Computational Physics: Modeling and Simulation

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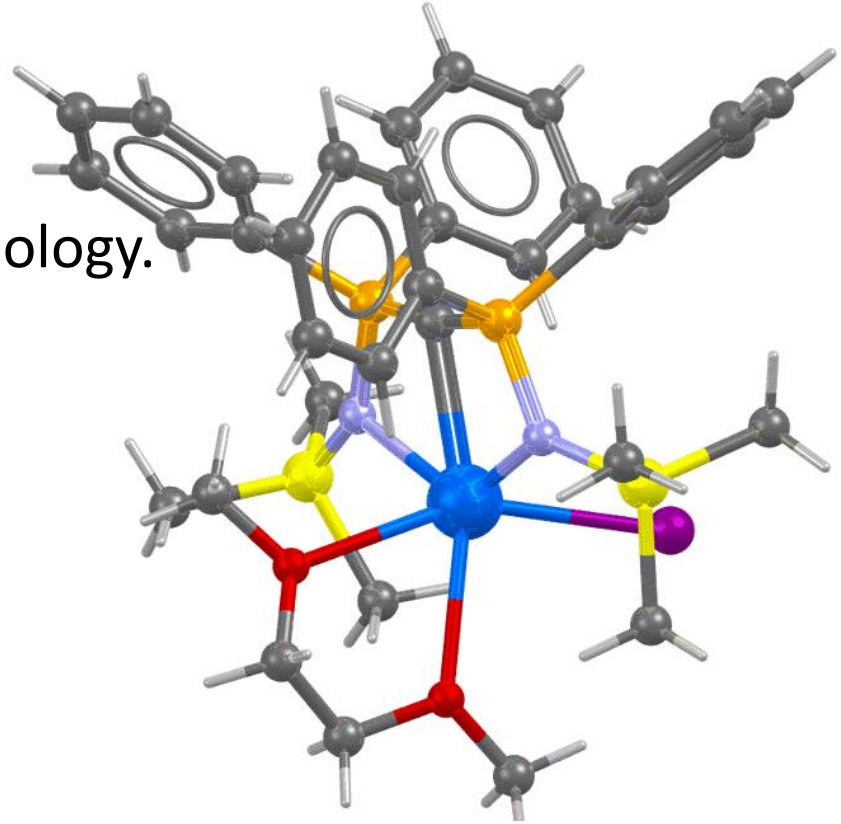
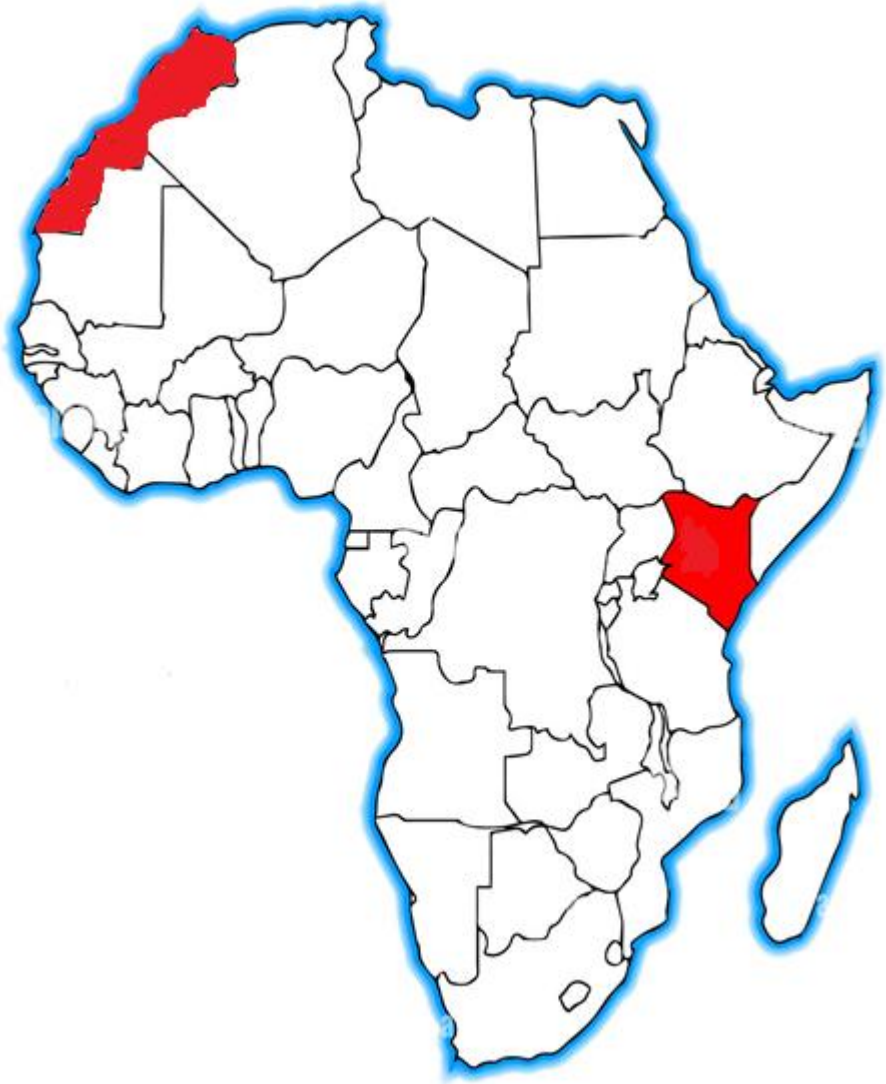
Materials Research Society of Kenya
https://mrsk.or.ke/



The African School of Fundamental Physics and Applications
and Biennial African Conference of Physics




Kenya
Masinde muliro university of science &...
Kisumu
Nakuru
Eldoret
Jinja
Bungoma
Meru
Nanyuki
Kisii
Migori
Thika
Nairobi
Kitui
Athi River
Lake Victoria
A109
A104
A1
A2
A3
Map data ©2021

ABOUT MASINDE MULIRO UNIVERSITY OF SCIENCE & TECHNOLOGY

- MMUST is a public university, located in Kakamega town in Western Kenya, about 400 km North-west Kenya's capital Nairobi and 50 km north of Kisumu city

- In the locality of Kakamega forest- a tropical rain forest unique of indigenous trees, avifauna and several other animals. Also famous of the "crying stones"

Learning outcomes for the session

- **Become familiar with the SCOUT software**.
  - Learn how to simulate optical properties of materials from experimental data using SCOUT software.
  - Learn how to simulate electrical properties of materials from experimental data using SCOUT software.
- **Become familiar with the crystallography software and database**.
  - Be familiar with crystallography database
  - Learn how to analyse data from an X-Ray Diffractometer.
- **Become familiar with SCAPS software**.
  - **Simulate** solar cell paramemeters using SCAPS software.

	Modeling	Simulation
Definition	Creating simplified representations or abstractions of physical systems using mathematical equations, rules, or conceptual frameworks.	The process of using a model to compute the behavior of a system over time or under different conditions by executing the model on a computer.
Purpose	Describe, understand, and predict the behavior of a physical system. Models can range from simple mathematical equations (e.g., Newton's laws of motion) to complex theoretical frameworks (e.g., quantum field theory).	Mimic the behavior of a real-world system in a virtual environment. It allows physicists to study complex systems, conduct experiments that are impractical or impossible in reality, and make predictions.
Examples	Using a mathematical model to describe the motion of planets in the solar system or the behavior of particles in a quantum system	Molecular dynamics simulations to study the behavior of atoms and molecules, computational fluid dynamics to model airflow around objects, or cosmological simulations to understand the evolution of the universe.

Importance of modeling and simulation in Physics

1. Understanding Complex Systems
2. Predictive Power
3. Hypothesis Testing
4. Education and Communication
5. Cost and Safety
6. Exploration of New Phenomena
7. Interdisciplinary Applications

Software for simulation and modeling

- Scout software
- Crystallography software
- DFT codes
- SCAPS software

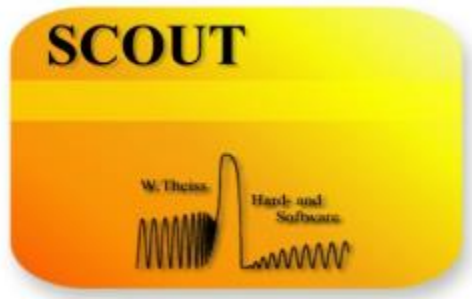
SCOUT Software

SCOUT downloads | WTheiss Hardware and Software

Spectrum interpretation by simulation

written by W.Theiss

W. Theiss – Hard- and Software for Optical Spectroscopy
Dr.-Bernhard-Klein-Str. 110, D-52078 Aachen, Germany
Phone: + 49 241 5661390 Fax: + 49 241 9529100
e-mail: theiss@mtheiss.com web: www.mtheiss.com



- The goal of optical spectroscopy is :
  - determination of microscopic quantities such as resonance frequencies of oscillating atoms,
  - impurity concentrations
  - thin film thicknesses from macroscopic experiments.
- This is possible if the microscopic phenomena are coupled to the electric fields of the probing radiation (***the dielectric function*** or its square root, the ***complex refractive index*** - both quantities are more generally called ***'optical constants***').

SCOUT Software

Software, hardware, problem solving for

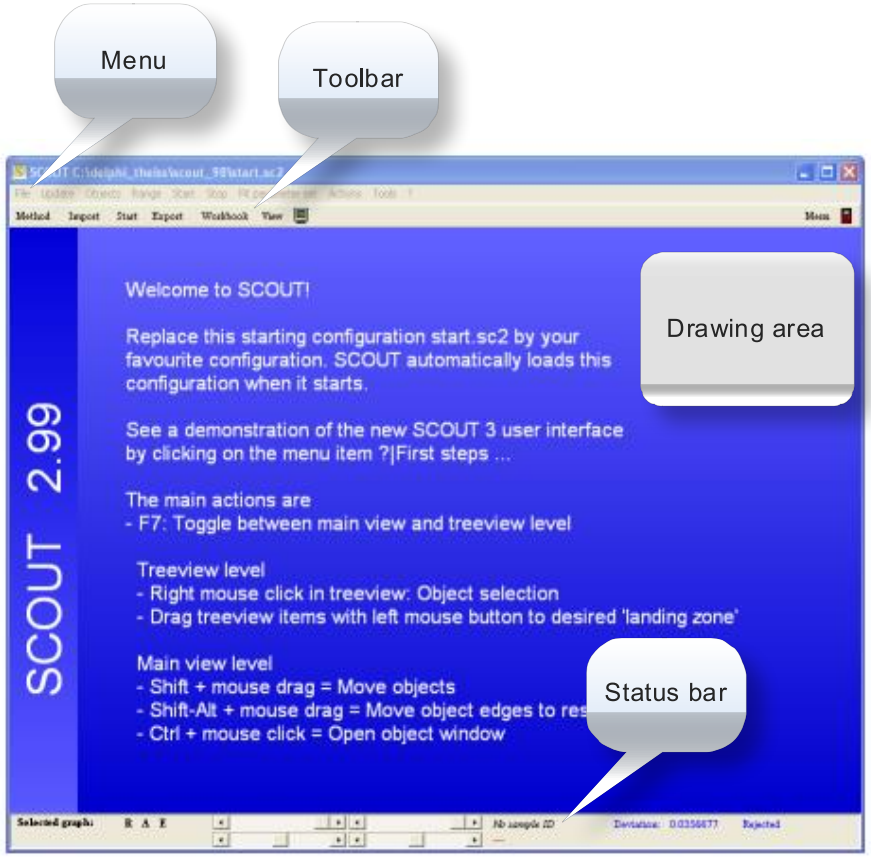
• Optics	**Research**
• Optical Spectroscopy	• Thin film analysis by spectrum simulation techniques
• Material Science	• Advanced models for optical constants
• Product Design	• Spectral ray-tracing investigations
• Production Control	• Direct determination of optical constants
	• Realistic modeling of diffuse reflectance spectra

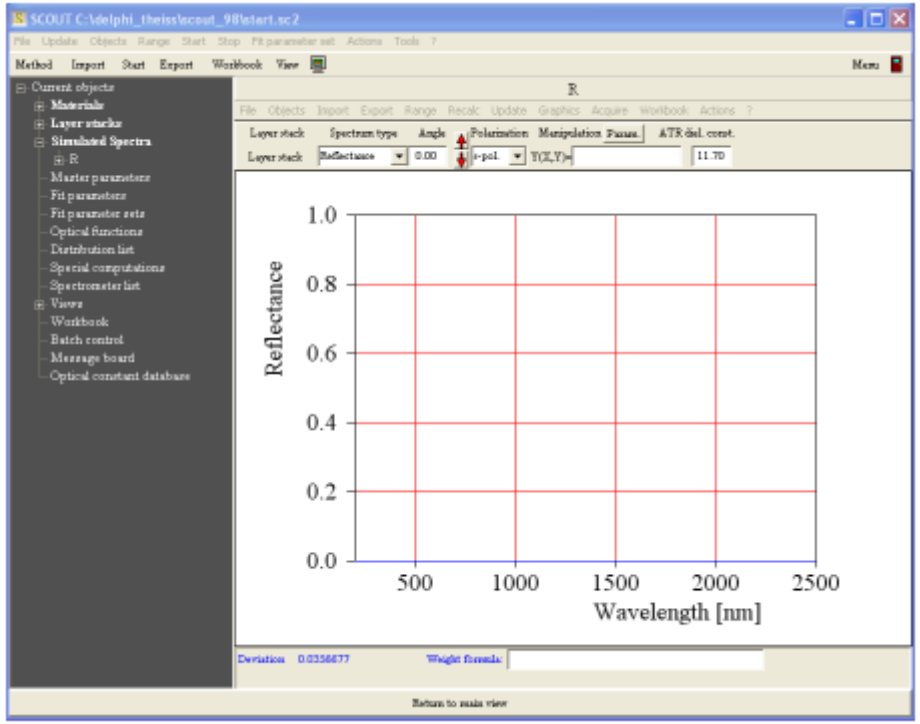
SCOUT Software

Software, hardware, problem solving for

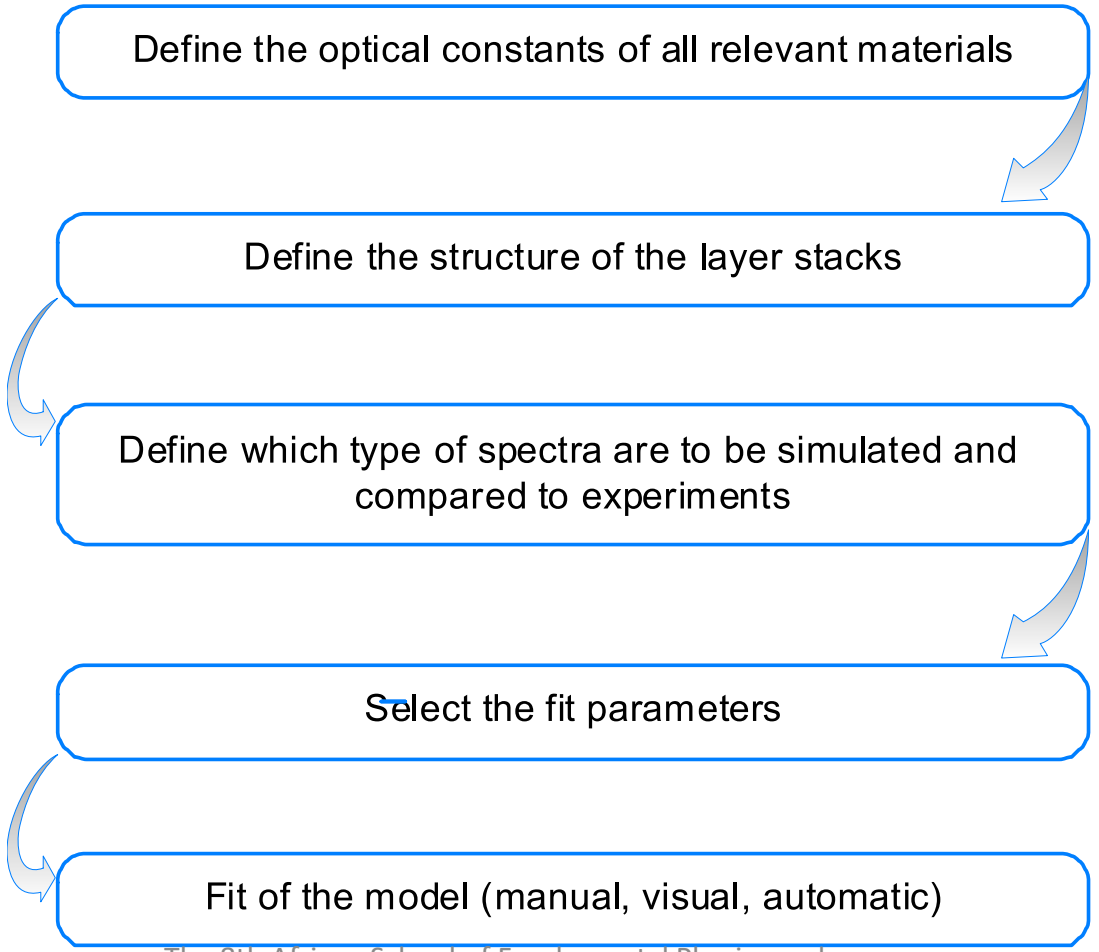
Design	Production Control
• Design of thin film systems with customized optical properties	• Thin film analysis by automatic spectrum simulation
• Architectural and car glass coatings	• Online monitoring
• Optimization of coatings for solar applications	• Thickness and composition determination of thin films
• Design and analysis of optical setups by high-level ray-tracing	• Optical inspection networks for large coating lines
• Prediction of the optical appearance of color prints and paints	• OLE automation servers for external control (LabView or other high level programming languages)

SCOUT Software



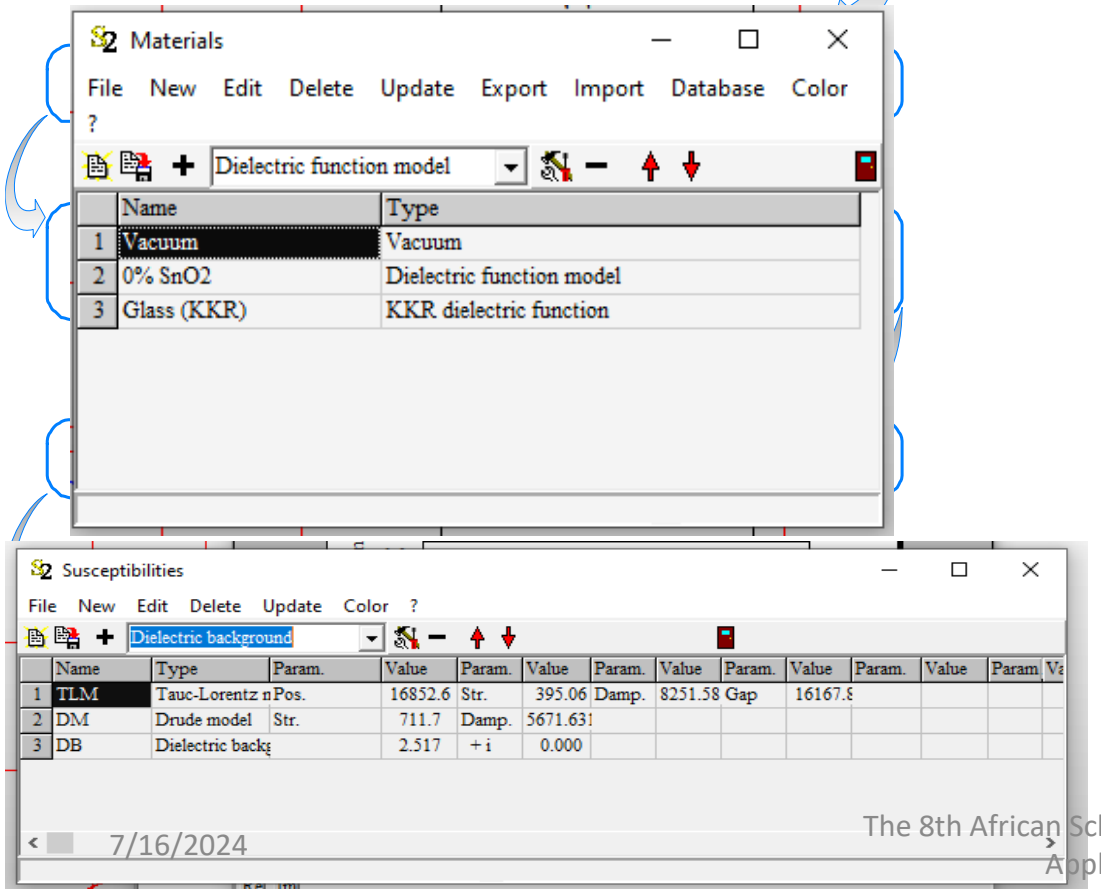


SCOUT Software: Required steps for developing optical models



SCOUT Software: Required steps for developing optical models

Define the optical constants of all relevant materials



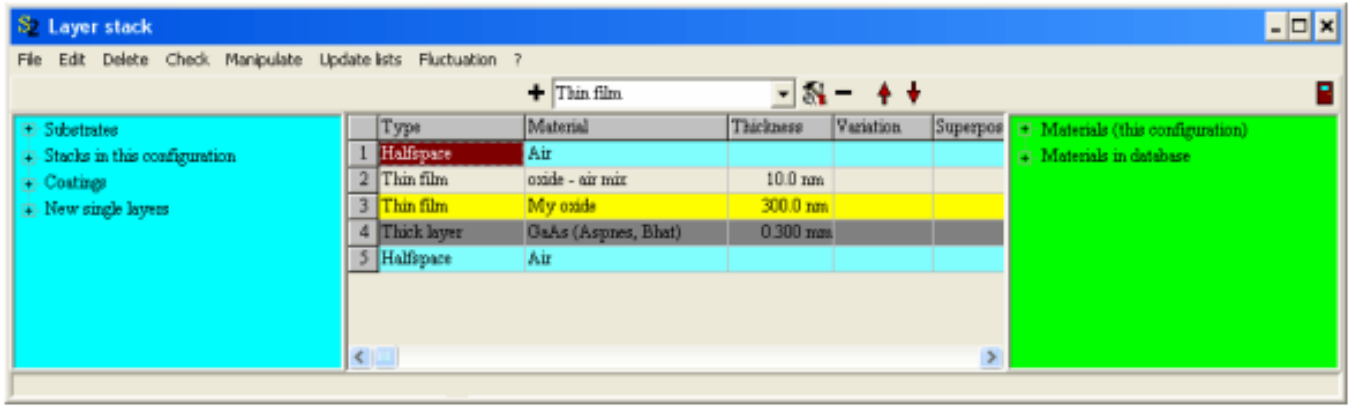
Materials are managed in the first branch of the object tree called **Materials**.
Define objects representing fixed optical constants (imported from files) or optical constant models that give you flexibility if you want to adjust optical constants to fit experimental data.

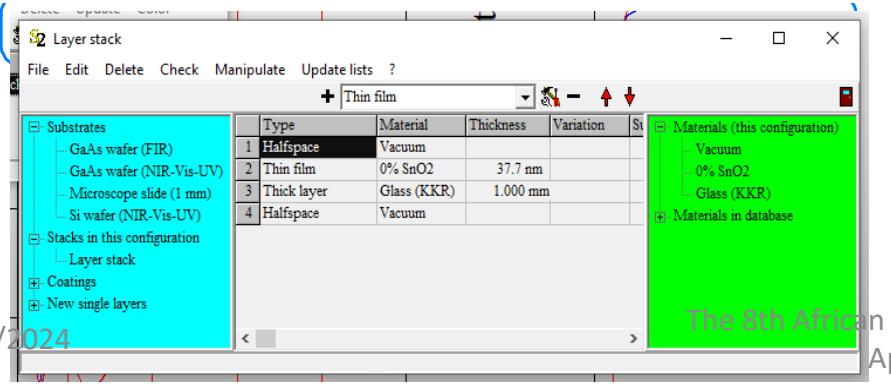
Optical constant models present are:
Drude model for free carriers
Extended Drude model for free carriers with frequency dependent damping harmonic oscillator
extended oscillator model suggested by Brendel
extended oscillator model suggested by Kim
oscillator model suggested by Gervais
OJL interband transition model
Campi-Coriasso interband transition model
Tauc-Lorentz interband transition model
user-defined expressions for optical constants

SCOUT Software: Required steps for developing optical models

Define the optical constants of all relevant materials

Define the structure of the layer stacks

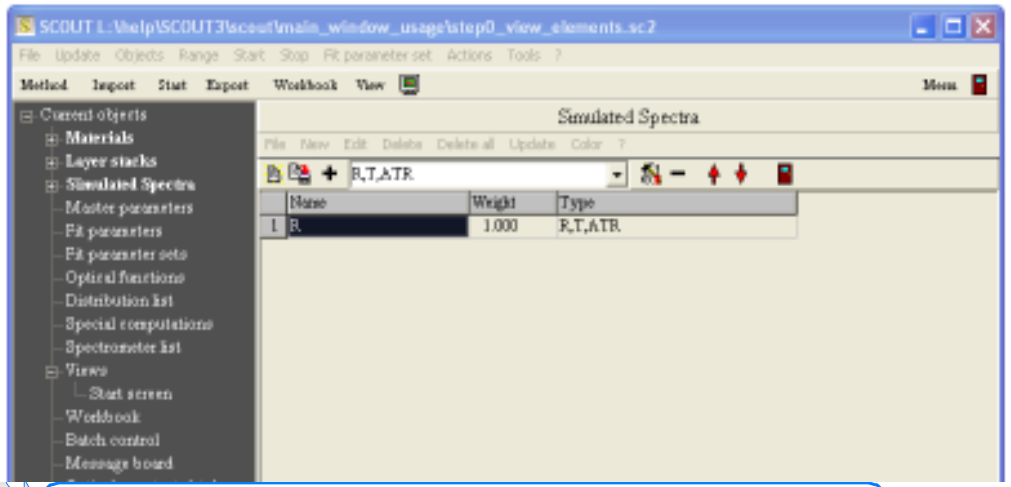




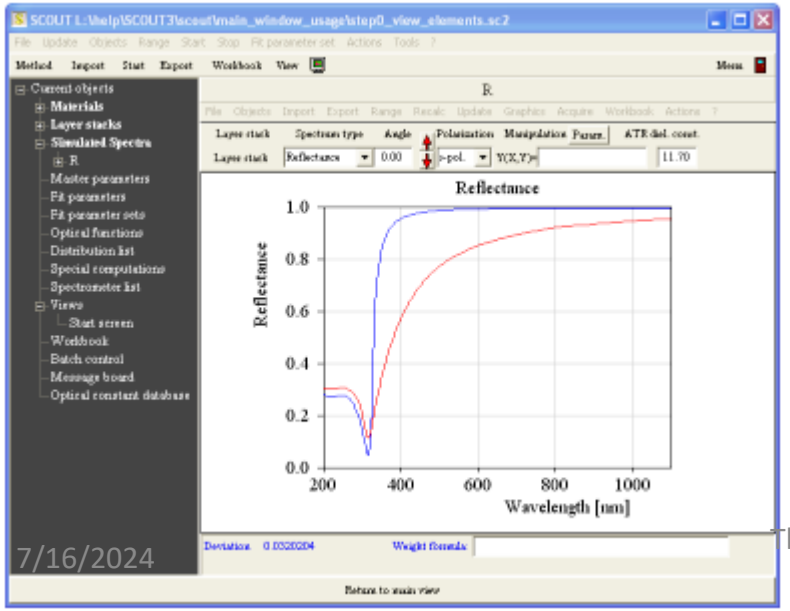
The tree branch **Layer stacks** shows the list of layer stacks.
In most cases you will investigate one layer stack only, but SCOUT lets you work with several stacks if you want to (or have to).
Each layer stack may consist of an unlimited number of layers which are again managed in lists, called layer stack.
For simple layers you can select coherent or incoherent superposition of partial waves.

A 'Thin film' is always handled with coherent superposition whereas a 'Thick layer' is treated with incoherent superposition. For cases in between full coherent or incoherent superposition we have implemented an efficient averaging algorithm for lateral layer thickness inhomogeneities.

SCOUT Software: Required steps for developing



Define which type of spectra are to be simulated and compared to experiments



These spectra are collected in the spectra list which is the **Simulated spectra** branch in the treeview. The following types of spectra can be used at present:

- Reflectance
- Transmittance
- Absorbance
- ATR
- Layer Mix (computes the average spectrum of a patterned sample)
- Ellipsometry
- Ellipsometry stack average
- PL spectrum
- EL spectrum
- Layer absorption (computes the absorbed fraction of incident light intensity in a certain layer in a stack)
- Charge carrier generation (computes the number of photon-generated charge carriers in a layer)

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Define which type
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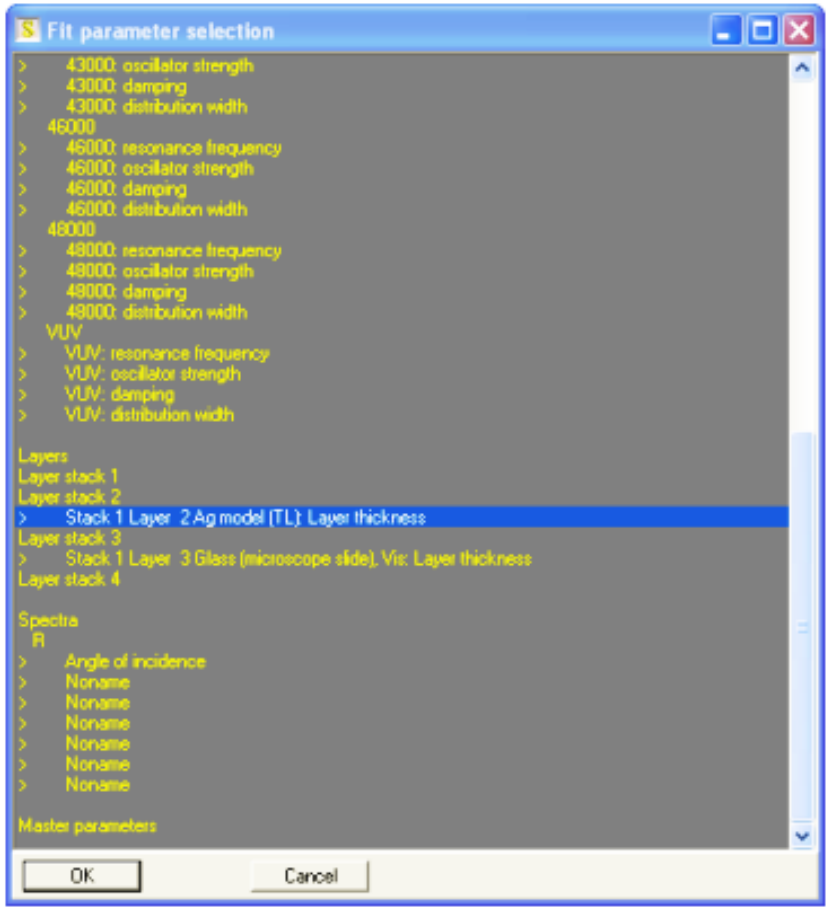
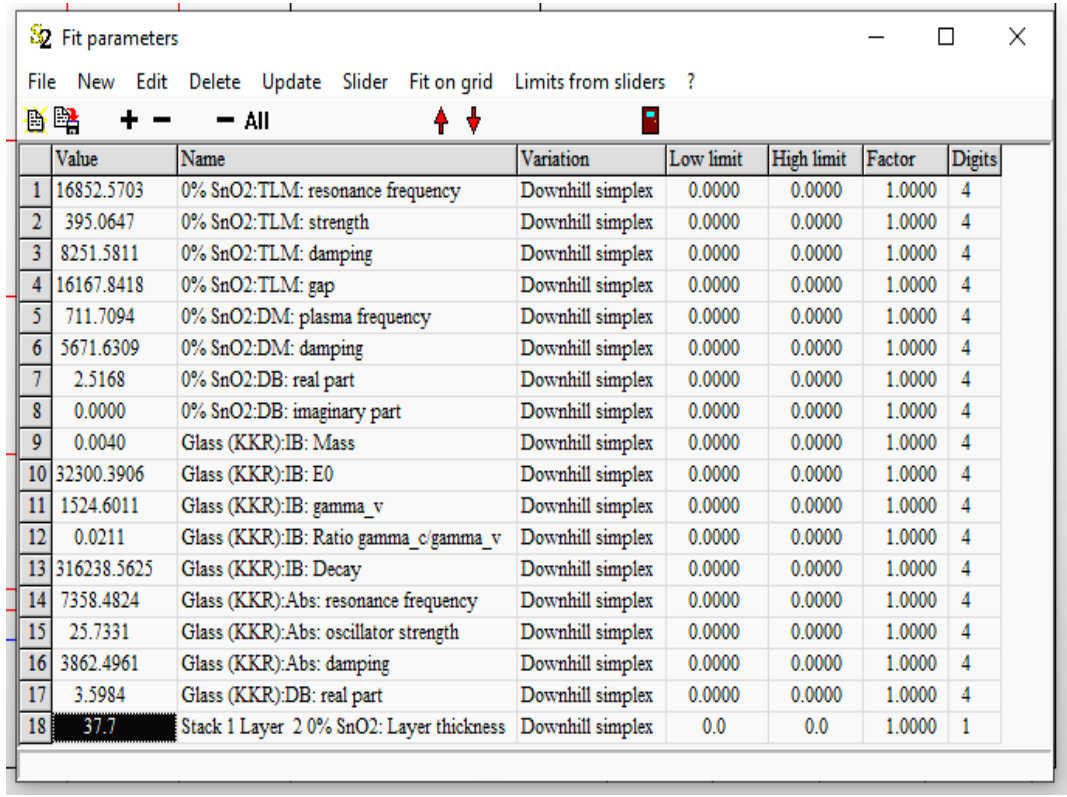




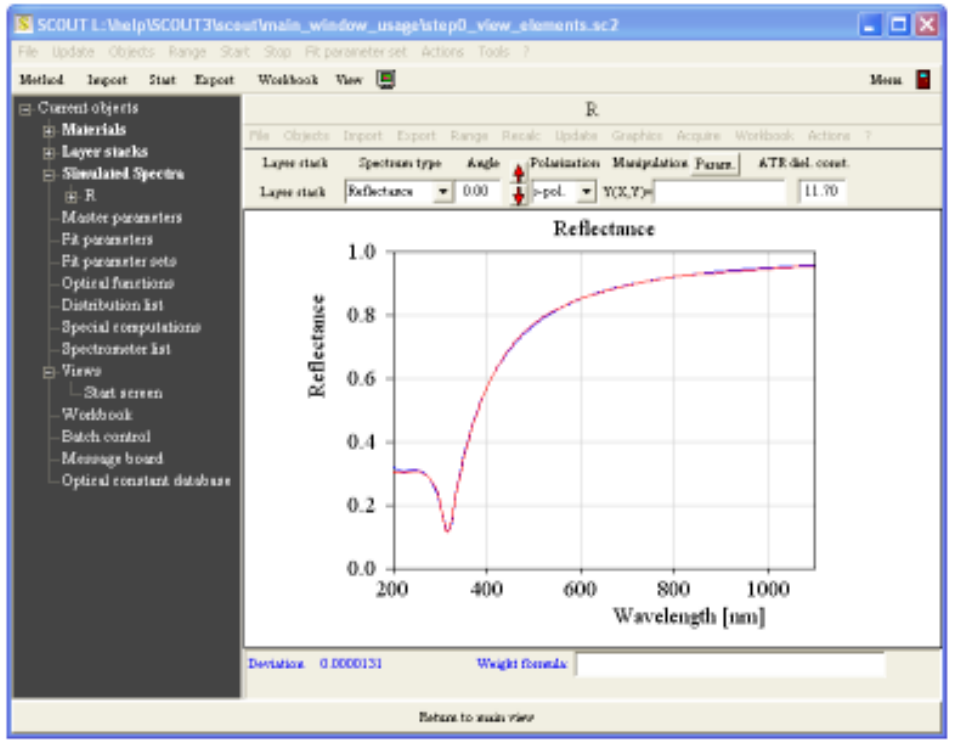
	Value	Name	Variation	Low limit	High limit	Factor	Digits
1	16852.5703	0% SnO2:TLM: resonance frequency	Downhill simplex	0.0000	0.0000	1.0000	4
2	395.0647	0% SnO2:TLM: strength	Downhill simplex	0.0000	0.0000	1.0000	4
3	8251.5811	0% SnO2:TLM: damping	Downhill simplex	0.0000	0.0000	1.0000	4
4	16167.8418	0% SnO2:TLM: gap	Downhill simplex	0.0000	0.0000	1.0000	4
5	711.7094	0% SnO2:DM: plasma frequency	Downhill simplex	0.0000	0.0000	1.0000	4
6	5671.6309	0% SnO2:DM: damping	Downhill simplex	0.0000	0.0000	1.0000	4
7	2.5168	0% SnO2:DB: real part	Downhill simplex	0.0000	0.0000	1.0000	4
8	0.0000	0% SnO2:DB: imaginary part	Downhill simplex	0.0000	0.0000	1.0000	4
9	0.0040	Glass (KKR):IB: Mass	Downhill simplex	0.0000	0.0000	1.0000	4
10	32300.3906	Glass (KKR):IB: E0	Downhill simplex	0.0000	0.0000	1.0000	4
11	1524.6011	Glass (KKR):IB: gamma_v	Downhill simplex	0.0000	0.0000	1.0000	4
12	0.0211	Glass (KKR):IB: Ratio gamma_c/gamma_v	Downhill simplex	0.0000	0.0000	1.0000	4
13	316238.5625	Glass (KKR):IB: Decay	Downhill simplex	0.0000	0.0000	1.0000	4
14	7358.4824	Glass (KKR):Abs: resonance frequency	Downhill simplex	0.0000	0.0000	1.0000	4
15	25.7331	Glass (KKR):Abs: oscillator strength	Downhill simplex	0.0000	0.0000	1.0000	4
16	3862.4961	Glass (KKR):Abs: damping	Downhill simplex	0.0000	0.0000	1.0000	4
17	3.5984	Glass (KKR):DB: real part	Downhill simplex	0.0000	0.0000	1.0000	4
18	37.7	Stack 1 Layer 2 0% SnO2: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1

Select the fit parameters

Fit of the model (manual, visual, automatic)

The treeview branch **Fit parameters** holds the list of fit parameters. These are the parameters of the model that are to be adjusted in order to reach optimal agreement between simulation and measurements. Besides fitting to experimental data, you can also select a model parameter as fit parameter if you want to compute its value by a user-defined function (which may contain master parameters, optical function values or the time).

SCOUT Software: Required steps for developing optical models



Fit of the model (manual, visual, automatic)

Fit parameters

File New Edit Delete Update Slider Fit on grid Limits from sliders ?

All

	Value	Name	Variation	Low limit	High limit	Factor	Digits
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2	395.0647	0% SnO2:TLM: strength	Downhill simplex	0.0000	0.0000	1.0000	4
3	8251.5811	0% SnO2:TLM: damping	Downhill simplex	0.0000	0.0000	1.0000	4
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18	37.7	Stack 1 Layer 2 0% SnO2: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1

Dielectric permeability

$$\boldsymbol{P} = \varepsilon_0(\varepsilon - 1)\boldsymbol{E} \quad (1.1)$$

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1.2)$$

$$N(\omega) = n(\omega) + ik(\omega) \quad (1.3)$$

$$\varepsilon = N^2 \quad (1.4a)$$

$$\varepsilon_1 = n^2 - k^2 \quad (1.4b)$$

$$\varepsilon_2 = 2nk \quad (1.4c)$$

$$\varepsilon = \chi^{VC} + \chi^{FC} + \cdots \quad (1.5)$$

$$R(\omega) = \left[\frac{(n(\omega) - 1)^2 + k^2(\omega)}{(n(\omega) + 1)^2 + k^2(\omega)}\right] \quad (1.6)$$

$$n(\omega) = \frac{1 + R(\omega)}{1 - R(\omega)} + \sqrt{\frac{4R(\omega)}{\left(1 - R(\omega)\right)^2} - k^2} \quad (1.7)$$

$\boldsymbol{P}$	Polarization
$\boldsymbol{E}$	Applied E-Field
ε_0	dielectric constant of free space
ε	the complex dielectric function
ω	Angular frequency
$N(\omega)$	Complex refractive index
n	the real index of refraction
k	the extinction coefficient
χ^{Vc}, χ^{FC}	susceptibilities of the valence electrons, the free carriers
$R(\omega)$	the bulk reflection coefficient
$n(\omega)$	refractive index

Determination of optical constants

Γ damping constant for the Drude term.

Ω_{TO} resonance frequency,

Ω_p oscillator strength,

Ω_τ damping constant,

σ Gauss–Lorentz-switch constant.

$\sigma = 0$, a Gaussian line shape, $\sigma > 5$, Lorentzian line shape

$$\varepsilon = \varepsilon_\infty + \chi_{VE} + \chi_{FC} \qquad (1.8)$$

$$\chi_{FC} = \frac{\omega_p^2}{\omega^2 + i\omega\Gamma} \qquad (1.9)$$

$$\omega_p^2 = \frac{ne^2}{m_e\varepsilon_0} \qquad (1.20)$$

$$\chi_{VE} = \frac{\Omega_p^2}{\Omega_{TO}^2 - \omega^2 - i\omega\tau(\omega)} \qquad (1.21)$$

$$\tau(\omega) = \Omega_\tau exp\left[-\frac{1}{1+\sigma^2}\left(\frac{\omega - \Omega_{TO}}{\Omega_\tau}\right)^2\right] \qquad (1.22)$$

$$\chi_{\text{Drude}} = -\frac{\Omega_P^2}{\tilde{\nu}^2 + i\tilde{\nu}\Omega_\tau}$$

$$n = \frac{4\pi^2 c_0^2 \varepsilon_0 m}{e^2}\Omega_P^2$$

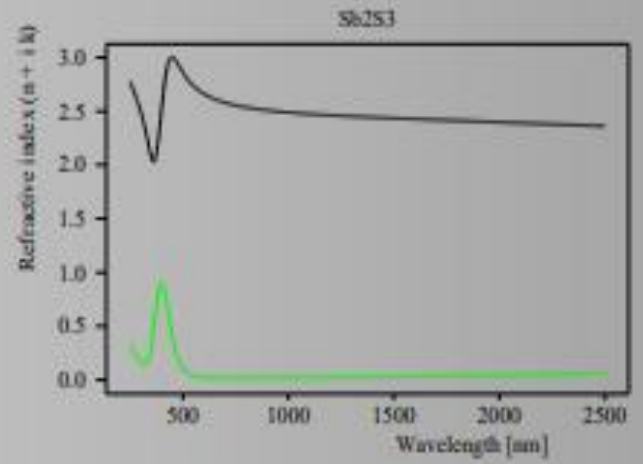
$$\mu = \frac{e}{m}\frac{1}{2\pi c_0}\frac{1}{\Omega_\tau} \qquad \rho = \frac{\Omega_\tau}{2\pi c_0 \varepsilon_0 \Omega_P^2}$$

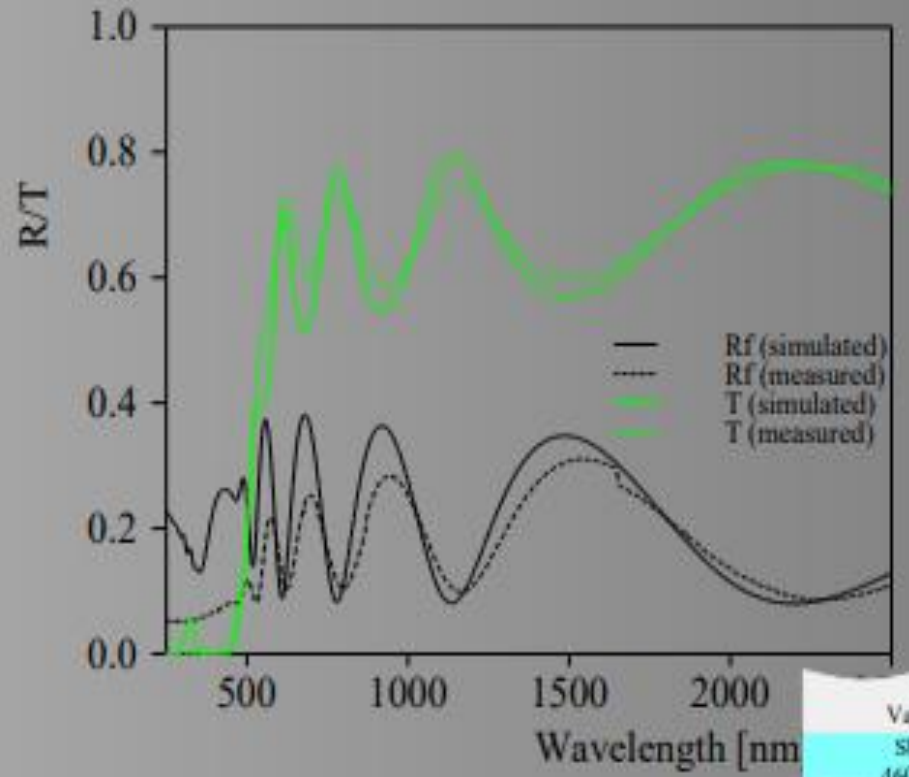
Sb2S3 model development

SCOUT
Sb2S3 model

Optical constant model composed of
- constant
- far UV oscillator (harmonic oscillator)
- 2 OJL interband transitions
- 1 Kim oscillator
- Drude model

The layer stacks for R and T differ in the thickness of the main Sb2S3 layer. This is of type "Thickness averaging" which means that it averages out interference patterns for slightly different thicknesses. This reduces the amplitude of interference structures in the spectra. Very likely the thickness of your layer differs from positon to position, and within the investigated sample spot there is a thickness distribution rather a constant thickness.

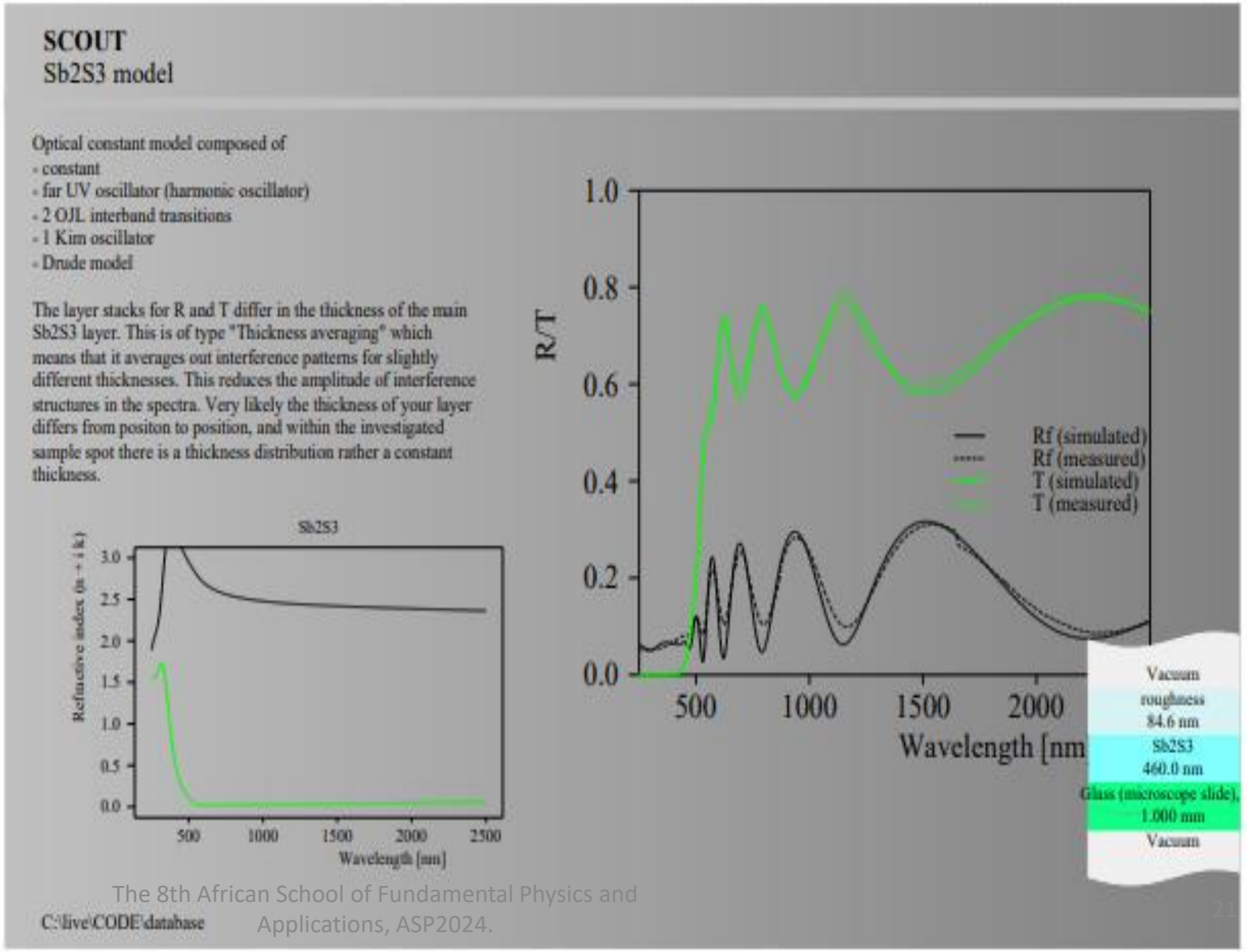




C:\live\CODE\database

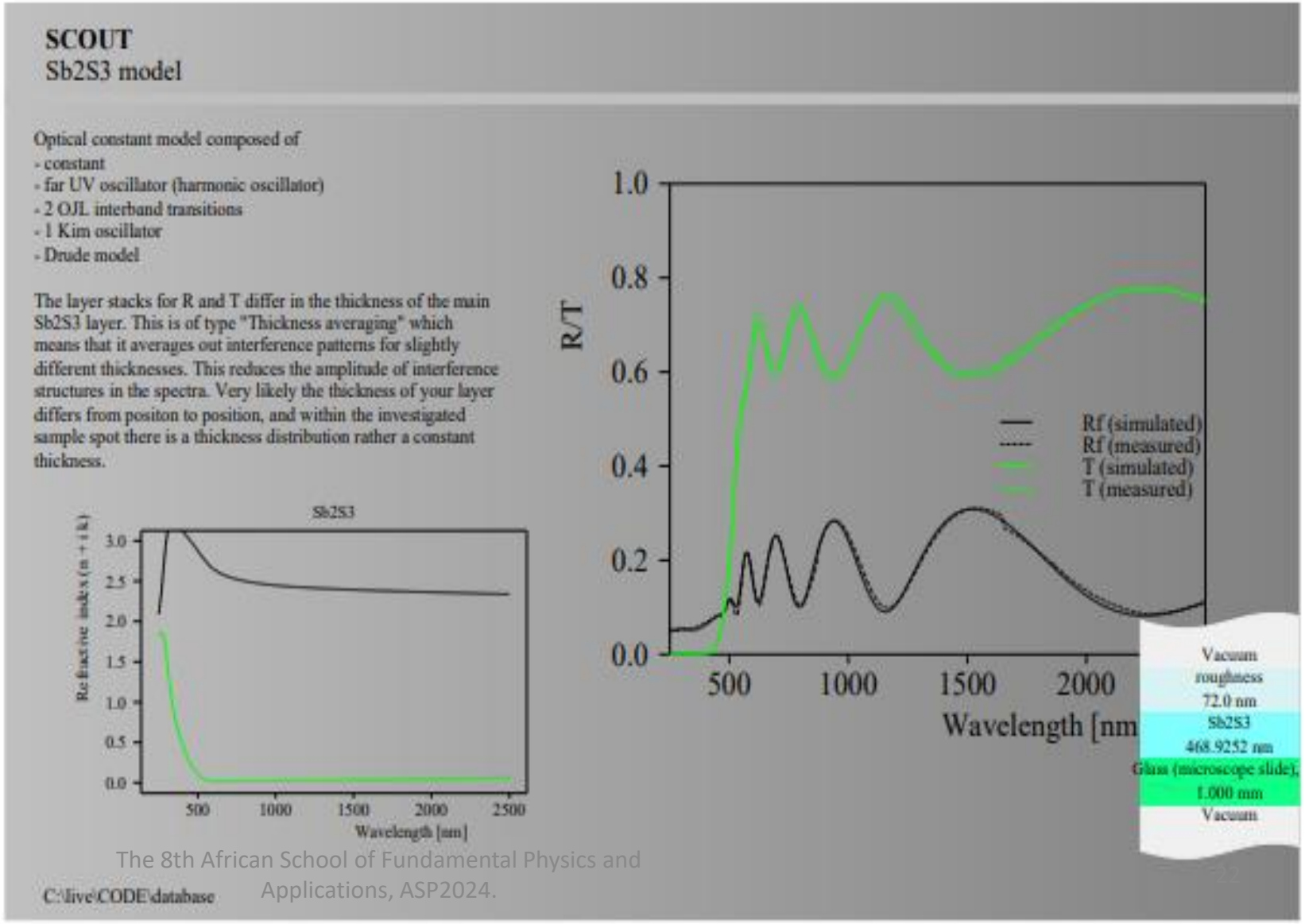
Sb2S3 model development

In order to reduce the reflectance in the UV one needs to introduces surface roughness (which acts like an anti-reflection layer at small wavelengths).



Sb2S3 model development

A small shift in the interference patterns for R and T noticed. Very likely the spectra have not been measured at exactly the same spot on the sample.



Sb2S3 model development

Allowing different thickness values for R and T gives the best solution up to now

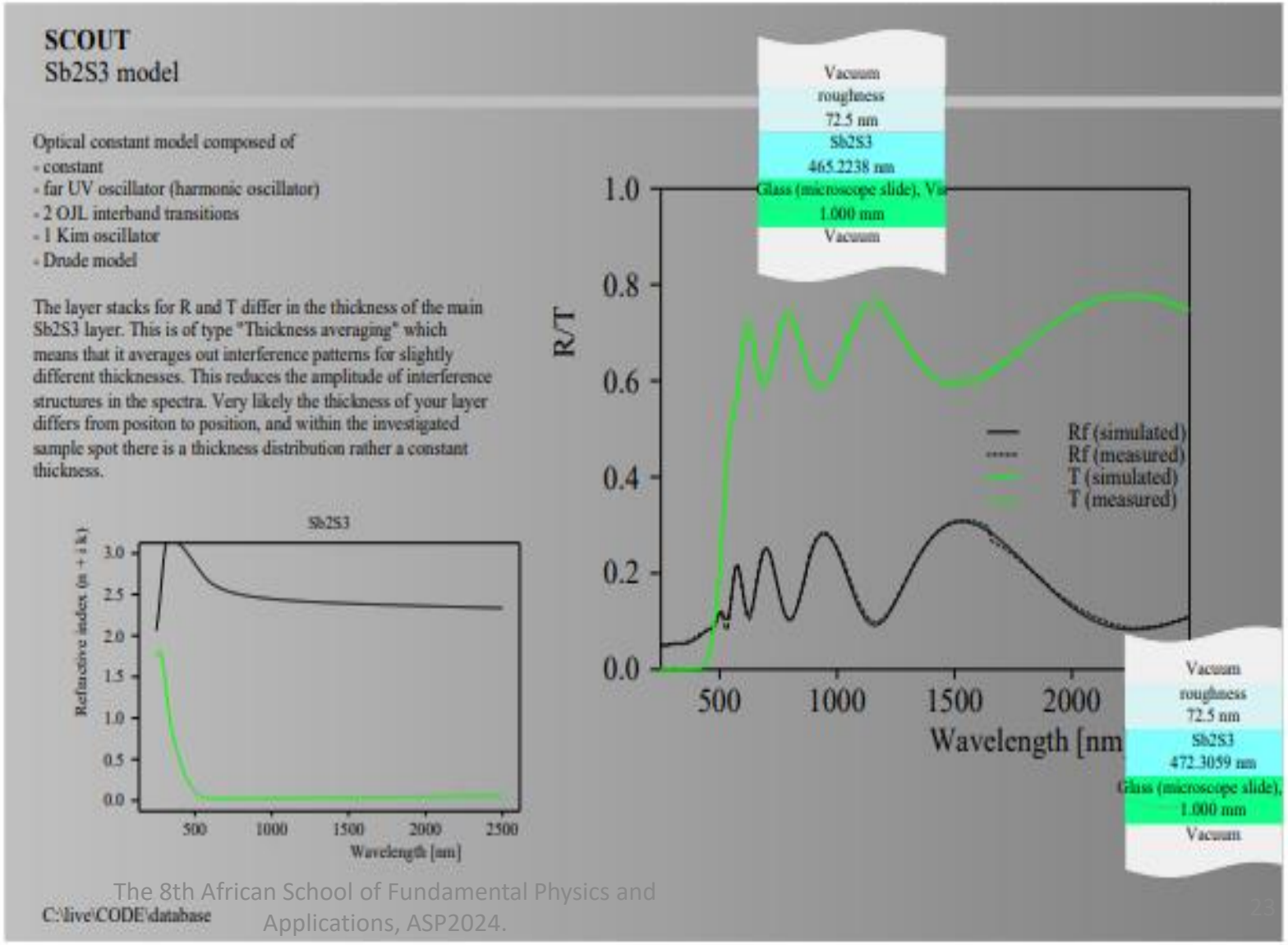
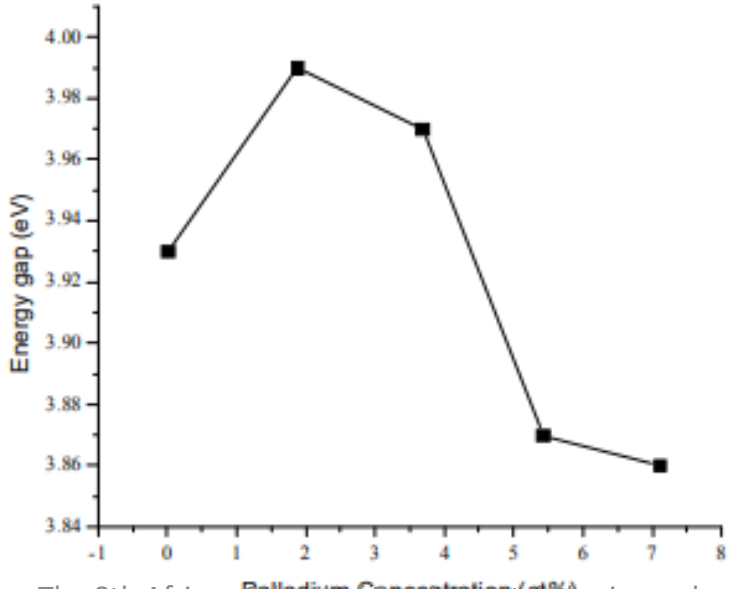


Table 1: Calculated values of carrier concentration (n), mobility (μ), resistivity (ρ) and conductivity (σ) of the undoped tin oxide and palladium doped tin oxide films

Film	Plasma frequency (Ω_p) cm^{-1}	Damping constant (Ω_τ) cm^{-1}	Carrier concentration (n) cm^{-3}	Mobility (μ) cm^2/Vs	Resistivity (ρ) Ωcm	Conductivity (σ) $\Omega^{-1}cm^{-1}$
0at% Pd:SnO_2	13809.9639	343585.625	6.38024E+22	5.69E-03	0.1080051	9.258821481
1.88at% Pd:SnO_2	23835.9805	631534.25	1.90072E+23	3.10E-03	0.0666385	15.00633867
3.68at% Pd:SnO_2	23082.4746	456856.8125	1.78245E+23	4.28E-03	0.0514055	19.45316349
5.42at% Pd:SnO_2	97.6613	160.2429	3.19078E+18	1.22E+01	1.0072289	0.992822968
7.10at% Pd:SnO_2	8.6206	1658.2019	2.48615E+16	1.18E+00	1337.6941	0.000747555



Enhancing your SCOUT work

- Customizing SCOUT for routine spectroscopy using Views and the toolbar
- Inspecting the influence of model parameters on optical spectra
  - Parameter variation action
- Working with databases
  - Contains materials with pre-defined optical constants and pre-defined layer stacks.
- Programming SCOUT by OLE automation
  - Create automated reports and batch operations with the Windows Scripting Host (WSH), MS Word, MS Excel, LabView or any other OLE automation controller.

Software for simulation and modeling

- ~~Scout software~~
- Crystallography software
- DFT codes
- SCAPS software

Crystallography Software

List at least five crystallography software that you are familiar with.

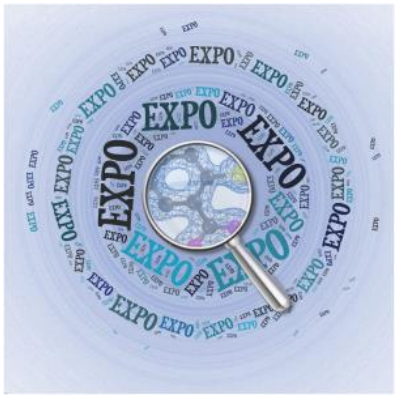
Crystallography Software

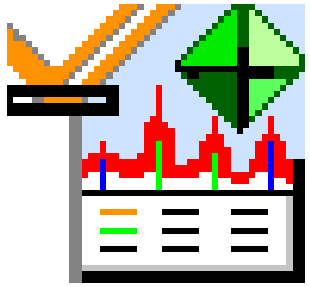
List at least five crystallography database that you are familiar with.

Crystallography Software

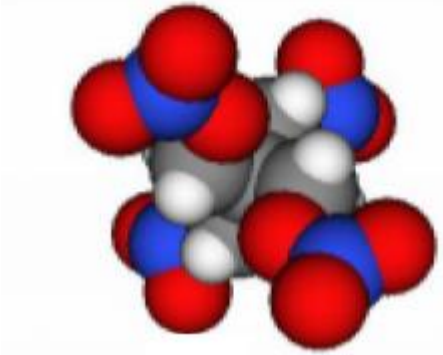
List at least five crystallography software that you are familiar with.

(IUCr) Crystallographic software list





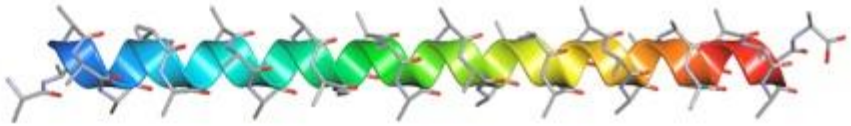
GSAS-II



FullProf Suite

Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

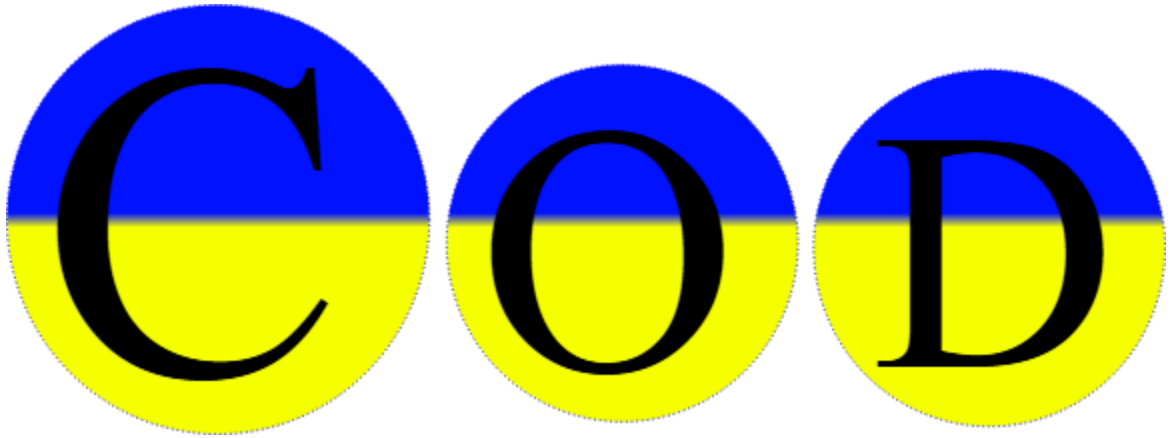
ArgusLab



Crystallography Software

List at least five crystallography database that you are familiar with.

https://www.iucr.org/resources/data/databases

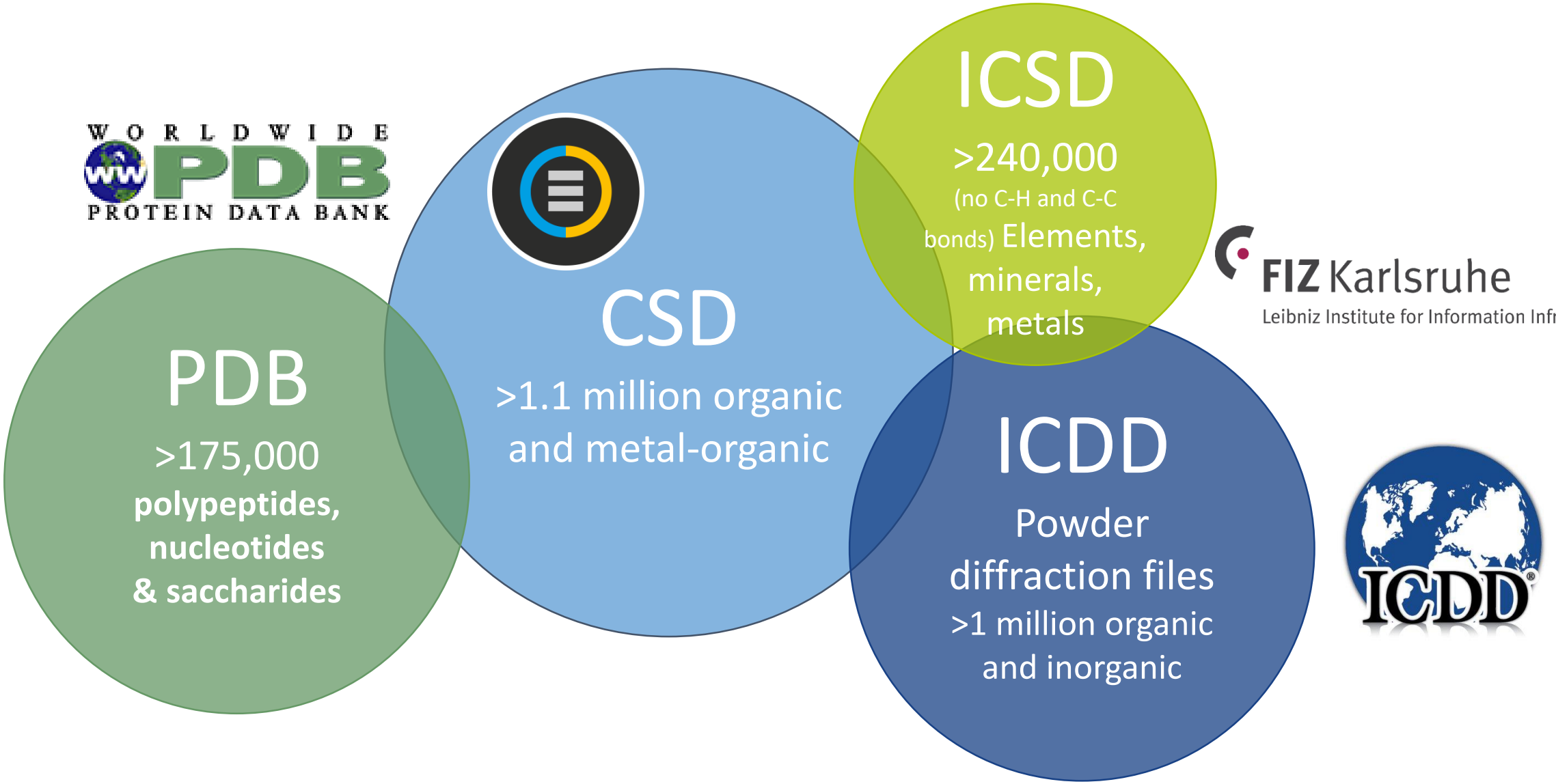


What is a crystallographic database?

- They usually include:
  - Bibliographic data
  - Crystallographic, chemical and experimental information
  - Atomic coordinates

- What makes a crystallographic data special?
  - Standard agreed file format
  - Every published structure is added to the appropriate database
  - There are established curated databases rather than just collections of data with some level of quality control through processing & validation
  - They enable you to learn from the wealth of data they contain

Structural databases



bilbao crystallographic server	BCS: Bilbao Crystallographic Server of crystallographic symmetry information
BMCD	BMCD: Biological Macromolecule Crystallization Database
COD	Crystallography Open Database: Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers
CCDC advancing structural science	CSD: Cambridge Structural Database of organic and metal-organic structures
FIZ Karlsruhe ICSD	ICSD: Inorganic Crystal Structure Database
NAKB Nucleic Acid Knowledgebase	NAKB: Nucleic Acids Knowledge Base (successor to the Nucleic Acid Database NDB)
	The Pauling File: Inorganic Materials Database containing Phase Diagram, Crystal Structure and Physical Property entries
PDB PROTEIN DATA BANK	PDB: Protein Data Bank
ICDD	PDF: Powder Diffraction File of the International Centre for Diffraction Data

Refcodes

CSD Refcode - JEKNOC16

What is JEKNOC16?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

Refcode families

- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
  - Polymorphs
  - New determinations or re-refinements of the same substance
  - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* refcode families

Some of my favourite refcodes are: KITTEN, BATMAN, DISNEY, GAUTAM, GLYCIN

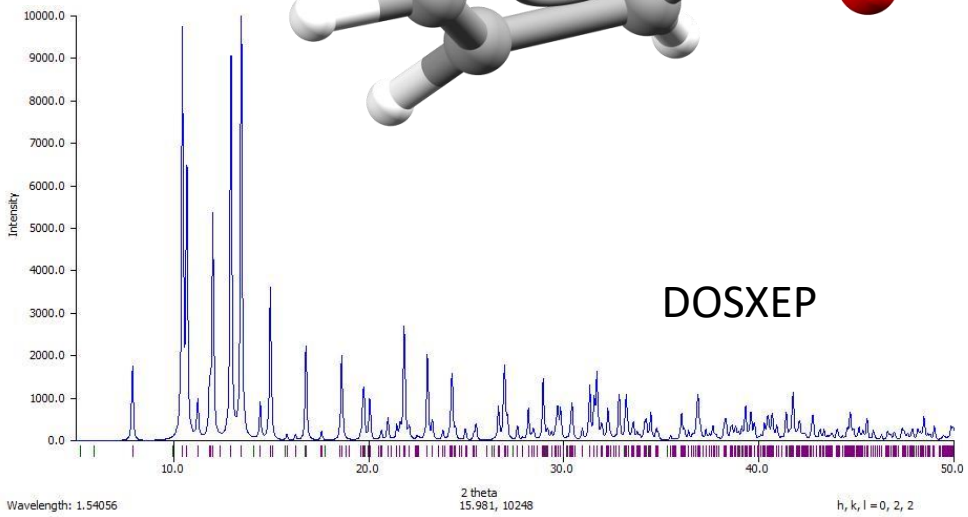
ICDD Code: 00-027-1402 Silicon

ICSD Code: ICSD:028767 Uranium Oxide

Powder data

$$R = \frac{\sum ||F_{\mathrm{obs}}| - |F_{\mathrm{calc}}||}{\sum |F_{\mathrm{obs}}|},$$

$$I_{hkl} \propto |F(hkl)|^2$$



DOSXEP

CSD deposition workflow looks for the presence of:

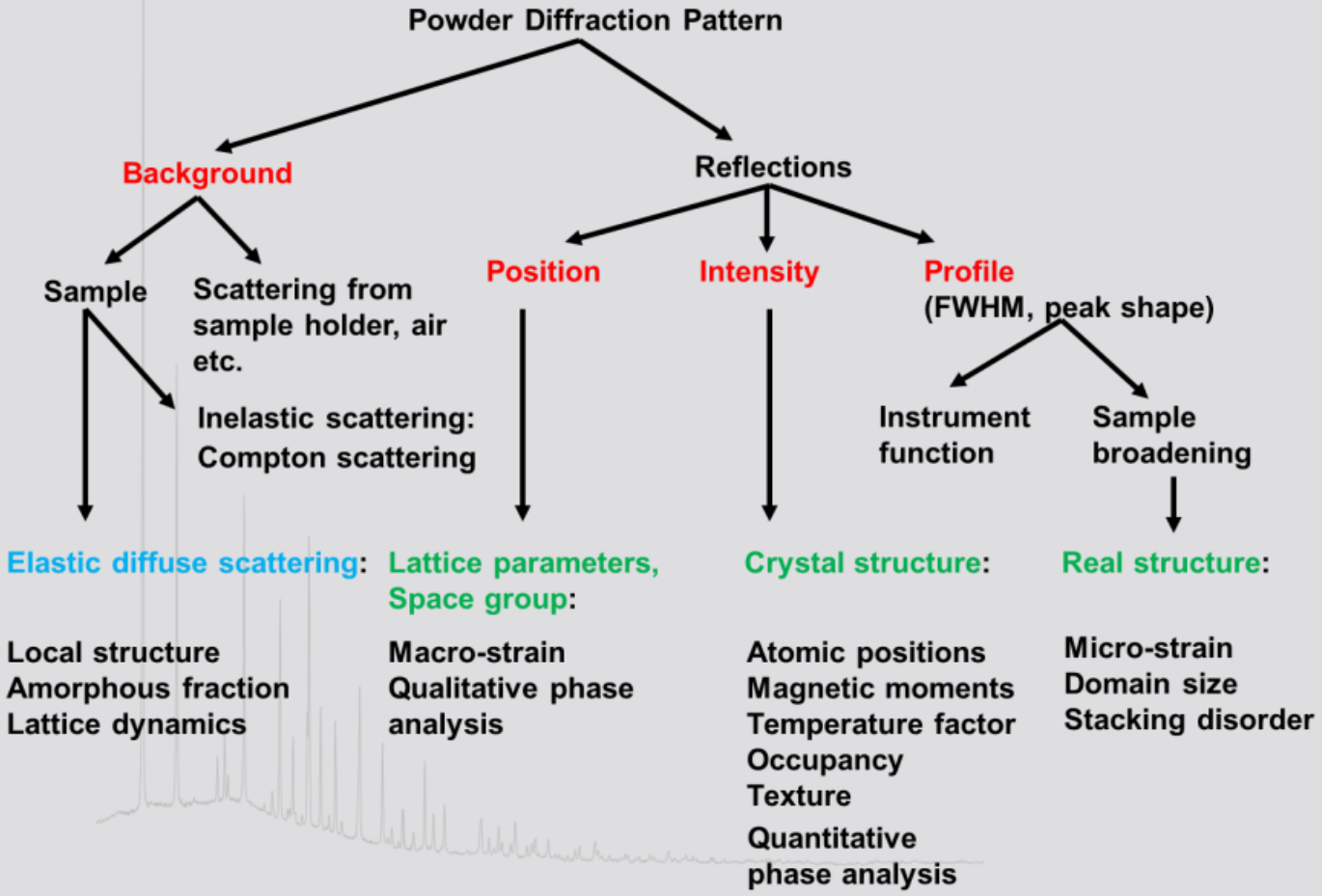
- _pd_calc_method
- _pd_block_id
- _pd_phase_block_id
- _pd_proc_ls_prof_wR_expected
- _pd_proc_ls_prof_R_factor
- _pd_proc_ls_prof_wR_factor

- Powder CIF dictionary: https://www.iucr.org/resources/cif/dictionaries/cif_pd

WHAT INFORMATION IS IN A POWDER PATTERN ?

From: Dinnebeir ISCoC Erice School, 2024

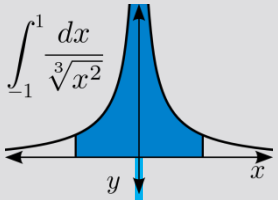
"Total" scattering = elastic incoherent (diffuse) scattering + elastic coherent (Bragg) scattering



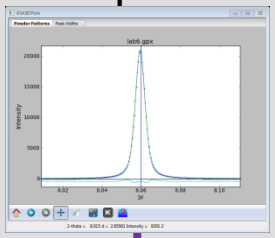
HOW TO MODEL A POWDER PATTERN:
- THE RIETVELD FORMULA -

From: Dinnebeir ISCoC Erice School, 2024

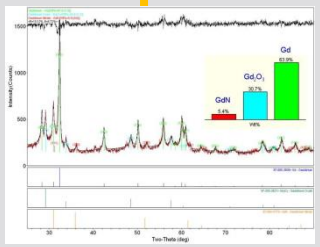
Peak intensity



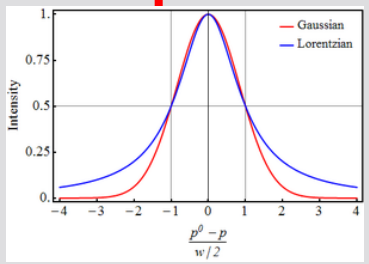
Peak position



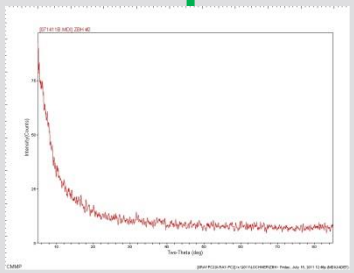
$$y_{calc}(2\theta_i) = \sum_p \left(S_p \sum_{(hkl)p} \left(|F_{calc}((hkl)p)|^2 \cdot \Phi_{(hkl)p}(2\theta_i - 2\theta_{(hkl)p}) \cdot Corr_{(hkl)p}(2\theta_i) \right) \right) + \mathrm{Bkg}(2\theta_i)$$



Scale factors



Peak profile

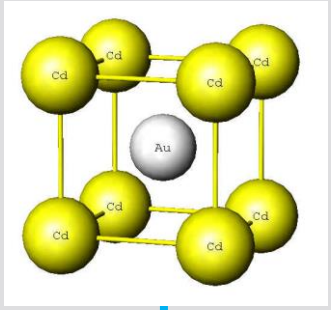


Background

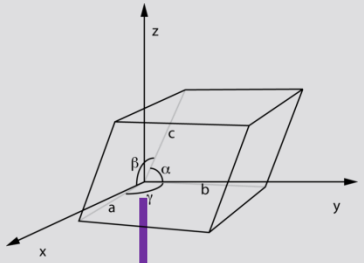
THE RIETVELD FORMULA

From: Dinnebeir ISCoC Erice School, 2024

Crystal structure

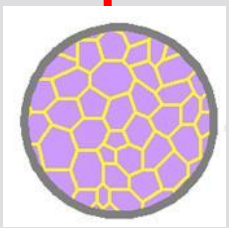


Unit cell & space group

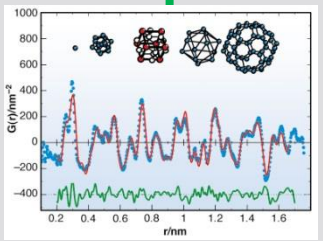


$$y_{calc}(2\theta_i) = \sum_p \left(S_p \sum_{(hkl)p} \left(|F_{calc}((hkl)p)|^2 \cdot \Phi_{(hkl)p}(2\theta_i - 2\theta_{(hkl)p}) \cdot Corr_{(hkl)p}(2\theta_i) \right) \right) + \mathrm{Bkg}(2\theta_i)$$

QPA



IRF & microstructure



Local order & instrument

Methods for QPA with XRPD

- Two categories:
  - Single peak intensities («traditional methods»)
  - Full profile fitting (Rietveld method)

- Absorption-diffraction method
  - External standard method (*Klug equation*)
  - Methods where mass absorption coeffiecient is known or can be determined
- [Spiking method]
- Internal standard method
  - "Reference Intensity Ratio" (RIR) method
    - Generalized, normalized [and with constraints] RIR
- The Rietveld method
  - standardless
  - with internal standard addition
  - with PONKS (Partial Or No Known Crystal Structure)

Some programs for the Rietveld method

Program name	*Website*
FULLPROF SUITE	www.ill.eu/sites/fullprof/php/downloads.html
GSAS + EXPGUI	subversion.xray.aps.anl.gov/trac/EXPGUI
GSAS-II	subversion.xray.aps.anl.gov/trac/pyGSAS
HIGH SCORE PLUS ($)	www.malvernpanalytical.com
MAUD	maud.radiographema.eu/
PDXL ($)	www.rigaku.com
PROFEX (BGMN)	profex.doebelin.org/
QUANTO	www.ba.ic.cnr.it/softwareic/
RIETAN-FP·VENUS	fujioizumi.verse.jp/download/download_Eng.html
SIROQUANT ($)	www.siroquant.com/
TOPAS ACADEMIC ($)	www.topas-academic.net/
TOPAS ($)	www.bruker.com
($) = commercial;	

Software for Rietveld analysis

FullProf Suite

- The FullProf Suite (for Windows and Linux) is formed by a set of crystallographic programs (FullProf, WinPLOTR, EdPCR, GFourier, etc...) mainly developed for Rietveld analysis (structure profile refinement) of neutron (constant wavelength, time of flight, nuclear and magnetic scattering) or X-ray powder diffraction data collected at constant or variable step in scattering angle 2theta.

https://www.ill.eu/sites/fullprof/

From: Software available for reitvelde refinement by Peter Tzvetkov

DDM

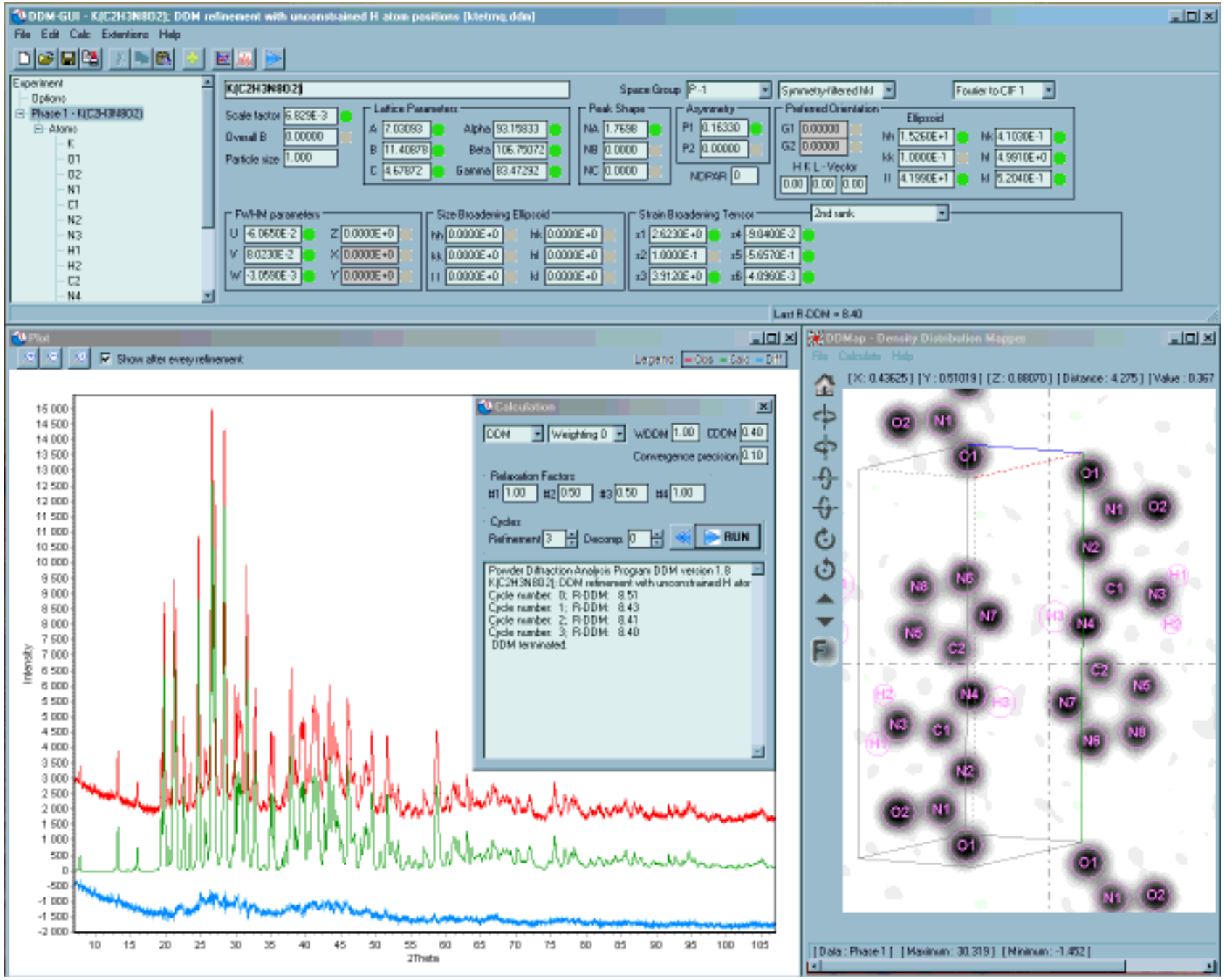
Derivative Difference Minimization Program

- Program for crystal structure analysis from powder diffraction data by making use of either Rietveld or Derivative Difference Minimization (DDM) method
- Does not require the background line modeling
- In the DDM method the refinement is aimed not at minimizing the absolute difference between the experimental and calculated profiles but at minimizing the oscillations (or curvature) of the difference curve.

Maintained by Leonid Solovyov, Institute of Chemistry and Chemical Technology, Krasnoyarsk

https://sites.google.com/site/ddmsuite/home

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

Al15.ddm - Notepad

File Edit Format View Help

```
New compound
Al15In05(WO4)3_Rietveld.dat
   0   5   1   0   0   0   3   1   0   <- JOB NPR NPH NBC NEX NSC INS IPR ISZ
   2   2   1   0   1   0   0   0   0   <- IWP IPL IPC MAT NXT LS1 LS2 LS3 LS4
 1.54060 1.54444   0.500  90.000  12.000   0.000   1.000 180.000   0.000  10.0
  20 0.10 0.50 0.50 0.50 1.00                    <- MCYCLE EPS RELAX[4]
   0   0   3.000   1.000    0                    <- NDEC MAXS WDDM CDDM IWGHT
 -.1037E-1 0.0000E+0 0.0000E+0  0.00000  0.00000  0.00000 <-DISP[3] ABSORP[3]
      1.00      0.00      0.00      0.00      0.00      0.00
  .00000    .00000    .00000    .00000    .00000    .00000
        0.00      0.00      0.00      0.00      0.00      0.00
90936-ICSD
  10   0   0  0.00  0.00  0.00    0.00       <- NATOM IFUR NDPAR PREF(hkl) PARS
P n c a                x         y         z       Biso      N     Anis Adist
Al1  Al             0.468306  0.378863  0.246812  0.000000    4.82211  0  2.200
                       11.00     21.00     31.00      0.00    41.0000
In1  In             0.468306  0.378863  0.246812  0.000000    3.17789  0  2.200
                       11.00     21.00     31.00      0.00   -41.0000
W1   W              0.250000  0.000000  0.473196  0.000000    4.00000  0  3.000
                        0.00      0.00      1.00      0.00     0.0000
W2   W              0.118221  0.355235  0.394383  0.000000    8.00000  0  2.200
                        1.00      1.00      1.00      0.00     0.0000
O1   O              0.095143  0.135760  0.076048  0.000000    8.00000  0  0.000
                        1.00      1.00      1.00      0.00     0.0000
O2   O              0.132780  0.069468  0.366380  0.000000    8.00000  0  0.000
                        1.00      1.00      1.00      0.00     0.0000
O3   O              0.008207  0.251898  0.319882  0.000000    8.00000  0  0.000
                        1.00      1.00      1.00      0.00     0.0000
O4   O              0.334987  0.405567  0.082287  0.000000    8.00000  0  0.000
                        1.00      1.00      1.00      0.00     0.0000
O5   O              0.064324  0.479474  0.326895  0.000000    8.00000  0  0.000
                        1.00      1.00      1.00      0.00     0.0000
O6   O              0.302662  0.336590  0.358630  0.000000    8.00000  0  0.000
                        1.00      1.00      1.00      0.00     0.0000
 .3277E-05   2.69655                                        <- Scale, Overall B
      1.00      1.00
 0.5685E+0 -.2937E-1 0.7269E-2 0.0000E+0 0.0000E+0 0.0000E+0    <- U V W Z X Y
      1.00      1.00      1.00      0.00      0.00      0.00
   9.27953  12.81317   9.17945  90.00000  90.00000  90.00000  0 <- Lattice LAUE
      1.00      1.00      1.00      0.00      0.00      0.00
   0.00000   0.00000   0.00000   0.00000   0.00000 <- Pref.Or[2] Asymm[3]
      0.00      0.00      0.00      0.00      0.00
 0.5435E+0 0.0000E+0 0.0000E+0                    <- Peak Shape NA, NB, NC
      1.00      0.00      0.00
 0.000000 0.000000  1                                    <- FWHMmin FWHMmax IANS
 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 <- Pref.Or.Ellips
      0.00      0.00      0.00      0.00      0.00      0.00
 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 <- Aniso-Size
      0.00      0.00      0.00      0.00      0.00      0.00
 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 0.0000E+0 <- Aniso-Strain
    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
```

From: Software available for reitvelde refinement by Peter Tzvetkov

GSAS

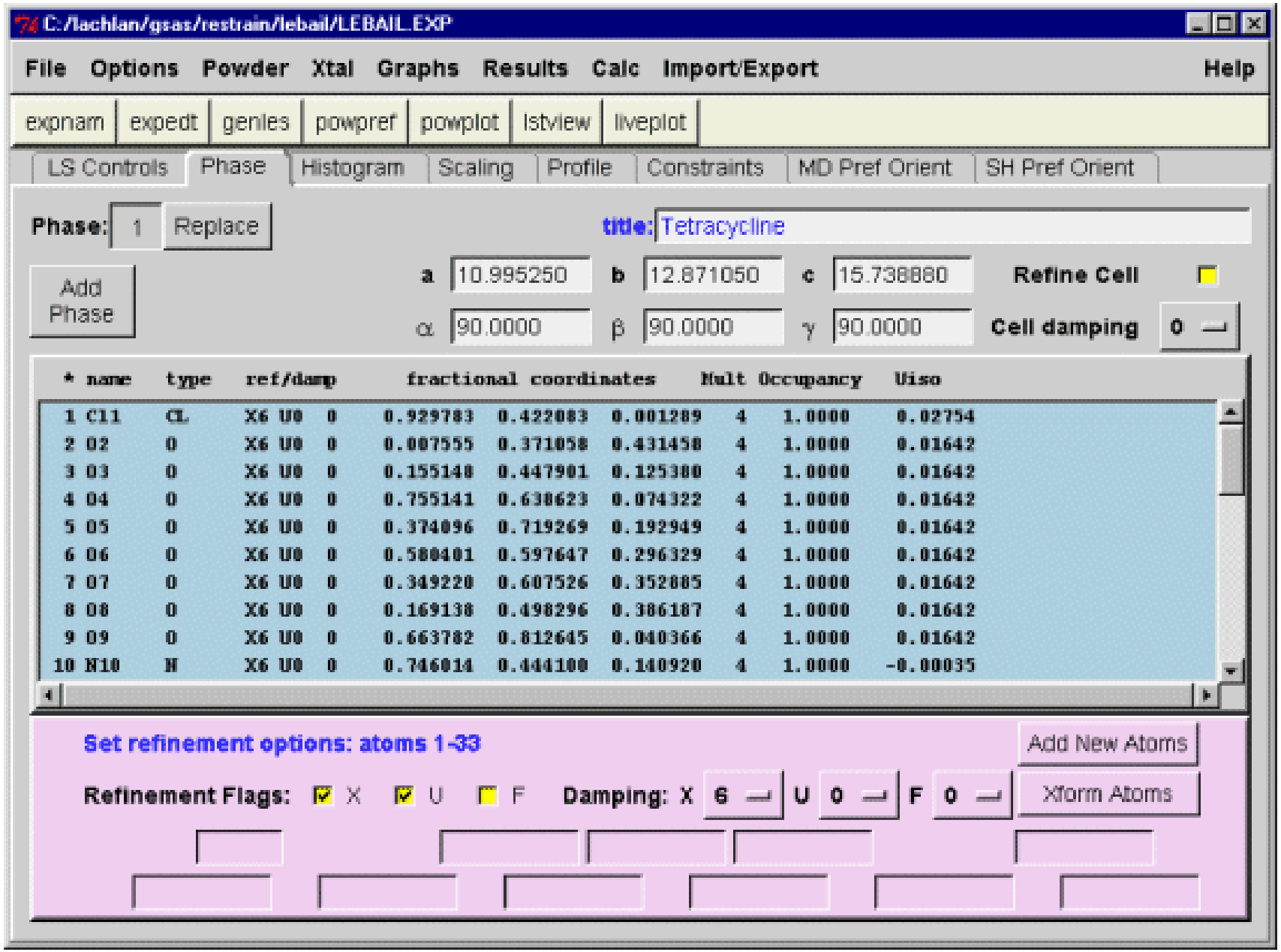
The General Structure Analysis System

- GSAS is a comprehensive system for the refinement of structural models to both x-ray and neutron diffraction data
- GSAS has been created by Allen C. Larson and Robert B. Von Dreele of Los Alamos National Laboratory
- GUI developed by Brian Toby
- Crystallographic analysis
- Quantitative phase determination
- Texture mapping
- Stress-strain measurements

https://subversion.xray.aps.anl.gov/trac/EXPGUI

http://www.aps.anl.gov/Xray_Science_Division/Powder_Diffraction_Crystallography/

From: Software available for reitvelde refinement by Peter Tzvetkov



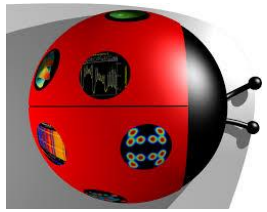
From: Software available for reitvelde refinement by Peter Tzvetkov

GSAS-II

- Open source Python project that addresses all types of crystallographic studies
- Include pretty much all the functionality of GSAS
- Extends the capabilities of GSAS and EXPGUI
- Area-detector data calibration
- Powder diffraction indexing
- Structure solution

https://subversion.xray.aps.anl.gov/trac/pyGSAS
https://www1.aps.anl.gov/Science/Scientific-Software/GSASII

From: Software available for reitvelde refinement by Peter Tzvetkov



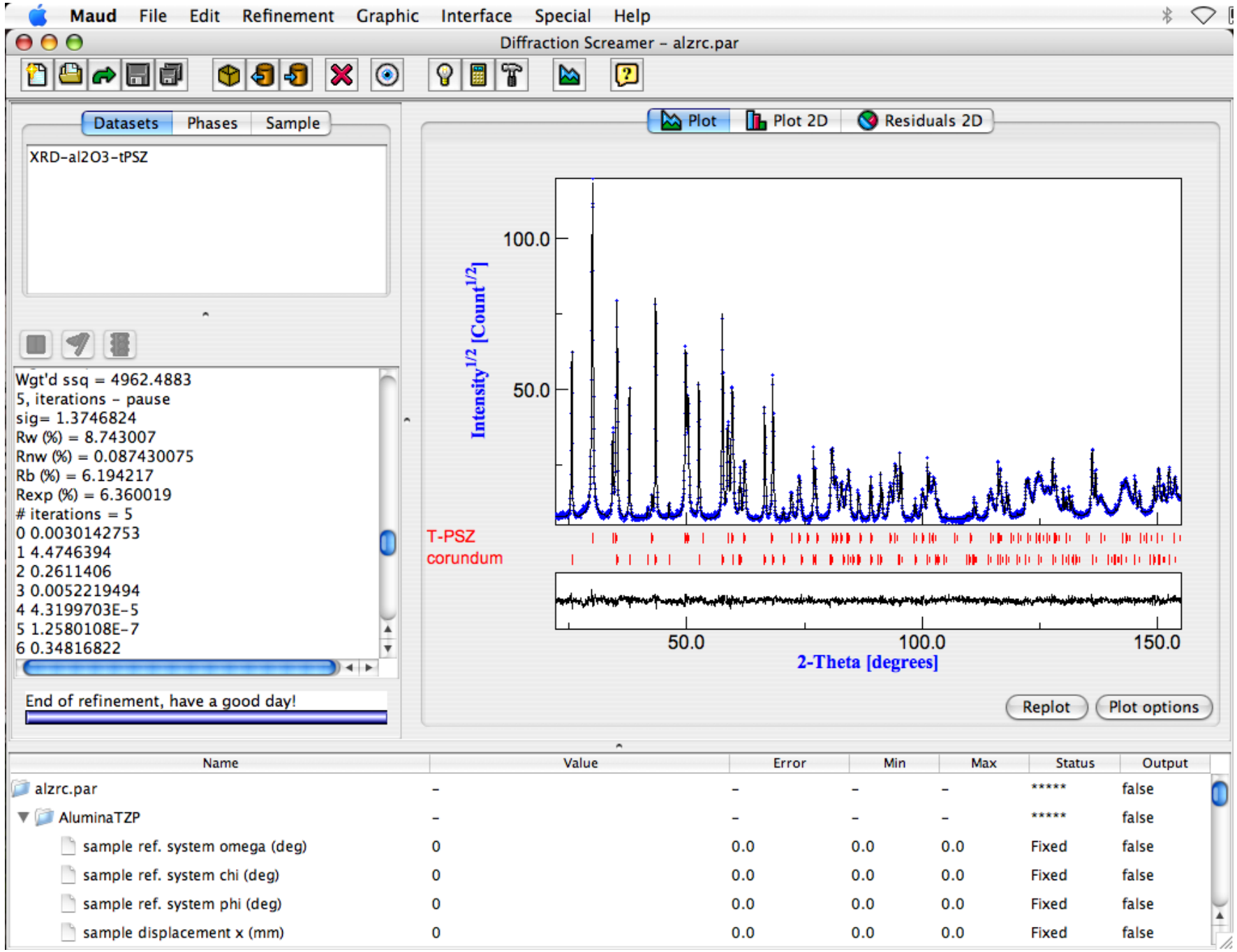
MAUD

Material Analysis Using Diffraction

- Written in Java can run on Windows, MacOSX, Linux, Unix
- Easy to use, every action is controlled by a GUI
- Ab-initio structure solution integration, from peak finding, indexing to solving
- Microstructure analysis (size-strain, anisotropy, planar defects, turbostratic disorder and distributions included)
- Texture and residual stress analysis
- Thin film and multilayer aware; film thickness and absorption models
- Works with TEM diffraction images and electron scattering
- Very well documented with video tutorials in YouTube

Maintained by Luca Lutterotti, Università degli Studi di Trento.

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

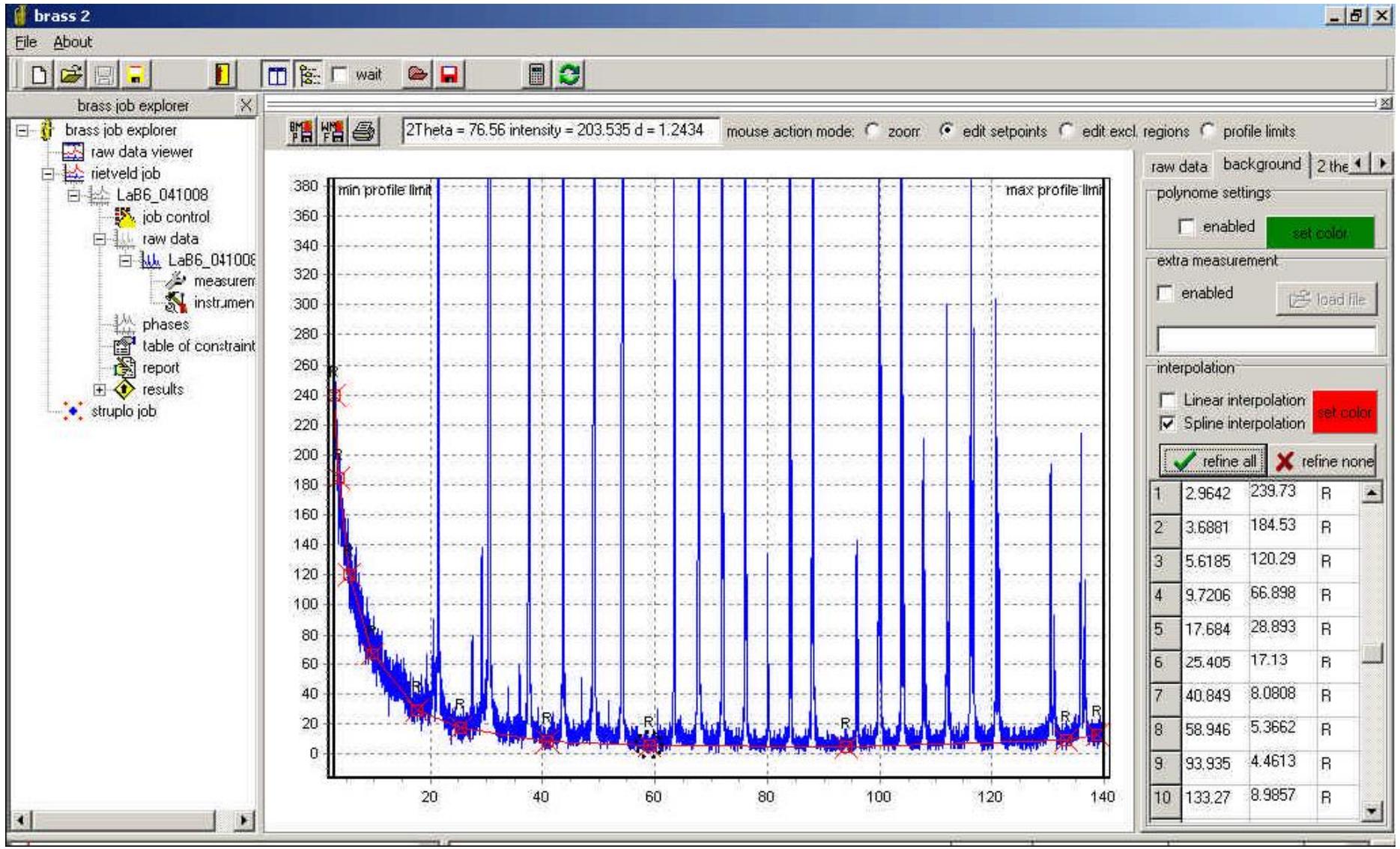
BRASS

Bremen Rietveld Analysis and Structure Suite

- It is a suite of programs covering tasks from raw data display over Rietveld refinement
- Structure completion via Fourier and Grid search methods
- Stress/ strain and crystallite size analysis
- Quantitative phase analysis
- Crystal chemical calculations

Maintained by:
Thomas Messner, Johannes Birkenstock, Reinhard Fischer,
Michael Wendschuh, Christoph Vogt

http://www.brass.uni-bremen.de/



Last version 2.0 (2006).

From: Software available for reitvelde refinement by Peter Tzvetkov

JANA

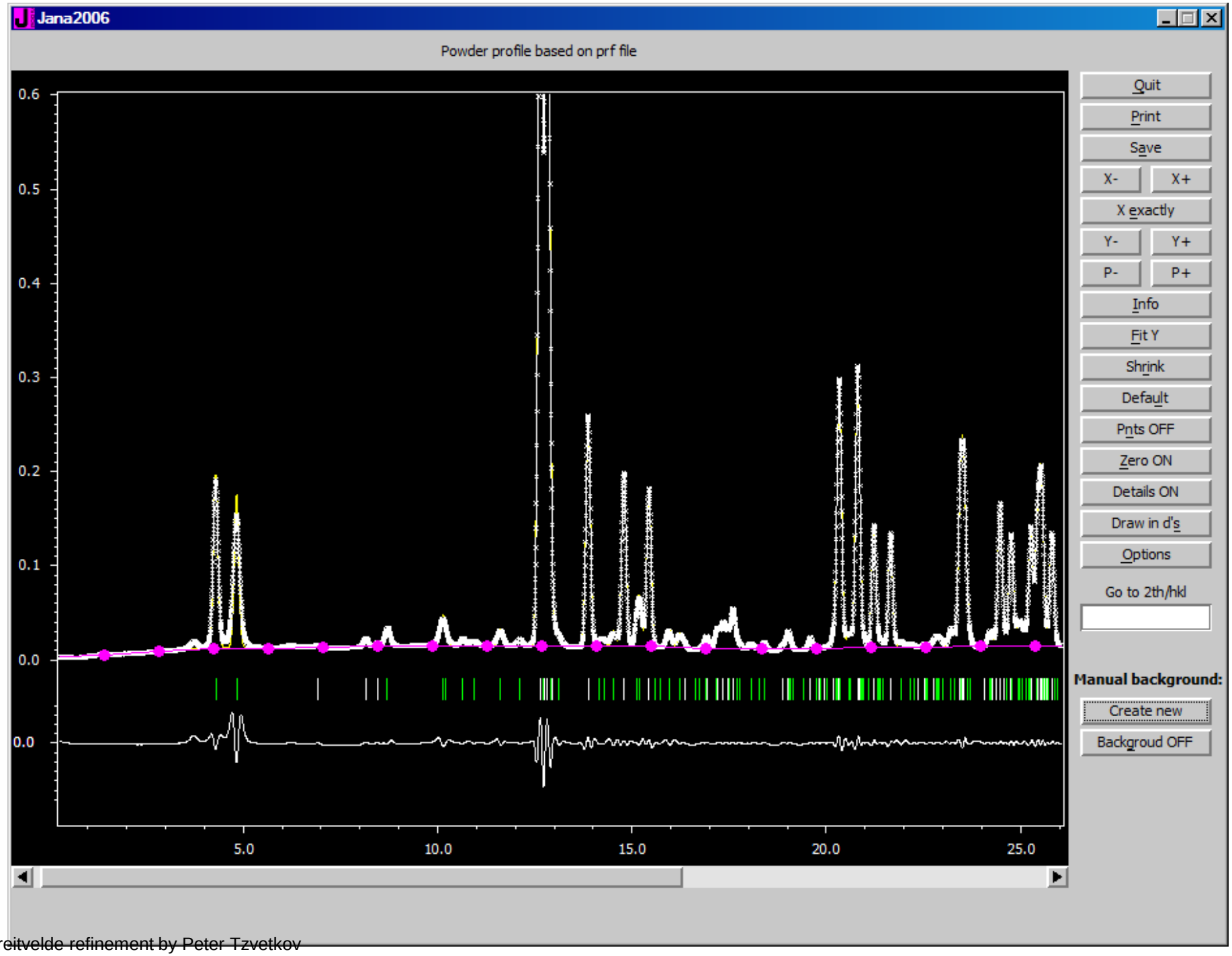
- Jana2006 is a crystallographic program focused to solution, refinement and interpretation of difficult, especially modulated structures
- Built-in charge flipping algorithm
- Commensurate and composite structures
- Transformations for group-subgroup relations and commensurate-supercell relations
- Magnetic structures

Maintained by: Vaclav Petricek, Michal Dusek, Lukas Palatinus

Development of Jana is continuously supported by Grant Agency of the Czech Republic and Academy of Sciences of the Czech Republic. Thanks to this support we can make the program freely available to everybody.

http://jana.fzu.cz/ ; http://www.xrayforum.co.uk/jana

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

EXPO2014

http://wwwba.ic.cnr.it/content/expo

From: Software available for reitvelde refinement by Peter Tzvetkov

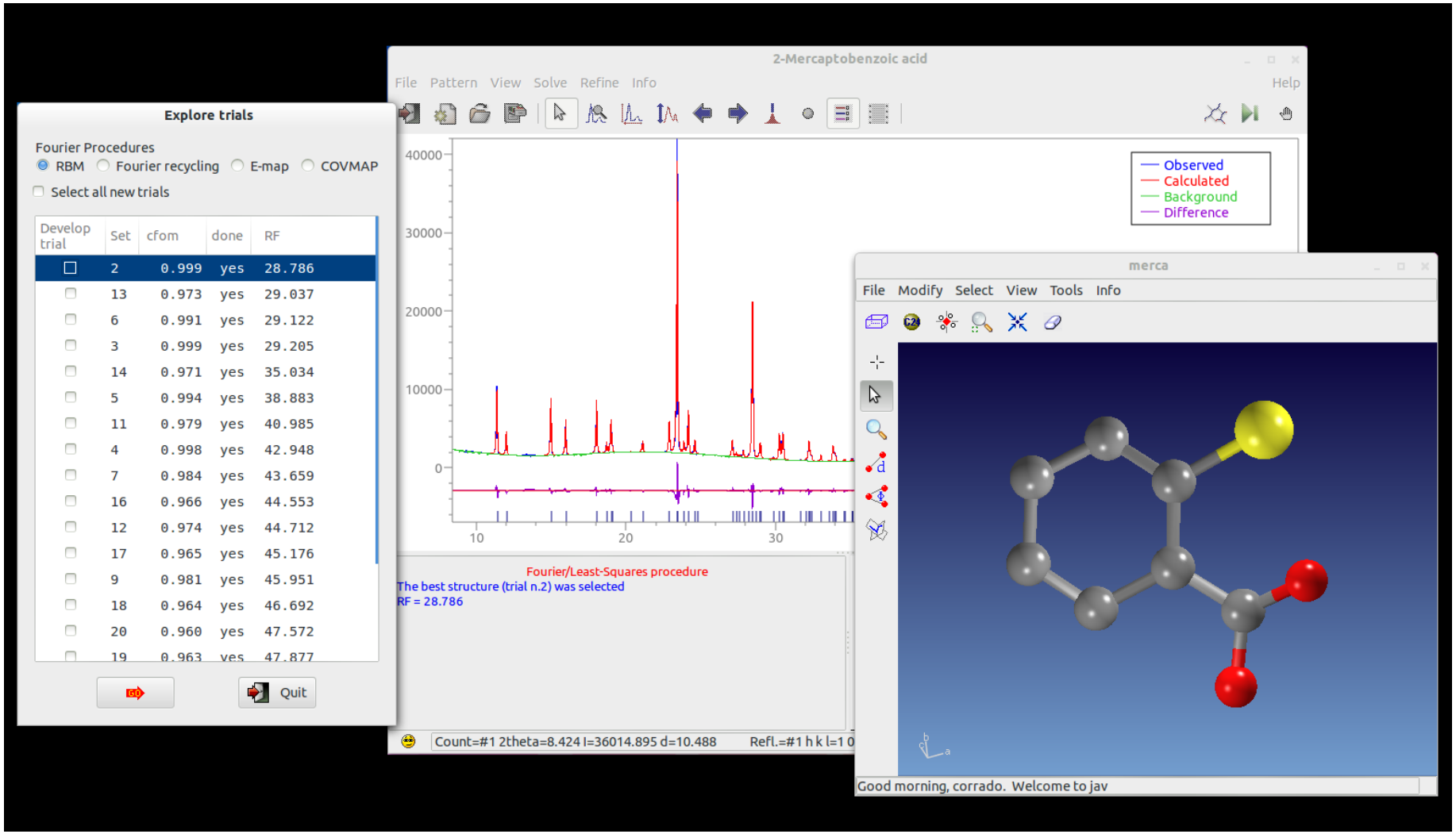
EXPO2014

- Solve crystal structures by powder diffraction data by using reciprocal as well as direct space methods
- Indexing, space group determination, estimation of the integrated intensities, ab-initio and non ab-initio structure solution
- Rietveld refinement
- The EXPO2014 graphical interface has been optimized and made very user friendly

Maintained by Institute of Crystallography, Bari.

http://wwwba.ic.cnr.it/content/expo

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

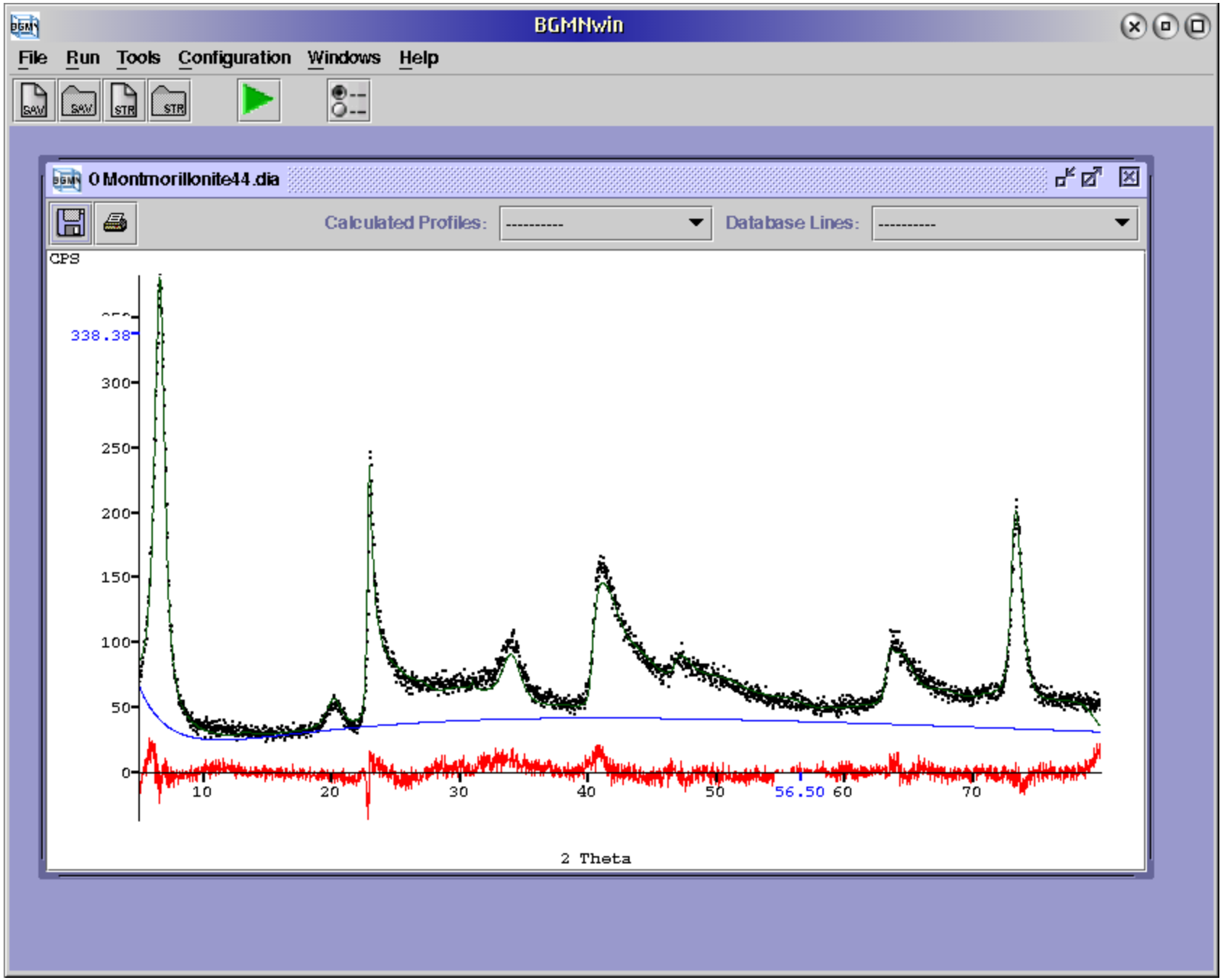
BGMN

- Correction of strong and multiple preferred orientation with spherical harmonics
- Pre-defined models for microstructure related line broadening effects
- Phase analysis of disordered layer silicates/clays
- Calculation of amorphous content by an internal standard method
- Structure interpreter language for free definition of new parameters and constraints between parameters

Sep 9 2010 Dr. Joerg Bergmann passed away.

http://www.bgmn.de/

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

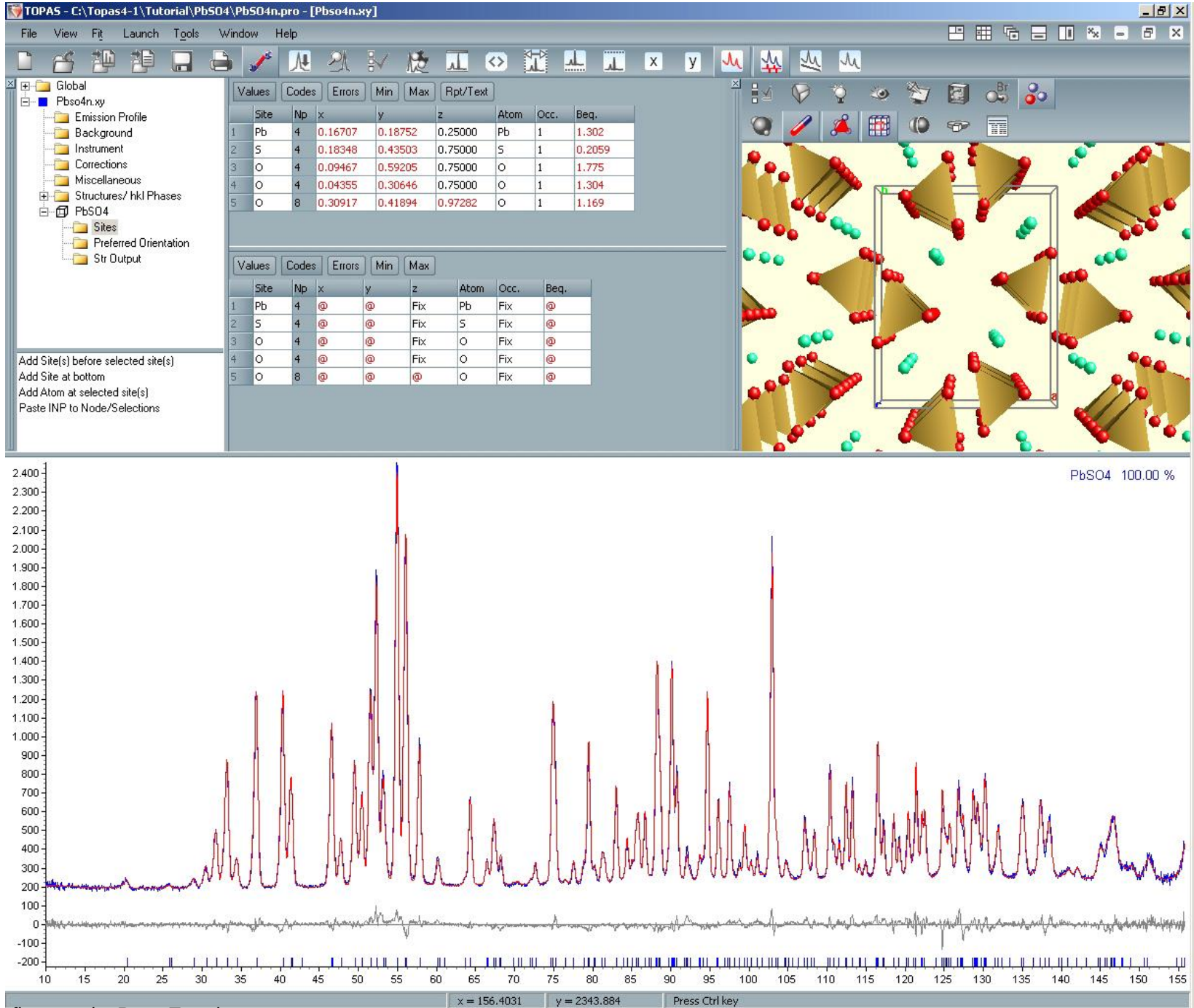
Topas
(DIFFRAC.SUITE Topas)

- Single Line Fitting
- Indexing (LSI and LP-Search methods)
- Whole Powder Pattern Decomposition
- Ab-initio structure determination in direct space from powder and single crystal data
- Rietveld structure refinement
- Magnetic structure

Written by Alan Coelho for Bruker-AXS.

http://www.bruker.com/

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

Mn1-sint3.inp - Notepad

File Edit Format View Help

```
r_exp  1.954 r_exp_dash  4.479 r_wp  6.703 r_wp_dash  15.366 r_p  4.900 r_p_dash  14.982 weighted_Durbin_Watson  0.270 gof  3.430
do_errors
xdd "Mn1-sint3-Rietveld.raw"
        r_exp  1.954 r_exp_dash  4.479 r_wp  6.703 r_wp_dash  15.366 r_p  4.900 r_p_dash  14.982 weighted_Durbin_Watson  0.270 go
        bkg @  2014.43544`_4.56687318 -856.414326`_6.97860072  746.486031`_5.60792133 -368.580635`_5.34107938  241.479248`_5.2791
        LP_Factor( 0)
        Zero_Error(@, -0.00601`_0.00067)
        Rp 217.5
        Rs 217.5
        Slit_Width( 0.1)
        Divergence( 0.3)
        axial_conv
                filament_length  12
                sample_length  15
                receiving_slit_length  12
                primary_soller_angle  2.3
                secondary_soller_angle  2.3
                axial_n_beta  20
                axial_del  0.0053
        lam
                ymin_on_ymax  0.001
                la  0.653817 lo  1.540596 lh  0.501844
                la  0.346183 lo  1.544493 lh  0.626579
        str
                CS_L(@, 77.49377`_8.13728)
                r_bragg  2.52830135
                scale @  0.000399799514`_1.8e-006
                phase_name "PbBaFeMnO5-sint3"
                MVW( 2144.869, 485.654679`_0.0191209841, 100.000`_0.000)
                space_group Pnma
                Phase_LAC_1_on_cm( 1735.49463`_0.06833)
                Phase_Density_g_on_cm3( 7.33369`_0.00029)
Out_CIF_STR(Mn1-sint3.cif)
                a @  5.80033`_0.00012
                b @  3.91074`_0.00010
                c @  21.40995`_0.00047
                site Pb1 num_posns  4 x @  0.04737`_0.00034 y  0.25 z @  0.57047`_0.00009 occ Pb+2  1 beq @  1.6037`_0.0572
                site Ba1 num_posns  4 x @  0.55885`_0.00048 y  0.25 z @  0.68507`_0.00014 occ Ba+2  1 beq @  1.3530`_0.0691
                site Fe1 num_posns  4 x @  0.45567`_0.00127 y  0.25 z @  0.44825`_0.00024 occ Fe+3  1 beq @  0.4360`_0.1533
                site Fe2 num_posns  4 x @  0.93408`_0.00124 y  0.25 z @  0.31408`_0.00037 occ Fe+3  1 beq @  1.5821`_0.1516
                site O1 num_posns  4 x @  0.94114`_0.00325 y  0.75 z @  0.31941`_0.00092 occ O-2  1 beq O1  1.1450`_0.1980
                site O2 num_posns  4 x @  0.65434`_0.00366 y  0.25 z @  0.25725`_0.00105 occ O-2  1 beq =O1; :  1.1450`_0.1980
                site O3 num_posns  4 x @  0.21275`_0.00331 y  0.25 z @  0.39240`_0.00107 occ O-2  1 beq =O1; :  1.1450`_0.1980
                site O4 num_posns  4 x @  0.71715`_0.00331 y  0.25 z @  0.38431`_0.00104 occ O-2  1 beq =O1; :  1.1450`_0.1980
                site O5 num_posns  4 x @  0.42105`_0.00382 y  0.75 z @  0.45658`_0.00086 occ O-2  1 beq =O1; :  1.1450`_0.1980
prm p1  0.00390`_0.01286 min 0.0001
spherical_harmonics_hkl sh
sh_order  6 load sh_Cij_prm {
                        y00   !sh_c00  1.00000
                        y20   sh_c20  -5.09477`_16.85446
```

From: Software available for reitvelde refinement by Peter Tzvetkov

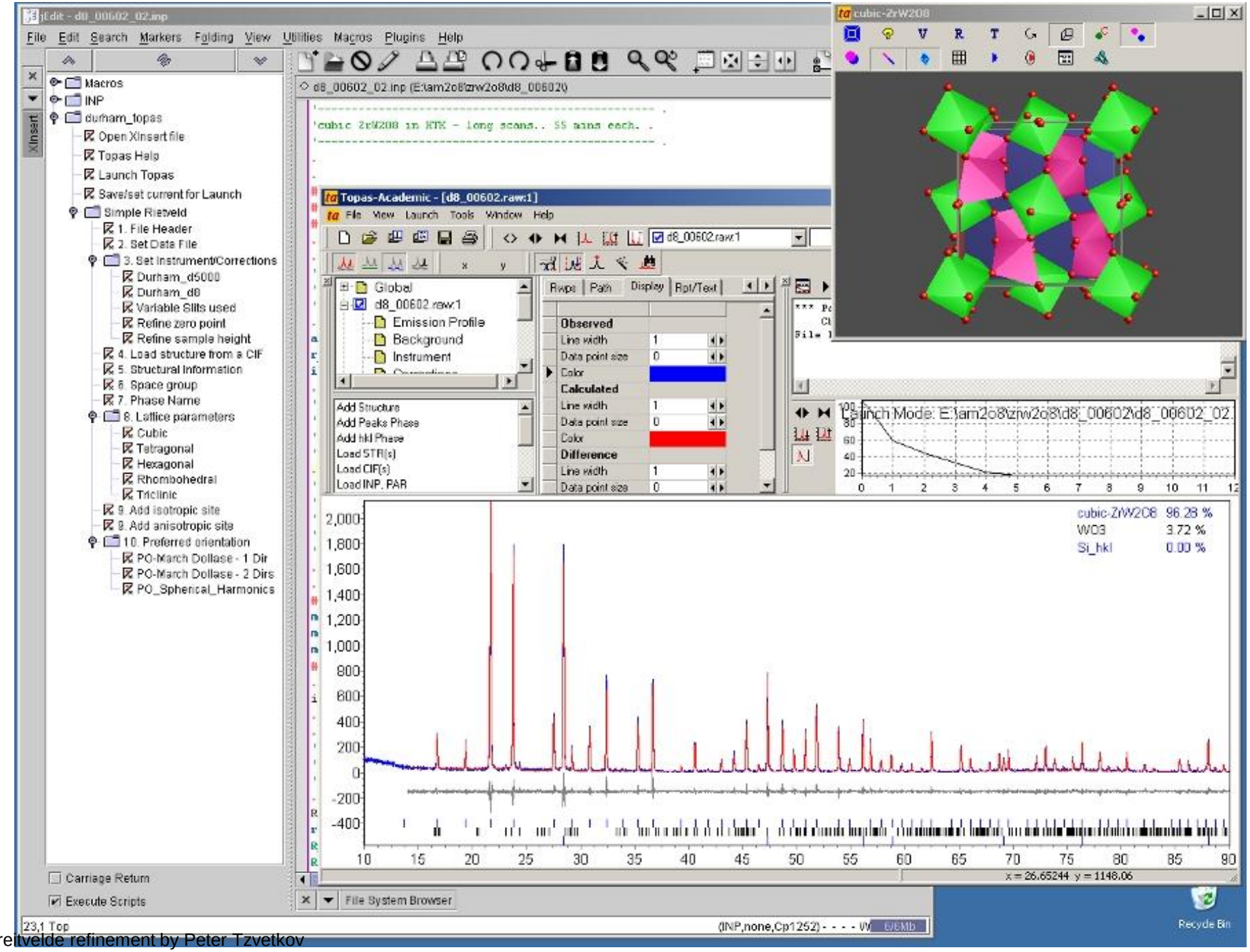
Topas academic

- Available to degree-granting institutions
- Academic comprises all the functionality of BRUKER-AXS TOPAS operating in Launch mode

http://www.topas-academic.net/

John S.O. Evans, Durham University
https://community.dur.ac.uk/john.evans/topas_academic/topas_main.htm

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

X’pert Highscore Plus

- Automated and semi automated Rietveld analysis
- Pawley and Le Bail fits
- Indexing by Dicvol, Treor, Ito and McMaile
- Integrated charge flipping algorithm and electron density display

- *www.panalytical.com*

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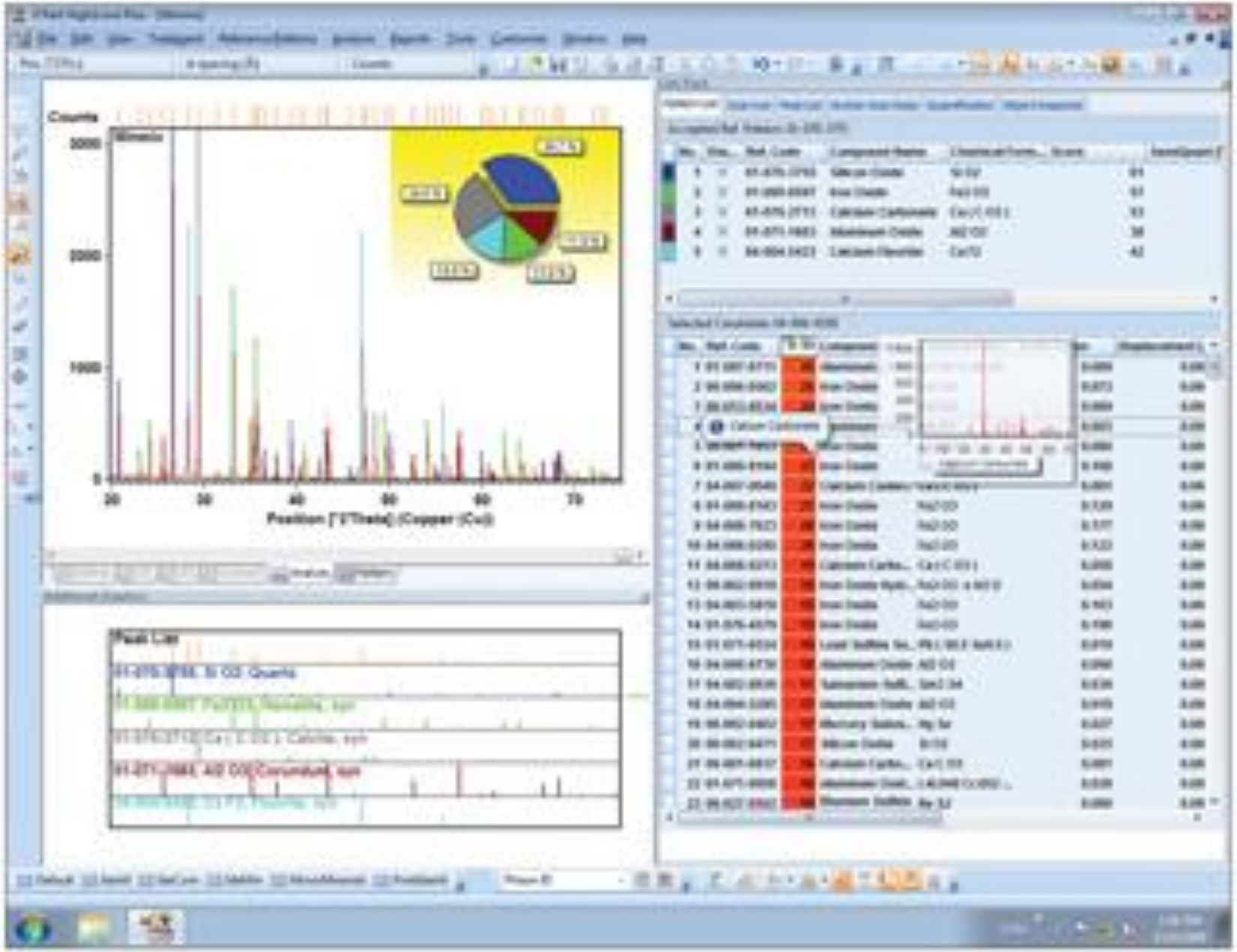

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Rietan

http://fujioizumi.verse.jp/download/download_Eng.html

Rietan-GUI

http://physonit.jp/en/services/rietan-gui/

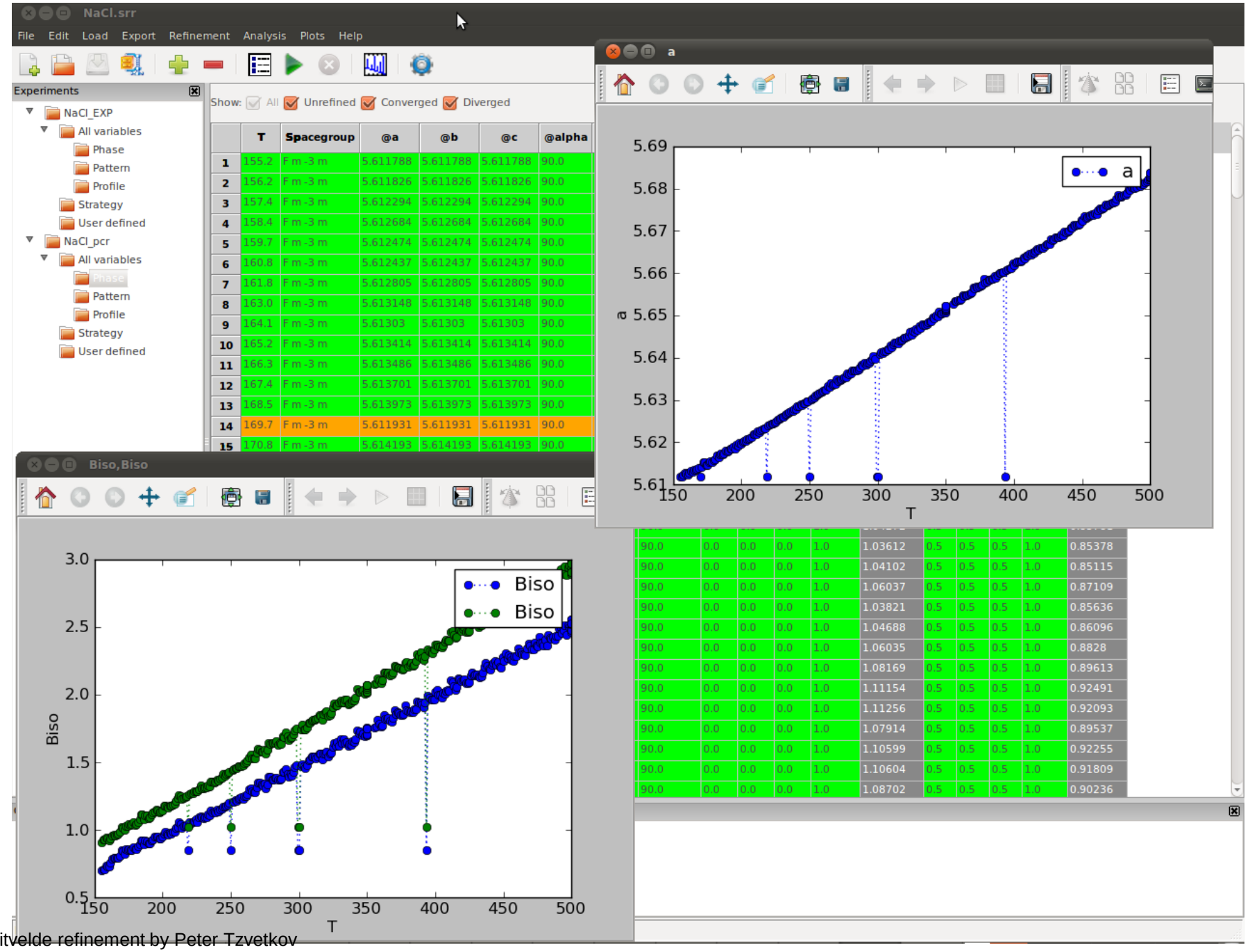
From: Software available for reitvelde refinement by Peter Tzvetkov

SrRietveld

- The program is distributed under the BSD License
- Makes use of the FullProf and GSAS Rietveld refinement engines

http://www.diffpy.org/doc/srrietveld/

From: Software available for reitvelde refinement by Peter Tzvetkov



From: Software available for reitvelde refinement by Peter Tzvetkov

Profex

- Profex is a graphical user interface for Rietveld refinement of powder X-ray diffraction data with the program BGMN
- Generic support for FullProf.2k as an alternative Rietveld backend to BGMN
- Profex runs on Windows, Linux, and Mac OS X

http://profex.doebelin.org/

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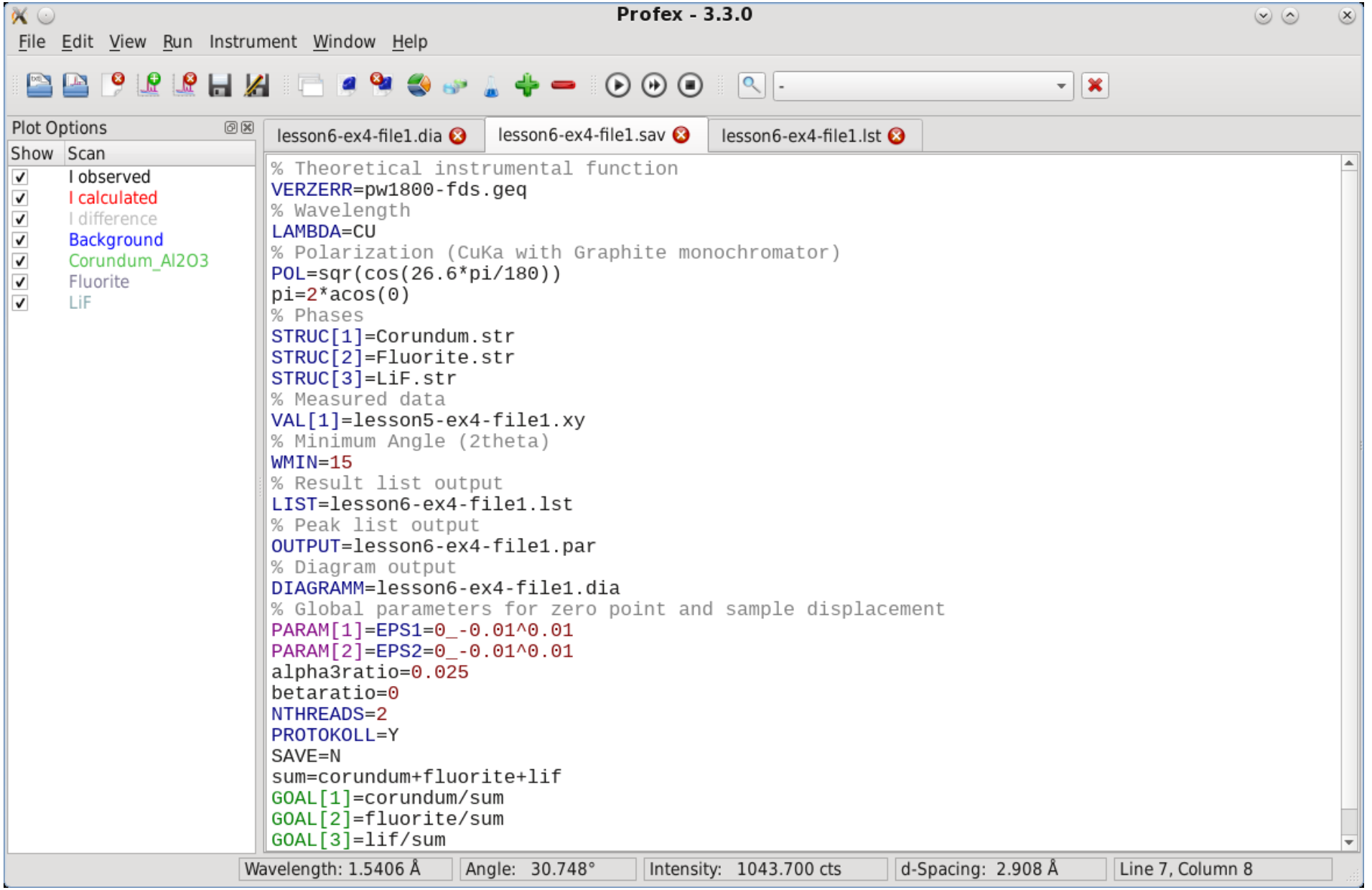

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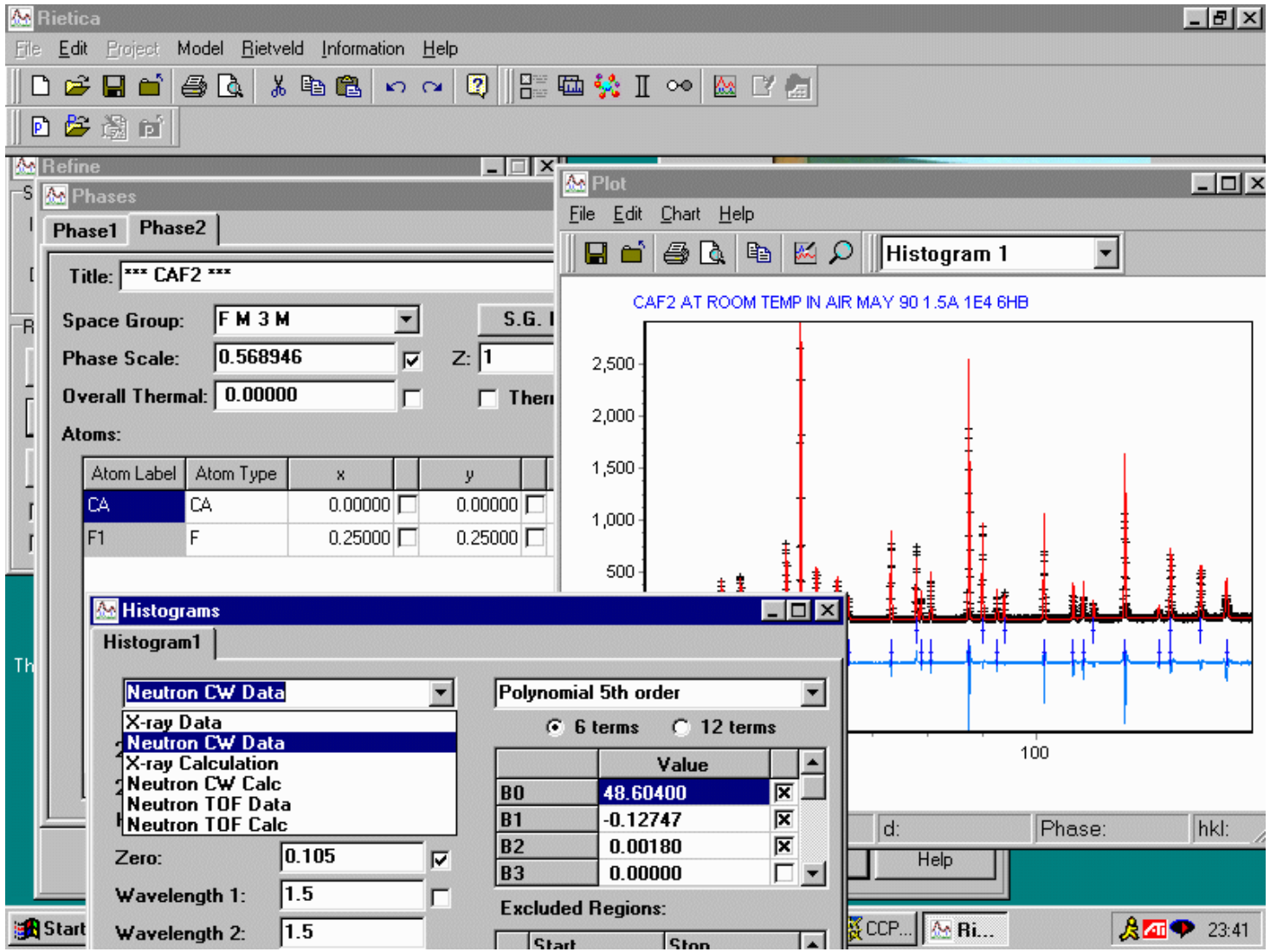

http://www.rietica.org/index.html

From: Software available for reitvelde refinement by Peter Tzvetkov

Xfit-Koalariet

- http://www.ccp14.ac.uk/tutorial/xfit-95/getxfit.htm

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DBWS-9807a

- http://www.ccp14.ac.uk/ccp/web-mirrors/dbws/downloads/young/download_dbws.html

- **DBWSTOOL**

From: Software available for reitvelde refinement by Peter Tzvetkov

Software for simulation and modeling

- ~~Scout software~~
- ~~Crystallography software~~
- DFT codes – Prof. Halima Zaari
- SCAPS software

SCAPS-1D (Solar Cell Capacitance Simulator)

simulation programme developed at the
Department of Electronics and Information Systems (ELIS) of the
University of Gent, Belgium.

Alex Niemegeers, Marc Burgelman, Koen Decock, Stefaan Degrave, Johan Verschraegen

https://scaps.elis.ugent.be/

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Contents lists available at ScienceDirect

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journal homepage: www.cell.com/heliyon

Research article

Numerical study of copper antimony sulphide ($CuSbS_2$) solar cell by SCAPS-1D

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journal homepage: www.elsevier.com/locate/ijleo

Numerical study of lead free $CsSn_{0.5}Ge_{0.5}I_3$ perovskite solar cell by SCAPS-1D

Milimo Amos Nalianya [a,*], Celline Awino [a], Henry Barasa [a], Victor Odari [a], Francis Gaitho [a], Benard Omogo [b], Maxwell Mageto [a]

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Results in Optics 12 (2023) 100470

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journal homepage: www.sciencedirect.com/journal/results-in-optics

Monolith $Cs_{1-x}Rb_xSnI_3$ perovskite – silicon 2T tandem solar cell using SCAPS-1D

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[b] Department of Physics, Masinde Muliro University of Science and Technology, P.O. Box 190-50100, Kakamega, Kenya
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http://journals.uonbi.ac.ke/index.php/ajps/index

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Device Simulation of Sb_2S_3 Solar Cells by SCAPS-1D Software

ODARI, Victor [1,2a*], MUSEMBI, Robinson [1, b] and MWABORA Julius [1, c]

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[2]Department of Physics, School of Natural and Applied Sciences, Masinde Muliro University of Science and Technology, P.O. Box 190-50100 Kakamega, Kenya.

OghmaNano (Organic and hybrid Material Nano Simulation tool)

https://www.oghma-nano.com/