NRIXS software

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

KCTL app screen shot: