Required Code for IXS Work on Single Crystals

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The following comment is based on long experience.

Modelling codes allowing the calculation of phonon energies (dispersion) and, in principle, intensities, are easily available. In nearly all cases it is ***required*** that a user have such code ***available during the IXS measurement***. The form this code should take is one where you can input any arbitrary (H K L) and temperature and get a ***text listing of all the phonon modes***, their energies, and their intensities, and if possible, maybe even calculate the spectral response assuming some resolution function. This form is dictated by the analyzer array configuration used at the SP8 IXS beamlines. I emphasize: code that makes nice 2D v plots of dispersion, or calculates dispersion along high symmetry directions, is ***NOT SUFFICIENT***.

You must easily access any arbitrary single HKL (not only integer HKL) to provide a text listing of energy and intensity for each phonon mode. An example is at the bottom of this page.

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 dropped or modified from the form given in eqn. 18. This phasing can be checked by making sure the intensity of the acoustic modes near gamma are reasonable.] It is acceptable, in many cases, to set the Debye-Waller factor to unity, as that makes the calculations easier/faster.

Also, as nearly goes without saying, you should have a listing of all the Bragg reflections from your sample (or, better, a cif file) to aid in sample alignment, and if you have multiple indexing schemes (e.g. pseudo-cubic & orthorhombic, etc.) you probably should come prepared with the transformation matrices for changing between different coordinate systems.

Sample output – the "Motion" and "Scattering" output requires additional inputs and can be skipped.

```
$ 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
#  48   66.58  0.00   O
Etc.
```