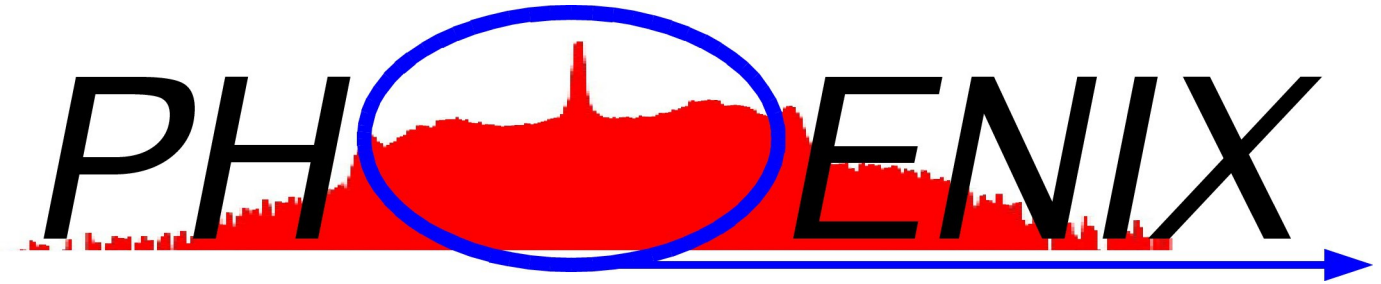
NRIXS software



PHOnon Excitation by Nuclear Inelastic X-ray scattering

Software for the evaluation of Nuclear Inelastic X-ray Scattering Spectra

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About PHOENIX:

- developed 1995 by W. Sturhahn at the APS
  - incoherent inelastic nuclear resonant scattering
  - explain first NRIXS experiments (Sturhahn et al. PRL 74, 1995)
  - FORTRAN code implemented on Sun UNIX
- improved 1995-2010 by W. Sturhahn at the APS
  - resolution function subtraction, 1997
  - ported to Linux in 2004
  - sound velocity treatment, 2007
  - visualization support, version 2.0.0 (2009)
- improved 2010- by W. Sturhahn and *NRIXS software*
  - inverse construction (DOS to spectrum), version 2.1.0 (2012)
  - API for variable data input formats, version 2.1.0, (2012)

publications related to PHOENIX:

W. Sturhahn, Hyperfine Interact 125 (2000)

PHOENIX now supports:

- all Mössbauer isotopes
- addition of raw data sets including normalization
- creation of energy scale from angle/temperature data
- flexible procedure for subtraction of elastic peak
- data normalization
- detailed balance, energy calibration, and moment calculation
- correction routine for limited-range spectra
- partial phonon density-of-states extraction with Fourier-Log method
- consistency checks of moment and PDOS results
- optional deconvolution with resolution function
- flexible extrapolation scheme for Debye sound velocity extraction
- aggregate compressional and shear sound velocities
- reconstruction of spectra from measured or theoretical PDOS
- calculation of various thermodynamic quantities from PDOS

More on PHOENIX:

- 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, PHOENIX-2.0.0, was released in 2009
  - ☆ simple installation procedure for Unix and Mac OS X
  - ☆ all previous capabilities of PHOENIX
  - ☆ run-time graphics
- PHOENIX-2.1.4
  - ☆ API for custom data input formats, e.g., SPEC or mda
  - ☆ inverse calculations, i.e., NRIXS spectra from DOS
  - ☆ options for output formats

PHOENIX modules:

- padd
  - interface between data acquisition and user evaluation
  - creates energy scale, adds scans, normalizes data
  - features customizable API for arbitrary data formats
- phox
  - extracts phonon DOS from NRIXS spectrum
  - calculates moments of NRIXS spectrum
  - performs consistency checks
- psvl
  - extracts aggregate sound velocities from partial phonon DOS
- psth
  - creates NRIXS spectrum from phonon DOS
  - calculates temperature dependent contractions of phonon DOS

PHOX app screen shot: