



COherent NUclear Scattering from Single crystals

**Software for the evaluation of
Synchrotron Mössbauer Spectra**

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About CONUSS:

- developed 1983-1986 by E. Gerdau and W. Sturhahn at the University of Hamburg
 - ☆ coherent elastic nuclear and electronic Bragg scattering
 - ☆ explain first NRS experiments (Gerdau et al. PRL 54, 1985)
 - ☆ FORTRAN code implemented on IBM 360 mainframe (MVS-VM)

- improved 1986-today by W. Sturhahn and supported by the University of Hamburg (1986-1993), ESRF (1992), APS (1992-2010), MPI-Halle (2012-2013)
 - ☆ forward scattering (SMS a.k.a. NFS) added in 1991
 - ☆ ported to Sun UNIX in 1992
 - ☆ extended data handling capability (fitting) added in 1996
 - ☆ ported to Linux in 2004, to OS X in 2011
 - ☆ grazing incidence scattering (GINS) added in 2014

publications related to CONUSS:

W. Sturhahn and E. Gerdau, Phys. Rev. B 49 (1994)

W. Sturhahn, Hyperfine Interact 125 (2000)

More on CONUSS:

- has been used for data evaluation in numerous publications
- distributed under GPL, source code public, evaluations traceable
- can be obtained at <http://www.nrixs.com> – no charge
- a major upgrade, CONUSS-2.0.0, was released in 2010
 - ☆ simple installation procedure for Unix and Mac OS X
 - ☆ all previous capabilities of CONUSS
 - ☆ enhanced fit capabilities & run-time graphics
 - ☆ new Monte Carlo approach to find start-values, explore the parameter space, and smart parameter optimization
- CONUSS-2.1.0 was released in 2015
 - ☆ support of grazing incidence geometry
 - ☆ input parameter simplifications
- CONUSS-2.1.1 is the present version
 - ☆ systematic output file naming
 - ☆ dual fit for isomer shift determination from SMS

CONUSS now supports:

- all Mössbauer isotopes
- forward scattering, grazing incidence, and Bragg/Laue reflections
- no limitations by sample structure
- combined hyperfine interactions
- distributions of hyperfine fields
- textures
- relaxation effects
- full polarization and directional dependences
- thickness effects
- time spectra (SMS) and energy spectra (trad. Mössbauer spectr.)
- sample combinations
- time, energy, and angle averaging
- sample thickness distributions
- comparison to experimental data including fitting
- flexible assignment and grouping of fit parameters

CONUSS provides solutions:

problem	program	SIF	examples
fitting data forward scattering dual fit Mössbauer spectroscopy grazing incidence Bragg/Laue diffraction	kctl	in_kctl in_kfor in_kfor in_kfor in_kgin in_kref	kctl-NFS1, kctl-NFS2 kctl-NFS3 kctl-MBS1, kctl-MBS2 kctl-GINS kctl-NBS1, kctl-NBS2
explore parameter space forward scattering or Mössbauer grazing incidence Bragg/Laue diffraction	kmco	in_kmco in_kfor in_kgin in_kref	kmco-NFS kmco-GINS kmco-NBS
calculate spectra forward scattering or Mössbauer grazing incidence Bragg/Laue diffraction	kfmf kgmf krmf	in_kfor in_kgin in_kref	kfmf-NFS, kfor-NFS kgmf-GINS, kgmf-GIS krmf-NBS

KCTL app screen shot:

The screenshot shows the KCTL application running on a Mac. The main window displays a plot of residuals (σ) and counts over time (ns). The plot shows a series of peaks and troughs, with the residuals fluctuating around zero. The counts are plotted on a logarithmic scale. The plot is titled "Iteration step 5 -- $\chi^2 = 2.782$ ".

The left panel shows the command-line interface with the following output:

```
[kctl-NFS1]: kctl
++ CONUSS-2.1.1 Copyright (C) 2016 Wolfgang Sturhahn
++ This program comes with ABSOLUTELY NO WARRANTY.
++ This is free software.
++ You may redistribute it under certain conditions.
++ For details see <http://www.gnu.org/licenses/>.

--- CONUSS module KCTL data section size: 1829.3 Mb
--- execution starting..

--- reading standard input file 'in_kctl'
--- reading file 'in_kfor'
--- reading file 'kforParams.txt'
--- reading file 'Fe.mif'
--- reading file 'in_kmix'
--- reading file 'in_kfit'

iteration   Quality   ChiA2
start      2.141E+02   124.130
# 1 N      9.562E+00   11.143
# 2 N      3.467E+00   4.670
# 3 N      1.794E-01   2.875
# 4 N      4.411E-04   2.782
Final      2.782

Results -->
Normalized ChiA2 value: 2.78 +- 0.08

parameter name  ##  value  +- error  % error
thickness (micron)  1  9.75540-01 +- 4.30-03  0.444
Bhf              2  3.26800+01 +- 3.40-03  0.010
[70,90] Theta    3  8.25860+01 +- 1.70-01  0.207
[-5,5] Phi       4  -1.16570+00 +- 1.90-01  16.373
[80,100] Texture  5  9.55920+01 +- 1.60-01  0.169
scaling factor    6  2.85350+04 +- 1.50+02  0.576
energy/time resolution FW  7  3.40870-01 +- 1.40-02  4.148

Error estimates give a 68% confidence interval.

Error correlation matrix -->
## | 1 2 3 4 5 6 7
1 | 1 -0.158 -0.017 -0.061 -0.201 -0.945 0.081
2 | -0.158 1 0.173 0.004 -0.104 0.145 0.847
3 | -0.017 0.173 1 0.247 -0.042 0.036 0.147
4 | -0.061 0.004 0.247 1 -0.141 0.059 -0.139
5 | -0.201 -0.104 -0.042 -0.141 1 0.069 -0.154
6 | -0.945 0.145 0.036 0.059 0.069 1 -0.084
7 | 0.081 0.847 0.147 -0.139 -0.154 -0.084 1

Smallest eigenvalues of Fisher information matrix -->
Fixed | none 1 2 3 4 5 6 7
none | 2 2 6 2 2 2 2 2
1 | 2 2 6 3 4 2 2 2
2 | 2 2 3 4 2 2 2 2
3 | 2 2 2 6 2 2 2 2
4 | 2 2 2 2 6 2 2 2
5 | 2 2 2 2 2 6 2 2
6 | 2 2 2 2 2 2 6 2
7 | 2 2 3 3 3 2 2 3 5 2

--- CPU time : user 0.43 s system 0.04 s
--- CONUSS module KCTL finished

[kctl-NFS1]2: █
```

The right panel shows a file browser window with the following table:

Name	Size	Access	Date Modified
Results		-- drwxr-xr-x (755)	11/19/2016, 13:32
Fe_exp.dat	21 KB	-rw-r--r-- (644)	11/19/2016, 14:40
Fe_fit.dat	15.4 KB	-rw-r--r-- (644)	11/19/2016, 14:40
Fe_fsh.dat	904 bytes	-rw-r--r-- (644)	11/19/2016, 14:40
Fe_kctl_ptl.txt	3.8 KB	-rw-r--r-- (644)	11/19/2016, 14:40
Fe_kctl.csv	2 KB	-rw-r--r-- (644)	11/19/2016, 14:40
Fe_kfor_log.txt	4.5 KB	-rw-r--r-- (644)	11/19/2016, 14:40
Fe_rsd.dat	15.1 KB	-rw-r--r-- (644)	11/19/2016, 14:40
Fe.dat	6.6 KB	-rw-r--r-- (644)	11/19/2016, 13:32
Fe.mif	1.7 KB	-rw-r--r-- (644)	11/19/2016, 14:22
Fe.mif~	1.7 KB	-rw-r--r-- (644)	11/19/2016, 13:32
in_kctl	851 bytes	-rw-r--r-- (644)	11/19/2016, 13:32
in_kfit	3.7 KB	-rw-r--r-- (644)	11/19/2016, 14:21
in_kfit~	3.7 KB	-rw-r--r-- (644)	11/19/2016, 14:21
in_kfitB	3.7 KB	-rw-r--r-- (644)	11/19/2016, 14:21
in_kfor	944 bytes	-rw-r--r-- (644)	11/19/2016, 13:32
in_kmix	3.2 KB	-rw-r--r-- (644)	11/19/2016, 13:32
kforParams.txt	490 bytes	-rw-r--r-- (644)	11/19/2016, 14:16

The bottom right panel shows the contents of the 'Fe.mif' file:

```

short material input file of program package CONUSS

fit parameters
=====
* first number: start value
* second number: optional, but if given then
  first number becomes prior
  second number becomes prior variation
* @ Bhf := 33
* @ [70,90] Theta := 80
* @ [-5,5] Phi := -1[]
* @ [80,100] Texture := 95
* -----1-----2-----3-----4-----5-----6-----7----->

Material
=====
(1) composition :: Fe
(2) density (g/cm^3) :: 8
(3) MB data file :: Fe57.mbt
(4) abundance of the MB atom :: 0.95
(5) Lamb-Mössbauer factor :: 0.796

--:-- Fe.mif Top (18,26) (Fundamental)
Wrote /Users/wolfgang/CONUSS-2.1.1/examples/kctl-NFS1/Fe.mif
  
```