

# The xrfSource Computer Program

version 2.0.0

## Users Guide

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Jan 02, 2020

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## Summary

The purpose of the program is to produce a description of the x-ray spectrum which is sent out from an x-ray tube. The spectrum data produced by the program defines the relative distribution at different wavelengths of the intensity (photons/sec.) sent out from the x-ray tube.

In the current version of the program three well known algorithms for the calculation of x-ray spectrums are implemented:

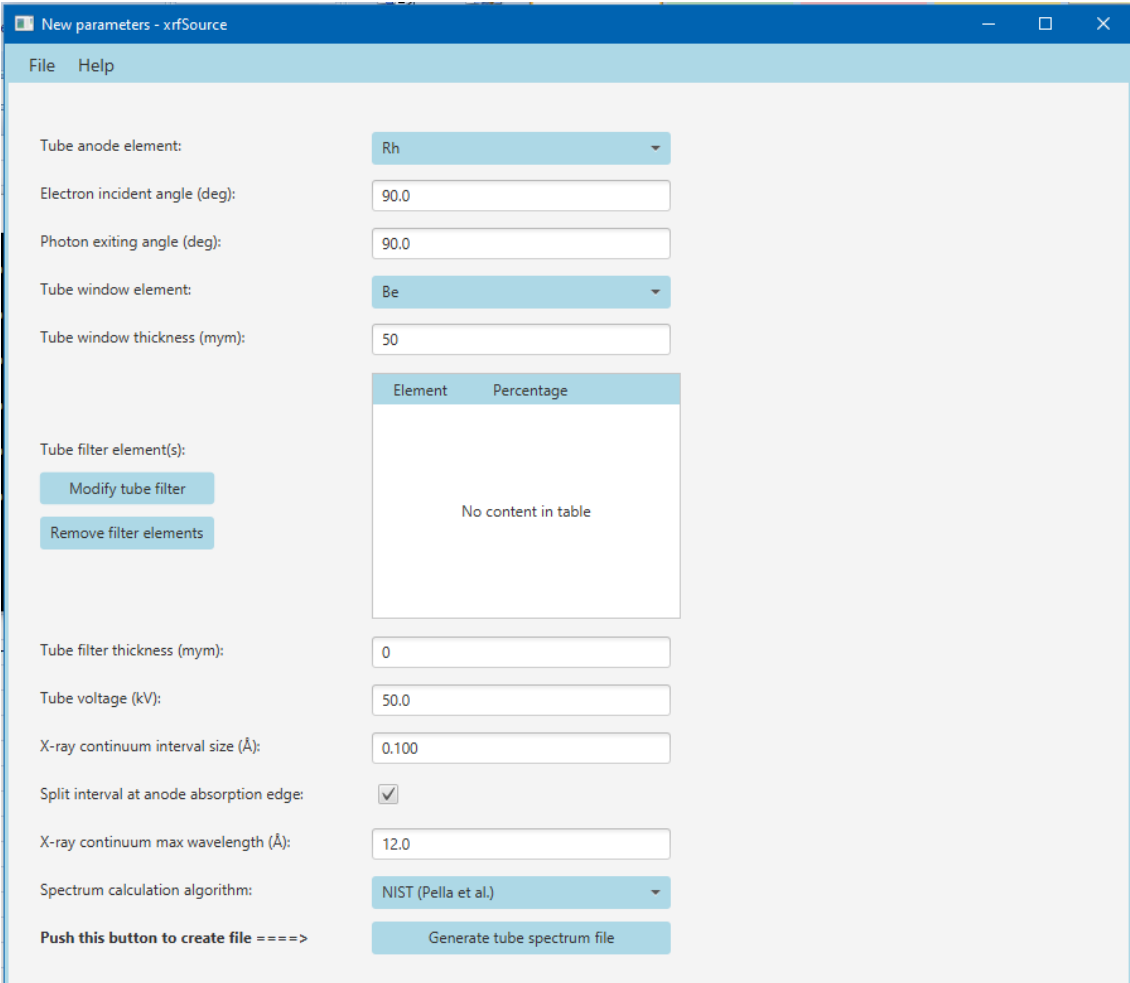
- a) The algorithm published by Pella, Feng and Small
- b) The algorithms published by Horst Ebel
- c) The algorithms published by Finkelshtein and Pavlova

The program is licensed under the open source MIT License. Executables can be downloaded from our website e2t.se for free. Source code can be downloaded from our GitHub repository.

## User Interface and Parameters

The program has a graphical user interface with a main menu with a File and Help alternative. The File submenu has menu alternatives to open or save parameters used for the generation of x-ray spectrums and an alternative to quit the program.

Parameters which control the generation of x-ray spectrums are input via the panel below.



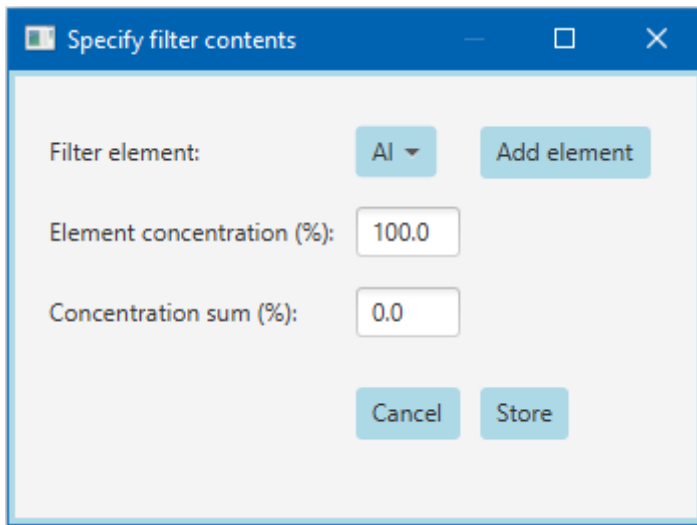
The screenshot shows a software window titled "New parameters - xrfSource" with a menu bar containing "File" and "Help". The main area contains several input fields and a table:

- Tube anode element: Rh (dropdown)
- Electron incident angle (deg): 90.0 (text input)
- Photon exiting angle (deg): 90.0 (text input)
- Tube window element: Be (dropdown)
- Tube window thickness (mym): 50 (text input)
- Tube filter element(s):
  - Buttons: "Modify tube filter" and "Remove filter elements"
  - Table with columns "Element" and "Percentage", containing "No content in table"
- Tube filter thickness (mym): 0 (text input)
- Tube voltage (kV): 50.0 (text input)
- X-ray continuum interval size (Å): 0.100 (text input)
- Split interval at anode absorption edge:
- X-ray continuum max wavelength (Å): 12.0 (text input)
- Spectrum calculation algorithm: NIST (Pella et al.) (dropdown)
- Buttons: "Push this button to create file ==>>>" and "Generate tube spectrum file"

Description of the parameters controlling the generation of an x-ray tube spectrum:

Tube anode element	The anode material of the x-ray tube. Cr, Rh or W can be selected.
Electron incident angle	The angle in degrees relative the anode surface of the incoming electrons. This parameter is used just by the Horst Ebel algorithm.
Photon exiting angle	The angle in degrees relative the anode surface of the photons exiting the x-ray tube. This parameter is 90 degrees for an end widow tube, less than 90 degrees for a side window tube.
Tube window element	The material of the tube window. Currently Be is the only alternative.
Tube window thickness	The thickness in micrometer of the tube window.
Modify tube filter	This button opens a sub window where the composition filter can be specified. The generated spectrum will take to account the attenuation of this filter. The filter may be a pure element or an alloy of Al, Cu, Zn and Pb.
Remove filter elements	This button removes the filter specification.
Tube filter thickness	The thickness in micrometer of the tube filter.
Tube voltage	The x-ray tube anode voltage in kV. This voltage will determine the start wavelength of the continuum. If for example the tube voltage is 50 kV the continuum start wavelength will be the wavelength corresponding to the energy 50 keV.
X-ray continuum interval size	The intensity of the continuum of the x-ray spectrum is normally (see below) done for wavelength intervals of equal size. The program will calculate the intensity per Angstrom of the center wavelength of each interval. This parameter specifies the size of this wavelength interval in Angstrom.
Split interval at anode absorption edges	If this check box is marked the program will start a new continuum interval at the wavelength above an absorption edge and reduce the interval at the wavelength below the absorption edge. This is to avoid that the spectrum discontinuity is inside a continuum interval. If this check box is unmarked all spectrum intervals will have equal size.
X-ray continuum max wavelength	The maximum wavelength of the generated spectrum. This parameter will affect the number of continuum intervals generated. The parameter may also affect the number of tube line intensities generated by the program.
Spectrum calculation algorithm	This parameter selects the algorithm used for the calculation of the x-ray tube spectrum. The selectable algorithms are described in the chapter below.
Generate tube spectrum file	This button starts the generation of the tube spectrum data and generates a data file with the calculated intensities. The program will open a dialog where the user selects the file format and the file name. A data file with the parameters used for the spectrum generation will also be stored together with the spectrum file.

The sub window for filter definition is shown below:



Description of the filter definition sub window parameters:

Filter element	The material of the filter or a component of a filter alloy. Al, Cu, Zn and Pb may be selected.
Element concentration	The weight percentage of the filter element to be added.
Add element	The combination of the filter element material and its percentage is added to the filter definition. This operation is possible if the concentration sum after this addition is below or up to 100 percent
Concentration sum	This field has the current sum of filter element weight percent.
Store	This button stores the filter definition and closes the sub window. This command succeeds if the concentration sum of the filter is 100 percent.
Cancel	This button cancels the filter definition operation and closes the sub window.

## Algorithms implemented

Three different algorithms for the calculation of x-ray tube spectrums have been implemented in the program.

- a) The algorithms developed by P.A. Pella, L. Feng and J.A. Small, here also called the NIST algorithm were published in two papers.
  - 1) An Analytical Algorithm for Calculation of Spectral Distributions of X-Ray Tubes for Quantitative X-Ray Fluorescence Analysis, published in X-Ray Spectrometry, vol. 14, no. 3, pages 125-135.
  - 2) Addition of M- and L-series Lines to NIST Algorithm for Calculation of X-Ray Tube Output Spectral Distributions, published in X-Ray Spectrometry, vol. 20, pages 109-110.

The tube voltage range mentioned in these papers is 10-60 kV. This algorithm does not take the angle of the incoming electrons to account.

- b) The algorithms developed by Horst Ebel were published in two papers.
  - 1) X-ray Tube Spectra, published in X-Ray Spectrometry, vol. 28, pages 255-266.

- 2)  $L_{\nu}$ ,  $L_{\alpha 1,2}$ ,  $L_{\eta}$ ,  $L_{\beta 1,2,3,4,5,6}$ ,  $L_{\gamma 1,2,3}$  spectra of x-ray tubes, published in X-Ray Spectrometry, vol. 32, pages 46-51.

This algorithm has been developed using relatively low tube voltages 5-30 kV. The angle of the incoming electrons relative the anode surface is taken to account here.

- c) The algorithm developed by A.L. Finkelshtein and T.O. Pavlova was published in X-Ray Spectrometry vol. 28, pages 27-32.

The tube voltage used in this work is 40-60 kV. This algorithm does not take the angle of the incoming electrons to account.

## Output Data

The program produces two types of data files, one file with the calculated spectrum data and one file with the parameters used for the calculation.

## X-ray Spectrum Data

The calculated spectrum is specified for a number of wavelength intervals. For each interval there is a center wavelength in Angstrom, an integrated intensity of the interval (photons/sec.), the width of the wavelength interval in Angstrom and the type of interval, a characteristic line of the tube or an interval of the continuum. For the characteristic lines the natural width of the corresponding line is specified as the width.

The produced spectrum which specifies the relative distribution in wavelength of tube intensity has been normalized to get the integrated intensity of the most intense characteristic line is equal to 1.0.

The program can produce two types of spectrum data formats, a comma separated format (csv) and an xml format. Below are examples of the two file types (truncated files)

csv format					xml format				
1	0.557	1.22e-01	2.11e-04	L	1	<code>&lt;?xml version="1.0" encoding="ISO-8859-1" standalone="yes"?&gt;</code>			
2	0.615	4.24e-01	2.52e-04	L	2	<code>&lt;!--This intensity file was created by program xrfSource Thu Jan 02 13:26:21 CET</code>			
3	3.685	1.62e-02	8.55e-03	L	3	<code>&lt;XrfSourceSpectrum</code>			
4	3.943	4.09e-02	2.73e-03	L	4	<code>&lt;TubeLines&gt;</code>			
5	4.131	1.18e-01	2.77e-03	L	5	<code>&lt;TubeLine intensity="1.22e-01" wavelength="0.557" width="2.11e-04"/&gt;</code>			
6	4.252	9.51e-02	9.11e-03	L	6	<code>&lt;TubeLine intensity="4.24e-01" wavelength="0.615" width="2.52e-04"/&gt;</code>			
7	4.288	5.85e-02	9.27e-03	L	7	<code>&lt;TubeLine intensity="1.62e-02" wavelength="3.685" width="8.55e-03"/&gt;</code>			
8	4.375	6.28e-01	4.23e-03	L	8	<code>&lt;TubeLine intensity="4.09e-02" wavelength="3.943" width="2.73e-03"/&gt;</code>			
9	4.597	1.00e+00	3.70e-03	L	9	<code>&lt;TubeLine intensity="1.18e-01" wavelength="4.131" width="2.77e-03"/&gt;</code>			
10	4.605	9.98e-02	4.40e-03	L	10	<code>&lt;TubeLine intensity="9.51e-02" wavelength="4.252" width="9.11e-03"/&gt;</code>			
11	4.922	1.16e-02	1.90e-02	L	11	<code>&lt;TubeLine intensity="5.85e-02" wavelength="4.288" width="9.27e-03"/&gt;</code>			
12	5.216	3.21e-02	2.10e-02	L	12	<code>&lt;TubeLine intensity="6.28e-01" wavelength="4.375" width="4.23e-03"/&gt;</code>			
13	0.298	1.56e-01	1.00e-01	C	13	<code>&lt;TubeLine intensity="1.00e+00" wavelength="4.597" width="3.70e-03"/&gt;</code>			
14	0.398	2.57e-01	1.00e-01	C	14	<code>&lt;TubeLine intensity="9.98e-02" wavelength="4.605" width="4.40e-03"/&gt;</code>			
15	0.491	2.28e-01	8.59e-02	C	15	<code>&lt;TubeLine intensity="1.16e-02" wavelength="4.922" width="1.90e-02"/&gt;</code>			
16	0.584	2.71e-01	1.00e-01	C	16	<code>&lt;TubeLine intensity="3.21e-02" wavelength="5.216" width="2.10e-02"/&gt;</code>			
17	0.684	2.53e-01	1.00e-01	C	17	<code>&lt;/TubeLines&gt;</code>			
18	0.784	2.33e-01	1.00e-01	C	18	<code>&lt;Continuum&gt;</code>			
19	0.884	2.14e-01	1.00e-01	C	19	<code>&lt;ContinuumSlice intensity="1.56e-01" wavelength="0.298" width="1.00e-01"/&gt;</code>			
20	0.984	1.95e-01	1.00e-01	C	20	<code>&lt;ContinuumSlice intensity="2.57e-01" wavelength="0.398" width="1.00e-01"/&gt;</code>			
21	1.084	1.77e-01	1.00e-01	C	21	<code>&lt;ContinuumSlice intensity="2.28e-01" wavelength="0.491" width="8.59e-02"/&gt;</code>			
					22	<code>&lt;ContinuumSlice intensity="2.71e-01" wavelength="0.584" width="1.00e-01"/&gt;</code>			
					23	<code>&lt;ContinuumSlice intensity="2.53e-01" wavelength="0.684" width="1.00e-01"/&gt;</code>			
					24	<code>&lt;ContinuumSlice intensity="2.33e-01" wavelength="0.784" width="1.00e-01"/&gt;</code>			
					25	<code>&lt;ContinuumSlice intensity="2.14e-01" wavelength="0.884" width="1.00e-01"/&gt;</code>			
					26	<code>&lt;ContinuumSlice intensity="1.95e-01" wavelength="0.984" width="1.00e-01"/&gt;</code>			
					27	<code>&lt;ContinuumSlice intensity="1.77e-01" wavelength="1.084" width="1.00e-01"/&gt;</code>			

The program has a plug-in design which allows user specific file formats to be easily added. Users can ask us for a plug-in to produce their specific file format. Contact us via an e-mail to [xrfSource@e2t.se](mailto:xrfSource@e2t.se).

## Parameter File

The program produces an xml file with the parameters used to calculate a tube spectrum. The file is stored in the same directory as the spectrum file and with the same name as the spectrum file except for the extension which is .xml. When the spectrum file produced is an xml file then \_par.xml is added for the parameter file name. This file documents the parameters used for the spectrum generation. The file can also be read into the user interface via an open menu alternative.

Below is an example of a parameter file:

```
1 <?xml version="1.0" encoding="ISO-8859-1" standalone="yes"?>
2 <!--This parameter file was created by program xrfSource Thu Jan 02 13:26:23 CET 2020-->
3 <XraySourceParameters anodeVoltage="50.0" filterThickness="0.0" inAngle="90.0" intervalSize="0.1" maxWavelength="12.0" outAngle="90.0" programVersion="2.0.0" splitAtEdge="true" windowThickness="50.0">
4   <AnodeElement atomicNumber="45" symbol="Rh"/>
5   <WindowElement atomicNumber="4" symbol="Be"/>
6   <FilterElements/>
7   <Algorithm calcModel="NIST" description="NIST (Palla et al.)"/>
8 </XraySourceParameters>
```

## Fundamental parameter references

The program uses various fundamental parameters for the calculations. The sources for the parameters are mostly according to the references in the published papers.

There is an exception for absorption data which is calculated by an incorporated version (in Java) of the Mucal program developed by Pathikrit Bandyopadhyay (initial development in Fortran) and Boyan Boyanov (converted to C). The Mucal calculations are based on data from: W.H. McMaster N.K. Del Grande, J.H. Mallett and J.H. Hubbell, "Compilation of x-ray cross sections", *Lawrence Livermore National Laboratory Report UCRL-50174* (section I 1970, section II 1969, section III 1969 and section IV 1969). Fluorescence yield data from: M. O. Krause, *J. Phys. Chem. Ref. Data*, 8, 307(1979).

The energies of characteristic lines are according to the NIST database X-ray Transition Energies Database.

Characteristic line widths have been calculated using the natural width of the atomic levels as tabulated in the paper "Widths of the atomic K.N7 levels", by J.H. Campbell and T. Papp. published in *Atomic Data and Nuclear Data Tables*, Vol. 77, No. 1. January 2001.

Absorption edge energies are calculated using the Mucal program.

Fluorescent yields are according to a paper, A Review, Bibliography, and Tabulation of K, L, and higher Atomic Shell X-Ray Fluorescence Yields, by J.H. Hubbell, P.N. Trehan, Nirmal Singh, B. Chand, D. Metha, L. Garg, R.R. Garg, Surinder Singh, S. Puri, published in *Journal of Physical and Chemical Reference Data* 23, 339-364 (1994).

Atomic weights are according to the NIST database Atomic Weights and Isotopic Compositions with Relative Atomic Masses. Developers and Contributors of the database: J.S. Coursey, D. J. Schwab, J. J. Tsai, and R. A. Dragoset, NIST Physical Measurement Laboratory.

Transition probabilities are according to Radiative Decay Rates of Vacancies in the K and L Shells, by J.H. Scofield, published in *Phys. Rev.* vol. 179, no. 1, pages 9-16, 1969.

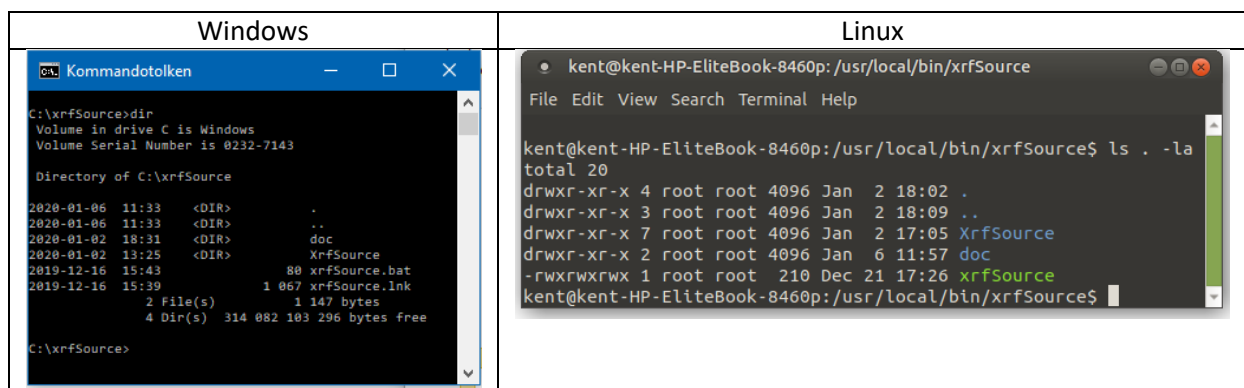
## Program installation

There are two versions of the program, one for Windows systems and one for Linux systems. The program is a self contained Java application which includes the Java runtime environment required for the program. A zip file containing the Windows or Linux version can be downloaded from the web site e2t.se.

To install the Windows version of the program the Zip file is unzipped to the c:\ folder creating a program directory c:\xrfSource.

After the Linux zip file has been downloaded, open a terminal window,  
first: `cd /usr/local/bin`, then: `sudo unzip your-zip-file-folder/xrfSourceLinux.zip`.

After installation the program folder should look like this:



## Program start

The program directory of the Windows versions has a shortcut file xrfSource.lnk which can be copied to the desktop to simplify program start. An alternative is to start a command window and input command `c:\xrfSource\xrfSource`.

The Linux version of the program is started from a terminal window (Ctrl+Alt+T) with the command `/usr/local/bin/xrfSource/xrfSource`.

## Program Source Code

The program source code can be downloaded from the GitHub account kente2t/xrfSource. The downloaded files can be modified but the copyright notice and the license text must be retained in all files.



## The Program License

The copyright notice and the license text (MIT license) is shown below. The executables of the program can be downloaded and copied with no restrictions. If the source files are downloaded and modified then the copyright notice and the license text must be retained.

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