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 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-2.1.0
  - API for custom data input formats, e.g., SPEC or mda
  - inverse calculations, i.e., NRIXS spectra from DOS
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

![Graph showing energy spectrum with logarithmic scale]

- 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

<table>
<thead>
<tr>
<th>counts</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^4</td>
</tr>
<tr>
<td>10^3</td>
</tr>
<tr>
<td>10^2</td>
</tr>
<tr>
<td>10^1</td>
</tr>
</tbody>
</table>

- 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

Command: phox

- construct the input file in_phox
- inspect output files
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](image)

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

Command:

```bash
psvl
```
example 3.2:

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

Command: 

```bash
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
```