Required Code for IXS Work on Single Crystals

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The following comment is based on long experience.

For measurement of phonons in crystalline materials, ***there must be code available during the IXS measurement to calculate phonon energies and IXS intensities***. The form this code should take is one where you can input any (HKL) and temperature and get a ***text listing of all the phonon modes***, their energies, and their intensities, and maybe even calculate the spectral response assuming some resolution function. I emphasize: code that makes nice plots along high symmetry directions is ***NOT SUFFICIENT*** during experiments (though may be useful in planning stages). The indicated form - text listing at arbitrary (HKL) - is dictated by the analyzer array configuration used at the SPring-8 IXS beamlines, where a lot of information is available from off-symmetry directions: how mode energies and intensities change as one moves off of a symmetry direction provides important, sometimes critical, information about what modes are appearing.

During experiments you must easily access any arbitrary single HKL to provide a text listing of energy and IXS intensity for each phonon mode.

If you like, you can find relevant formula for the phonon intensity from its eigenpolarization in eqns. 17 and 18 of my review https://arxiv.org/abs/1504.01098 [Sometimes the phasing of the eigenpolarization – the exp[i **Q.r**$_d$] term - is absorbed in the eigenvector, so it should be modified from the form given in eqn. 18. The phasing can be checked by making sure the intensity of the acoustic modes near gamma are reasonable.] It is acceptable, sometimes, to set the Debye-Waller factor (DWF) to unity, as that makes the calculations easier/faster, though if at higher temperature, or if specific atoms are known to have different (e.g. larger/softer) motion, then better to include it. (It can be useful to have a flag for setting the DWF to unity or doing a harmonic estimate for the atom/Q/T dependent value. Of course, for MD results at finite T, the DWF already included.)

Note: in the event that more than one coordinate system is used for the system (e.g. tetragonal vs pseudo-cubic, primitive vs unit cell, *etc.*), come prepared with the relevant transformation matrices in the calculation code.

Sample output – the "Motion" and "Scattering" output requires additional inputs and can be skipped. For clarity the example was chosen along a fairly high symmetry direction but the interesting output is often to compare with what happens if one goes off the direction: what modes increase/decrease, harden/soften, how much, etc.

```
$ Enter H K L T:  3 0 -3 300.
# Force constants from :./LaFeAsO_mag_3.d08
# EPC matrix constants from :./none
# Mode summary for (hkl) = (   3.00,  0.00, -3.00 ) at T = 300.00 K
# Struct. fact electrons^2/unit cell - Sigma pol.  Modes with small intensity are not listed for clarity.
#
# Mode# E(meV) HWHM   Motion        sf2    rel_sf2  Scatt.     Stks/Anti@300K  Rel%
#   1    0.10  0.00   All
#   2    0.12  0.00   All
#   3    0.34  0.00   All
#   4    9.69  0.00   All
#   5    9.80  0.00   All
#   6   11.86  0.00   FeAs          8.96     2.75   As         24.36/ 15.40    4.11
#   7   12.41  0.00   All
#   8   12.87  0.00   FeAs
#   9   14.30  0.00   La
#  10   14.31  0.00   La
#  11   14.33  0.00   La           77.36    23.74   La        181.83/104.47   29.62
#  12   14.72  0.00   FeAs          0.14     0.04   La          0.33/  0.19    0.05
#  13   14.81  0.00   La           98.59    30.25   La        226.09/127.50   36.58
#  14   15.15  0.00   La
#  15   15.58  0.00   FeAs
#  16   15.82  0.00   La            0.04     0.01   La          0.10/  0.05    0.02
#  17   16.06  0.00   FeAs
#  18   17.58  0.00   FeAs         33.83    10.38   As         68.58/ 34.75   10.69
#  19   20.87  0.00   As
#  20   23.39  0.00   Fe
#  21   23.95  0.00   As
#  22   24.07  0.00   As
#  23   24.68  0.00   As
#  24   25.31  0.00   La
#  25   25.34  0.00   La
#  26   26.59  0.00   Fe
#  27   26.94  0.00   Fe
#  28   30.59  0.00   FeAs
#  29   30.79  0.00   FeAs
#  30   32.47  0.00   FeAs
#  31   32.71  0.00   FeAs         53.55    16.43   FeAs       74.60/ 21.04    9.89
#  32   32.92  0.00   FeAs
Etc.
```