CONUSS

***CO**herent **NU**clear **S**cattering from **S**ingle crystals*

Software for the evaluation of Synchrotron Mössbauer Spectra

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Scattering channels:

initial state → intermediate state → final state

$$|\gamma_i\rangle|\Psi_i\rangle \longrightarrow |\Psi_n\rangle \longrightarrow |\gamma_f\rangle|\Psi_f\rangle$$

$$|\gamma_i\rangle|\Psi_i\rangle = |\chi_i\rangle\Pi_j|\phi_j^{(i)}\rangle \qquad |\gamma_f\rangle|\Psi_f\rangle = |\chi_f\rangle\Pi_j|\phi_j^{(f)}\rangle$$

lattice nucleus & core electrons

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incoherent

$$|\phi_j^{(i)}\rangle \neq |\phi_j^{(f)}\rangle$$

coherent elastic

$$|\Psi_i\rangle = |\Psi_f\rangle$$

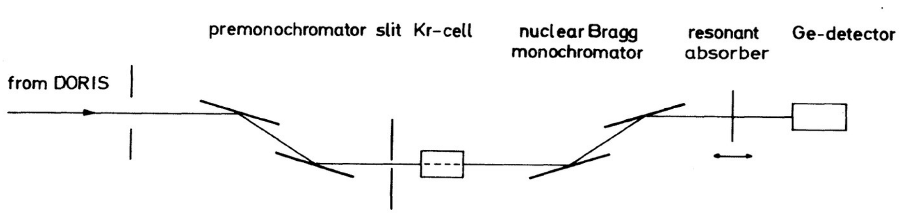
- PHOENIX software
  - ☆ supported since 1995, 29 years
  - ☆ tutorials in 2008, 2012, 2014, 2016, 2018
- CONUSS software
  - ☆ supported since 1985, 39 years
  - ☆ tutorials in 2005, 2012, 2014, 2016, 2017, 2023

Coherent elastic scattering:

➢ NBS – Nuclear Bragg Scattering

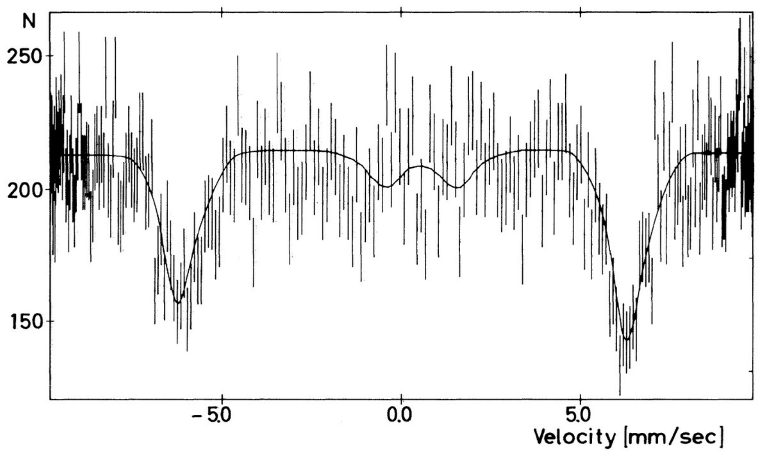
- introduced in 1985
  E.Gerdau et al., Phys.Rev.Lett. 54 (1985)
- uses (pure) nuclear Bragg reflections
- few applications due to need for high-quality single crystals

experimental setup



E.Gerdau et al., Phys.Rev.Lett. 54 (1985)

first Mössbauer spectrum using synchrotron radiation



https://www.nrixs.com/pdf/nrs_hamburg_2015.pdf

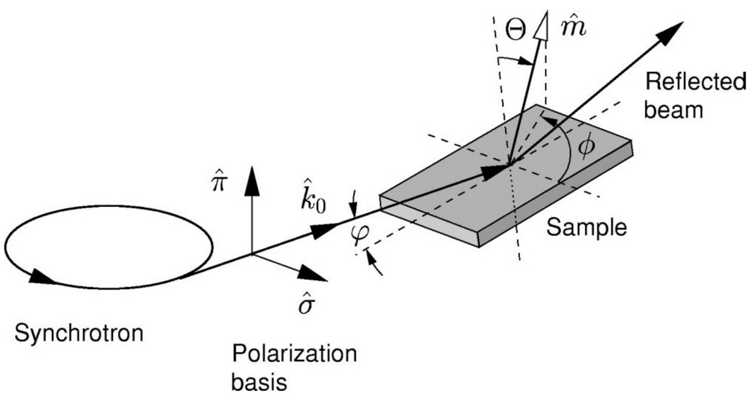
Coherent elastic scattering:

- GINRS – Grazing Incidence Nuclear Resonant Scattering

  - introduced in 1991

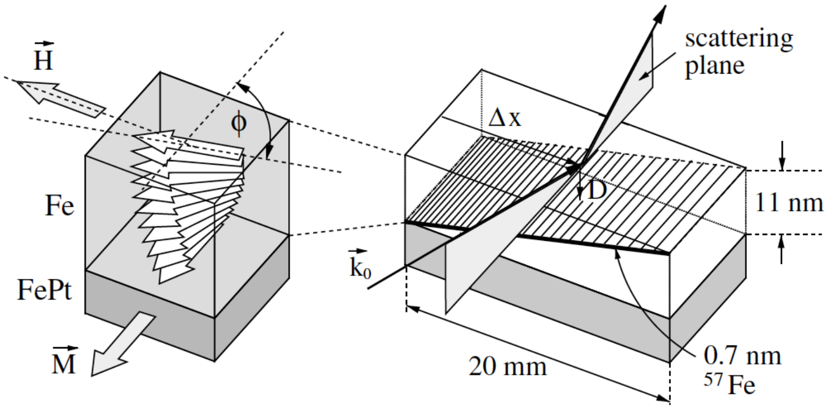
    M.Grote et al., Europhys.Lett. 17 (1991)
  - uses specular reflection off thin films containing Mössbauer isotopes
  - applications in magnetism of nano-structures

experimental setup



R.Röhlsberger et al., Phys.Rev. B 67 (2003)

study of spin structures

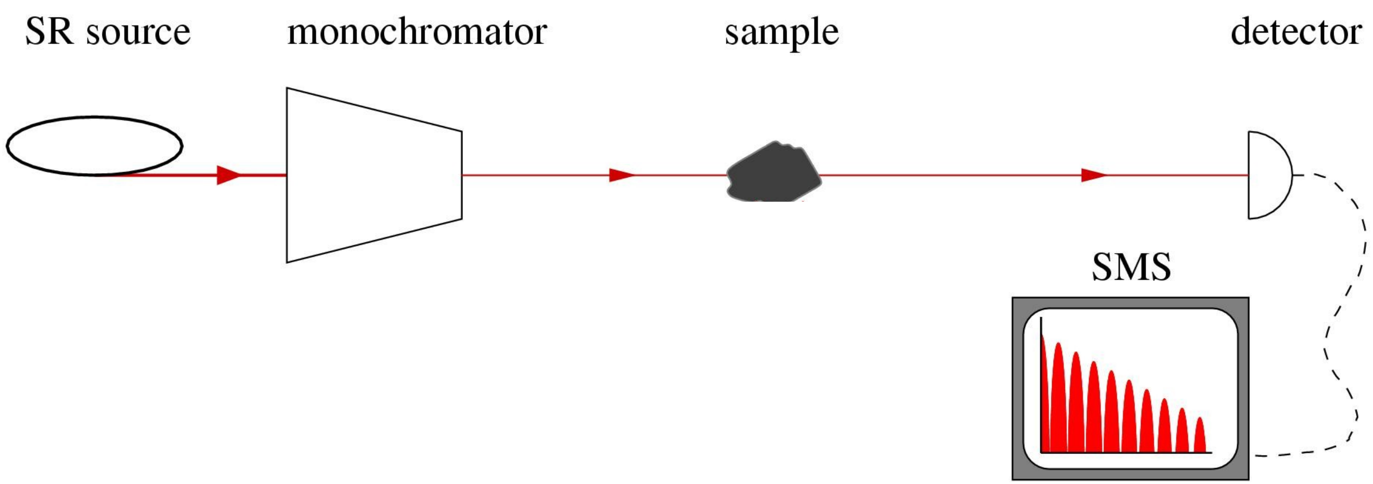


R.Röhlsberger et al., Phys.Rev.Lett. 89 (2002)

Coherent elastic scattering:

- tSMS – time-resolved Synchrotron Mössbauer Spectroscopy
  (a.k.a. NFS)

  - ✰ introduced in 1991
    J.Hastings et al., Phys.Rev.Lett. 66 (1991)
  - ✰ internal magnetic fields, electric field gradients, isomer shifts
  - ✰ applications include magnetic phase transitions,
    determination of spin & valence states, and melting studies
  - ✰ requires appropriate time structure



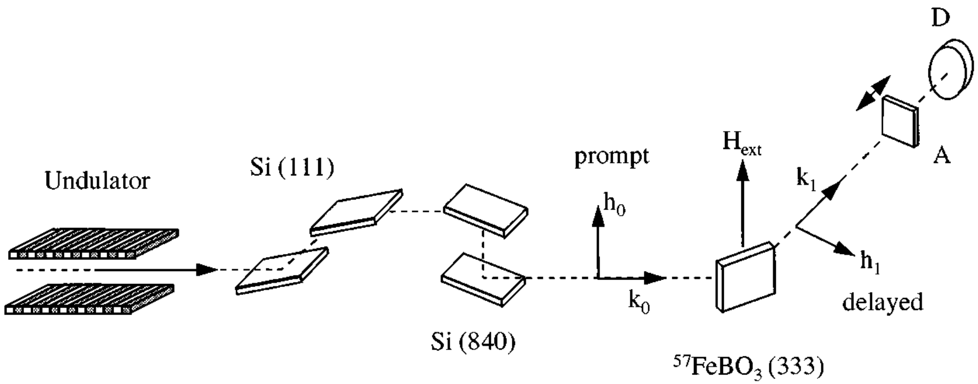
https://www.nrixs.com/pdf/sms_intro17.pdf

Coherent elastic scattering:

➢ eSMS – energy-resolved Synchrotron Mössbauer Spectroscopy

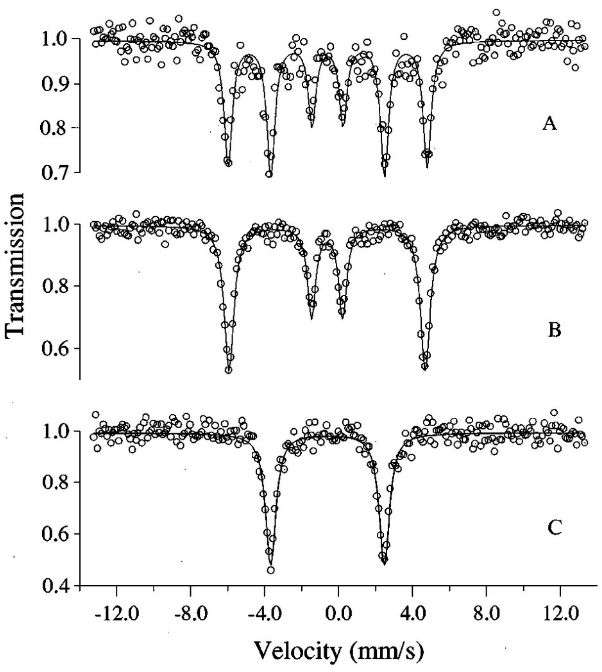
- introduced in 1997
  G.V.Smirnov et al., Phys.Rev. B 55 (1997)
- pure nuclear Bragg reflections create narrow-bandwidth x-ray
- polarization filtering methods are now developed (see talk by T.S.Toellner)

experimental setup



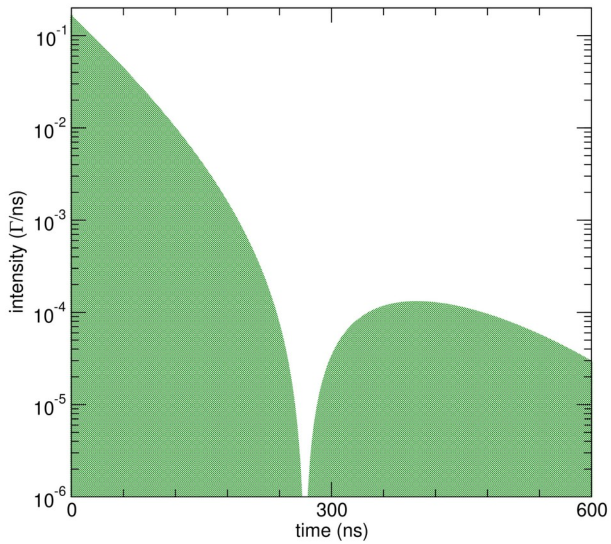
G.V.Smirnov et al., Phys.Rev. B 55 (1997)

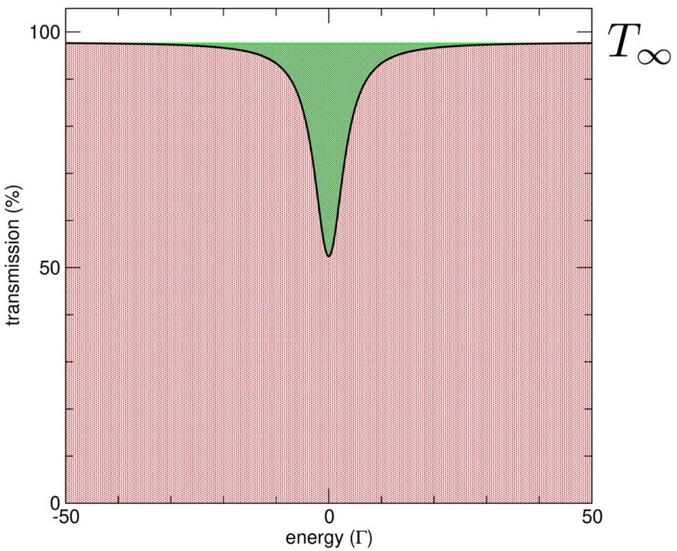
velocity spectrum



tSMS versus eSMS:

- time structure of storage ring: tSMS requires special timing modes
- statistical quality (inverse relative error) of a measured spectrum





$$Q_t = \sqrt{N_{t,tot}}$$

$$Q_e = \sqrt{N_{e,tot}\,\frac{(T_\infty - \langle T \rangle)^2}{T_\infty \langle T \rangle}}$$

$$\Delta = 0.002$$

- evaluation capabilities → CONUSS

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 MacOS in 2011
  - ✰ grazing incidence scattering (GINS) added in 2015

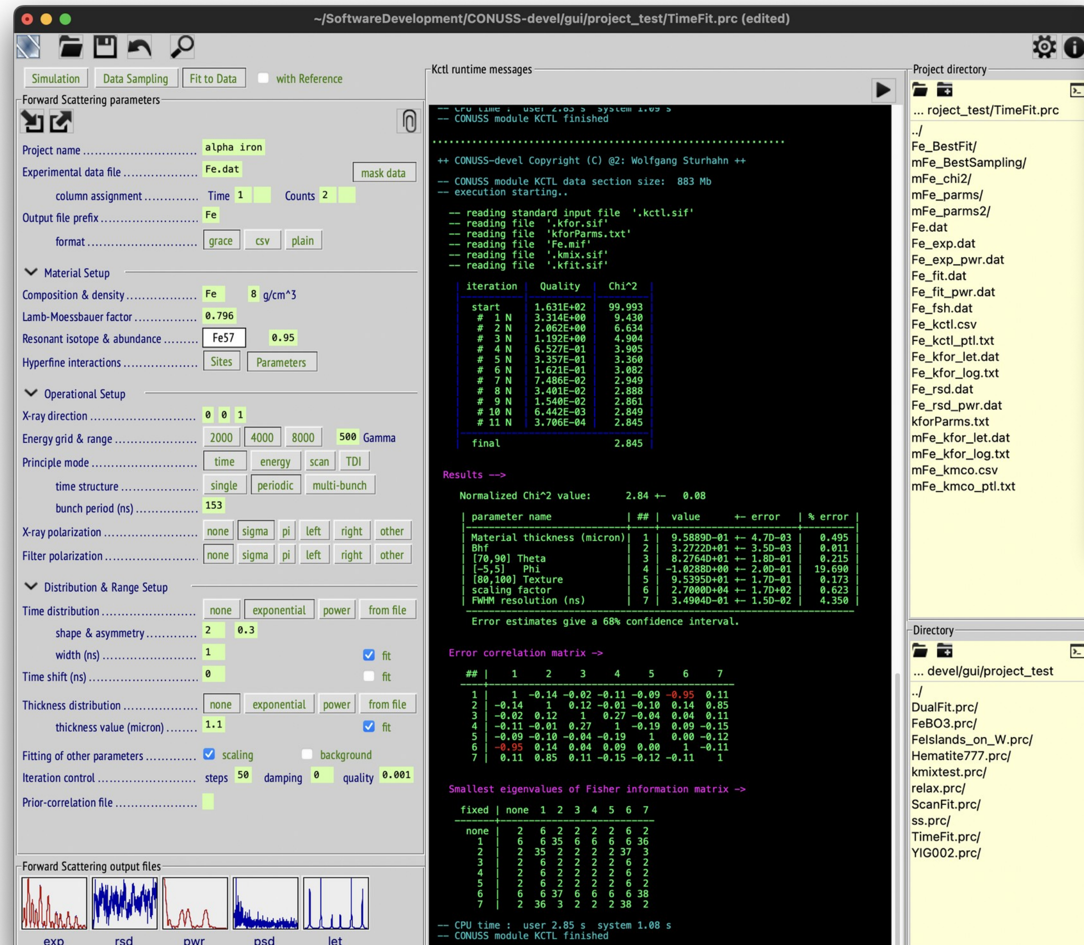
publications related to CONUSS:
W. Sturhahn and E. Gerdau, Phys. Rev. B 49 (1994)
W. Sturhahn, Hyperfine Interact 125 (2000)

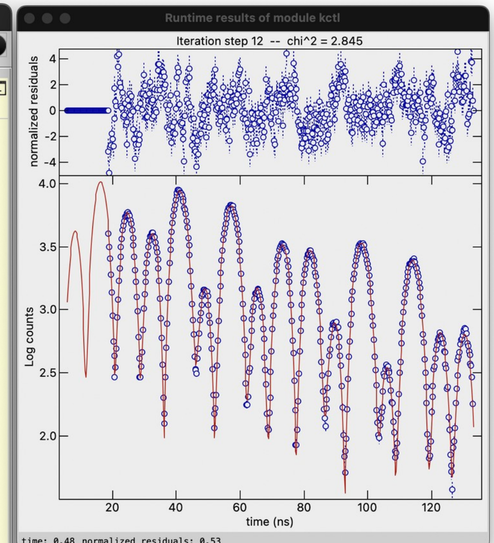
More on CONUSS:

- has been used for data evaluation in numerous publications
- distributed under GPL, source code public, evaluations traceable
- can be obtained at https://www.nrixs.com – no charge
- a major upgrade, CONUSS-2.0.0, was released in 2010
  - ☆ simple installation procedure for Linux and MacOS
  - ☆ all previous capabilities of CONUSS
  - ☆ enhanced fit capabilities & run-time graphics
  - ☆ new Monte Carlo approach to find fit start-values, explore the parameter space, and perform smart parameter search
- CONUSS 2.1.0, 2.1.1, 2.2.0, 2.2.1, 2.3.0 released 2015 to 2023
  - ☆ support of grazing incidence geometry
  - ☆ input parameter simplifications
  - ☆ dual fit mode, absorber scan modes
  - ☆ user-defined source profiles
  - ☆ kdec module for deconvolution of multi-line source profiles
  - ☆ time-domain-interferometry mode
- CONUSS-3.0.0 with GUI released 2024

The CONUSS GUI:

- GUI upgrade, CONUSS-3.0.0, supported by Caltech
  - ☆ translates functionality into Tcl/Tk for Unix and MacOS
  - ☆ maintains all previous capabilities of CLI
  - ☆ enhancements of core modules





- Thanks to Jennifer Jackson and her group at Caltech for ongoing tests of the software and discussions regarding improvements

CONUSS now supports:

- all Mössbauer isotopes, user-defined isotope data
- forward scattering, grazing incidence, and Bragg/Laue reflections
- no limitations by sample structure
- combined hyperfine interactions
- distributions of hyperfine fields
- orientational distributions (textures)
- Blume-Tjon magnetic hyperfine field relaxation
- full polarization and directional dependences
- thickness effects
- time-resolved Mössbauer spectra (tSMS)
- energy-resolved Mössbauer spectra (eSMS and traditional)
- sample combinations with optional scanning, TDI mode
- 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	example directory
fitting data	kctl	in_kctl	
forward scattering, time spectra		in_kfor	kctl-NFS1, kctl-NFS2
dual fit		in_kfor	kctl-NFS3
forward scattering, energy spectrum		in_kfor	kctl-NFS4
forward scattering, TDI spectrum		in_kfor	kctl-TDI
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-NBS1, krmf-NBS2