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:
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 per e-mail from Wolfgang Sturhahn, no charge
- a major upgrade, PHOENIX-2.0.0, was released in 2009

PHOENIX-2.0.0

- has a simple installation procedure for Unix and Mac OS X
- offers all previous capabilities of PHOENIX
- features run-time graphics

PHOENIX-2.1.0

- API for custom data input formats, e.g., SPEC or mda
- inverse calculations, i.e., NRIXS spectra from DOS
PHOX app screen shot:
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
example 1.1:

- add data of several NRIXS scans on bcc-Fe, ASCII input format

- construct the input file `in_padd`
- inspect output files `*.shf, *.mon, *.ptp`

Command:

`padd`
**example 1.2:**

- add data of several NRIXS scans on hcp-Fe, ASCII input format, simultaneous creation of resolution function

![Graph showing energy vs. counts]

- construct the input file `in_padd`
- inspect output directories/files

**Command:**

```
mpadd NRIXS:11 NFS:9
```
example 2.1:

- extract phonon DOS from bcc-Fe spectrum created in exp. 1.1

- construct the input file in_phox

- inspect output files

Command: phox
example 2.2:

- extract phonon DOS from hcp-Fe spectrum created in exp. 1.2 using data and resolution function

Command:

```
phox
```

- construct the input file in_phox
- inspect output files
example 3.1:

- extract sound velocities from phonon DOS created in exp. 2.1

![Graph showing Debye sound velocity vs. energy (meV)]

- construct the input file `in_psvl`
- inspect output files

Command:

`psvl`
example 3.2:

- extract sound velocities from phonon DOS created in exp. 2.2

![Graph showing Debye sound velocity vs. energy (meV)]

- construct the input file in_psvl
- inspect output files

Command:

```plaintext
psvl
```
example 4.1:

- calculate temperature dependent functions from phonon DOS created in exp. 2.1

☆ construct the input file `in_psth`

☆ inspect output files

Command:

`psth`
example 4.2:

- calculate normalized NRIXS spectrum from a theoretical phonon DOS
- construct the input file `in_psth`
- inspect output files

Command:

`psth`