTH - A DEDICATE USER INTERFACE

Visit the Nimloth web page for more information and download: www.nimloth.app.

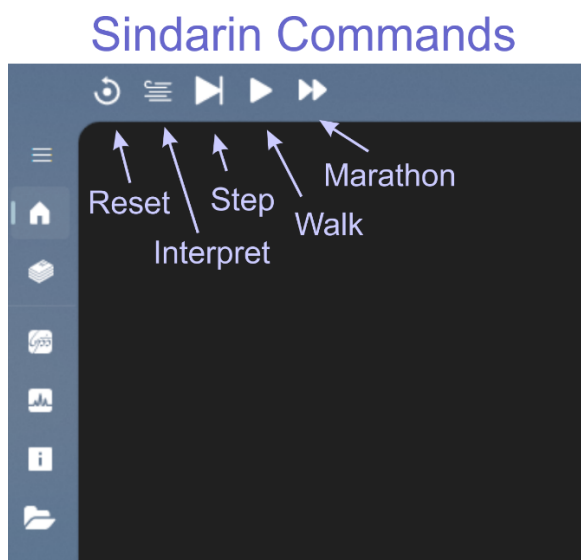


Nimloth is a program designed to simplify the use of Sindarin with several useful tools, making it the best choice for Sindarin users:

- Organize your diffraction works
- Keep all files and information about the diffraction experiment in one place
- Text editor
 - Text highlighting
 - Several tools to facilitate text typing
 - comment/uncomment
 - code completion
 - Sindarin text generators
- Results view
 - Detailed results
 - Export results to several file formats
 - Diffractogram functionality to enhance details visibility
- Feature-rich graphics for viewing, evaluating, correcting, and exporting
- Crystallographic tools
- Import crystallographic structure from CIF
 - Build a personal crystallographic database

The Nimloth is still in development, with a release coming soon, follow the official website.

The Sindarin invocations can be accessed from the buttons in the top right corner of the application window. See the figure below.



2.4 SINDARIN INSCRIPTION

A Sindarin inscription is a plain text file (or manuscript) that contains the input information for the Sindarin Interpreter to do calculations. The text has to follow the Sindarin grammar rules to be interpreted correctly. We recommend using the “.sin” extension for Sindarin manuscripts, because some user interfaces use this extension to activate some features or to sort files.

3 SPEAKING SINDARIN TO THE INTERPRETER

You might be wondering why we use text as input for calculations in Sindarin. Or you might think that this is old-fashioned, boring or difficult. If so, I suggest you read the section on Why "Sindarin language"? I hope that after reading it and doing some tutorials, you will feel differently about this topic.

Sindarin is a written form that aims to be simple, easy, flexible, intelligible and concise. It has some words and some rules that you need to follow to write correctly in Sindarin. You can find a comprehensive list of Sindarin words in the Sindarin Vocabulary section (page 63). In the following sections, we will introduce the rules that form the Sindarin grammar.

3.1 SPEAKING SINDARIN: A QUICK REFERENCE

This section gives a quick reference to the Sindarin grammar before the detailed chapters that follow. It introduces the six elements you will use to write any Sindarin inscription: data types, sentences, the Sindarin vocabulary, blocks and nesting, marking decimal data to optimize, and annotations. Each element is presented with a short definition and one or two examples; the full reference for every word and rule is given in the remaining sections of this chapter and in the Sindarin Vocabulary chapter.

3.1.1 Data types

Every piece of information in a Sindarin inscription belongs to one of six data types: integer, decimal, string, boolean, enumerator, and array. A short example of each:

```
1                // integer
0.005            // decimal
"sample.xye"     // string
true             // boolean
Reflection       // enumerator (one of a fixed set of words)
[1 0 0]          // array
```

The full definition of each type, including the accepted notations and conversion rules, is given in the Data Type (page 20) section below.

3.1.2 Sentences and declarations

A Sindarin inscription is a sequence of sentences. A sentence is one line of text that provides a piece of information. The general form of a sentence is:

```
Word data1 data2 ...
```

The first word identifies what kind of information the sentence provides; the words that follow are the data attached to it, separated by white space. For example:

```
Experimental "sample.xye"
Cell "P m -3 m" 4.0
```

The first sentence declares Experimental information and points to the data file sample.xye. The second declares Cell information with a space group and a lattice parameter.

Many words also accept a declarative form, in which one or more pieces of data are written directly on the same line instead of inside the block below.

3.1.3 Looking up the vocabulary

The words you may use as the first word of a sentence are listed in the Sindarin Vocabulary chapter (page 63). The vocabulary is organized in two ways: by topic (Calculation Control, Experimental data, Diffraction, Crystallographic, Background Function, Profile, and the decimal operators, functions and constants), and alphabetically. Each entry states what the word does, which data it accepts, which blocks it must sit inside, and what may sit inside its own block. When in doubt about which word to use, search the alphabetic entries first; when planning the overall structure of an inscription, the by-topic listing is usually more convenient.

3.1.4 Blocks and nesting

A block is the set of sentences that belong to a parent sentence. Blocks are marked by indentation: each level of nesting is one TAB character at the beginning of the line. The number of leading TABs determines the nesting level and therefore which parent the sentence belongs to. For example:

```
Experimental "sample.xye"  
  Displacement 0.005  
  Phase  
    Cell "P m -3 m" 4.0  
    Scale 1.0
```

Displacement and Phase sit at nesting level 1, so they belong to the Experimental block. Cell and Scale sit at level 2, so they belong to the Phase block. Each entry in the Sindarin Vocabulary chapter lists which blocks the word may appear (Parent/owner) inside and what may appear inside its own block (Properties and Children), those rules determine where a sentence is allowed to go.

3.1.5 Marking decimal data to optimize

Decimal value may be marked for optimization by prefixing it with an @ (at sign). A marked value is one that the optimization routine is allowed to adjust to fit the experimental data. For example:

```
Displacement @0.005
```

declares that 0.005 is the starting value of the displacement and that this value should be refined by the next optimization invocation. A decimal that is not marked with @ is held fixed at the value written in the inscription. Marked values may also be named and reused across several sentences, with optional limits; the Variables section (page 25) covers the full syntax, including the special values the Interpreter exposes during the calculation.

3.1.6 Annotations

An annotation is any text that the Interpreter ignores. Annotations begin with // (two forward slashes) and continue to the end of the sentence. They may stand on their own line or follow content on the same line:

```
// This whole line is an annotation
```

```
Experimental "sample.xye" // and so is everything after the slashes
Displacement @0.005      // refine this value
```

Use annotations to record decisions, label sections of the inscription, or temporarily disable a sentence without deleting it. A second kind of annotation, enclosed in braces { }, is reserved for the Interpreter's own use (calculated values and standard deviations); it is described in the Annotations section (page 28).

The remaining sections of this chapter expand each of these elements in detail. The Sindarin Vocabulary chapter is the reference for every available word.

3.2 SPEAKING SINDARIN: DETAILED TECHNICAL REFERENCE

3.2.1 Data Type

Data is the term for specific information that can be used for calculations. It can either be involved in calculations directly or affect how objects behave. The interpreter recognizes six types of data: Integer, Decimal, String, Boolean, Enumerator and Array.

3.2.1.1 Integer

Integer data is a number that can represent positive and negative whole numbers, without decimal parts.

Examples:

```
1| 0
2| -1
3| 103
```

3.2.1.2 Decimal

The decimal data is a number, negative or positive, that can have fractional component, represented by digits after decimal point. The decimal data can alternatively be written in scientific notation, using the letter “e” (or “E”) to indicate the exponential part of the number. Internally, the Sindarin uses a double-precision float number to handle decimal numbers to archive good precision in calculations.

Examples:

```
1| 3.14
2| 0.0015
3| -3E+5
4| 6.4e-7
```

The third and fourth examples use scientific notation, where -3E+5 means -3×10^5 , and 6.4e-7 means 6.4×10^{-7} .

Decimals are important for calculating crystal diffraction and have a special form in Sindarin. They can be used with math operations like addition (+), subtraction (-), multiplication (*), division (/), and functions like logarithm (log()), trigonometry (sin(), tan()), etc. Use parentheses to show the order of operations. See the Decimal Operators section for more details. The results of these operations and functions are decimals and can be used

wherever decimals are needed. A list of all functions and operations of decimals can be found in Decimal Operators (page 66).

Examples:

```
1| (1.2 + 3) * 2
2| 2 / log(21.5 - 3)
3| sin(3.141592)
```

3.2.1.3 String

A string is a sequence of characters written between quotes “”

Examples:

```
1| "datafile.xye"
2| "Something written between quotes!"
3| "I a -3 d"
```

3.2.1.4 Boolean

A boolean is a binary data type that can be either true or false.

Examples:

```
1| true
2| false
```

3.2.1.5 Enumerator

An enumeration is a data type that has a fixed set of values. These values are words made of alphanumeric characters only.

Examples:

The Stabilization property can have one of three values: Marquardt, Dumping or None:

```
1| Stabilization Marquardt
2| Stabilization Dumping
3| Stabilization None
```

3.2.1.6 Array

An array is a sequence of one or more values of the same data type. In Sindarin, arrays can be decimal or integer. The numbers are separated by white space and enclosed in brackets []. For example, an integer array of length 3 can represent a Miller index (h, k and l) of a crystallographic plane, and a decimal array of length 2 can represent a point (x and y).

Examples:

```
1| [2 0 -1]
2| [20.52 505.8]
```

The first example is an array of three integers: 2, 0 and -1. The second example is an array of two decimal numbers: 20.52 and 505.8.

3.2.2 Objects

Objects store data and perform actions. The class of an object defines the types and number of data it stores and the actions it can do. Objects of different classes have different data and actions. One can have multiple objects of the same class, but each one has its own values for its data.

Experimental is an object class that one will use a lot to calculate diffraction. One data stored in an Experimental object is the file name that contains the experimental diffraction data, which is a string. One action of this object is to access the file and load the experimental data. Two objects of the Experimental class with different file names will load different experimental data. They belong to the same Experimental class, but they are different objects with different data. The object class can be thought of as the object type, similar to how there are data types (string, integer, etc.).

The Sindarin sentence for declaring an object follows this pattern: the first word of the line is the object class followed by zero or more data separated by white space. The Sindarin text below shows a generic declaration of an object:

```
1| Class Data1 Data2 Data3...
```

The object class defines the type, number and order of the data one writes. For example, the Experimental declaration is:

```
1| Experimental (String)filename[1..n]
```

The first word of the line is the Experimental object class and the data in this declaration is a string that must be written one or more times. The data name is filename and it is the name of a file that has experimental data to be loaded when the Interpret is run

To declare Experimental objects, write this sentence:

```
1| Experimental "data.xye"  
2| Experimental "data2.xye" "data3.dat"
```

Here, two objects of the Experimental class are declared. The first one loads the experimental data from the file "data.xye" and the second one loads the experimental data from two files named "data2.xye" and "data3.xye".

One class that is frequently used is the Cell. The sentence for declaring this class follows this pattern:

```
1| Cell (string)spaceGroup (decimal)latticeParameter[1,2,3,4,6]
```

The first word of the line is the Cell object class, the second word is a string named spaceGroup and the next word is a decimal named latticeParameter. The decimal can be written one, two, three, four or six times. Here are two examples of Cell object declarations:

```
1| Cell "P 1" 6.2 4.3 3.4 89.7 121.2 80.6  
2| Cell "I a -3 d" 5.232
```

The first Cell object has a string data that corresponds to P 1 Space Group, number 1 from the International Union of Crystallography (IUCr) table, and six decimal data that represent the six lattice parameters of triclinic lattice: the edges a, b and c and the angles alpha, beta and gamma. The second Cell object has a string data that corresponds to I a -3 d Space Group, number 230 from the IUCr table, and one decimal data that is the lattice parameter for Cubic lattice: the edge a. The number of decimal parameters of the Cell object is determined by the first string data, as it must match the number of lattice parameters for the unit cell.

3.2.2.1 Parameters

Data written on the same line as the object declaration are called parameters. The parameters must be separated by white space.

3.2.2.2 Object Parenting

Children are objects that belong to another object, which is called their parent. The class and number of children depend on the class of the parent. The declarative form is the same for any object, but the children are declared inside the parent's block. See the Object's Block section for more details. An object that has no parent is called a root object.

3.2.2.3 Nesting

In Sindarin, nesting is shown by leading whitespace at the start of each line. The default character for nesting is the tab, but the whitespace character can also be used. However, it is not possible to mix these two characters within an object block (see the Object's Block section). The nesting depth of a line is given by the number of leading whitespace characters, and depths can be compared to establish the parent-child relationship between objects. For example, if the first line has two tabs and the second line has one tab, then the first line has a greater nesting depth than the second line.

3.2.2.4 Object's Block

An object's block consists of all the lines below the object's declaration that have a greater nesting depth than the declaration line. Consider the following Sindarin text:

```

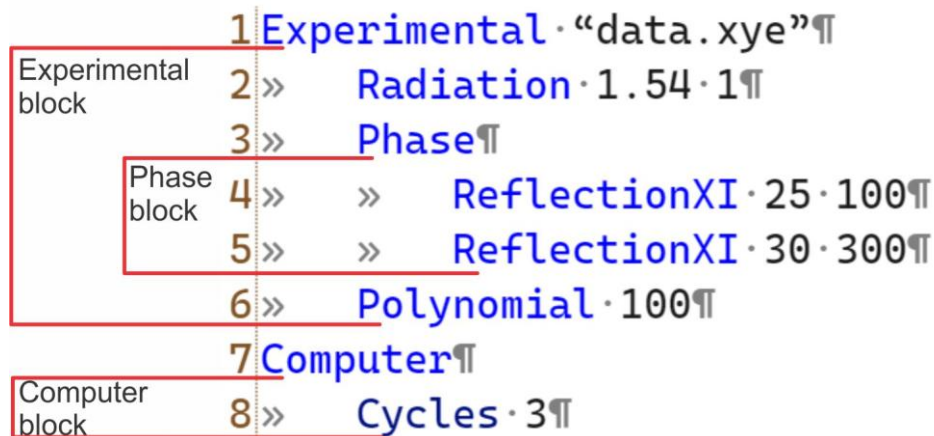
1| Experimental "data.xye"
2|     Radiation 1.54 1
3|     Phase
4|         ReflectionXI 25 100
5|         ReflectionXI 30 300
6|     Polynomial 100
7| Calculation
8|     Cycles 3

```

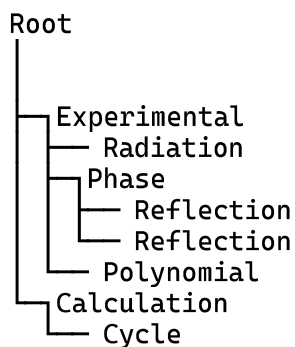
The declaration line of the Experimental object (line 1) has no space at the beginning and all the following lines that start with one or more tabs are inside the Experimental object's block, so lines 2 to 6 belong to the Experimental object. Experimental objects are root objects. The declaration line of the Radiation object (line 2) starts with one tab, so this Radiation object is a child of the Experimental object. For the same reason, the Phase object (line 3) is also a child of the Experimental object. The two declaration lines of the ReflectionXI objects (lines 4 and 5) start with two tabs, so they are inside the block of the Phase object and both are children of the Phase object. The next line (line 6) with the declaration of the Polynomial object starts with only one tab and therefore this line is not

inside the Phase object's block but is inside the Experimental object's block. So, the Experimental object has three children: one Radiation object, one Phase object and one Polynomial object. And the Phase object has two children: two ReflectionXI objects.

The line that declares the Calculation object (line 7) has no space at the beginning, so this line is outside the Experimental block and the Calculation object is a root object. The last line (line 8) has a tab at the start, so this line is inside the Calculation object's block and is a property (Cycles is a property, not an object) of the Calculation object. The following image shows graphically the block of each object:



The hierarchy structure of the object from the example can be represented as follow:



Properties and variables declarations cannot have blocks.

3.2.2.5 Properties

Data written inside the object's block (see the Object's Block section) are called properties. The sentence for assigning a property is similar to the sentence for declaring an object, except that the first word of the line is the property name (instead of the object class) followed by the property value. So, a property-assignment sentence reads:

1| PropertyName Data

The sentence for assigning the Displacement property to the Experimental object is:

```

1| Experimental "data.xye"
2|     Displacement 0.00578
  
```


3.2.2.6 *Implicit Objects and default values of parameters and properties*

Some objects or properties are created or assigned a value even if they are not declared in the text. Calculation is an example of an object that is always created by the interpreter with default values for its properties. Cutoff is a property of the Experimental object that always has a default value if it is not declared in the text. To see the default values of each property and parameter, consult the Sindarin dictionary entries for each object class.

3.2.2.7 *Some details of children*

Some classes can be declared only once per parent, others can be declared as many times as the user wants, and others cannot be declared together with other classes. Some classes cannot be children of any other objects; these are root objects, like the Experimental class. Other object classes can only be children of a specific object class, like Cell, which can only be a child of a Phase object. Some other classes can be children of different parents, like the profile classes, which can be children of Radiation, Experimental, Phase, ReflectionXI, ReflectionHKL or PeakXI. This information for each class is available in the specific entries in the Sindarin Vocabulary (page 63).

3.2.3 Variables

A variable is a special kind of object that stores a decimal value and can be used in any parameter or property of decimal type of any object. A variable has two parts: an identifier and a decimal value. An identifier is a sequence of characters that must be unique in the Sindarin text, no other variable can have the same identifier and it cannot match any reserved Sindarin word such as object class, property name, constant and so on. The allowed characters for an identifier are alphanumeric and “_”, but the first character cannot be a number. The basic sentence for declaring a variable is:

```
1| variableIdentifier = decimal
```

The character “=” is used to assign a decimal value to an identifier. When the interpreter reads this pattern, a variable is created in the memory. The decimal value can be a number or an expression.

Examples:

```
1| Var_1 = 2.0  
2| IDENT = 4.2 + 3.1 * 0.25
```

The identifier of a declared variable can be used like any other decimal value, directly in properties or parameters or inside expressions. To use an identifier of a declared variable is the same as using its decimal value and it can be used anywhere that a decimal value is expected.

Examples:

```
1| Displacement Var_1  
2| Cell “I a -3 d” IDENT  
3| Var2_ = 2 * 0.4 + Var_1 + 1
```

In the first example (line 1), the variable Var_1 is directly assigned to the Displacement property. In the second example (line 2), the variable IDENT is assigned to a

parameter of the Cell object. And in the third example (line 3), Var_1 is used within an expression to declare the variable Var2_. In these examples, it is assumed that two variables with identifiers Var_1 and IDENT are declared elsewhere in the Sindarin text. A variable can be declared in a single line, inside the block of an object or directly in an assignment property, parameter or expression. In the latter case, the variable must be enclosed in parentheses “()”.

Examples

```
1| Displacement (Var_1 = 2.0)
2| Cell "I a -3 d" 4.975
3|     Var_2 = 2.0
4| Var2_ = 2 * 0.4 + (Var_3 = 2.0) + 1
```

In the first example (line 1), the variable Var_1 is declared in the assignment of the Displacement property. In the second example (line 3), the variable Var_2 is declared within the block of a Cell object. And in the third example (line 4), Var_3 is declared inside the declaration of the variable Var2_.

When a value of a variable is written as an expression, after some Sindarin interpretation invocation is executed, the interpreter will write the calculated value of the variable after the identifier and between braces “{}”. For example, the variable Var2_, after an interpretation command, will appear in the text like this:

```
1| Var2_{3.8} = 2 * 0.4 + (Var_1 = 2.0) + 1
```

This means that the value of Var2_ is 3.8, which is the result of multiplying 2 by 0.4 and adding it to the value of Var_1, which is 2.0, and to 1

3.2.3.1 *Fitting*

Variables can be set to adjust their value in an optimization routine (see the Optimization invocations section) to make the theoretical data closer to the experimental data. To mark a variable for adjustment, simply write the “@” character before the decimal number in the variable declaration, as shown in the following example:

```
1| Var_1 = @2.0
```

This means that the value of Var_1 can be changed by the optimization routine to find the best fit for the data.

The variable Var_1 is marked for adjustment and its value can be modified to reach the minimum residual value of the data when the optimization routine runs. After the optimization routine, the new values of all the variables marked for adjustment are written by the interpreter in the Sindarin text, replacing the old values. The standard deviation calculated for each adjusted variable value is also written by the interpreter after the numeric value, enclosed in braces “{}”, like this:

```
1| Var_1 = @1.999998{±0.00005}
```

This means that the value of Var_1 after the optimization is 1.999998, with a standard deviation of 0.00005. You can use this information to evaluate the quality and uncertainty of your fit.

3.2.3.2 Limits values

It is possible to declare the minimum and maximum value that a variable can reach in an optimization routine. If the new value of the variable is outside the limits, the algorithm will return to the previous value and try to change it again in the next optimization cycle. If the user writes the value of a variable outside the declared limits, the interpreter will return an error and the calculation will not be performed. Minimum and maximum are properties of the variable object, but the sentence for assigning them is different from other object properties. To declare the minimum and maximum limits of a variable, just write the reserved words “min” or “max” and the decimal value at the end of the variable declaration. Some examples of declaring constraints are:

```
1| Var_1 = 2 min 1.1
2| Var_2 = 2 max 3.5
3| Var_3 = 2 min 1.1 max 3.5
4| Var_4 = 2 max 3.5 min 1.1
```

In these examples, the variable Var_1 has a minimum value of 1.1, Var_2 has a maximum value of 3.5 and Var_3 has both a minimum value of 1.1 and a maximum value of 3.5. Var_4 is identical to Var_3; the order of min and max is not important.

Some parameters and properties have internal limits. For example, the two parameters of the ReflectionXI object are the x-position in the diffractogram and the intensity. Both of them must be greater than zero, and the x-position also has a maximum limit: it must be less than 180. If a parameter or property has a value outside the internal bounds, the interpreter will do the same as for a constrained variable: it will return the variable (or variables) of that parameter or property to the previous value if it has been changed by the optimization routine, or it will return an error if the value was written by the user.

3.2.3.3 Implicit Variables

It is possible to declare a variable without an identifier; these are the implicit variables. You just need to write “@” before a decimal value. This way, the decimal value is transformed into an implicit variable and marked for adjustment in the optimization routine. This is very useful for optimizing the value of a parameter or property, but its value is not useful elsewhere.

The implicit variable cannot have constraints. Some examples of implicit variables are:

```
1| Displacement @2.0
2| Cell “I a -3 d” @4.975
```

In these examples, the values of the Displacement property (@2.0) and the numeric parameter of the Cell (@4.975) are implicit variables that can be adjusted by the optimization routine.

Examples:

```
1| Displacement (1.9 + @0.1)
2| Cell "I a -3 d" (@4.970 * 1.001)
3| Var2_ = 2 * 0.4 + @2.0 + 1
```

In the first and second examples, @0.1 (line 1) and @4.970 (line 2) are implicit variables declared within the expressions of assignment of the Displacement property and a parameter of the Cell object, respectively. In the third example (line 3), @2.0 is an implicit variable declared within the expression of declaration of the variable Var_1.

3.2.3.4 Internal Variables

The Sindarin framework exposes several internal variables that can be utilized within decimal data in appropriate contexts. Unlike user-defined variables, internal variables are not refinable and may assume different values depending on the context. For instance, the internal variable xPeak may take on varied values for distinct reflections. Should an internal variable be employed within decimal data where it is prohibited, the interpreter returns an error. For example, the AbsorptionFunction cannot depend on the internal variable IPeak. In cases where an internal variable is used in permissible decimal data but its value cannot be deduced, the internal variable yields a NaN value. As an illustration, the Zero property may depend on dReflection; however, if the diffraction model does not utilize the Radiation object, dReflection cannot be calculated, resulting in Zero being NaN.

A complete list of the internal variables can be found in Internal variables at page 67.

3.2.4 Annotations

Annotations are parts of the text that are not interpreted by the interpreter and do not affect the calculation. They are user notes within the Sindarin text. Annotations start with a double slash “//” and end at the end of the sentence, such as:

```
1| // some notes
```

Example:

```
2| // This is an annotation
3| Experimental "data.xye" // This is another annotation
4|     Displacement 0.005 // This is an annotation after a property
    assignment
```

These annotations are ignored by the interpreter and do not change the value of the Displacement property. You can use annotations to document your Sindarin text, explain your choices, or remind yourself of something. Annotations can make your Sindarin text more readable and understandable.

There is a special type of annotation that the Interpreter uses to write some information about variables, such as calculated value and standard deviation, when applicable. These annotations are only possible in specific places in the text, after identifiers or values of implicit variables. The user should not use this type of annotation. They are enclosed in braces “{}”. Some examples:

```

1| Displacement @0.0879371124{±0.00029}
2| Var_1{7.2} = 2.0 + 5.2
3| Var_2{±0.00029} = @2.0

```

The standard deviation (SD) calculated after the optimization algorithm have shown inside braces and start with “±”.

3.2.5 Case Insensitive

Sindarin is fully case insensitive, which means that upper and lower case letters do not distinguish one word from another. So experimental, Experimental, EXPERIMENTAL and ExPeRiMeNtAl are the same word for the Interpreter. The same rule applies to string data, where “I a -3 d” is equivalent to “I A -3 D”. The only exception is with strings that represent file names in Linux operating system, where the file name is case sensitive. Therefore, it is necessary to pay attention to the letter case of file names. For example, a file named Data.xye must have the string “Data.xye” because the string “data.xye” (or other string with different letter case) will return an error that the file was not found. For the other operating systems, Windows and macOS, it doesn’t matter, because the same file can be found with strings like “DaTa.XyE” or any variety of letter case.

3.2.6 In what order should it be written?

The order of declaration of objects does not matter. The Interpreter will read the full text and instantiate all objects and variables and only then calculate each object in a specific internal order. Therefore, no matter which object, variable or property is written before or after in the text. The only logic that matters is the object block that impose the parentage relationship of objects.

Consider the examples 1 and 2, after executing the interpret invocation, they will return the same results.

Example 1:

```

1| Var1 = 2
2| Var2 = 1
3| DataSimulation
4|     Polynomial Var1 Var2
5|     Interval -10 10 0.1 “dataTest.xye”
6| Data “dataTest.xye”
7|     Polynomial Var1 Var2

```

Example 2:

```

1| Data “dataTest.xye”
2|     Polynomial Var1 Var2
3| Var2 = 1
4| DataSimulation
5|     Interval -10 10 0.1 “dataTest.xye”
6|     Polynomial Var1 Var2
7| Var1 = 2

```

3.2.7 Custom User Formulas

In Sindarin, there are objects and properties dedicated to customizing equations to describe peak shift, peak absorption, background function, and peak profile. These objects

or properties are simple, each having just a decimal parameter. However, their great capability lies in the flexibility of decimal data with operators, functions, internal constants and especially the internal variables that Sindarin exposes to the user. For more information on this decimal flexibility, refer to the chapters: Decimal Operators and Functions (page 66), Decimal Constants (page 67) and Internal variables (page 67).

To correct peak positions, the Zero property of Experimental object can be used. Its value is directly added to the peak positions without other internal functions, as shown Equation 1 (page 35). To exemplify the use of Zero property as a custom user formula to correct the peak position, the following Sindarin text uses the Zero property to correct the displacement of the sample relative to the goniometer center:

```
1|      disp = -0.00005
2|      Zero (deg(-2 * disp * cos(rad(xPeak / 2))))
```

The equation of decimal data in line 2 of the example uses the internal variable xPeak which is the value of the peak position calculated from the interplanar distance. This equation is the same as that used to calculate the displacement, and the text is similar to the next line:

```
1|      Displacement disp
```

The AbsorptionFunction property of Experimental object is dedicated to customizing functions to correct peak intensity. Its decimal value is directly multiplied by the peak intensity, as shown in Equation 2 (page 36). In the next example, the equation of the decimal value of this property is used to calculate the Lorenz factor and also uses the internal variable xPeak:

```
1| AbsortionFunction (1.0 + cos(rad(xPeak)) ^ 2 / 2)
```

For background description, the Function object can be used with the internal variable x. The following example describes a polynomial function of order 3:

```
1| a0 = 4
2| a1 = 3
3| a2 = 2
4| a3 = 1
5| Function (a0 + a1 * x + a2 * x ^ 2 + a3 * x ^ 3)
```

The results are identical to using the following Polynomial object:

```
1| Polynomial a0 a1 a2 a3
```

The Function is calculated outside of phase and cell objects, so it is not possible to use some internal variables like xPeak and dReflection.

To describe peak profiles, there are two objects: ProfileFunction and ProfileFunctionFT. The ProfileFunction is used to describe the profile in the same space as the experimental data and usually uses two internal variables to describe the peak profile: x

and xpeak. The following example describes a Gaussian function with an FWHM of 0.1 °2θ using ProfileFunction object:

```
1|      h = 0.1
2|      ProfileFunction ((0.9394 / h) * e ^ (-2.7725 * ((x - xpeak)
   / h) ^ 2))
```

That it is identical to using Gauss object with a parameter of 0.1:

```
1|      Gauss 0.1
```

Alternatively, it is possible to use the declarative form of the ProfileFunction object with two parameters, where the second parameter is used to describe the internal variable fwhm:

```
1| ProfileFunction ((0.9394 / fwhm) * e ^ (-2.7725 * ((x - xpeak) /
   fwhm) ^ 2)) 0.1
```

The ProfileFunction can have a Split object as a child to introduce asymmetry effects in the profile.

It is possible to use the ProfileFunctionFT to describe the profile directly in Fourier space, using the internal variable xl instead of x. The next example the same gaussian function is described directly in Fourier space.

```
1| lamb = 1.540598
2| h = 0.1
3| hxl = 4 * cos(rad(xpeak / 2)) * sin(rad(h / 4)) / lamb
4| ProfileFunctionFT (e ^ (-3.5597 * (hxl * xl) ^ 2))
```

The first line declares a variable with the value of the wavelength of the radiation, which is necessary to computer Fourier space, and it is used to calculation the FWHM of the Gaussian in Fourier space units, stored in variable hxl (line 3).

The ProfileFunctionFT object has an alternative declarative form with two parameters, where the second parameter represents the imaginary portion of the complex number of the profile in Fourier space.

The use of equations or function in decimal parameters or properties is not restricted to specialized objects or properties for user customization, it can be applied to any decimal data. For example, the Gauss object has a declarative form with one parameter, which is the FWHM of the profile. This parameter's value is not used in any internal function but is directly applied as the FWHM in the Gaussian function. Therefore, to describe the modified Caglioti dependence of the FWHM on the peak position (see The pseudo-Voigt function section, page 40), the following can be used:

```
1| Gauss (sqrt(gu * tan(rad(xpeak / 2)) ^ 2 + gv * tan(rad(xpeak /
   2)) + gw + gz / cos(rad(xpeak / 2)) ^ 2))
```

The results will be the same as using the declarative form of Gauss object with four parameters:

1| Gauss gu gv gw gz

4 SPECIFIC INFORMATION

This section is dedicated to presenting some information and details about the various aspects of Sindarin, especially related to the calculations.

4.1 THE SINDARIN INTERPRETER

The Sindarin Interpreter is a part of the Sindarin program that receives the text from a Sindarin inscription and reads the source text, instantiates the appropriate objects and data (see Objects) in the memory, calculates the theoretical diffractogram, executes the optimization routine, and returns the results or related errors.

4.2 SINDARIN INVOCATIONS

The Sindarin is executed by some invocations: Interpret, Step, Walk, Marathon, Result and Reset. To know how to execute these invocations, see the User Interface section.

4.2.1 Interpret invocation

The interpret invocation performs the basic operations in Sindarin, the interpreter reads the text, instantiates all objects and calculates each of them in a specific internal order to calculate the theoretical diffractogram and write the value of each calculated variable (equations) in the text.

4.2.2 Optimization invocations

The Step, Walk and Marathon invocations are the optimization invocations, they do the same as the interpret invocation and, in addition, perform the optimization routine (see the Optimization Routine section) and finally write the new values of the refined variables in the text. The difference between these three commands is the number of cycles of the optimization routine, Step is only one cycle, Walk is the number defined by the Cycles property of the Calculation object (the default is 3) and Marathon executes cycles until a convergence or divergence criterion is reached.

4.2.3 Results invocation

The results invocation can be executed after the interpret invocation or any optimization invocation to get the results of the calculation.

4.2.4 Reset invocation

The Reset invocation cleans all memory, all objects and variables are erased. All objects and variables will be instantiated and assigned in the next interpret invocation. This command has effect only on the Nimloth interface.

4.3 OPTIMIZATION ROUTINE

Sindarin uses the nonlinear least squares (nlls) approach to approximate the theoretical diffractogram to the experimental diffractogram by optimizing the values of the parameters of the mathematical model. The Gauss–Newton algorithm is used to estimate the new parameter values and the Marquardt modification (Marquardt, 1963) to stabilize the refinement process when it tends to diverge.

The user controls the choice of which parameters are optimized by marking/unmarking the variables to refine in the text (see the section 3.2.3.1).

Sindarin automatically selects the optimal cycle when the optimization routine diverges or encounters issues, and returns the results of this cycle at the end of refinement. If divergence occurs in the first cycle, all refinable variables revert to their initial values. This feature enhances the reliability and stability of Sindarin, ensuring that a set of poorly static or error-generating variables are never returned.

Furthermore, Sindarin's optimization routine possesses a unique characteristic: when variables exhibit high correlation within the covariance matrix, they are automatically addressed to prevent divergence while they continue to be refined. All other variables proceed with optimization, and only thereafter, the highly correlated variables are refined individually. This approach eliminates the need for manual alternation in optimizing these highly correlated variables.

4.4 ERRORS RETURNED BY THE INTERPRETER

When the Interpreter cannot read the Sindarin text properly or cannot evaluate the theoretical diffractogram calculation correctly, it will return one or more errors with information about the impediment of the calculations. An error can occur for several reasons, some examples: grammar error, wrong number of parameters, unrecognized words, value of a parameter or property is outside the internal constraints, value of a variable is outside the constraints, some data calculated internally is wrong (like negative FWHM of a specific peak). The returned error has five parts of information that help the user to correct the text:

1. Error Code: A unique numeric code that corresponds to the type of error
2. Description: A brief description of the type of error
3. Object: The object that generated the error, if applicable.
4. Line: Text line of the object or property that generated the error, if applicable.
5. Message: More details about the error, e.g., the file name that cannot be found.

4.5 EXPERIMENTAL DATA FILE

The experimental data file used in Sindarin is a plain text file with a series of experimental points. The data in the file can be of two different arrangements:

- 1) Each point is written on a line and can have three numbers: x , the position on the horizontal axis, y , the position on the vertical axis and e , the experimental error of measuring that point. On the line, they are separated by white space, comma or tab. Measurement error information is optional, so lines can only have two numbers. The points must be in ascending order and the step in x , the difference between the sequential x 's, does not need to be constant for all points.

Example:

1	4.00	1023.45	3.52
2	4.02	1020.91	6.1
3	4.04	1019.38	4.93
4	4.06	1021.44	2.04

- 2) The first line of the text file has three decimal data: x_i , x_{step} and x_f , where x_i is the horizontal coordinate of the first point, x_{step} is the value of the difference between

each sequential x and x_f is the horizontal coordinate of the last point in the series. The other lines must have only one decimal value, which is the value of the vertical coordinate (y) of each point in ascending order of x . Therefore, it is not possible to have experimental error information and the step in x is constant for all points. The number of lines of y must match the number of x generated from the first line.

Example:

```
1| 4.00  0.02  4.06
2| 1023.45
3| 1020.91
4| 1019.38
5| 1021.44
```

The two examples above have the same data written in two different arrangements. The decimal data can also be written in scientific notation, so the y coordinate of the first point in the examples above can be written as 1.02345E3.

It is possible to write annotations in data files with the same rules as annotations in Sindarin texts (see the Annotations section, page 28).

4.6 AN OVERVIEW OF PEAK DIFFRACTION CALCULATION

The diffraction peaks of the theoretical diffractogram are calculated by the PeakXI objects. Reflection objects (ReflectionHKL and ReflectionXI) always create PeakXI objects to perform the calculations. The number of PeakXI objects created by each reflection object is equal to the number of declared Radiation objects. If no Radiation object is declared, ReflectionHKL object cannot be used and ReflectionXI will only have one PeakXI object. The position of each PeakXI of a reflection object is calculated by the Bragg equation using the interplanar distance (d) of the reflection and the wavelength (λ) of each Radiation object.

Reflection objects are created by the user by declaring them directly in the Sindarin text or a list of ReflectionHKL objects is created automatically from the crystallographic information of the Cell object (see more details in section 4.7).

The diffraction peaks must have three pieces of information to be calculated: position (x_{ref}), intensity (I_{ref}) and profile. The next sections are devoted to explaining the various ways in which this information is provided to calculate the theoretical diffractogram. Sindarin was designed to be flexible, there are a lot of possibilities to model the theoretical diffractogram, this allows the user to obtain the desired information from the calculation.

4.6.1 General equations for calculating the position and intensity of reflections

The position of reflections in the diffractogram is calculated by the ReflectionHKL, ReflectionXI or PeakXI objects. The following equation shows the calculation of the position of reflections:

$$\text{Equation 1} \quad x_{Ref} = Bragg(d) + x_{obj} + Zero + Disp(x) + Shift$$

The $Bragg(d)$ term is the Bragg function to calculate the diffraction angle from the interplanar distance (d) of the ReflectionHKL object and the x_{obj} term is the diffraction angle directly from the parameter of the ReflectionXI or PeakXI objects. The default value of all terms in Equation 1 is 0. For the ReflectionHKL object, the $Bragg(d)$ is different from zero

and x is zero, for the ReflectionXI or PeakXI objects, the x is different from zero and $Bragg(d)$ is zero. The decimal terms $Zero$ and $Displ(x)$ are position corrections, properties of the Experimental object, and the $Shift$ term is an arbitrary position correction, a property of the ReflectionHKL object. The calculation of Specimen Displacement depends on the diffraction geometry.

The intensity of reflections is calculated by the ReflectionHKL, ReflectionXI or PeakXI objects. The following equation shows the general equation for the intensity calculation:

Equation 2
$$I_{ref} = S|F(HKL)|^2 I_{obj} M_{HKL} L_P(x) P_O(HKL) Abs(x) I_{rad}$$

The $|F(HKL)|^2$ term is the structure factor calculated for each reflection with the crystallographic information of the Cell object when Atom objects are declared. The M term is the reflection multiplicity which depends on the Miller indices of the reflection and the Laue symmetry. The I_{obj} term is the intensity declared by the user as a parameter of the ReflectionHKL, ReflectionXI or PeakXI objects. The S term is the phase scale factor, a property of the Phase object. The $L_P(x)$ term contains the polarization and Lorentz factors, including the monochromator polarization correction. The $P_O(HKL)$ term is the preferred orientation correction when a preferred orientation object is declared. The $Abs(x)$ term is the absorption correction term. The I_{rad} term is the relative intensity of the radiation line. The default value of all terms in Equation 2 is 1.

The next sections will use the terms of Equation 1 and Equation 2 to explain details about the calculation of the diffraction peak.

4.7 REFINEMENT WITH DIFFERENT STRUCTURE DETAILS

The calculation of the theoretical diffractogram can be performed by providing different details about the crystal structure: Complete structure information (Rietveld Refinement), Only lattice parameter information (Pawley method) or No structure information. The last two approaches are also called Whole Powder Pattern Fitting (WPPF).

4.7.1 Complete structure information (Rietveld Refinement)

Classical Rietveld refinement is performed when the diffraction model has complete crystallographic information, with cell geometry and all atoms in the cell. In this case, a list of ReflectionHKL objects is created internally by the Cell object, which calculates the interplanar distance (d) for all ReflectionHKL using the lattice parameters. The structure factor ($|F(HKL)|^2$) is calculated using information about all Atoms objects and the multiplicity (M_{HKL}) is determined using Miller indices and the Laue symmetry. Therefore, the x_{ref} is calculated using the $Bragg(d)$ function and the x_{obj} term is zero in Equation 1, and the I_{ref} is calculated using $|F(HKL)|^2$ and M_{HKL} and the I_{obj} term is 1 by default in Equation 2.

The crystal structure can be refined to obtain accurate crystallographic information using Rietveld refinement. In general, this refinement uses fewer refinable variables among the three different structure detailing models and has no problem with overlapping peaks.

Sindarin text example:

```
1|      Phase
2|      Scale 0.001
```

```

3|          Cell "F D -3 M" 5.432117
4|          Si "Si1" 0 0 0 1 0.05

```

4.7.2 Only lattice parameter information (Pawley method)

It is possible to refine a theoretical diffraction model without atomic information, only with unit cell geometry; this is the Pawley method. The reflection position (x_{ref}) is calculated in the same way as in Rietveld Refinement, but the intensity of each reflection needs an arbitrary refinable scale factor. Instead of writing a list of Atom objects in the Cell object block, a list of ReflectionHKL objects with two parameters (Miller index and intensity scale factor (I)) should be written. The I_{ref} is calculated with I_{obj} and M_{HKL} ; $|F(HKL)|^2$ term has the default value 1 in Equation 2. The S term can't be refined simultaneously with all ReflectionHKL intensity parameters because there is a high correlation and it makes the optimization routine unstable.

In this refinement, the cell geometry can be fitted and in general has more refinable variables than Rietveld refinement and less than in the refinement without any structure information. This method is useful for obtaining information from profiles and cell geometry or when intensities are used to solve the structure.

Different overlapping reflections, with the same position (x_{ref}) or very close, can't have their intensity individually fitted, as these intensities have a high correlation, which would make the optimization routine unstable.

Sindarin text example:

```

1|          Phase
2|          Cell "F D -3 M" 5.432117
3|          ReflectionHKL [1 1 1] 1000
4|          ReflectionHKL [2 0 2] 880
1|          ReflectionHKL [1 1 3] 530
2|          ReflectionHKL [4 0 0] 140

```

4.7.3 No structure information

It is still possible to have the refinement of the theoretical diffractogram without any crystal cell information. In this case, the cell object is not declared; it is necessary to write a list of ReflectionXI objects in the Phase object block with two refinable parameters: position (x_{obj}) and an intensity scale factor (I_{obj}). The x_{ref} is calculated with x_{obj} ($Bragg(d) = 0$) and the I_{ref} is calculated using I_{obj} ($|F(HKL)|^2 = 1$ and $M_{HKL} = 1$ by default).

No structure information is refined and, in general, this method has more refinable variables. This method is useful when only peak profile information is of interest or when the peak position information is used to find the lattice parameters and the space group.

The same observations about the S term and overlapping reflections of the Pawley method are valid for this refinement.

Example:

```

1|          Phase
2|          ReflectionXI 28.43 1000
3|          ReflectionXI 47.28 880
4|          ReflectionXI 56.10 530
5|          ReflectionXI 69.11 140

```

4.8 PROFILES

The profile is the shape that the peaks take on the diffractogram. A correct analysis of the diffractogram peak profiles can provide important information about the sample, such as crystal size and its mean and distribution, mean crystal shape, defects in terms of microstrain or more specific ones, such as dislocation and stacking fault. Many approaches have been proposed to fit the profile of diffraction peaks and Sindarin can perform several of them, allowing the user to choose the most suitable approach for their experimental data and samples. Some aspects of profiles calculation in Sindarin are explained in the next sections.

4.8.1 Profile level

PeakXI objects are used to calculate the profiles, which can be declared at different levels: Radiation, Experimental, Phase, Reflection/Peak. Each profile object will be assigned to the corresponding PeakXI objects based on the parent/children relationship. So:

- Experimental: a profile object declared on an Experimental block will be computed on all peaks of all its child Phases.
- Phase: a profile object declared on a Phase block will be computed only on its peaks.
- Reflections: if profile objects are declared in blocks of ReflectionXI or ReflectionHKL objects, they will be computed only on peaks derived from them.
- Peaks: if a profile object is declared in a PeakXI block, it will be computed only for that peak.
- Radiation: profile objects declared on a Radiation block will be computed on corresponding peaks of all phases that are children of the Experimental object.

4.8.2 Convolution of peak profiles

The profiles are calculated at the PeakXI object. If there are two or more profile objects, they are convoluted. The convolution can be calculated by three different mathematical methods: analytical convolution, FFT convolution and special numerical convolution.

- Analytical convolution

Analytical convolution is possible when there is a known function that represents the convolution of the initial functions. It is the fastest convolution method. Sindarin performs analytical convolutions for Gauss, Lorentz, Voigt and psVoigt functions. In Sindarin, these functions and others derived from them are called Voigtian functions.

- Fast Fourier Transform (FFT) Convolution

The convolution in the reciprocal FFT space is performed quickly because it is a simple operation of multiplying each point. The convoluted data in the reciprocal FFT space is transformed to the direct space by the Inverse Fast Fourier Transform (IFFT). This procedure is very fast, especially when the functions can be evaluated directly in the reciprocal FFT space.

- Special numeric convolutions

The conventional numerical convolution is very computationally intensive and time-consuming, but some functions can be convoluted with a special numerical method that is

very fast, comparable to the FFT convolution. In Sindarin, the following functions and their derivatives can be convoluted by special numerical methods: Box, InverseProfile, Exponential and Circle.

- Microstructure Voigtians

The profile objects VoigtianSize and VoigtianStrain undergo a special process before they can be convoluted with other profile functions. If there are two or more VoigtianSize objects, they are transformed into a single VoigtianSize object with a weighted average size property related to that specific crystallographic direction of reflection. The same is done with VoigtianStrain objects. This operation will return an average apparent microstructure, which is useful for modeling a complex anisotropic microstructure, for example, when the sample has a mixture of different crystal shapes. It is important to take into account that this approach is only meaningful for the average apparent microstructure, but not for the real value of the microstructure.

4.8.3 Fundamental Parameters Approach (FPA)

Sindarin can compute the instrumental profile by the Fundamental Parameters Approach (FPA) (Cheary & Coelho, 1992). The principle is to model the profile of the diffracted peak by the optical and instrumental effects of the radiation in the diffraction experiment. This is accomplished by convoluting the original profile of the emitted radiation by the source with functions that describe these effects. FPA calculation can achieve a very accurate instrumental line profile of the diffracted peaks. The following corrections are available:

- Target Width: The width of the x-ray beam at the radiation source. See TargetWidth, page 121.
- Axial Divergence: The effect generated by the difference in the radiation path due to the length of the incident beam on the sample when viewed perpendicularly to the diffractometer axis (or parallel to the rotational axis of the goniometer). Currently, only the simple correction function is available, as shown in (Cheary & Coelho, 1992). More complex functions for correction of axial divergence will be included to describe more accurate instrumental settings. See AxialDivergence, page 71.
- Equatorial Divergence: The effect generated by the difference in radiation path due to the height of the incident beam on the sample when using a flat specimen. See EquatorialDivergence, page 88.
- Receiving Slit Width: The effect generated by the width of the receiving slit. See ReceivingSlitWidth, page 112.
- Transparency: When the sample has a small linear attenuation coefficient and/or small thickness, the diffracted radiation can come from below the center of the diffraction circle of the diffractometer. Transparency123
- Tilt: When the specimen surface is tilted with respect to the diffractometer axis. See Tilt, page 122.
- Defocusing: When the receiving slit is not on the focusing circle. See Defocusing, page 82.

The Sindarin also exposes the main base functions of FPA corrections: Box, also known as the top hat function (page 72), Circle (page 76), Exponential (page 90) and InverseProfile (page 98).

In addition, Sindarin has Voigtian functions with FWHM described in units of wavelength for use with Radiation objects to describe the profile of each discrete emission line radiation. The FWHM profile of these functions follows the optical dependence with the diffraction angle (Section Radiation modeling, page 45).

4.8.4 Whole powder pattern modelling (WPPM)

The Whole Powder Pattern Modeling (WPPM) is an approach to model the peak profiles of the diffractogram according to a physical model of the sample, without using biased analytical functions (Scardi & Leoni, 2002). Some characteristics of the sample can be modeled by this method:

- Crystal size distribution
- Surface relaxation (not implemented yet)
- Dislocation
- Microstrain as a distance-dependent strain field in the crystal
- Stacking and Twin Fault

Although the WPPM method was initially developed to be used without crystallographic information, it can also be used for peak profile calculation in Rietveld refinement, combining the structural and microstructural analysis of the two methods.

4.8.5 The pseudo-Voigt function

Among the many functions that have been used to fit the diffraction peak profile, the pseudo-Voigt (psVoigt) has received great attention in the last decades. psVoigt can adequately describe the experimental diffraction peak profile in most cases, it is light to be computed, it has analytical convolution, it can be calculated directly in Fourier space and it has some approach to describe peak asymmetry. These characteristics make this function widely used, and it is implemented in many software for diffraction calculation. In Sindarin, it is a base function to describe the peak profile.

The psVoigt function (psV) is a linear combination of: Lorentzian (L(x)), and Gaussian (G(x)) functions.

Equation 3 $psV = \eta L(x) + (1 - \eta)G(x)$

The parameter η represents the linear combination coefficient for mixing the two functions, with its value ranging from 0 to 1.

The Lorentz function normalized by area is:

Equation 4
$$L(x) = \frac{2}{\pi} \frac{\frac{1}{H_L}}{1 + 4\left(\frac{x - x_{hkl}}{H_L}\right)^2}$$

Where x_{hkl} is the Bragg position of the diffracted peak and H_L is the Full Width at Half Maximum (FWHM) of the Lorentz's function.

The Gauss function normalized by area is:

Equation 5

$$G(x) = 2 \sqrt{\frac{\ln(2)}{\pi}} \frac{\frac{1}{H_G}}{e^{4 \ln(2) \left(\frac{x-x_{hkl}}{H_G}\right)^2}}$$

Where H_G is the FWHM of the Gauss's function.

The psVoigt is a simplification of the Voigt function, that is a convolution of the Lorentzian and Gaussian with different FWHM. However, this convolution doesn't have an analytical result, and the numeric convolution is heavy to computer. The psVoigt can describe totally the Voigt profile, and is very light to computer. In the psVoigt, H_L and H_G are assumed to have the same FWHM as the FWHM of psVoigt (H_{psV}). The value of H_L and H_G of the equivalent Voigt, can be calculated by a semiempirical equation (Wertheim et al., 1974).

To define the psVoigt, two parameters are necessary. Some approaches use η and the H_{psV} , the parameters H_L and H_G of equivalent Voigt are a function of η and H_{psV} . On the other hand, some approaches define H_L and H_G of the equivalent Voigt and η and H_{psV} parameters are calculated as a function of H_L and H_G . In both cases, the two parameters can be parameterized as a function of x_{hkl} in Whole Profile Fit approach to significantly reduce the number of refined parameters. The parametrization of H_{psV} may adhere to the Caglioti equation¹ (Caglioti et al., 1958):

Equation 6

$$H_{psV}^2 = U \tan^2 \left(\frac{x_{hkl}}{2} \right) + V \tan \left(\frac{x_{hkl}}{2} \right) + W + \frac{P}{\cos^2 \left(\frac{x_{hkl}}{2} \right)}$$

Equation 7

$$\eta = \eta_0 + \eta_1 \frac{x_{hkl}}{2} + \eta_2 \left(\frac{x_{hkl}}{2} \right)^2$$

Where U , V , W and P^2 are refinable parameters of H_{psV} and η_0 , η_1 and η_2 are refinable parameters of η .

The parameterization of H_L and H_G of Thompson-Cox-Hastings psVoigt (TCHZ) (Thompson et al., 1987) are stable in optimization routine and therefore it is the more commonly used in most of software. The H_L and H_G are calculated following the equations:

Equation 8

$$H_G^2 = U \tan^2 \left(\frac{x_{hkl}}{2} \right) + V \tan \left(\frac{x_{hkl}}{2} \right) + W + \frac{Z}{\cos^2 \left(\frac{x_{hkl}}{2} \right)}$$

Equation 9

$$H_L = X \tan \left(\frac{x_{hkl}}{2} \right) + \frac{Y}{\cos \left(\frac{x_{hkl}}{2} \right)}$$

Where U , V , W and Z^2 are refinable parameters of H_G and X and Y are refinable parameters of H_L .

In Sindarin, it is possible to use different approaches. In the simplest one, without FWHM bias dependence with x_{hkl} , each peak profile is fitted independently without parameterization, and for this case, a psVoigt object with two decimal parameters is used in

¹ Historically, the parameters U and W in the Caglioti equation have been constrained to positive values due to underlying physical relationships. In contrast, the parameter V is permitted to assume negative values, as no physical relationship prescribes its sign. Nonetheless, given the empirical (or semi-empirical) nature of the equation, there are no inherent limitations on the individual values of these parameters.

² The P parameter, while not present in the original publications, was subsequently introduced to establish a correlation with the Scherrer equation for determining crystal size (Young & Desai, 1989).

the block of the following objects: RefelctionHKL, ReflectionXI or PeakXI. A Sindarin text example is shown below:

```

1|      Phase
2|      Cell "Cubic" 5.4321
3|      ReflectionHKL [1 0 0] 200
4|      psVoigt 0.054 0.41
5|      ReflectionHKL [1 0 1] 150
6|      psVoigt 0.089 0.52
7|      ReflectionHKL [2 1 0] 100
8|      psVoigt 0.12 0.63

```

On the other hand, it is possible to use the parametrization approach to use fewer parameters and achieve stabilization in the optimization routine. The TCHZ approach, which uses six parameters in the object declaration (Equation 8 and Equation 9):

```

1| psVoigt 0.0003542 -0.00179 0.00257 0 0.04275 0.00842

```

Alternatively, using the parametrization of FWHM and eta, with seven parameters in object declaration (Equation 6 and Equation 7):

```

1| psVoigt 0.08044 0.001293 0.08138 -0.07885 0.3083 0.01257 -3.5208E-
05

```

4.8.6 Peak asymmetry

The diffraction profile often assumes an asymmetrical shape, when one side of the profile is wider than the other. The asymmetry has different origins, both from geometry of the diffractometer and from the effects of the samples. There are two approaches for modeling the asymmetry in diffractogram analysis: a physic modeling of the effect from the instrument and the sample, or a simple and phenomenological modeling.

The first approach is made by the Fundamental Parameters Approach (FPA) and the Whole Powder Pattern Modeling (WPPM). FPA has functions that can model each effect of the geometry of the x-ray beam in the diffractometer, such equatorial and axial divergence, and WPPM has functions that can model the microstructure of the sample, such stacking-fault. These approaches can be very accurate and detailed. In Sindarin, three functions are available to address asymmetry through the FPA approach: AxialDivergence (page 71), EquatorialDivergence (page 88) and Transparency (page 123).

On the other hand, for general purposes, a simple and empirical function can be introduced to modify the profile function and describe the asymmetry. In Sindarin, Split (page 120) functions offer an alternative means to rectify asymmetry using a straightforward and empirical approach.

In Sindarin, the Circle (page 76) function constitutes the basis for axial divergence correction. However, it is possible to directly use the Circle object, whose parameter is calculated according to the diffraction angle by an empirical function. This delineates a compromise between the empirical approach's simplicity and the precision afforded by the rapid convolution algorithm intrinsic to the FPA method.

Symmetric Voigtian functions possess an analytical convolution. However, when a split function is employed to correct asymmetry, the convolution of this asymmetric Voigtian peak profile is assessed through FFT convolution.

4.9 DIFFRACTION GEOMETRIES

Sindarin can perform X-ray diffraction calculations with different experimental geometries: transmission, reflection, symmetric, asymmetric, with or without monochromator and different samples: flat specimen, capillary and thin film. Additionally, it is possible to set the polarization of the incident beam (useful for synchrotron radiation) and the variable receive slit. Each geometry has specific corrections for the intensity and position of the peaks.

The following sections show some Sindarin text examples for different diffraction setups. These Sindarin texts only cover the diffraction setup, and do not include other necessary declarations for the calculation, such as Radiation and background. It is useful to keep in mind that the default diffraction setup in Sindarin is reflection, symmetric, flat specimen, unpolarized incident beam and Lorentz factor not applied.

When either the `MonochromatorTwoTheta` or the `Polarization` property of the `Experimental` object is declared, the Lorentz factor is automatically applied to the intensity calculation. These properties will modify the $L_p(x)$ term of the intensity equation (Equation 2).

The `SpecimenThickness` and `IncidentAngle` properties of the `Experimental` object and the `Capillary` object will modify the $Abs(x)$ term of the intensity equation. The `Capillary` object can also modify the $DispI(x)$ term of the position equation (Equation 1).

To correct the shift of the diffraction reflections due to the displacement of the sample, there is the `Displacement` property of the `Experimental` object. Just declare it as: “Displacement -0.00123”. Another available intensity correction ($Abs(x)$ term of equation) is the variable divergence slit. Set the `VariableSlit` property of the `Experimental` object to `True` as: “VariableSlit True”.

4.9.1 Diffraction Setup: Reflection, Symmetric, Flat Specimen, without Lorentz-Polarization correction

Sindarin text:

```
1| Experimental "dataFile.xye"
```

All the properties and objects related to the diffraction setup are set to default. The $L_p(x)$ and $Abs(x)$ terms are equal to 1 in Equation 2. In this setup, the intensity of the reflection objects, when declared by the user, is directly the value of the intensity observed in the diffractogram (I_{ref})

4.9.2 Diffraction Setup: Reflection, Symmetric, Flat Specimen

Sindarin text:

```
1| Experimental "dataFile.xye"
2| Polarization 0 // to apply the Lorentz factor
```

For this setup, it is only necessary to declare the Polarization property. The other properties and objects related to the diffraction setup are set to default. When the Polarization property is declared, even if it is zero, the Lorentz factor is applied in the calculation. The $L_P(x)$ term is different from 1 and the $Abs(x)$ term is 1.

4.9.3 Diffraction Setup: Reflection, Symmetric, Flat Specimen, Polarized incident beam

Sindarin text:

```
1| Experimental "dataFile.xye"
2|     Polarization 0.95 //polarization fraction of incident beam
```

The code is very similar to the previous example, but the Polarization property is set to a value other than zero.

4.9.4 Diffraction Setup: Reflection, Symmetric, Flat Specimen, Monochromator

Sindarin text:

```
1| Experimental "dataFile.xye"
2|     MonochromatorTwoTheta 28.44 //2θ of monochromator
```

For this setup, it is only necessary to declare the MonochromatorTwoTheta property. The other properties and objects are set to default. When the MonochromatorTwoTheta property is declared, the Lorentz factor and the polarization of the monochromator are applied in the calculation. It is not necessary to declare "Polarization 0". The $L_P(x)$ term is different from 1 and the $Abs(x)$ term is 1.

4.9.5 Diffraction Setup: Reflection, Symmetric, Flat Specimen, Monochromator, Polarized incident beam

Sindarin text:

```
1| Experimental "dataFile.xye"
2|     Polarization 0.95 //polarization fraction of incident beam
3|     MonochromatorTwoTheta 28.44 //2θ of monochromator
```

The Lorentz factor is applied in the calculation. The $L_P(x)$ term is different from 1 and the $Abs(x)$ term is 1.

4.9.6 Diffraction Setup: Reflection, Symmetric, Thin Film

Sindarin text:

```
1| Experimental "dataFile.xye"
2|     Polarization 0 //to apply the Lorentz factor
3|     SpecimenThickness 0.1 //MuT
```

The value of the SpecimenThickness property is the linear absorption coefficient multiplied by the thin film thickness. The intensity correction in this case is applied by the $Abs(x)$ term, which is different from 1.

If a polarized incident beam or a monochromator is used, just declare the appropriate property, as in the previous examples. The $L_P(x)$ term is different from 1.

4.9.7 Diffraction Setup: Reflection, Asymmetric, Flat specimen

Sindarin text:

```
1| Experimental "dataFile.xye"  
2|     Polarization 0 //to apply the Lorentz factor  
3|     IncidentAngle 4
```

The value of the IncidentAngle property is the fixed angle of the incident beam on the sample. The intensity correction is applied by the $Abs(x)$ term, which is different from 1.

If a polarized incident beam or a monochromator is used, just declare the appropriate property, as in the previous examples. The $L_p(x)$ term is different from 1.

4.9.8 Diffraction Setup: Reflection, Asymmetric, Thin Film

Sindarin text:

```
1| Experimental "dataFile.xye"  
2|     Polarization 0 //to apply the Lorentz factor  
3|     SpecimenThickness 0.1 //MuT  
4|     IncidentAngle 4
```

For this diffraction setup, just declare both the SpecimenThickness and IncidentAngle properties.

The $Abs(x)$ and $L_p(x)$ terms are different from 1. If a polarized incident beam or a monochromator is used, just declare the appropriate property, as in the previous examples.

4.9.9 Diffraction Setup: Transmission, Capillary

Sindarin text:

```
1| Experimental "dataFile.xye"  
2|     Polarization 0 //to apply the Lorentz factor  
3|     Capillary 0.7 -0.31 0.047 //MuR, dispL, dipV
```

The three parameters of the Capillary object are: linear absorption coefficient multiplied by capillary radius, displacement in direction of incident beam and displacement in perpendicular direction of incident beam, respectively. The Capillary object will apply intensity correction through the $Abs(x)$ term (Equation 2) and position correction through the $Displ(x)$ term (Equation 1).

If a polarized incident beam or a monochromator is used, just declare the appropriate property, as in the previous examples.

4.10 RADIATION MODELING

The modeling of radiation is very flexible in Sindarin. You can use any wavelength, any number of discrete lines, any relative intensity of each discrete line, incident beam polarization fitting and individual discrete line profile modeling with physical parameters. The incident beam polarization is an intensity correction described in section 4.9.3.

A Radiation object can be a child of Experimental and Simulation objects. The basic declaration sentence has two parameters: the wavelength and relative intensity:

```
1|      Radiation 1.540598 1
```

One can declare as many Radiation objects as needed. For example, to describe the two copper K_α lines:

```
1|      Radiation 1.540598 1
2|      Radiation 1.544426 @0.455
```

The intensity of the K_{α2} Radiation is about half of the main discrete line, the K_{α1}. In the Sindarin text example above, the intensity of the second Radiation object is a refinable variable, which means that this decimal data will be fitted in the optimization routine.

Each Radiation object will create one PeakXI object in each reflection object (see section 4.6).

The profile of each discrete radiation can be modeled by declaring Profile objects in each Radiation object block. There are several Voigtian profile objects with the FWHM parameter described in terms of wavelength unit and the dependence with the diffracted angle follows the diffraction optics. These peak profiles are very useful for modeling the physical profile of X-ray generated at the radiation source and are used in conjunction with FPA analyses.

The radiation generated by a Cu cathode X ray tube in a typical laboratory diffractometer can be described in detail by 5 discrete radiation lines as reported in (Cheary et al., 2004). The Sindarin text below shows how to use this radiation model in Sindarin:

```
1|      Radiation (Lambda1 = 1.53475) 0.0137
2|      LorentzWavelength Lambda1 3.686E-3
3|      Radiation (Lambda2 = 1.540591) 0.5710
4|      LorentzWavelength Lambda2 0.437E-3
5|      Radiation (Lambda3 = 1.541065) 0.0789
6|      LorentzWavelength Lambda3 0.643E-3
7|      Radiation (Lambda4 = 1.544399) 0.2328
8|      LorentzWavelength Lambda4 0.513E-3
9|      Radiation (Lambda5 = 1.544686) 0.1036
10|     LorentzWavelength Lambda5 0.687E-3
```

4.11 CRYSTALLOGRAPHIC INFORMATION

A Cell object stores all crystallographic information of a phase. The first parameter is a string and represents the symmetry space group. The next parameters are decimal numbers and are the lattice parameters. The number of decimal parameters depends on the lattice type. For instance, only one decimal parameter is required for a cubic lattice, and six decimal parameters are required for a triclinic lattice.

Space-group identifiers may be provided in Hermann-Mauguin notation, as a Hall symbol, or as the space-group number listed in the International Tables for Crystallography, Volume A (ITC-A), published by the International Union of Crystallography (IUCr) (Aroyo, 2016). When a space group admits multiple lattice settings and the setting parameter is not explicitly specified in the string parameter, the following defaults are assumed: for monoclinic lattices, the unique axis is b ($\beta \neq 90^\circ$); for trigonal lattices, the hexagonal (:H) setting is used;

and for orthorhombic lattices, the centrosymmetric origin choice, “choice 2” (:2) in ITC-A, is adopted. The string parameter is case insensitive.

In the block of a Cell object, it is possible to declare two types of objects: ReflectionHKL and atoms. Atoms are declared using the symbol of the chemical element in the first word of the line followed by five decimal parameters: three for relative space position inside the cell (x, y, z), occupation of the crystallographic site (occ) and isotropic atomic displacement factor (uiso). ReflectionHKL is used mainly to describe diffraction reflection without atoms information (see Only lattice parameter information (Pawley method)).

The rutile is a typical structure of TiO_2 (COD 1530150) and the crystallographic information is:

- Cell type: tetragonal
- Lattice parameters: $a = b = 4.594$, $c = 2.959$ and $\alpha = \beta = \gamma = 90^\circ$.
- Space Group (Hermann-Mauguin): $P 4_2 / m n m$ (number 136)
- Oxygen atom position (x, y, z): 0.327, 0.327, 0
- Titanium atom position (x, y, z): 0, 0, 0
- Oxygen and Titanium site occupation: 1
- Oxygen atomic displacement parameter (Uiso): 0.0115
- Titanium atomic displacement parameter (Uiso): 0.00909

So, the Sindarin text for this structure is:

```
1|          Cell "P 42/m n m" 4.594 2.959
2|          O2- 0.327 0.327 0 1 0.0115
3|          Ti4+ 0 0 0 1 0.00909
```

4.12 EXAMPLE OF SINDARIN TEXT TO RIETVELD REFINEMENT

This section presents a typical example of Sindarin text to Rietveld refinement. The experimental setup consists of a diffractometer with Bragg-Bretano geometry, copper x-ray tube and a graphite monochromator. The sample is a single-phase rutile (TiO_2):

```
1| Experimental "data.xye"
2|      Radiation 1.540560 1
3|      Radiation 1.544390 0.5
4|      MonochromatorTwoTheta 28.44
5|      Polynomial 227.2 -115.96 15.5 209.5 -106.58 -330.5 309.3
6|      psVoigt 0.013623 -0.00884 0.00283 0 0.0525 0.00489
7|      split -0.1968 0.0232 0
8|      Displacement -2.105E-5
9|      zero 0.0104
10|     Phase
11|      Scale 0.00173
12|      Cell "P 42/M N M" 4.59366447 2.95956998
13|      O2- 0.327 0.327 0 1 0.09576
14|      Ti4+ 0 0 0 1 0.0478
```

Line by line comments:

Line 1: Create an Experimental object with the data from the file data.xye. All other information below this line belongs to the block of this Experimental object. For more information, see section Experimental.

Line 2: Create a Radiation object for the $K\alpha_1$ line of copper: wavelength 1.54056Å and relative intensity of 1. For more information, see sections Radiation modeling and Radiation.

Line 3: Create a Radiation object for the $K\alpha_2$ line of copper: wavelength 1.54439Å and relative intensity of 0.5.

Line 4: The 2θ angle of the crystal monochromator used, to graphite is 28.44 °2 θ . The Lorentz correction is applied when the monochromator is specified. For more information, see sections Diffraction Setup: Reflection, Symmetric, Flat Specimen, Monochromator and MonochromatorTwoTheta.

Line 5: Use a polynomial function with seven parameters to model the background. For more information, see section Polynomial.

Line 6: Use a pseudo-Voigt function with parametrized FWHM as function of 2θ to model the diffraction profile. Six parameters are informed: U, V, W and Z for Gaussian FWHM and X and Y for Lorentzian FWHM. Apply this profile to all peaks of calculated diffractogram. For more information, see sections Profile level, The pseudo-Voigt function and psVoigt.

Line 7: Create a Split object inside the psVoigt block that modifies the pseudo-Voigt function to model asymmetry of diffraction profile. For more information, see sections Peak asymmetry and Split.

Line 8: Correct the sample displacement from goniometer center. The decimal number is the ration of the displacement and the diffractometer radius. For more information, see sections General equations for calculating the position and intensity of reflections and Displacement.

Line 9: Correct the zero angle of the diffractometer. For more information, see sections General equations for calculating the position and intensity of reflections and Zero.

Line 10: Create a Phase object. For more information, see section Phase.

Line 11: Set the Scale factor of the phase. For more information, see sections General equations for calculating the position and intensity of reflections and Scale.

Line 12: Define the Cell object of the space group $P 4_2 / m n m$ (number 136), with tetragonal lattice, $a = 4.59366447\text{\AA}$ and $c = 2.95956998\text{\AA}$. For more information, see sections Crystallographic Information and Cell

Line 13: Define an atom object of the oxygen element with an oxidation number of -2. The relative position inside the cell is 0.327, 0.327 and 0 (x, y, z), the relative site occupation is 1 and the atomic displacement factor is 0.09576. For more information, see sections Crystallographic Information (page 46) and Atoms (page 70)

Line 14: Define an atom object of the titanium element with an oxidation number of +4. The relative position inside the cell is 0, 0 and 0 (x, y, z), the relative site occupation is 1 and the atomic displacement factor is 0.0478.

5 TUTORIAL

In this chapter, you will learn how to use Sindarin to calculate information on crystalline solid samples from X-ray diffraction experimental data. The data files that you need are located in the Sindarin folder (on Nimloth, a Work Library is created for these tutorials). These files are based on real experimental measurements, but they have been simulated for the purpose of these tutorials. The tutorials will guide you in writing the Sindarin text that sets up the calculations, adjusting the parameters of the theoretical model to fit the experimental data, running the Sindarin invocations that perform the calculations, and checking the results that you obtain. The tutorials are designed to walk you through the calculations step by step. You will see different examples of calculations that cover various user needs and experimental measurement settings. The following are some examples: quantitative phase analysis, lattice parameter calculation, and microstructural analysis; measurements in a laboratory diffractometer with an X-ray tube using Bragg-Brentano geometry and measurements with synchrotron light; refinement with full crystallographic information and refinement with only lattice parameters and a reflection list.

5.1 GENERAL INFORMATION

All necessary files, including the data file, Sindarin inscription and crystallographic information files (CIF), required for following the tutorials are located in a folder named “Tutorials” inside of Sindarin program directory. These files are systematically organized into separate subfolders corresponding to each tutorial.

To edit the Sindarin inscriptions within the tutorial folder, one may utilize a preferred text editor (refer to “User Interface” chapter). It is to be noted that a Sindarin inscription is essentially a simple text file. Hence, any text file can be created, edited, and utilized to execute calculations in Sindarin using Sindarin invocations. It is recommended that the file extension be “.sin” (refer to the Sindarin inscription chapter for details, page 17).

In instances where Nimloth is employed, a “Tutorials” entry is generated within the Works library upon the initial launch of the application. This entry contains all the tutorials present in this manual. One should select the desired tutorial Work to access and edit the corresponding Sindarin inscription and other files.

For instructions on executing Sindarin invocations, consultation of the “User Interface” chapter is advised. Each user interface presents a unique method for execution.

Attention must be paid to the nesting of lines, that is the tab characters at the beginning of each line. The nesting depth delineates the hierarchical relationship among objects. For further details, please consult the chapters on Nesting and Object’s Block (page 23).

All text presented in these tutorials, formatted as code, may be copied and pasted into the Sindarin text file within the text editor. The nesting is appropriately structured. The following text serves as an example of the code format.

This line is in code format

Each tutorial encompasses the complete set of steps and explanations, as it is designed to be conducted independently. Consequently, there is a considerable amount of information and text that is reiterated across them. Feel free to omit certain paragraphs, not the steps, if the user has completed other tutorial beforehand.

All CIF files are obtained from Crystallography Open Database (COD).

5.2 TUTORIAL 0: FIRST CONTACT WITH SINDARIN

This tutorial provides an initial exposure to Sindarin text and the fundamental principles of Sindarin invocations. The accompanying experimental data file contains a simulated dataset that delineates a polynomial function. This function is defined within the horizontal coordinate range of -10 to 10. The polynomial, characterized by the equation below, is of the third degree:

$$y = 3.2 + 2.5x + 1.75x^2 + 0.5x^3$$

Open the Sindarin inscription “sample.sin” located in the Tutorial 0 directory using a text editor. On Nimloth, access the corresponding Work and proceed to Sindarin Editor.

To commence the text, input the following line without any leading whitespace. This instruction instantiates a Data object within the memory, which utilizes the file “sample.xye”, containing the experimental data, as its parameter. The primary function of this object is to load the data from the aforementioned file:

```
Data "sample.xye"
```

Subsequent lines belong to the Experimental object block, where the nesting depth of these lines is greater than that of the Experimental line.

For the subsequent line, begin with a single tab character to mark its nesting. This line initializes a Polynomial object that models a polynomial function. The parameters of this object correspond to the coefficients of the function. Given that there is only one parameter, the polynomial is of degree 0, which is represented as a horizontal line on the graph:

```
Polynomial 0
```

Execute the interpret command to perform the calculations. At this point, the value of χ^2 is 48738, indicating substantial deviation of the calculated function from the experimental data. The graphical representation of the calculated function is a horizontal line at Y=0.

To illustrate the optimization command in decimal data, put a “@” on left side of the number 0 of Polynomial object. This line should look like this:

```
Polynomial @0
```

Proceed by executing the Marathon command.

After finishing the optimization routine, the χ^2 is 45104. The original text is updated with the new optimized value of the first parameter of Polynomial, which is written with the estimated standard deviation enclosed in braces “{}”:

```
Polynomial @61.9953451{±15}
```

At this stage, the function represents a horizontal line at Y=54.35. To refine the model further, add an additional parameter to the Polynomial object with a value of “0” and designate it for optimization by prefixing it with an “@” symbol:

```
Polynomial @61.9953451{±15} @0
```

Re-run the Marathon command. The χ^2 value is now reduced to 8749, and the text is updated accordingly:

```
Polynomial @62.116637{±6.6} @32.7909924{±1.1}
```

The theoretical function now represents an inclined line, indicative of a first-degree polynomial.

Include more two parameters with initial value 0, sign to refine each parameter at a time and execute the Marathon command:

```
Polynomial @3.22876789{±5.5} @32.7989961{±0.94} @1.74914551{±0.12}  
// Chi2 = 5975  
Polynomial @3.20000022{±4.2E-05} @2.50023116{±7.2E-06}  
@1.74999999{±9.2E-07} @0.499996185{±1.1E-07} // Chi2 = 0
```

Ultimately, the function impeccably describes the experimental data, with a χ^2 is 0 (and the r^2 is 1.0). The final function is a third-degree polynomial, with the calculated parameters being: 3.20000(2), 2.500116(4), 1.7500000(5), 0.49999809(5). The numbers in parentheses following the value of each decimal number represent the ESD for the last significant digit.

5.3 TUTORIAL 1: QUANTITATIVE PHASE ANALYSIS

Tutorial 1 encompasses a standard quantitative phase analysis utilizing X-ray diffraction. The specimen comprises a binary mixture of titanium oxide phases: rutile and anatase. The analytical apparatus employed is a laboratory diffractometer equipped with an X-ray tube, featuring copper as the anode material. The diffractometer’s arms are configured symmetrically, accommodating a flat specimen in reflection mode. Additionally, a graphite monochromator is situated preceding the point detector.

Open the Sindarin inscription “sample.sin” located in the Tutorial 1 directory using a text editor. On Nimloth, access the corresponding Work and proceed to Sindarin Editor.

To initiate the text, type the above line without leading whitespace. This line instantiates the Experimental object in memory, utilizing the file “sample.xye” containing experimental data as a parameter. This object is responsible to load the data from the specified file:

Experimental "sample.xye"

Subsequent lines belong to the Experimental object block, where the nesting depth of these lines is greater than that of the Experimental line.

Input the next lines with a single tab character at the beginning to mark nesting. These lines generate two Radiation objects, each representing a K α radiation line of the copper element:

```
Radiation 1.540598 1
Radiation 1.544426 0.5
```

The ensuing command is employed to account for the monochromator's influence on the polarization of the diffracted X-ray beam. The specified value, 28.44, corresponds to the angle of the graphite analyzer crystal. Notably, the Lorentz correction is automatically applied upon assigning this property (for further information, refer to the "Diffraction Setup: Reflection, Symmetric, Flat Specimen, Monochromator" Chapter):

```
MonochromatorTwoTheta 28.44
```

To adjust for background, input the following line. The decimal parameter of 100 serves as an arbitrary starting point, approximating the minimum intensity observed in the experimental data:

```
Polynomial 100
```

The following lines initialize the Phase object, within whose block the information about the phase, including crystallographic information, is specified. The string parameter is optional and serves merely as an identifier for this phase and does not influence the calculation:

```
Phase "Anatase"
```

The nesting of the subsequent three lines, marked by two tab characters, signifies their inclusion within the Phase block.

The line below sets the scale factor of the phase:

```
Scale 0.01
```

The next line instantiates a psVoigt object and associates it with the current phase. This pseudo-Voigt profile function applies to all peaks of this phase:

```
psVoigt 0 0 0.01 0 0 0
```

The crystallographic information for the anatase phase is obtained from COD code 1530151. The correspondent CIF file is located in the tutorial directory.

The ensuing line generates a Cell object with space group $I 4_1 / a m d$ and tetragonal lattice parameters of 3.78 and 9.51 Å:

```
Cell "I 41/A M D:1" 3.78 9.51
```

The cell encompasses two crystallographic sites: one occupied by Ti^{4+} at the origin, and the other by O^{2-} at relative coordinates $x = 0$, $y = 0$ and $z = 0.1775$. To declare an atom within the Cell block, the atom (or ion) symbol followed by an optional string label, three decimal values representing the atom's relative position within the cell, a decimal for the site occupation, and a final decimal for the atomic displacement parameter. The nesting of these lines uses three tab characters:

```
Ti4+ "Ti1" 0 0 0 1 0.01
O2- "O1" 0 0 0.1775 1 0.01
```

For the rutile phase, COD code 9004141 was utilized. The Sindarin text for this phase is as follows:

```
Phase "Rutile"
Scale 0.01
psVoigt 0 0 0.01 0 0 0
Cell "P 42/M N M" 4.593 2.959
Ti4+ "Ti1" 0 0 0 1 0.01
O2- "O1" 0.3051 0.3051 0 1 0.01
```

The initial Sindarin text is complete and the refinement of the parameters could be started.

Execute the interpret command to perform the calculations. At this point, the χ^2 is 90.59 and the calculated diffractogram differs significantly from the experimental diffractogram, especially in the intensity and width of each peak. However, all peaks of the two phases and the background are present in calculated diffractogram.

To illustrate the optimization command in decimal data, put a "@" on left side of the number 100 of Polynomial object. This line should look like this:

```
Polynomial @100
```

Execute the walk command.

After finishing the optimization routine, the χ^2 is 89.17. The original text is updated with the new optimized value of the first parameter of Polynomial, which is written with the estimated standard deviation enclosed in braces "{}":

```
Polynomial @87.6222027{±1.2}
```

Next, refine the scale of the two phases, write the "@" on left side of the decimal data of Scale property of both phases and run the walk command. The χ^2 is now 33.19. The new values are written in the text:

Scale of the anatase phase after optimization:

```
Scale @0.0109021647{±0.00017}
```

Scale of the rutile phase after optimization:

Scale @0.0159739102{±0.0005}

Note that all decimal data marked with “@” are optimized, and the first parameter of Polynomial object was optimized and updated to 98.6615345{±0.73}.

Refine each psVoigt parameter, one by one, for each phase at a time. Be care with parameter Z of the gaussian (the fourth parameter of psVoigt), as it frequently has high correlation with others gaussian parameters. Therefore, if the model does not use the Z parameter to relate to a physical model, set it to zero and do not refine it.

The refined value of each parameter of psVoigt for the anatase phase is:

```
psVoigt @0.0381318006{±0.0011} 0 0.01 0 0 0 // Chi2 = 27.58
psVoigt @0.0489453603{±0.0048} @0.164330713{±0.0038} 0.01 0
0 0 // Chi2 = 19.63
psVoigt @0.238433982{±0.035} @0.0607873592{±0.033}
@0.0429714632{±0.0064} 0 0 0 // Chi2 = 18.13
psVoigt @105260.284 @-0.0227346743{±0.042} @105260.065 @-
105259.98 0 0 // Chi2 = 17.88
psVoigt @0.0744250566{±0.035} @-0.0318636216{±0.021}
@0.0680701336{±0.0037} 0 @0.240396799{±0.0081} 0 // Chi2 = 17.29
psVoigt @0.0965209583{±0.011} @-0.107362767{±0.0018}
@0.0299537624{±0.00077} 0 @0.23981764{±0.018} @0.107330071{±0.0041}
// Chi2 = 14.89
```

The refined value of each parameter of psVoigt for the rutile phase is:

```
psVoigt @0.0193763101{±0.0012} 0 0.01 0 0 0 // Chi2 = 14.30
psVoigt @0.0044609696{±0.0087} @0.124702209{±0.0061} 0.01 0
0 0 // Chi2 = 12.60
psVoigt @0.611946509{±0.1} @-0.249795637{±0.092}
@0.10906531{±0.019} 0 0 0 // Chi2 = 12.01
psVoigt @0.395158677{±0.13} @-0.126122406{±0.095}
@0.0899133819{±0.024} 0 @0.0587679881{±0.055} 0 // Chi2 = 11.97
psVoigt @0.520128357{±0.19} @-0.143441323{±0.14}
@0.0209692495{±0.029} 0 @-0.202308611{±0.11} @0.198369517{±0.035} //
Chi2 = 11.77
```

Next, refine all the lattice parameters of each phase.

The results for the anatase phase are:

```
Cell "I 41/A M D:1" @3.78742119{±8.7E-05}
@9.50876958{±0.00046} // Chi2 = 4.86
```

The result for the rutile phase is:

```
Cell "P 42/M N M" @4.59571811{±0.00028}
@2.95885313{±0.00032} // Chi2 = 4.75
```

A XRD standard was not measured for this study and the alignment of the diffractometer arms (the Zero property of Experimental object) was not corrected, so the results of the lattice parameters are not accurate and should be used with caution.

At this point, increase the number of parameters of the Polynomial object by three, one by one:

```
Polynomial @83.1878913{±0.3} @-8.28929491{±0.49} // Chi2 = 4.53
Polynomial @66.8613854{±0.2} @-7.57916089{±0.37}
@50.4954739{±0.23} // Chi2 = 2.56
Polynomial @65.9889957{±0.31} @7.31406166{±0.43}
@51.3298022{±0.68} @-24.8639752{±0.54} // Chi2 = 2.45
```

At this point, the refinement can be considered finished. The χ^2 is low and the theoretical diffractogram is very similar to the experimental diffractogram. Other parameters, such as zero, peak asymmetry, bisection and position of each atom, can be refined, but they will not have significant impact on the main result, which is amount of each phase.

Execute the command to write the result to a file (or, if in Nimloth, go to the result panel). The relative amount of each phases is shown, the anatase phase is 78(2)% and the rutile is 22(2)%

5.4 TUTORIAL 2: LATTICE PARAMETERS ANALYSIS

Tutorial 2 encompasses a lattice parameters analysis utilizing X-ray diffraction. The specimen comprises a pure cerium oxide. The analytical apparatus employed is a laboratory diffractometer equipped with an X-ray tube, featuring copper as the anode material. The diffractometer's arms are configured symmetrically, accommodating a flat specimen in reflection mode. No monochromator is used.

For precise lattice parameters values, it is essential to measure the X-ray diffraction of a line position standard under identical diffractometer conditions as those used for the sample measurement. In this tutorial, the NIST standard SRM 640 (silicon) is employed for this purpose. The objective is to obtain the Zero correction for the position of the diffractometer arms. The diffractogram of the standard must be analyzed first.

The theoretical refinement model employed in this tutorial does not incorporate atom information. This is due to the fact that the lattice parameters, which are the sole focus of interest, are unrelated to the positions or types of atoms.

Open the Sindarin inscription “stand.sin” located in the Tutorial 2 directory using a text editor. On Nimloth, access the corresponding Work and proceed to Sindarin Editor.

To initiate the text, type the above line without leading whitespace. This line instantiates the Experimental object in memory, utilizing the file “stand.xye” containing experimental data as a parameter. This object is responsible to load the data from the specified file:

```
Experimental "stand.xye"
```

Subsequent lines belong to the Experimental object block, where the nesting depth of these lines is greater than that of the Experimental line.

Input the next lines with a single tab character at the beginning to mark nesting. These lines generate two Radiation objects, each representing a K α radiation line of the copper element:

```
Radiation 1.540598 1
Radiation 1.544426 0.5
```

To adjust for background, input the following line. The decimal parameter of 100 serves as an arbitrary starting point, approximating the minimum intensity observed in the experimental data:

```
Polynomial 100
```

The next line instantiates a psVoigt object and associates it with Experimental object. This pseudo-Voigt profile function is applicable to all peaks of all phases (in this instance, there is only one phase):

```
psVoigt 0 0 0.01 0 0 0
```

The following lines initialize the Phase object, within whose block the information about the phase, including crystallographic information, is specified. The string parameter is optional and serves merely as an identifier for this phase and does not influence the calculation:

```
Phase "Silicon"
```

The nesting of the subsequent lines, marked by two or more tab characters, signifies their inclusion within the Phase object block.

The ensuing line generates a Cell object with space group $Fd\bar{3}m$ and tetragonal lattice parameter of 5.431179 Å, information obtained from standard NIST certificate:

```
Cell "F D -3 M:1" 5.431179
```

Within the Cell object block, the ReflectionHKL objects are defined. Each object contains two parameters: the first is an array of three integers representing the Miller indices of the reflection; the second parameter corresponds to the reflection's intensity. To circumvent refinement instability caused by a high correlation between the intensities of reflection (1 1 5) and (3 3 3), which have identical position, only reflection (3 3 3) is incorporated into this theoretical model:

```
ReflectionHKL [1 1 1] 10000
ReflectionHKL [2 0 2] 10000
ReflectionHKL [1 1 3] 10000
ReflectionHKL [4 0 0] 10000
ReflectionHKL [1 3 3] 10000
ReflectionHKL [2 2 4] 10000
ReflectionHKL [3 3 3] 10000
ReflectionHKL [4 0 4] 10000
ReflectionHKL [1 3 5] 10000
```

The initial Sindarin text has been finalized, allowing for the commencement of parameter refinement. It should be noted that polarization corrections are unnecessary, as the peak intensities are considered arbitrary parameters within the context of this study.

Execute the interpret command to perform the calculations. At this point, the χ^2 is 201.50 and the calculated diffractogram differs significantly from the experimental diffractogram. However, all peaks of the phase and the background are present in calculated diffractogram.

To illustrate the optimization command in decimal data, put a “@” on left side of the number 100 of Polynomial object. This line should look like this:

```
Polynomial @100
```

Execute the walk command.

After finishing the optimization routine, the χ^2 is 151.52. The original text is updated with the new optimized value of the first parameter of Polynomial, which is written with the estimated standard deviation enclosed in braces “{}”:

```
Polynomial @205.47025{±2.6}
```

Next, refine the intensity of all ReflectionHKL objects, write the “@” on left side of the second parameter of the ReflectionHKL objects and run the walk command. The χ^2 is now 23.48. The new values are written in the text:

```
ReflectionHKL [1 1 1] @5995.32463{±1.1E+02}
ReflectionHKL [2 0 2] @8654.82694{±2E+02}
ReflectionHKL [1 1 3] @3576.26452{±1.1E+02}
ReflectionHKL [4 0 0] @6197.85158{±4.3E+02}
ReflectionHKL [1 3 3] @2577.52875{±1.5E+02}
ReflectionHKL [2 2 4] @3652.0958{±1.9E+02}
ReflectionHKL [3 3 3] @6004.72356{±4.7E+02}
ReflectionHKL [4 0 4] @1969.87625{±2.5E+02}
ReflectionHKL [1 3 5] @820.60419{±68}
```

Note that all decimal data marked with “@” are optimized, and the first parameter of Polynomial object was optimized and updated to 217.363{±1}.

Refine each psVoigt parameter, one by one, for each phase at a time, starting with the nonzero parameter. Be care with parameter Z of the gaussian (the fourth parameter of psVoigt), as it frequently has high correlation with others gaussian parameters. Therefore, if the model does not use the Z parameter to relate to a physical model, set it to zero and do not refine it.

The refined value of each parameter of psVoigt for the anatase phase is:

```
psVoigt 0 0 @0.00570526344{±0.00033} 0 0 0 // Chi2 = 21.67
psVoigt @0.000787828174{±0.00034} 0 @0.0051298818{±0.00018} 0 0 0
// Chi2 = 21.60
psVoigt @-7.80473866E-05{±0.0014} @0.00177900855{±0.002}
@0.00439349088{±0.00062} 0 0 0 // Chi2 = 21.58
```

```

psVoigt @-0.000360177851{±0.00028} @-0.000604181858{±0.00021}
@0.00431652518{±0.00011} 0 @0.0235936942{±0.0018} 0 // Chi2 = 21.40
psVoigt @-0.00148008535{±0.00095} @0.0031518711{±0.0017}
@0.000921536495{±0.0006} 0 @-0.00667311968{±0.0075}
@0.0262950318{±0.0034} // Chi2 = 20.34

```

Increase the number of parameters of the Polynomial object by three, one by one:

```

Polynomial @220.054177{±0.87} @-54.3038548{±1.5} // Chi2 = 16.06
Polynomial @215.864116{±1.3} @-55.3302255{±1.5} @12.5163189{±2.9}
// Chi2 = 16.00

```

Include the following line in the Experimental object block (one tab character as nesting) to correct the Zero of the diffractometer:

```
Zero @0
```

Upon assigning the decimal value for refine and executing the Walk command, the value of the Zero is $-0.0185934561 \pm 0.00068$ with the χ^2 currently 8.17.

Subsequently, assign the Displacement property within the Experimental object block (one tab character as nesting):

```
Displacement @0
```

After refining the decimal value and executing the walk command, the value of the Displacement is $0.000806775035 \pm 6.2\text{E-}05$ and χ^2 equals 5.95.

To rectify the asymmetry of the peaks, incorporate the Split object within the psVoigt object block:

```
Split 0 0 0
```

Refine the decimal parameters of this object sequentially:

```

Split @-0.281082231{±0.01} 0 0 // Chi2 = 4.93
Split @0.222740225{±0.021} @-0.160045594{±0.006} 0 // Chi2 =
4.17
Split @0.583183299{±0.085} @-0.412158248{±0.057}
@0.0386203397{±0.0088} // Chi2 = 4.13

```

Run walk command some time to have sure that the refinement reached the local minimum. The χ^2 is 4.11 now.

At this point, the refinement of the standard is complete, the requisite information for refining the sample diffractogram is the Zero parameter, recorded as 0.0103501339 ± 0.0041 . The psVoigt object, inclusive the Split object, of the standard refinement serves as an advantageous starting point for refining the sample peak profile and will therefore be utilized in the Sindarin inscription of the sample.

Open the “sample.sin” Sindarin inscription located in the Tutorial 2 directory using a text editor. On Nimloth, access the corresponding Work and proceed to Sindarin Editor.

To initiate the text, type the above line without leading whitespace, utilizing the file name "sample.xyc" as parameter:

```
Experimental "sample.xyc"
```

Several sentences are analogous to those in the Sindarin inscription used for the standard refinement, hence many explanations are identical and are not presented here. The subsequent four lines are replicated from the initial Sindarin text of the standard:

```
Radiation 1.540598 1
Radiation 1.544426 0.5
Polynomial 100
```

The next three are derived from the final Sindarin inscription of the standard. It is important to note that none of the decimal parameters in these lines are designated for refinement. These values must remain fixed during the refinement of the sample:

```
psVoigt 0.0118750657{±0.00066} -0.0197128428{±0.0009}
0.00975592006{±0.00029} 0 0.0250685294{±0.0032}
0.00490697953{±0.0013}
Split 0.607769983{±0.084} -0.431540361{±0.057}
0.0412900759{±0.0088}
Zero 0.0103501339{±0.0041}
```

The next lines are to instantiate the Phase and the Cell objects. The space group and the lattice parameter are obtained from the COD code 4343161:

```
Phase "Ce O2"
Cell "F M -3 M" 5.40972
```

The objective of this tutorial is to obtain the lattice parameters accurately, so it is not necessary information of atoms. Instead, atoms objects in this case are utilized ReflectionsHKL objects within Cell object block. For this phase and inside the range of 2 of the experimental diffractogram the following ReflectionsHKL must be

```
ReflectionHKL [1 1 1] 100
ReflectionHKL [2 0 0] 100
ReflectionHKL [2 0 2] 100
ReflectionHKL [1 1 3] 100
ReflectionHKL [2 2 2] 100
ReflectionHKL [4 0 0] 100
ReflectionHKL [1 3 3] 100
ReflectionHKL [2 0 4] 100
ReflectionHKL [2 2 4] 100
ReflectionHKL [3 3 3] 100
```

The reflection (1 1 5) was excluded from the analysis, despite being within the experimental measurement's angular range, due to its diffraction angle being identical to that of the reflection (3 3 3), which would result in a significant correlation of intensity between these two reflections. While this does not affect the present study, for scenarios involving

anisotropic functions reliant on the Miller index, employing Rietveld refinement is advisable as it allows for the determination of each reflection's intensity based on the structure factor.

Execute the interpret command to perform the calculations. At this point, the χ^2 is 2010. Refine two parameters of the Polynomial, the χ^2 is 1912 and the parameters are:

```
Polynomial @290.842687{±13}
```

Now, refine the intensity of each reflection of the phase. All reflection intensity may be refined simultaneously because the peaks are not overlapped. The χ^2 is 50.36 and the text updated shows:

```
ReflectionHKL [1 1 1] @105.880983{±3.1}
ReflectionHKL [2 0 0] @46.9633986{±2.6}
ReflectionHKL [2 0 2] @34.5458605{±1.5}
ReflectionHKL [1 1 3] @12.6961116{±0.66}
ReflectionHKL [2 2 2] @7.85052572{±1.1}
ReflectionHKL [4 0 0] @9.46162236{±1.5}
ReflectionHKL [1 3 3] @5.83805556{±0.49}
ReflectionHKL [2 0 4] @4.27182168{±0.45}
ReflectionHKL [2 2 4] @6.02336315{±0.51}
ReflectionHKL [3 3 3] @19.3517603{±1.6}
```

Signed to refine the lattice parameter of the Cell object and run walk command. The χ^2 is 35.58 and the new text look like this:

```
Cell "F M -3 M" @5.41188004{±5.9E-05}
```

Now include a line with Displacement property inside the Experimental object block (nesting depth with one tab character) with value 0:

```
Displacement @0
```

Signed the value of Displacement to refine and run the walk command. The χ^2 is 12.25 and the new value of this property is 0.000386001063{±5.7E-06}.

Introduce a new line for the psVoigt object within the Phase object block, ensuring it is nested with two tab characters. This function models the sample profile, whereas the first psVoigt object, located in the Experimental object block, represents the instrumental profile. For the propose of this tutorial, the physical significance of the sample's width is not considered. The initial value is set to be minimal, yet non-zero:

```
psVoigt 0.00001 0 0 0 0 0 //Chi2 = 13.33
```

Refine one by one parameters of psVoigt of phase object:

```
UZXY
```

```
psVoigt @0.00488009921{±0.00015} 0 0 0 0 0 // Chi2 = 5.84
psVoigt @-0.0102314085{±0.0005} @0.0140221237{±0.00036} 0 0
0 0 // Chi2 = 3.14
```

```

psVoigt @0.0105859687{±0.0014} @-0.0130335453{±0.0018}
@0.00770203257{±0.0005} 0 0 0 // Chi2 = 2.80
psVoigt @0.00975037281{±0.0012} @-0.0156928683{±0.0014}
@0.00756024322{±0.0004} 0 @0.0211451598{±0.0012} 0 // Chi2 = 2.49
psVoigt @0.0068569538{±0.0012} @-0.0110027286{±0.0015}
@0.0055735064{±0.00044} 0 @0.017010966{±0.00092}
@0.00415227817{±0.00057} // Chi2 = 2.45

```

Include more two parameters to Polynomial object and refine them. The χ^2 is 2.25 and the new values can be seen in the updated text:

```

Polynomial @347.177776{±0.69} @-8.0171543{±0.79} @16.1335562{±1.5}
// Chi2 = 2.25

```

To conclude the refinement process, execute the walk command several times ascertain that the local minimal of the refinement has been attained.

The lattice parameter obtained from this process is $5.40890 \pm 2 \text{ \AA}$, with the estimated standard deviation in fifth decimal place.

6 SINDARIN VOCABULARY

A Dictionary with all “words” used in Sindarin is presented. Here, word means object classes and property names.

6.1 WORDS BY OBJECT TYPE

In this section, terminology is organized according to the classification of object types, accompanied by an explanation of the general aspects pertinent to each category. Only objects, which are capable of containing a block, are classified herein; their properties are not delineated. Concluding this section is a comprehensive enumeration of operations, internal constants, internal variables and functions applicable to decimal data.

6.1.1 Calculation Control

<i>Entry</i>	Section	Page
<i>Calculation</i>	6.2.7	73

6.1.2 Experimental data

<i>Entry</i>	Section	Page
<i>Data</i>	6.2.20	80
<i>DataSimulation</i>	6.2.21	81
<i>ExcludeRegion</i>	6.2.34	88
<i>Experimental</i>	6.2.35	89
<i>Interval</i>	6.2.46	96
<i>Simulation</i>	6.2.82	117

6.1.3 Diffraction

<i>Entry</i>	Section	Page
<i>Ellipsoidal</i>	6.2.30	86
<i>MarchDollase</i>	6.2.55	102
<i>PeakXI</i>	6.2.61	105
<i>Phase</i>	6.2.62	106
<i>POSphericalHarmonic</i>	6.2.65	107
<i>Radiation</i>	6.2.71	111
<i>ReflectionXI</i>	6.2.75	113

6.1.4 Crystallographic

<i>Entry</i>	Section	Page
<i>Atoms</i>	6.2.3	70
<i>Cell</i>	6.2.10	74
<i>ReflectionHKL</i>	6.2.74	113

6.1.5 Background Function

In Sindarin, a variety of functions are available to compute the intensity (denoted as y in the chart) at each experimental point. In instances where the background is irregular and challenging to correct, the amalgamation of certain functions can facilitate this task and simplify the accurate modeling of the diffractogram background. Sindarin allows for the combination of any number of functions; one simply needs to declare multiple background objects within the Sindarin text.

Entry		Section	Page
<i>BackgroundFile</i>		6.2.5	72
<i>Chebyshev</i>		6.2.12	76
<i>CosineFourier</i>		6.2.17	78
<i>DebyeLike</i>		6.2.22	81
<i>Function</i>		6.2.39	92
<i>FunctionArctangent</i>		6.2.40	92
<i>FunctionPsVoigt</i>		6.2.41	93
<i>Interpolation</i>		6.2.45	96
<i>Inverse</i>		6.2.47	97
<i>LogDistribution</i>		6.2.50	99
<i>Logistic</i>		6.2.51	99
<i>Polynomial</i>		6.2.64	107

6.1.6 Profile

6.1.6.1 Basic Profile

Entry		Section	Page
<i>ProfileFunction</i>		6.2.66	108
<i>ProfileFunctionFT</i>		6.2.67	109
<i>ShiftFT</i>		6.2.80	116
<i>Split</i>		6.2.86	120

6.1.6.2 Voigtian function

6.1.6.2.1 Basic Voigtian functions

Entry		Section	Page
<i>Gauss</i>		6.2.42	94
<i>Lorentz</i>		6.2.52	100
<i>psVoigt</i>		6.2.69	110
<i>Voigt</i>		6.2.94	125

6.1.6.2.2 Voigtian in Wavelength

Entry	Section	Page
<i>GaussWavelength</i>	6.2.43	95
<i>LorentzWavelength</i>	6.2.53	101
<i>psVoigtWavelength</i>	6.2.70	111
<i>VoigtWavelength</i>	6.2.97	129

6.1.6.2.3 Voigtian Microstructure

Entry	Section	Page
<i>VoigtianSize</i>	6.2.95	126
<i>VoigtianStrain</i>	6.2.96	128

6.1.6.3 FPA function

6.1.6.3.1 FPA base functions

Entry	Section	Page
<i>Box</i>	6.2.6	72
<i>Circle</i>	6.2.13	76
<i>Exponential</i>	6.2.36	90
<i>InverseProfile</i>	6.2.48	98

6.1.6.3.2 Specific aberration correction

Entry	Section	Page
<i>AxialDivergence</i>	6.2.4	71
<i>Defocusing</i>	6.2.23	82
<i>EquatorialDivergence</i>	6.2.33	88
<i>ReceivingSlitWidth</i>	6.2.73	112
<i>TargetWidth</i>	6.2.88	121
<i>Tilt</i>	6.2.90	122
<i>Transparency</i>	6.2.91	123

6.1.6.4 WPPM function

Entry	Section	Page
<i>Dislocation</i>	6.2.26	83
<i>DislocationPopa</i>	6.2.27	84
<i>Fault</i>	6.2.37	91
<i>MicrostrainPAH</i>	6.2.57	103
<i>MicrostrainWUAH</i>	6.2.58	104

Entry	Section	Page
<i>SizeDistribution</i>	6.2.83	117

6.1.7 Decimal Operators and Functions

Decimal data can be utilized with mathematical operators and functions. Operators are placed between two decimals data, such as the addition operator:

1| 1 + 1

Functions are indicated by a specific term followed by parentheses. The decimal value(s) are placed inside the parentheses. For instance, the square root function:

1| Sqrt(4)

The subsequent section will enumerate all operators and functions in Sindarin, categorized by type.

6.1.7.1 Decimal operators

Entry	Short Description
<i>Division (/)</i>	Divides two decimal data
<i>Multiplication (*)</i>	Multiplies two decimal data
<i>Parentheses ()</i>	Parentheses in mathematics, used to order operations
<i>Power (^)</i>	A number raised to a power
<i>Subtraction (-)</i>	Subtract two decimal data
<i>Sum (+)</i>	Add two decimal data

6.1.7.2 General functions

Entry	Short Description
<i>Sqrt</i>	Square Root
<i>Abs</i>	Absolute
<i>ln</i>	The natural logarithm
<i>log</i>	The common logarithm
<i>rad</i>	Calculates the angle in radians from the angle in degrees
<i>deg</i>	Calculates the angle in degrees from the angle in radians

6.1.7.3 Trigonometric functions

Entry	Short Description
<i>Acos</i>	Arccosine
<i>Asin</i>	Arcsine
<i>Atan</i>	Arctangent
<i>Cos</i>	Cosine
<i>Sin</i>	Sine
<i>Tan</i>	Tangent

6.1.7.4 Special functions

Entry	Short Description
<i>psVoigtH</i>	Calculation of psVoigt FWHM from the Gaussian and Lorentzian FWHM
<i>psVoigtEta</i>	Calculation of psVoigt Eta from the Gaussian and Lorentzian FWHM
<i>psVoigtBeta</i>	Calculation of psVoigt integral breadth from the Gaussian and Lorentzian FWHM
<i>psVoigtHBeta</i>	Calculation of psVoigt FWHM from integrated breadth and eta of the psVoigt
<i>psVoigtHGaus</i>	Calculation of Gaussian FWHM from integrated breadth and eta of the psVoigt
<i>psVoigtHLorentz</i>	Calculation of Lorentzian FWHM from integrated breadth and eta of the psVoigt
<i>randon(mean sd)</i>	This function generates a random value with equal probability, centered around a specified base value (mean) with a given standard deviation (sd)
<i>randonGauss(mean sd)</i>	This function generates a random value following a Gaussian distribution, centered around a specified base value (mean) with a given standard deviation (sd)
<i>logDist(mean sd x)</i>	

Special functions require two decimal parameters, separated by space, within the function parentheses. An example is:

```
1| psVoigtH(0.43 0.184)
```

6.1.8 Decimal Constants

Entry	Short Description
<i>E</i>	The Euler number
<i>CLight</i>	The speed of light in vacuum
<i>NaN</i>	Not a Number
<i>PI</i>	The π constant
<i>hPlanck</i>	The Planck constant
<i>NAvog</i>	The Avogadro constant

6.1.9 Internal variables

Entry	Short Description
<i>x</i>	A decimal data representing the variable independent of the diffractogram derived from the experimental data, utilized in functions.

<i>xl</i>	A decimal data representing a point in one-dimensional Fourier space, calculated from the experimental data and the wavelength of the radiation. The unit of measurement is the same as that of the wavelength, which is angstrom.
<i>xmin</i>	A decimal array of length two denotes the point with the minimum x-value in the experimental data; the first decimal represents the x-coordinate, and the second indicates the intensity.
<i>xmax</i>	A decimal array of length two denotes the point with the maximum x-value in the experimental data; the first decimal represents the x-coordinate, and the second indicates the intensity.
<i>ymin</i>	A decimal array of length two denotes the point with the minimum y-value in the experimental data; the first decimal represents the x-coordinate, and the second indicates the intensity.
<i>ymax</i>	A decimal array of length two denotes the point with the maximum y-value in the experimental data; the first decimal represents the x-coordinate, and the second indicates the intensity.
<i>xpeak</i>	A decimal value corresponds to the peak's position in 2θ (or another horizontal unit of the diffractogram).
<i>ipeak</i>	The decimal value signifies the peak's intensity in diffractogram units.
<i>dref</i>	The interplanar spacing of the reflection, denoted as d, is measured in Å units.
<i>fwhm</i>	A decimal data is employed to compute the Profile Function with two or more parameters.
<i>hkl</i>	An integer array of length three represents the Miller indices of a reflection.

When an internal variable constitutes an array, its value may be utilized either as an array or by accessing the value at a specific array position. For instance, `hkl[0]` retrieves the value of h in the Miller index, while `xmax[1]` obtains the intensity value of the point with the maximum x-coordinate in the experimental data.

6.2 ALPHABETIC ENTRIES

In this section the words are presented in alphabetic order with systematic information useful to use these entries in Sindarin document and to understanding of behavior or action of each object and property. Each entry in dictionary has the following information, when applied: Declarative form; Parameters; Description; Equations; Parents or owners; Children; Properties; References; Specific information; Internal Variables dependences. The decimal function and operators, decimal constants and internal variables it is not present here, they are in 6.1.7, 6.1.8 and 6.1.9 sections.

Common information table:

Declarative form

Type

Parent(s)/Owner(s)

References

Short description

Object-specific information table:

Object classification

Parameters

***Internal variables
dependences for
parameters***

Properties

Children

Specific information

Property-specific information table:

Data type

***Internal variables
dependences***

Specific information

Default value

6.2.1 AbsorptionFunction

Declarative form

AbsorptionFunction (decimal)

Type

Property

Parent(s)/Owner(s)

Experimental 89
Simulation 117

References

Short description

A generic decimal data that is used in calculation of intensity reflection.

Data type

Decimal

***Internal variables
dependences***

Specific information

Default value

0

6.2.2 AngularDependency

Declarative form	AngularDependency (enum)[SinLike, QuadraticLike, FPALike]
Type	Property
Parent(s)/Owner(s)	Split 120 Circle 76
References	(Cheary & Coelho, 1992; Enzo et al., 1988; Toraya, 1986)
Short description	Defines the x-dependent function type with three parameters for asymmetry peak correction.
Data type	bool
Internal variables dependences	-
Specific information	The AngularDependency property can only be assigned when there are three or four object parameters of the asymmetry correction object.
Default value	SinLike

If the property is SinLike, the dependency is a Quadratic function:

$$asym(x) = \mu_0 + \frac{\mu_1}{\sin\left(\frac{x}{2}\right)} + \frac{\mu_2}{\sin^2\left(\frac{x}{2}\right)}$$

If it is QuadraticLike:

$$asym(x) = \mu_0 + \mu_1[x - (90 + \mu_2)]^2$$

And, if it is FPALike:

$$asym(x) = \frac{\mu_0}{\sin(x)} + \mu_1\sqrt{\tan\left(\frac{x}{2}\right)} + \mu_2 \tan(x)$$

6.2.3 Atoms

Declarative form	AtomSymbol (decimal)x (decimal)y (decimal)z (decimal)occ (decimal)uiso AtomSymbol (string)label (decimal)x (decimal)y (decimal)z (decimal)occ (decimal)uiso
Type	Object
Parent(s)/Owner(s)	Cell 74

References	
Short description	Object that represents an atom inside the cell
Object classification	Crystallographic 63
Parameters	The label is an optional string data utilized for atom identification. The initial three decimal values represent the atom's relative position within the cell (x, y and z). This is succeeded by a decimal value indicating the atom's site occupancy in the crystallographic cell (occ). Subsequently, a decimal value denotes the isotropic atomic displacement parameter (uiso) in Å ² .
Internal variables dependences for parameters	
Properties	-
Children	-
Specific information	First word must be the atom symbol, for example, for oxygen atom must write O, or for sodium cation must write Na1+

6.2.4 AxialDivergence

Declarative form	AxialDivergence (decimal)laxial
Type	Object
Parent(s)/Owner(s)	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	Profile correction due the axial divergence of X-ray beam on the sample
Object classification	Profile 64
Parameters	Axial length of the X-ray beam on the sample divide by diffractometer radius
Internal variables dependences for parameters	
Properties	ConvolutionType (page 77)
Children	-
Specific information	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.5 BackgroundFile

Declarative form	BackgroundFile (string)file_[1..n]
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117 Data 80 DataSimulation 81
References	-
Short description	Load a data from file(s) and apply it(them) to background
Object classification	Background Function 64
Parameters	File names to be load
Internal variables dependences for parameters	
Properties	-
Children	-
Specific information	Multiple background objects can be used simultaneously

6.2.6 Box

Declarative form	Box (decimal)wBox
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	A box profile shape
Object classification	Profile 64
Parameters	The width of the box in 20 units

<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	ConvolutionType (page 77)
<i>Children</i>	-
<i>Specific information</i>	The Box function is the base of the Defocusing, ReceivingSlitWidth, TargetWidth and Tilt profile functions.

6.2.7 Calculation

<i>Declarative form</i>	Calculation
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Root
<i>References</i>	-
<i>Short description</i>	This object has several data that control the calculation of diffractogram and the optimization routine

<i>Object classification</i>	Calculation Control 63
<i>Parameters</i>	-
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	Cycles 79 DerivationBothSide 82 CalculeProfileInPeak 73 RapidYRecalcule 112 Stabilization 121
<i>Children</i>	-
<i>Specific information</i>	This object is always instantiated. If the user does not attribute explicitly in the text, the object assumes default values of the properties

6.2.8 CalculeProfileInPeak

<i>Declarative form</i>	CalculeProfileInPeak (bool)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Calculation 73

References	-
Short description	Enable the calculation of the profiles in each peak in the diffractogram. Otherwise, the calculation is performed in each Reflection.
Data type	Boolean
Internal variables dependences	-
Specific information	-
Default value	false

6.2.9 Capillary

Declarative form	<p>Capillary (decimal)mur</p> <p>Capillary (decimal)mur (decimal)displ (decimal)dispv</p>
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	(Gozzo et al., 2010; Sabine et al., 1998)
Short description	Enable corrections due the capillary sample in transmission diffraction geometry. These corrections are applied to the intensity and position of reflections due sample absorption. Additionally, capillary displacement can also be corrected.
Object classification	Diffraction 63
Parameters	A decimal data that is the effective linear absorption of the sample multiplied by capillary radius (muR). The other two decimal data that is the displacement of the sample form the goniometry center in two directions divided by diffractometer radius (dispL and dispV).
Internal variables dependences for parameters	
Properties	EnableIntensity 87 EnableShift 87
Children	-
Specific information	-

6.2.10 Cell

<i>Declarative form</i>	Cell (string)spaceGroup (decimal)latticeParameter _[1,2,3,4,6]
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Phase 106
<i>References</i>	(Aroyo, 2016)
<i>Short description</i>	Create an object that represents the crystallographic cell
<i>Object classification</i>	Crystallographic 63
<i>Parameters</i>	The string represents the space group symbol, which can be expressed in either Hermann-Mauguin notation, Hall notation or number, as established by the International Table (IUCR). Accompanying this, the lattice parameters are provided in units of angstroms (Å), the number of decimal parameters depends on the lattice system.
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	Z 131
<i>Children</i>	Atoms 70 ReflectionHKL 113 Z 131
<i>Specific information</i>	See more information in 4.11 Crystallographic Information section, page 46

6.2.11 CenteredInMiddle

<i>Declarative form</i>	CenteredInMiddle (bool)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Polynomial 107
<i>References</i>	
<i>Short description</i>	Set if the polynomial is calculated centered in the middle of the x range of experimental data
<i>Data type</i>	Bool
<i>Internal variables dependences</i>	
<i>Specific information</i>	
<i>Default value</i>	True for Experimental and Simulation root objects False for Data and DataSimulation root objects

6.2.12 Chebyshev

<i>Declarative form</i>	Chebyshev (decimal)coefficient _[1..n]
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117 Data 80 DataSimulation 81
<i>References</i>	
<i>Short description</i>	Chebyshev polynomial of the first kind
<i>Object classification</i>	Background Function 64
<i>Parameters</i>	Coefficients of the Chebyshev polynomial function
<i>Internal variables</i>	
<i>dependences for parameters</i>	
<i>Properties</i>	-
<i>Children</i>	-
<i>Specific information</i>	Multiple background objects can be used simultaneously

6.2.13 Circle

<i>Declarative form</i>	Circle (decimal)cutcir Circle (decimal)mu0 (decimal)mu1 (decimal)mu2 Circle (decimal)mu0 (decimal)mu1 (decimal)mu2 (decimal)xmaxasy
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	(Cheary & Coelho, 1992)
<i>Short description</i>	The Circle profile function
<i>Object classification</i>	Profile 64

Parameters	<p>The cutCir parameter is the limit of the calculation of Circle function.</p> <p>The parameters mu0, mu1, mu2 are used to calculate the limit of the circle function as a function of the 2θ. The parameter xMaxAsy is the maximum angle in 2θ that the Circle function is applied.</p>
Internal variables dependences for parameters	
Properties	<p>ConvolutionType 77</p> <p>AngularDependency 70</p>
Children	-
Specific information	The Circle is the base function of the AxialDivergence profile function

6.2.14 ConvolutionSMax

Declarative form	ConvolutionSMax (decimal)
Type	Property
Parent(s)/Owner(s)	<p>Experimental 89</p> <p>Simulation 117</p>
References	
Short description	The maximum distance from the peak center (in Å) at which the profile in Fourier space is calculated for use in convolution.
Data type	Decimal
Internal variables dependences	
Specific information	<p>ConvolutionXMax and ConvolutionSMax can not be instantiated simultaneously.</p> <p>If ConvolutionXMax and ConvolutionSMax is not signed by the user, it is used the ProfileXMax to calculate the convolution space of the profile</p>
Default value	-

6.2.15 ConvolutionType

Declarative form	ConvolutionType (enum)[FFT, Numerical]
-------------------------	--

Type	Property
Parent(s)/Owner(s)	Profile 64
References	
Short description	Set the type of convolution that is performed for the profile function
Data type	Enumerator
Internal variables dependences	-
Specific information	Numerical convolution can only be applied for profiles that has this possibility, the FPA functions. All profile functions can be convoluted by FFT approach.
Default value	Each profile has a default value

6.2.16 ConvolutionXMax

Declarative form	ConvolutionXMax (decimal)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	The maximum distance from the peak center (in units of the x-axis) at which the profile in diffraction space is calculated for use in convolution.
Data type	Decimal
Internal variables dependences	
Specific information	ConvolutionXMax and ConvolutionSMax can not be instantiated simultaneously. If neither ConvolutionXMax nor ConvolutionSMax is specified by the user, ProfileXMax will be utilized to calculate the convolution space of the profile
Default value	-

6.2.17 CosineFourier

Declarative form	CosineFourier (decimal)coefficient _[1..n]
-------------------------	--

Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117 Data 80 DataSimulation 81
References	
Short description	A cosine Fourier series
Object classification	Background Function 64
Parameters	Coefficients of each term in the cosine Fourier series
Internal variables dependences for parameters	
Properties	-
Children	-
Specific information	Multiple background objects can be used simultaneously

6.2.18 CutOff

Declarative form	CutOff (decimal)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	The relative intensity used as a threshold for profile calculation
Data type	Decimal
Internal variables dependences	
Specific information	In Sindarin, profile calculation is restricted by two main terms: the CutOff and the ProfileXMax, whichever is reached first
Default value	0.001

6.2.19 Cycles

Declarative form	Cycles (int)
Type	Property

<i>Parent(s)/Owner(s)</i>	Calculation 73
<i>References</i>	
<i>Short description</i>	The number of steps of optimization routine will be performed for walk command
<i>Data type</i>	Integer
<i>Internal variables dependences</i>	-
<i>Specific information</i>	The number of steps of the others optimization command is not modified
<i>Default value</i>	3

6.2.20 Data

<i>Declarative form</i>	<pre>Data (string)file_[1..n] Data (string)label (string)file_[1..n]</pre>
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Root
<i>References</i>	
<i>Short description</i>	The Data object serves as the primary entity for proposed calculations in general terms. Unlike the Experimental object, Data object can only have function objects (background objects). The main responsibility of the Data object includes importing experimental data from files outlined in the parameters
<i>Object classification</i>	Experimental data 63
<i>Parameters</i>	The label is an optional string data utilized to identify the experimental data and calculations. Following this, the file name of the experimental data, which is to be imported for calculation, is provided as a string data
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	WeightPoint
<i>Children</i>	Background Function 64 ExcludeRegion 88
<i>Specific information</i>	

6.2.21 DataSimulation

<i>Declarative form</i>	DataSimulation
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Root
<i>References</i>	
<i>Short description</i>	Although the DataSimulation object bears resemblance to the Data object, its functionality diverges; it does not import data from files but instead exports computed data to files

<i>Object classification</i>	Experimental data 63
<i>Parameters</i>	-
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	-
<i>Children</i>	Background Function 64 Interval 96
<i>Specific information</i>	Simulation and DataSimultaion objects can not have any refinable variable. Relevant data file information is contained within the Interval object.

6.2.22 DebyeLike

<i>Declarative form</i>	DebyeLike (decimal)length (decimal)w
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117
<i>References</i>	
<i>Short description</i>	A function based in Debye equation to x ray diffraction of two scatters.
<i>Object classification</i>	Background Function 64
<i>Parameters</i>	The distance between the scatters (length) and an arbitrary weight of the function to contribute to the background (w).
<i>Internal variables dependences for parameters</i>	

Properties	-
Children	-
Specific information	This function necessitates the inclusion of a radiation object. Multiple background objects can be used simultaneously

The equation is:

$$Y_i = w \frac{\sin \left[4\pi \frac{\sin(x_i)}{\lambda} \text{length} \right]}{4\pi \frac{\sin(x_i)}{\lambda}}$$

6.2.23 Defocusing

Declarative form	Defocusing (decimal)delr
Type	Object
Parent(s)/Owner(s)	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	Correction profile for defocus aberration, which arises when the receiving slit is not positioned within the focusing circle.
Object classification	Profile 64
Parameters	The decimal parameter delr represents the divergent equatorial angle (α), in degrees, multiplied by the ratio of the distance of the receiving slit to the goniometer circle (ΔR) to the radius of the diffractometer (R).
Internal variables dependences for parameters	
Properties	ConvolutionType 77
Children	-
Specific information	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.24 DerivationBothSide

Declarative form	DerivationBothSide (bool)
Type	Property
Parent(s)/Owner(s)	Calculation 73
References	
Short description	This property enables the use of double-sided calculation (plus and minus a delta) in the numerical calculation of the derivative of the diffractogram calculated with respect to a variable. While this increases the computation time, it significantly enhances the accuracy of the calculation. Therefore, it is highly recommended to keep this property set to true.
Data type	Boolean
Internal variables	
dependences	
Specific information	
Default value	true

6.2.25 Direction

Declarative form	Direction (arrayInt[3])
Type	Property
Parent(s)/Owner(s)	VoigtianSize 126 VoigtianStrain 128
References	
Short description	The index of the main crystallographic direction of an anisotropic function.
Data type	Array of Integer
Internal variables	
dependences	
Specific information	
Default value	-

6.2.26 Dislocation

Declarative form	Dislocation (decimal)rho (decimal)re (decimal)burgers (decimal)disla (decimal)dislb Dislocation (decimal)rho (decimal)re (decimal)burgers (decimal)dislaedge (decimal)dislbedge (decimal)dislascrew (decimal)dislbedgscrew (decimal)fractedge
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Scardi & Leoni, 2002)
Short description	Peak Profile Function for Modeling Dislocation Defects This model employs Wilkens' function to describe the peak profile associated with dislocation-induced broadening and Wilson and Ungár approach to account for anisotropy through the contrast factor.
Object classification	Profile 64
Parameters	Dislocation density (rho): expressed in \AA^{-2} Cutoff radius of the strain field (re): expressed in \AA Modulus of the Burgers vector (burgers): expressed in \AA Contrast factor parameters (disla, dislb, dislaedge, dislbedge, dislascrew, dislbscrew): a set of coefficients to describe the contrast factor Dislocation edge fraction (fractedge): fraction of the edge component of dislocations; a value of 1 represents a purely edge character, whereas 0 represents a purely screw character.
Properties	-
Children	-
Specific information	This implementation can be used only for cubic lattice.

6.2.27 DislocationPopa

Declarative form	DislocationPopa (decimal)rho (decimal)re (decimal)burgers (decimal)es _[2..15]
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89

	Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Leoni et al., 2010; Popa, 1998)
Short description	Peak Profile Function for Modeling Dislocation Defects This model employs Wilkens' function to describe the peak profile associated with dislocation-induced broadening and Popa's approach to account for anisotropy through the contrast factor.
Object classification	Profile 64
Parameters	Dislocation density (rho): expressed in \AA^{-2} Cutoff radius of the strain field (re): expressed in \AA Modulus of the Burgers vector (burgers): expressed in \AA Contrast factor parameters (es): a set of coefficients determined by the Laue symmetry of the crystal
Properties	-
Children	-
Specific information	This implementation is available for all Laue symmetries and the amount parameters <i>es</i> depend on Laue symmetry

6.2.28 Displacement

Declarative form	Displacement (decimal)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	Displacement of the sample from the diffractometer circle center. It is used to peak position correction. The decimal value is the displacement of sample divided by diffractometer radius.
Data type	Decimal
Internal variables dependences	
Specific information	
Default value	0

6.2.29 DistributionType

Declarative form	DistributionType (enum)[Lognormal, Gamma]
Type	Property
Parent(s)/Owner(s)	SizeDistribution 117
References	
Short description	Set the distribution function for the microstructure.
Data type	Enumerator
Internal variables dependences	
Specific information	
Default value	Lognormal

6.2.30 Ellipsoidal

Declarative form	Ellipsoidal (arrayInt[3])uvw (decimal)tau (decimal)k
Type	Object
Parent(s)/Owner(s)	Phase 106
References	(Pecharsky & Zavalij, 2009)
Short description	A ellipsoidal function to correct preferred orientation of the sample
Object classification	Diffraction 63
Parameters	The uvw parameter denotes the crystallographic direction associated with the preferred orientation. The Tau parameter represents the factor within the function that delineates the correlation between the correction in the principal direction and the perpendicular direction. The k parameter serves as a weighting factor employed when multiple preferred orientation functions are utilized.
Properties	-
Children	-
Specific information	Take careful to use this function, especially in quantitative phase analyses (QPA). Use MarchDollase object for QPA. Multiple preferred orientation objects can be used simultaneously.

The ellipsoidal function:

$$T_{hkl} = \frac{1}{N} \sum_{i=1}^N [1 + (\tau^2 - 1) \cos^2(\phi_{hkl}^i)]^{-\frac{1}{2}}$$

Where N is the total number of equivalent reflections, τ is the ratio between the length (or scaling factor) along the principal axis of the ellipsoid and the length along the perpendicular direction ($\tau = \frac{T_{\parallel}}{T_{\perp}}$) and ϕ_{hkl}^i is the angle between the principal axis of the ellipsoid and the direction of the i-th reflection of the equivalent reflection.

6.2.31 EnableIntensity

Declarative form

EnableIntensity (bool)

Type

Property

Parent(s)/Owner(s)

Capillary 74

References

Short description

Enable absorption intensity correction of reflections for capillary specimens

Data type

Boolean

**Internal variables
dependences**

Specific information

Default value

true

6.2.32 EnableShift

Declarative form

EnableShift (bool)

Type

Property

Parent(s)/Owner(s)

Capillary 74

References

Short description

Enable shift correction of reflections due to the absorption for capillary specimens

Data type

Boolean

<i>Internal variables dependences</i>	
<i>Specific information</i>	
<i>Default value</i>	true

6.2.33 EquatorialDivergence

<i>Declarative form</i>	EquatorialDivergence (decimal)alphaeqdiv
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	(Cheary & Coelho, 1992)
<i>Short description</i>	Profile function to correct the effect of equatorial divergence of flat specimens.
<i>Object classification</i>	Profile 64
<i>Parameters</i>	The alphaeqdiv parameter represents the equatorial angle divergence of the primary beam in degrees.
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	ConvolutionType (page 77)
<i>Children</i>	
<i>Specific information</i>	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.34 ExcludeRegion

<i>Declarative form</i>	ExcludeRegion (arrayDecimal[2])range _[1..n]
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117 Data 80 DataSimulation 81

References	
Short description	Exclude experimental points in specific regions of the experimental data
Object classification	Experimental data 63
Parameters	The parameters (range) are decimal arrays of length 2, where the two numbers in the array define the limits on the x-axis within which the experimental points are excluded.
Internal variables dependences for parameters	
Properties	
Children	
Specific information	

6.2.35 Experimental

Declarative form	<code>Experimental (string)file_[1..n]</code> <code>Experimental (string)label (string)file_[1..n]</code>
Type	Object
Parent(s)/Owner(s)	Root
References	
Short description	For diffraction computations, the pivotal entity is the Experimental object. It encapsulates all ancillary data and objects utilized in the theoretical model to calculate the diffractogram. This object's chief role encompasses the importation of experimental data from files outlined in the parameters
Object classification	Experimental data 63
Parameters	The label is an optional string data utilized to identify the experimental data and calculations. Following this, the file name of the experimental data, which is to be imported for calculation, is provided as a string data
Internal variables dependences for parameters	-
Properties	AbsorptionFunction 69 UseAnomalousScattering 124 ConvolutionSMax 77 ConvolutionXMax 78 CutOff 79 Displacement 85

	FFTResolution 91 IncidentAngle 95 MonochromatorTwoTheta 105 Polarization 106 ProfileXMax 109 SpecimenThickness 119 UseAnomalousScattering 124 VariableSlit 124 WeightPoint 130 Zero 131
<i>Children</i>	Background Function 64 Capillary 74 ExcludeRegion 88 Phase 106 Profile 64 Radiation 111 ScatteringFactor 114
<i>Specific information</i>	

6.2.36 Exponential

<i>Declarative form</i>	Exponential (decimal)wexp Exponential (decimal)wexp (decimal)cutexp
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	(Cheary & Coelho, 1992)
<i>Short description</i>	The exponential profile function
<i>Object classification</i>	Profile 64
<i>Parameters</i>	Falta escrever
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	ConvolutionType 77
<i>Children</i>	
<i>Specific information</i>	The Exponential is the base function of the Transparency profile function

6.2.37 Fault

Declarative form	Fault (decimal)alpha (decimal)beta
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Scardi & Leoni, 2002)
Short description	This model describes the stacking and twin fault as peak profile.
Object classification	Profile 64
Parameters	alpha: stacking fault probability. beta: twin fault probability.
Properties	-
Children	-
Specific information	This model is only applicable to FCC structures.

6.2.38 FFTResolution

Declarative form	FFTResolution (int)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	This property pertains to the relative point density used in calculating profiles for convolution via the Fast Fourier Transform approach, in relation to experimental data point density. If this property is set to 1, the point density matches the experimental data. If set to 2, the point density is double that of the experimental data.
Data type	Integer
Internal variables dependences	

Specific information
Default value

4

6.2.39 Function

Declarative form

Function (decimal)func

Type

Object

Parent(s)/Owner(s)

Experimental 89
Simulation 117
Data 80
DataSimulation 81

References

Short description

A user-defined function for background description.

Object classification

Background Function 64

Parameters

Func is a decimal parameter used to define the function and can use the expression capabilities of decimal data such as operators, functions, internal variables and internal constants.

Internal variables dependences for parameters

Properties

Children

Specific information

Multiple background objects can be used simultaneously

6.2.40 FunctionArctangent

Declarative form

FunctionArctangent (decimal)x0 (decimal)imax
(decimal)w
FunctionArctangent (decimal)x0 (decimal)imax
(decimal)wl (decimal)wr

Type

Object

Parent(s)/Owner(s)

Experimental 89
Simulation 117
Data 80
DataSimulation 81

References

Short description	A arctangent function for background modeling. It is particularly useful for describing step-like features in the background.
Object classification	Background Function 64
Parameters	x0: position of the inflection point or maximum slope (center of the transition). imax: maximum intensity. w: transition width, which defines how smooth or abrupt the step is. wl: transition width parameter for the left-hand branch of an asymmetric function. wr: transition width parameter for the right-hand branch of an asymmetric function.
Internal variables	
dependences for parameters	
Properties	
Children	
Specific information	Multiple background objects can be used simultaneously

Arctangent function:

$$y = I_{max} \left[\frac{1}{2} + \frac{1}{\pi} \arctan \left(\frac{x - x_0}{w} \right) \right]$$

6.2.41 FunctionPsVoigt

Declarative form	<pre>FunctionPsVoigt (decimal)x0 (decimal)int (decimal)fwhm (decimal)eta FunctionPsVoigt (decimal)x0 (decimal)int (decimal)fwhm (decimal)eta (decimal)mu</pre>
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117 Data 80 DataSimulation 81
References	
Short description	The psVoigt function can be utilized without a Peak object, such as ReflectionHKL, ReflectionXI, or PeakXI. This function is computed across the entire x-space.

Object classification	Background Function 64
Parameters	x0: the position of the maximum of the function int: the intensity, proportional to the area fwhm: the full width at half maximum eta: the linear combination parameter of Lorentz and Gauss functions mu: the asymmetry of the function. See Split (page 120) for more information about mu.
Internal variables	
dependences for parameters	
Properties	
Children	
Specific information	Multiple background objects can be used simultaneously

6.2.42 Gauss

Declarative form	Gauss (decimal)fwhm Gauss (decimal)gu (decimal)gv (decimal)gw (decimal)gz
Type	Object
Parent(s)/Owner(s)	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	
Short description	The Gaussian function for profile peak

Object classification	Profile 64
Parameters	fwhm: the full width at half maximum gu, gv, gw and gz: the Caglioti parameters to angular dependency of fwhm (See The pseudo-Voigt function, page 40)
Internal variables	
dependences for parameters	
Properties	ConvolutionType 77
Children	Split 120
Specific information	

6.2.43 GaussWavelength

Declarative form	GaussWavelength (decimal)lambda (decimal)fwhmLambda
Type	Object
Parent(s)/Owner(s)	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	
Short description	The Gaussian function in terms of wavelength of the radiation
Object classification	Profile 64
Parameters	lambda: The wavelength of the radiation in Å unit. fwhmLambda: the full width at half maximum in Å unit.
Internal variables dependences for parameters	
Properties	ConvolutionType 77
Children	Split 120
Specific information	For more information on profiles in terms of wavelength, see the Radiation modeling chapter, page 45

6.2.44 IncidentAngle

Declarative form	IncidentAngle (decimal)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	Defines the angle of the incident beam in an asymmetric diffractometer geometry.

<i>Data type</i>	Decimal
<i>Internal variables dependences</i>	
<i>Specific information</i>	IncidentAngle can not be simultaneously declared with the Capillary object
<i>Default value</i>	-

6.2.45 Interpolation

<i>Declarative form</i>	<code>Interpolation (arrayDecimal[1,2])points_[2..n]</code>
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117 Data 80 DataSimulation 81
<i>References</i>	
<i>Short description</i>	Describe the background in terms of interpolation of points.
<i>Object classification</i>	Background Function 64
<i>Parameters</i>	points: arrays of one or two elements that describe points in the chart. When the array contains only one decimal data, it represents the x-coordinate, and the y-coordinate is obtained from experimental data. When the array contains two decimal data, they represent the x and y coordinates, respectively.
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	
<i>Children</i>	
<i>Specific information</i>	Multiple background objects can be used simultaneously. The Interpolation must have at least two parameters.

6.2.46 Interval

<i>Declarative form</i>	<code>Interval (decimal)xi (decimal)xf (decimal)step Interval (decimal)xi (decimal)xf (decimal)step (string)filename</code>
-------------------------	---

	Interval (decimal)xi (decimal)xf (decimal)step (string)fileName (decimal)noise
Type	Object
Parent(s)/Owner(s)	Data 80 DataSimulation 81
References	
Short description	Describes the information for simulated data to be written to a file.
Object classification	Experimental data
Parameters	xi: the initial x-coordinate of the data xf: the final x-coordinate of the data step: the difference between two consecutive points in x-coordinate filename: the name of the file where the simulated data is written. noise: to include noise in simulated data. Its value is the standard deviation of the Gaussian distribution.
Internal variables dependences for parameters	
Properties	
Children	
Specific information	More the one Interval object can be declared

6.2.47 Inverse

Declarative form	Inverse (decimal)coeff
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117 Data 80 DataSimulation 81
References	
Short description	An inverse function, proportional to 1/x, to describe the background.
Object classification	Background Function 64
Parameters	coeff: A multiplier of the function
Internal variables dependences for parameters	
Properties	

Children	
Specific information	Multiple background objects can be used simultaneously

The inverse function:

$$\text{inverse}(x) = \text{coeff} \frac{1}{x}$$

6.2.48 InverseProfile

Declarative form	InverseProfile (decimal)cutInv
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	The inverse profile function
Object classification	Profile 64
Parameters	cutInv: is the limit on x-coordinate to calculate the function
Properties	
Children	
Specific information	The Inverse is the base function of the EquatorialDivergence profile function.

6.2.49 KSphere

Declarative form	KSphere (decimal)
Type	Property
Parent(s)/Owner(s)	VoigtianSize 126
References	
Short description	The Scherrer constant to calculate the size with Sphere shape.

<i>Data type</i>	Decimal
<i>Internal variables dependences</i>	
<i>Specific information</i>	
<i>Default value</i>	4/3

6.2.50 LogDistribution

<i>Declarative form</i>	LogDistribution (decimal)mu (decimal)sigma
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117 Data 80 DataSimulation 81
<i>References</i>	
<i>Short description</i>	The lognormal distribution function.
<i>Object classification</i>	Background Function 64
<i>Parameters</i>	mu: the mean of the Distribution sigma: the standard deviation of the Distribution
<i>Internal variables dependences for parameters</i>	
<i>Properties</i>	
<i>Children</i>	
<i>Specific information</i>	Multiple background objects can be used simultaneously

6.2.51 Logistic

<i>Declarative form</i>	Logistic (decimal)x0 (decimal)inten (decimal)w Logistic (decimal)x0 (decimal)inten (decimal)wl (decimal)wr
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117 Data 80 DataSimulation 81
<i>References</i>	
<i>Short description</i>	A logistic function for background modeling. It is particularly useful for describing step-like features in the background.

Object classification	Background Function 64
Parameters	<p>x0: position of the inflection point or maximum slope (center of the transition).</p> <p>imax: maximum intensity.</p> <p>w: transition width, which defines how smooth or abrupt the step is.</p> <p>wl: transition width parameter for the left-hand branch of an asymmetric function.</p> <p>wr: transition width parameter for the right-hand branch of an asymmetric function.</p>
Internal variables	
dependences for parameters	
Properties	
Children	
Specific information	Multiple background objects can be used simultaneously

Logistic function:

$$y = I_{max} \left[\frac{1}{1 + e^{-\frac{x-x_0}{w}}} \right]$$

6.2.52 Lorentz

Declarative form	<p>Lorentz (decimal)fwhm</p> <p>Lorentz (decimal)lx (decimal)ly</p>
Type	Object
Parent(s)/Owner(s)	<p>Radiation111</p> <p>Experimental 89</p> <p>Simulation 117</p> <p>Phase 106</p> <p>ReflectionXI 113</p> <p>ReflectionHKL 113</p> <p>PeakXI 105</p>
References	
Short description	The Lorentzian function for profile peak
Object classification	Profile 64
Parameters	<p>fwhm: the full width at half maximum</p> <p>lx and ly: the parameters to angular dependency of fwhm (See The pseudo-Voigt function, page 40)</p>

<i>Properties</i>	ConvolutionType 77
<i>Children</i>	Split 120
<i>Specific information</i>	

6.2.53 LorentzWavelength

<i>Declarative form</i>	LorentzWavelength (decimal)lambda (decimal)fwhmLamb
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	
<i>Short description</i>	The Lorentzian function in terms of wavelength of the radiation.
<i>Object classification</i>	Profile 64
<i>Parameters</i>	lambda: The wavelength of the radiation in Å unit. fwhmLambda: the full width at half maximum in Å unit.
<i>Properties</i>	ConvolutionType 77
<i>Children</i>	Split 120
<i>Specific information</i>	For more information on profiles in terms of wavelength, see the Radiation modeling chapter, page 45

6.2.54 ManageHighCorrelation

<i>Declarative form</i>	ManageHighCorrelation (bool)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Calculation 73
<i>References</i>	
<i>Short description</i>	Enable the automatic management of variables with high correlation.
<i>Data type</i>	Bool
<i>Internal variables dependences</i>	

<i>Specific information</i>	
<i>Default value</i>	true

6.2.55 MarchDollase

<i>Declarative form</i>	MarchDollase (arrayInt[3])uvw (decimal)tau (decimal)k
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Phase 106
<i>References</i>	(Dollase, 1986)
<i>Short description</i>	March-Dollase function to correct preferred orientation of the sample
<i>Object classification</i>	Diffraction 63
<i>Parameters</i>	The uvw parameter denotes the crystallographic direction associated with the preferred orientation. The Tau parameter represents the factor within the function that delineates the correlation between the correction in the principal direction and the perpendicular direction. The k parameter serves as a weighting factor employed when multiple preferred orientation functions are utilized.
<i>Properties</i>	-
<i>Children</i>	-
<i>Specific information</i>	Multiple preferred orientation objects can be used simultaneously

6.2.56 MeanStandardDeviation

<i>Declarative form</i>	MeanStandardDeviation (bool)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	SizeDistribution 117
<i>References</i>	
<i>Short description</i>	When this property is enabled, the two parameters of the SizeDistribution object directly represent the mean and the standard deviation of the distribution. When it is disabled, they correspond to the parameters used directly in the distribution equation. See the equations below for more details.
<i>Data type</i>	bool
<i>Internal variables dependences</i>	-

Specific information**Default value**

true

In the disabled case, the mean and standard deviation of the distribution can be calculated as follows:

For Lognormal distribution:

$$mean = e^{\mu + \frac{\sigma^2}{2}}$$

$$sd = \sqrt{e^{2\mu + \sigma^2}(e^{\sigma^2} - 1)}$$

For Gamma distribution:

$$mean = \mu$$

$$sd = \frac{\mu}{\sigma}$$

6.2.57 MicrostrainPAH**Declarative form**

MicrostrainPAH (decimal)alpha (decimal)beta
(decimal)es_[2..15]

Type

Object

Parent(s)/Owner(s)

Radiation 111
Experimental 89
Simulation 117
Phase 106
ReflectionXI 113
ReflectionHKL 113
PeakXI 105

References

(Adler & Houska, 1979; Popa, 1998; Scardi et al., 2018)

Short description

This model describes microstrain as a strain field that varies throughout the crystal volume. The peak broadening is characterized by two adjustable parameters associated with the Lorentzian (alpha) and Gaussian (beta) components of the strain broadening profile. The Popa's approach is employed to account for anisotropy through the contrast factor.

Object classification

Profile 64

Parameters

Lorentzian component (alpha): parameter describing the Lorentzian contribution to strain broadening.
Gaussian component (beta): parameter describing the Gaussian contribution to strain broadening.

Properties	Contrast factor parameters (es): a set of coefficients determined by the Laue symmetry of the crystal
Children	-
Specific information	This implementation is available for all Laue symmetries and the amount parameters <i>es</i> depend on Laue symmetry The microstrain is modeled as a strain field that decays within the crystal. For a detailed explanation of this behavior and its theoretical background, consult the cited references.

6.2.58 MicrostrainWUAH

Declarative form	MicrostrainWUAH (decimal)alpha (decimal)beta (decimal)e1 (decimal)e2
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Adler & Houska, 1979; Scardi et al., 2015)
Short description	This model describes microstrain as a strain field that varies throughout the crystal volume. The peak broadening is characterized by two adjustable parameters associated with the Lorentzian (alpha) and Gaussian (beta) components of the strain broadening profile. The Wilson and Ungár approach is employed to account for anisotropy through the contrast factor.
Object classification	Profile 64
Parameters	Lorentzian component (alpha): parameter describing the Lorentzian contribution to strain broadening. Gaussian component (beta): parameter describing the Gaussian contribution to strain broadening. Contrast factor parameters (e1, e2): a set of coefficients to describe the contrast factor
Properties	-
Children	-
Specific information	This implementation can be used only for cubic lattice. The microstrain is modeled as a strain field that decays within the crystal. For a detailed explanation of this behavior and its theoretical background, consult the cited references.

6.2.59 MonochromatorTwoTheta

<i>Declarative form</i>	MonochromatorTwoTheta (decimal)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117
<i>References</i>	
<i>Short description</i>	The angle of the crystal monochromator corresponds to a specific parameter utilized in the calculation of peak intensity
<i>Data type</i>	Decimal
<i>Internal variables dependences</i>	
<i>Specific information</i>	Automatically enable the Lorentz correction
<i>Default value</i>	-

6.2.60 Multiplicity

<i>Declarative form</i>	Multiplicity (int)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	ReflectionHKL 113
<i>References</i>	
<i>Short description</i>	Manually define the multiplicity of a reflection.
<i>Data type</i>	Integer
<i>Internal variables dependences</i>	
<i>Specific information</i>	If the space group of the cell is specified, the multiplicity of the reflection is automatically calculated. However, this property allows the user to manually define the multiplicity.
<i>Default value</i>	-

6.2.61 PeakXI

<i>Declarative form</i>	PeakXI (decimal)x0 (decimal)inten
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Phase 106

References	
Short description	Represents a diffraction peak in the diffractogram.
Object classification	Diffraction 63
Parameters	x0: the position of the peak, measured in units along the horizontal axis of the diffractogram inten: intensity of the peak related to the area.
Properties	
Children	
Specific information	Unlike ReflectionXI, PeakXI ignores all information regarding radiation objects, such as the number of radiation lines, relative intensities, and profiles.

6.2.62 Phase

Declarative form	<p>Phase</p> <p>Phase (string)label</p>
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	Object that represents a phase in the sample
Object classification	Diffraction 63
Parameters	The optional string parameter is a label to identify the phase
Properties	Scale 114
Children	Cell 74 Scale 114 MarchDollase 102 PeakXI 105 POSphericalHarmonic 107 Profile 64 ReflectionXI 113
Specific information	

6.2.63 Polarization

Declarative form	Polarization (decimal)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117

References	
Short description	The degree of polarization of the incident beam is quantified on a scale where a value of 0 indicates no polarization, and a value of 1 denotes complete polarization. It is used in calculation of peak intensity
Data type	Decimal
Internal variables dependences	
Specific information	If Polarization is declared, the Lorentz correction is automatically enabled
Default value	-

6.2.64 Polynomial

Declarative form	<code>Polynomial (decimal)coeff[1..n]</code>
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117 Data 80 DataSimulation 81
References	
Short description	A polynomial function
Object classification	Background Function 64
Parameters	The decimal parameters are the coefficients of the polynomial.
Properties	CenteredInMiddle 75
Children	
Specific information	Multiple background objects can be used simultaneously

6.2.65 POSphericalHarmonic

Declarative form	<code>POSphericalHarmonic (decimal)cs_[1..27]</code>
Type	Object
Parent(s)/Owner(s)	Phase 106
References	(Järvinen, 1993)
Short description	Symmetrized spherical harmonic function used to correct preferred orientation of the sample.
Object classification	Diffraction 63

Parameters	The cs parameters represent the coefficients of each spherical harmonic function for a given order. The number of required parameters depends on the Laue class of the space group declared in the Cell object, as well as on the harmonic order. For cubic systems, the harmonics are defined up to order 8, while for other crystal systems they are defined up to order 6.
Properties	SpecimenAngle 119 Weight 130
Children	-
Specific information	Multiple preferred-orientation objects may be applied simultaneously. The k property acts as a weighting factor when more than one preferred-orientation function is used. The order of spherical harmonic is determined from the number of supplied parameters. If the number of parameters is incorrect, Sindarin returns an error specifying how many parameters are required for the order and Laue class. For precise d The Alpha property depends on the diffraction geometry; see the corresponding dictionary entry for more information.

6.2.66 ProfileFunction

Declarative form	ProfileFunction (decimal)func ProfileFunction (decimal)func (decimal)fwhm
Type	Object
Parent(s)/Owner(s)	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	
Short description	A user-defined function for peak profile
Object classification	Profile 64
Parameters	func: A decimal parameter used to define the function, utilizing the expression capabilities of decimal data, including operators, functions, variables, internal variables, and internal constants. fwhm: The Full Width at Half Maximum, which can be described in terms of a decimal function and referenced in the main function of the profile using the internal variable fwhm
Properties	
Children	Split 120
Specific information	

6.2.67 ProfileFunctionFT

<i>Declarative form</i>	ProfileFunctionFT (decimal)funcreal ProfileFunctionFT (decimal)funcreal (decimal)funcimag
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	
<i>Short description</i>	A user-defined function for peak profile in fourier space.
<i>Object classification</i>	Profile 64
<i>Parameters</i>	funcreal and funcimag: Decimal parameters used to define the functions of real and imaginary parts. It possible to use the expression capabilities of decimal data, including operators, functions, variables, internal variables, and internal constants.
<i>Properties</i>	
<i>Children</i>	
<i>Specific information</i>	

6.2.68 ProfileXMax

<i>Declarative form</i>	ProfileXMax (decimal)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117
<i>References</i>	
<i>Short description</i>	The maximum distance from the peak center used as a threshold value for profile calculation
<i>Data type</i>	Decimal
<i>Internal variables dependences</i>	

<i>Specific information</i>	In Sindarin, profile calculation is restricted by two main terms: the CutOff and the ProfileXMax, whichever is reached first
<i>Default value</i>	4

6.2.69 psVoigt

<i>Declarative form</i>	<pre>psVoigt (decimal)fwhm (decimal)eta psVoigt (decimal)gu (decimal)gv (decimal)gw (decimal)gz (decimal)lx (decimal)ly psVoigt (decimal)psu (decimal)psv (decimal)psw (decimal)psz (decimal)eta0 (decimal)eta1 (decimal)eta2</pre>
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	(Caglioti et al., 1958; Thompson et al., 1987; Wertheim et al., 1974; Young & Desai, 1989)
<i>Short description</i>	The pseudo-Voigt function to profile modeling. It is a linear combination of Gaussian function and Lorentzian function to perform a numeric approximate of Voigt function.

<i>Object classification</i>	Profile 64
<i>Parameters</i>	<p>The decimal parameter fwhm represents the Full Width at Half Maximum, while the decimal parameter eta signifies the linear combination factor of Gaussian and Lorentzian functions.</p> <p>The FWHM can be computed as a function of 2θ. In second Declarative form, according to Thompson et al., 1987 (pseudo-Voigt TCHZ), the first four parameters calculate the FWHM of the Gaussian component, and the following two parameters determine the Lorentzian FWHM.</p> <p>The third declaration utilizes the relationship between the FWHM of the peak (the final FWHM, H_{psV}) and 2θ, as described by Caglioti et al., 1957, and the linear mixing factor η is a quadratic function of 2θ.</p> <p>Further details can be found in The pseudo-Voigt function chapter on page 40.</p>

<i>Properties</i>	ConvolutionType 77
<i>Children</i>	Split 120
<i>Specific information</i>	

6.2.70 psVoigtWavelength

<i>Declarative form</i>	psVoigtWavelength (decimal)lambda (decimal)fwhmLamb (decimal)eta
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	
<i>Short description</i>	The pseudo-Voigt function in terms of wavelength of the radiation

<i>Object classification</i>	Profile 64
<i>Parameters</i>	lambda: The wavelength of the radiation in Å unit. fwhmLambda: the full width at half maximum in Å unit. eta: the linear combination parameter of Lorentzian and Gaussian functions
<i>Properties</i>	ConvolutionType 77
<i>Children</i>	Split 120
<i>Specific information</i>	For more information on profiles in terms of wavelength, see the Radiation modeling chapter, page 45

6.2.71 Radiation

<i>Declarative form</i>	Radiation (decimal)lambda (decimal)intensity
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117
<i>References</i>	
<i>Short description</i>	An X-ray radiation.
<i>Object classification</i>	Diffraction 63

Parameters	The lambda parameter signifies the wavelength of the radiation in decimal form. The intensity parameter quantifies the relative intensity of this spectral line, applicable when multiple radiations are employed.
Properties	
Children	Profile 64
Specific information	Multiples radiation objects can be instantiated per Experimental object

6.2.72 RapidYRecalcule

Declarative form	RapidyRecalcule (bool)
Type	Property
Parent(s)/Owner(s)	Calculation 73
References	[ref]
Short description	Use numerical approximation calculation to estimate the theoretical diffractogram after a full calculation cycle.
Data type	Boolean
Internal variables dependences	
Specific information	This significantly increase the performance but decrease the accuracy, so use this with caution.
Default value	false

6.2.73 ReceivingSlitWidth

Declarative form	ReceivingSlitWidth (decimal)wslitrec
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	Function to correct the effect of the width of the receive slit on diffraction peak profile.

Object classification	Profile 64
Parameters	The wslitrec parameter is width of the receive slit divided by diffractometer radius.
Properties	ConvolutionType (page 77)
Children	
Specific information	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.74 ReflectionHKL

Declarative form	ReflectionHKL (arrayInt[3])hkl (decimal)inten
Type	Object
Parent(s)/Owner(s)	Cell 74
References	
Short description	Represent a reflection in a cell in terms of Miller index

Object classification	Crystallographic 63
Parameters	The hkl parameter is an array consisting of three integers that represent the Miller indices of the reflection. The inten parameter denotes an arbitrary value of the reflection's intensity.
Properties	Multiplicity 105 Shift 115
Children	Profile 64
Specific information	

6.2.75 ReflectionXI

Declarative form	ReflectionXI (decimal)x0 (decimal)inten
Type	Object
Parent(s)/Owner(s)	Phase
References	
Short description	Represent a reflection in a phase in terms of diffraction angle.

Object classification	Diffraction 63
Parameters	The x0 parameter represents the position of the reflection in decimal form, measured in units along the horizontal axis of the diffractogram. The inten parameter indicates an arbitrary value corresponding to the intensity of the reflection related to the area.

Properties	Multiplicity 105
Children	Profile 64
Specific information	<p>The horizontal position of the reflection in the diffractogram is determined in relation to the main radiation line. The peaks from other radiation lines of this reflection are calculated relative to this position.</p> <p>Unlike PeakXI, ReflectionXI uses all information regarding radiation objects, such as the number of radiation lines, relative intensities, and profiles.</p>

6.2.76 Scale

Declarative form	Scale (decimal)
Type	Property
Parent(s)/Owner(s)	Phase 106
References	
Short description	An arbitrary scale factor. Its value multiplies the intensity of all peaks in the phase.
Data type	Decimal
Internal variables	
dependences	
Specific information	
Default value	1

6.2.77 ScatteringFactor

Declarative form	ScatteringFactor (string)atom (decimal)fn1 (decimal)fn2
Type	Object
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	User defined anomalous scattering factor for a specific atom
Object classification	Diffraction 63
Parameters	<p>atom: a string to identify the chemistry element, must be the symbol of the chemical element.</p> <p>fn1 and fn2: atomic scattering factor components (dispersion coefficients).</p>
Properties	
Children	

Specific information

The fn1 and fn2 coefficients are, by default, obtained from the data of (Henke et al., 1993) when not declared by the user.

6.2.78 Shape**Declarative form**

```
Shape (enum)[Sphere, Ellipsoidal, Cylinder, Jarvinen] //for VoigtianSize
```

```
Shape (enum)[Sphere, Ellipsoidal] //for VoigtianStrain
```

```
Shape (enum)[Sphere, Cube, Tetrahedron, Octahedron] //for SizeDistribution
```

Type

Property

Parent(s)/Owner(s)

SizeDistribution 117

VoigtianSize 126

VoigtianStrain 128

References**Short description**

The shape of the crystals or of the spatial distribution of microstrain.

Data type

Enumerator

Internal variables**dependences****Specific information****Default value**

Sphere

6.2.79 Shift**Declarative form**

```
Shift (decimal)
```

Type

Property

Parent(s)/Owner(s)

ReflectionHKL

References**Short description**

An arbitrary shift of the reflection position in x-coordinate units.

Data type

Decimal

Internal variables**dependences****Specific information****Default value**

0

6.2.80 ShiftFT

Declarative form	ShiftFT (decimal)deltax
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Mendenhall et al., 2015)
Short description	A profile function in Fourier space to apply an arbitrary shift of the reflection position.
Object classification	Profile 64
Parameters	deltax: the shift in the position in x-coordinate units.
Properties	
Children	
Specific information	

6.2.81 SHParameters

Declarative form	SHParameters (decimal)cs
Type	Object
Parent(s)/Owner(s)	VoigtianSize 126
References	(Järvinen, 1993; Popa, 1998)
Short description	Used to declarer the coefficients of symmetrized spherical harmonic functions for VoigtianSize profile when Jarvinen is used as Shape property.
Object classification	Profile 64
Parameters	The coefficients of spherical harmonic. For more detail see explanation about the parameters in POSphericalHarmonic (page 107)
Properties	
Children	
Specific information	Use symmetrized spherical harmonics as describe in (Järvinen, 1993) to model anisotropic size (Popa, 1998).

6.2.82 Simulation

<i>Declarative form</i>	Simulation
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Root
<i>References</i>	
<i>Short description</i>	Although the Simulation object bears resemblance to the Experimental object, its functionality diverges; it does not import data from files but instead exports computed data to files
<i>Object classification</i>	Experimental data 63
<i>Parameters</i>	-
<i>Properties</i>	AbsorptionFunction 69 UseAnomalousScattering 124 ConvolutionSMax 77 ConvolutionXMax 78 CutOff 79 Displacement 85 FFTResolution 91 IncidentAngle 95 MonochromatorTwoTheta 105 Polarization 106 ProfileXMax 109 SpecimenThickness 119 UseAnomalousScattering 124 VariableSlit 124 Zero 131
<i>Children</i>	Background Function 64 Capillary 74 Interval 96 Phase 106 Profile 64 Radiation 111 ScatteringFactor 114
<i>Specific information</i>	Simulation and DataSimultaion objects can not have any refinable variable. Relevant data file information is contained within the Interval object.

6.2.83 SizeDistribution

Declarative form	SizeDistribution (decimal)mu (decimal)sigma
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Scardi & Leoni, 2002)
Short description	Peak profile function to model crystal size distribution
Object classification	Profile 64
Parameters	The mean cristal size (mu) in Å unit and the standard deviation of the distribution (sigma) in Å unit.
Properties	Shape 115 DistributionType 86 MeanStandardDeviation 102
Children	-
Specific information	The crystal size is defined as the cube root of the volume of the geometric object.

Lognormal distribution, t is the crystal size space:

$$g(t) = \frac{1}{\sigma(2\pi)^{1/2}t} \exp\left(-\frac{(\ln(t) - \mu)^2}{2\sigma^2}\right)$$

μ and σ are terms related to mean ($\langle t \rangle$) and standard deviation ($sd(t)$) of the distribution:

$$\langle t \rangle = \exp\left(\mu + \frac{1}{2}\sigma^2\right)$$

$$sd(t) = \exp(2\mu + \sigma^2)[\exp(\sigma^2) - 1]$$

and Gamma distribution:

$$g(t) = \frac{\sigma}{\mu\Gamma(\sigma)} \left(\frac{\sigma L}{\mu}\right)^{\sigma-1} \exp\left(-\frac{\sigma L}{\mu}\right)$$

where:

$$\langle t \rangle = \mu$$

$$sd(t) = \frac{\mu}{\sqrt{\sigma}}$$

6.2.84 SpecimenAngle

Declarative form	SpecimenAngle (decimal)
Type	Property
Parent(s)/Owner(s)	POSphericalHarmonic 107
References	(Järvinen, 1993)
Short description	Define the angle between the polar axis and diffraction vector for different diffraction geometries, expressed in degrees.
Data type	decimal
Internal variables dependences	-
Specific information	This angle takes on different values depending on the diffraction geometry, as shown in the table below. Refer to the cited reference for further details.
Default value	0

Diffraction geometry	α
Symmetric reflection	0
Symmetric transmission	90
Debye-Scherrer	90
Conventional neutron diffraction	90
Seeman-Bohlin	$\theta - \gamma$
Asymmetric reflection	$\theta - \gamma$
Asymmetric transmission	$\theta + \gamma$

In the table, θ represents the Bragg angle, and γ denotes the angle between the incident beam and the specimen surface. These expressions can be written using Sindarin text:

Alpha (xPeak/2 - 4)

Where $\theta = \text{xPeak}/2$ and $\gamma = 4$.

6.2.85 SpecimenThickness

Declarative form	SpecimenThickness (decimal)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	

Short description	It is the effective linear absorption coefficient multiplied by specimen thickness. It is used for intensity correction, specifically the absorption term, when the specimen is thin.
Data type	Decimal
Internal variables dependences	
Specific information	SpecimenThickness can not be simultaneously declared with the Capillary object
Default value	-

6.2.86 Split

Declarative form	<pre>Split (decimal)mu Split (decimal)mu (decimal)twoThetaMax Split (decimal)mu0 (decimal)mu1 (decimal)mu2 Split (decimal)mu0 (decimal)mu1 (decimal)mu2 (decimal)twoThetaMax</pre>
Type	Object
Parent(s)/Owner(s)	Voigtian function 64 ProfileFunction 108
References	
Short description	An empirical function used to modify the profile function and describe profile asymmetry
Object classification	Profile 64
Parameters	<p>The Decimal parameter μ (mu) represents the asymmetry factor, which is defined as the relative difference between the Half Width at Half Maximum (HWHM) on the right side and left side of the peak.</p> <p>The three decimal parameters μ_0 (mu0), μ_1 (mu1) and μ_2 (mu2) are used to calculate the asymmetry factor as a function of the peak position. The type of peak position dependence function is determined by the QuadraticLike property. For more information, refer to the description of this property in the dictionary entry.</p> <p>The decimal parameter twoThetaMax is the maximum peak position at which the asymmetry is applied.</p>
Properties	AngularDependency 70
Children	-
Specific information	μ must be between -1 and 1, excluding.

Definition of the asymmetry factor μ :

$$\mu = \frac{HWHM_{right} - HWHM_{left}}{FWHM}$$

Where FWHM é the Full Width at Half Maximum of the peak and $HWHM_{right}$ and $HWHM_{left}$ are the Half Width at Half Maximum of each side of the peak. If $\mu = 0$ the peak is symmetric.

6.2.87 Stabilization

<i>Declarative form</i>	Stabilization (enum)[Marquardt, Damping, None]
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Calculation 73
<i>References</i>	(Marquardt, 1963)
<i>Short description</i>	Definition of Stabilization Routines for Divergent Nonlinear Least Squares (NLLS) Procedures
<i>Data type</i>	Enumerator
<i>Internal variables dependences</i>	-
<i>Specific information</i>	Marquardt: the Marquardt routine is employed to try find new values for the fit variables within the current NLLS cycle. Damping: a successive reduction of the variable delta is performed to try find a new values for the fit variables within the current NLLS cycle.
<i>Default value</i>	None: no stabilization routine is applied. Marquardt

6.2.88 TargetWidth

<i>Declarative form</i>	TargetWidth (decimal)wtar
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	(Cheary & Coelho, 1992)

Short description	Function to correct profile effect from x ray source with a specific width.
Object classification	Profile 64
Parameters	The wtar parameter represents the ratio between the X-ray tube target's projected focal-line width and the diffractometer radius.
Properties	ConvolutionType (page 77)
Children	
Specific information	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.89 Tau

Declarative form	Tau (decimal)
Type	Property
Parent(s)/Owner(s)	VoigtianSize 126 VoigtianStrain 128
References	
Short description	Tau is the ratio defined as the quotient of the value of microstructures in the direction perpendicular to a given reference direction to that in the reference direction itself. A ratio of 1 denotes isotropy within the microstructure. A ratio greater than 1 suggests that the spatial form assumes a disc-like shape, whereas a ratio less than 1 indicates a needle-like spatial characteristic.
Data type	Decimal
Internal variables dependences	
Specific information	
Default value	-

6.2.90 Tilt

Declarative form	Tilt (decimal)delt
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117

	Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	The function to correct profile effect due specimen tilt.
Object classification	Profile 64
Parameters	delt: represents the ratio between the variation in the height of the sample surface and the diffractometer radius.
Properties	ConvolutionType (page 77)
Children	
Specific information	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.91 Transparency

Declarative form	Transparency (decimal)mu Transparency (decimal)mu (decimal)thickness
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Cheary & Coelho, 1992)
Short description	The function to correct profile effect due specimen transparency.
Object classification	Profile 64
Parameters	mu: represents the effective linear absorption coefficient multiplied by the diffractometer radius. thickness: represents the ratio between the thickness of the sample and the diffractometer radius. This parameter is used only if the sample is thin relative to the depth of the X-ray beam
Properties	ConvolutionType (page 77)
Children	
Specific information	For more information, see the Fundamental Parameters Approach (FPA) section, page 39

6.2.92 UseAnomalousScattering

Declarative form	UseAnomalousScattering (bool)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	
Short description	Enable the anomalous atomic scattering to be applied in structure factor calculation

Data type	Boolean
Internal variables dependences	-
Specific information	
Default value	true

6.2.93 VariableSlit

Declarative form	VariableSlit (bool)
Type	Property
Parent(s)/Owner(s)	Experimental 89 Simulation 117
References	(Bowden & Ryan, 1991; Kimmel, 1987)
Short description	When activated, a correction attributable to a variable divergence slit is implemented on the peak intensity. Within the Sindarin, this adjustment is incorporated into the absorption term of Equation 2 (page 36).

Data type	Boolean
Internal variables dependences	
Specific information	
Default value	false

6.2.94 Voigt

Declarative form	<pre>Voigt (decimal)fwhmG (decimal)fwhmL Voigt (decimal)gu (decimal)gv (decimal)gw (decimal)gz (decimal)lx (decimal)ly Voigt (decimal)vu (decimal)vv (decimal)vw (decimal)vz (decimal)eta0 (decimal)eta1 (decimal)eta2</pre>
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	
Short description	The Voigt function as peak profile.
Object classification	Profile 64
Parameters	<p>The decimal parameter fwhmG denotes the Full Width at Half Maximum (FWHM) of the Gaussian function. Similarly, the decimal parameter fwhmL indicates the FWHM of the Lorentzian function.</p> <p>The second declaration uses the first four parameters to calculate the Gaussian FWHM based on the Caglioti angular dependency, and the last two parameters to compute the Lorentzian FWHM. The third declaration uses the first four parameters to calculate the Voigt FWHM based on the Caglioti angular dependency, and the last three parameters are used to compute the η parameter, that is the mixture of Lorentz and Gauss functions. The definition and significance of η are provided below.</p>
Properties	ConvolutionType 77
Children	-
Specific information	

The parameter η is calculated according to the following expression:

$$\eta = \frac{FWHM_L}{FWHM_L + FWHM_G}$$

Where $FWHM_L$ is the full width at half maximum of the Lorentzian component and $FWHM_G$ is that of Gaussian component.

Attention: Despite the limit values of η be pure Lorentzian for $\eta = 1$ and pure Gaussian for $\eta = 0$, the η parameter in the Voigt function differs from that in the pseudo-Voigt function and is not numerically equivalent.

In case of the third declaration, the values of $FWHM_L$ and $FWHM_G$ are calculated using an empirical equation designed to compute the FWHM of the Voigtian function ($FWHM_V$) with a maximum relative error of 0.02% (Olivero & Longbothum, 1977):

$$FWHM_V = \frac{1}{2} \left(C_1 FWHM_L + \sqrt{C_2 FWHM_L^2 + 4C_3 FWHM_G^2} \right)$$

Where $C_1 = 1.0692$, $C_2 = 0.86639$ and $C_3 = 1$.

6.2.95 VoigtianSize

Declarative form	VoigtianSize (decimal)size (decimal)eta VoigtianSize (decimal)size (decimal)eta (decimal)k
Type	Object
Parent(s)/Owner(s)	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
References	(Baizar & Ledbetter, 1994; Balzar et al., 2004; Balzar & Ledbetter, 1993; Langford, 1980; Popa, 1998; Stokes & Wilson, 1942)
Short description	A Voigt-type function (Voigt or pseudo-Voigt) is used, whose angular dependence follows the crystallite size contribution to peak broadening. This model assumes that size-induced broadening may contain both Gaussian and Lorentzian components. The peak breadth employed for microstructural analysis is the integral breadth.
Object classification	Profile 64
Parameters	The size decimal parameter is the volume weighted mean crystal size or volume weighted apparent mean crystal size, depend on Shape property value (see below), in Å unit. The decimal parameters η (eta) is the linear combination factor of Gaussian and Lorentzian functions. The decimal parameter k is used as weight when more the one VoigtianSize is used in the model.
Properties	ConvolutionType 77 Direction 83

Children

Specific information

Shape 115
Tau 122
Width 131
SHPParameters 116
Split 120
The Tau and Width properties are mutually exclusive. KSphere can only be specified when Sphere shape is used.

The size parameter is a measurement that depends on the shape property:

1. Sphere: Refers to the particle diameter, assuming a Scherrer constant $K_\beta = 4/3$ calculated by integral breadth method (Stokes & Wilson, 1942). To apply alternative constant for sphere geometry, specify the property KSphere. For example, when the size is defined as the cubic root of the particle volume, $K_\beta = 1.07466130$.
2. Ellipsoidal: Corresponds to the length of the principal axis of the ellipsoid, in terms of the apparent mean size. The length of the direction perpendicular to principal axis is defined by the Width property.
3. Cylinder: Refers to the length of the principal axis, i.e., the height of the cylinder (Langford & Louër, 1982). The diameter of the cylinder is defined by the Width property. In this model, the size is the true size of the particle, not the apparent size.
4. Jarvinen: Use symmetrized spherical harmonics as describe in (Järvinen, 1993) to model anisotropic size. The size parameter in VoigtianSize is the apparent mean size in relation to all directions, correspond to R_o in (Popa, 1998) and to C_{00} in (Järvinen, 1993). The others spherical harmonic coefficients must be declared in SHParameters object.

For further considerations regarding the Scherrer constant and size distribution, see (Langford & Wilson, 1978).

The integral breadth (β_S) of the Voigt function is computed from the volume weighted mean size specified by the user in Sindarin text using the Scherrer equation (below). An appropriated Scherrer constant is applied. The corresponding Gaussian and Lorentzian widths are then derived from β_S and the mixing parameter η , assuming a linear combination of Gaussian and Lorentzian components, as described by Thompson et al. (1987). For further details, refer to the cited references.

The relationship between apparent mean size (τ), real mean size (T) and the diffraction angle (2θ , x_{peak}) of the reflection is given by:

$$\tau = \frac{1}{\beta_S \cos\left(\frac{x_{peak}}{2}\right)}$$
$$T = K_{Sch} \tau$$

Where K_{Sch} is the Scherrer constant.

Note on anisotropy and equivalent reflections:

An observed reflection in a diffractogram corresponds to a set of equivalent reflections aligned along different crystallographic directions. When using an anisotropic model for microstructure, except in the case of symmetrized spherical harmonics, this can lead to the issue that reflections within the same family may exhibit varying microstructural values due to their directional differences. Typically, the tridimensional object and its spatial orientation are chosen to conserve the symmetry between equivalent reflections in specific lattice system.

6.2.96 VoigtianStrain

<i>Declarative form</i>	VoigtianStrain (decimal)strain (decimal)eta VoigtianStrain (decimal)strain (decimal)eta (decimal)k
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	(Baizar & Ledbetter, 1994; Balzar et al., 2004; Balzar & Ledbetter, 1993; Thompson et al., 1987)
<i>Short description</i>	A Voigtian function (Voigt or pseudo-Voigt) whose angular dependence follows the effect of lattice microstrain for peak width. This model assumes that the effect of microstrain on broadening can have both a Gaussian and a Lorentzian part.
<i>Object classification</i>	Profile 64
<i>Parameters</i>	The strain decimal parameter is the maximum (upper-limit) microstrain (MMS). The decimal parameters η (eta) is the linear combination factor of Gaussian and Lorentzian functions. The decimal parameter k is used as weight when more the one VoigtianStrain is used in the model.
<i>Properties</i>	ConvolutionType 77 Direction 83 Shape 115 Tau 122 Width 131
<i>Children</i>	Split 120
<i>Specific information</i>	The Tau and Width properties are mutually exclusive.

See the note on anisotropy of VoigtianSize.

The relationship between apparent microstrain (AMS, η), maximum (or upper limit) microstrain (MMS, ϵ) and the diffraction angle (2θ , x_{peak}) of the reflection is given by:

$$\eta = \frac{\beta_D}{\tan\left(\frac{x_{peak}}{2}\right)}$$

$$\epsilon = \frac{\eta}{4}$$

Where β_D is the integral breadth associated with.

The mean square microstrain (MSMS, $\langle \epsilon^2 \rangle^{\frac{1}{2}}$) can only be evaluated if the peak profile is purely gaussian (i.e. the pseudo-Voigt mixing parameter $\eta = 0$):

$$\langle \epsilon^2 \rangle^{\frac{1}{2}} = \frac{1}{2\sqrt{2\pi}} \eta$$

The integral breadth (β_D) of the Voigt function is computed from the maximum microstrain (ϵ) specified by the user in Sindarin text. The corresponding Gaussian and Lorentzian widths are then derived from β_D and the mixing parameter η , assuming a linear combination of Gaussian and Lorentzian components, as described by Thompson et al. (1987). For further details, refer to the cited references.

6.2.97 VoigtWavelength

<i>Declarative form</i>	VoigtWavelength (decimal)lambda (decimal)fwhmLamb (decimal)eta
<i>Type</i>	Object
<i>Parent(s)/Owner(s)</i>	Radiation 111 Experimental 89 Simulation 117 Phase 106 ReflectionXI 113 ReflectionHKL 113 PeakXI 105
<i>References</i>	
<i>Short description</i>	The Voigt function in terms of wavelength of the radiation
<i>Object classification</i>	Profile 64
<i>Parameters</i>	lambda: The wavelength of the radiation in Å unit. fwhmLambda: the full width at half maximum in Å unit. eta: the linear mixture parameter of Lorentz and Gauss functions as described in Voigt function (pag. 125)
<i>Properties</i>	ConvolutionType 77

Children	Split 120
Specific information	The eta parameter is calculated according to the equation described in the Voigt entry one page 125. For more information on profiles in terms of wavelength, see the Radiation modeling chapter, page 45.

6.2.98 WeightPoint

Declarative form	WeightPoint (enum)[Unit, InverseY, InverseE, Weight]
Type	Property
Parent(s)/Owner(s)	Experimental 89 Data 80
References	
Short description	Specify the type of weight of each point in optimization routine.
Data type	Integer
Internal variables dependences	-
Specific information	
Default value	Assign by default 'Unit' weighting to the Data object and 'InverseY' weighting to the Experimental object. Should the experimental data error be available, the default setting is 'InverseE' for both objects.

6.2.99 Weight

Declarative form	Weight (decimal)
Type	Property
Parent(s)/Owner(s)	POSphericalHarmonic 107
References	
Short description	The weight of the preferred orientation.
Data type	Decimal
Internal variables dependences	
Specific information	
Default value	1

6.2.100 Width

<i>Declarative form</i>	Width (decimal)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	VoigtianSize 126 VoigtianStrain 128
<i>References</i>	
<i>Short description</i>	The value of the microstructure in the perpendicular direction to the specified direction

<i>Data type</i>	Decimal
<i>Internal variables dependences</i>	
<i>Specific information</i>	
<i>Default value</i>	-

6.2.101 Z

<i>Declarative form</i>	Z (int)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Cell
<i>References</i>	
<i>Short description</i>	The multiplicity of the chemical formula denoted by the total number of atoms contained within the unit cell.

<i>Data type</i>	Integer
<i>Internal variables dependences</i>	
<i>Specific information</i>	This property is not employed in the calculations of the diffractogram but is reserved for the interpretation of results.
<i>Default value</i>	1

6.2.102 Zero

<i>Declarative form</i>	Zero (decimal)
<i>Type</i>	Property
<i>Parent(s)/Owner(s)</i>	Experimental 89 Simulation 117
<i>References</i>	
<i>Short description</i>	Correction of the angular position of the diffractometer arms.
<i>Data type</i>	Decimal
<i>Internal variables dependences</i>	
<i>Specific information</i>	
<i>Default value</i>	0

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