



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:

The screenshot displays the PHOX software interface on a Mac OS X desktop. The interface is divided into several windows:

- Terminal (left):** Shows the execution of the PHOX module. It displays the version (2.1.4), copyright (© 2016 Wolfgang Sturhahn), and license information. The terminal output includes:


```
[bccFe]10: phox
++ PHOENIX-2.1.4 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/>.

--- PHOENIX module PHOX execution starting.
--- reading standard input file 'in_phox'
--- reading data file 'Fe_sum.csv'
--- reading resolution file 'mono.res'

Input parameters -->
Nuclear transition energy : 14.412 keV
Recoil energy of free atom : 1.956 meV
Temperature of the material : 297.00 K
Constant background : 0.50 cnts/channel
Normalization correction : 0.00 %/10meV
Linear E-scale correction : 0.00 0.1%
Quadratic E-scale correction : 0.00 1E-6/meV

Fit of the elastic peak -->
shape function unprocessed from file
peak : 1.00E+00
valid range (meV) : -9.90 to 9.90
fit range (meV) : -5.08 to 5.08 centered at 0.08
ChiA2 peak FWHM pos. %bgr. asm.
start: 8.85E+03 2.54 0.080 2.364 1.03
final: 2.19 9.23E+03 0.99 0.009 2.285 1.03
errors: 0.27 4.05E+02 0.04 0.016 0.244

smoothing range (meV) : -2.919 to 3.062

Quantities derived directly from the data -->
Lamb-Moessbauer factor : 0.7980 +- 0.0019
kinetic energy / atom : 14.0742 +- 0.0880 meV
mean force constant : 178.5420 +- 4.9993 N/m

Decomposition into n-phonon contributions -->
FFT-Filter smoothing : 0.00 meV

Quantities derived after refinement -->
Lamb-Moessbauer factor : 0.7981 +- 0.0019
kinetic energy / atom : 14.0827 +- 0.0881 meV
mean force constant : 180.4126 +- 5.0506 N/m
isotope fractionation : 1.5074 +- 0.1032 perMille/%
high T isotope frac. : 1.5758 +- 0.0441 perMille/%

Consistency tests using the refined data -->
tested quantity %deviation norm.dev. status
detailed balance -0.25 +- 0.50 0.50 ok
energy/temp. calib. 0.63 +- 0.73 0.86 ok

Consistency tests using the partial DOS -->
tested quantity %deviation norm.dev. status
negativity of DOS 0.20 +- 0.10 1.56 acceptable
norm of DOS 0.02 +- 0.44 0.03 ok
Lamb-Moessbauer factor 0.00 +- 0.26 0.00 ok
kinetic energy / atom 0.13 +- 0.80 0.17 ok
mean force constant -0.25 +- 3.31 0.07 ok
rms average -> 0.88 ok

Quantities calculated from the partial DOS -->
Lamb-Moessbauer factor : 0.7981 +- 0.0009
kinetic energy : 14.1014 +- 0.0709 meV/atom
mean force constant : 179.9701 +- 3.1856 N/m
Lamb-Moessbauer factor at T=0 : 0.9235 +- 0.0003
kinetic energy at T=0 : 6.8861 +- 0.0507 meV/atom
vibrational specific heat : 2.7105 +- 0.0112 k_B/atom
vibrational entropy : 3.0750 +- 0.0118 k_B/atom
resilience : 34.5639 +- 0.1724 N/m
Lamb-Moessbauer temperature : 1407.8 +- 7.02 K
isotope fractionation : 1.5293 +- 0.0831 perMille/%
high T isotope frac. : 1.5719 +- 0.0278 perMille/%

--- CPU time : user 0.17 s system 0.00 s
--- PHOENIX module PHOX Finished
[bccFe]11: █
```
- Grace Plotting Program (center):** Displays two plots. The top plot, titled "peak subtraction --> Fe_pst.dat", shows counts versus energy (meV) with a green data series and a red fit line. The bottom plot, titled "partial phonon DOS --> Fe_dos.dat", shows PDOS (1/eV) versus energy (meV) with blue data points and a red fit line.
- File Browser (bottom center):** Shows a directory listing for "/Users/wolfgang/PHOENIX-2.1.4/examples/bccFe". The listing includes files such as Results, Fe_1ph.dat, Fe_2ph.dat, Fe_3ph.dat, Fe_dos.dat, Fe_mon.csv, Fe_padd_ptl.txt, Fe_phox_ptl.txt, Fe_psn.dat, Fe_pst.dat, Fe_rfc.dat, Fe_shf.csv, Fe_sum.csv, in_padd, in_phox, in_psvl, mono.res, scan112.raw, scan115.raw, scan118.raw, and scan119.raw.
- in_phox Module Window (right):** Displays the standard input file for the PHOX module. It includes general information (transition energy, recoil energy), input data specific information (sample temperature), and output data specific information (syntax of data field, prefix, and option file names).