Letter to IXS Phonon Users

15 June 2007
Updated 2016

Re: **Advance calculations of complex crystalline systems.**

Dear Potential User,

In recent years, too many users have arrived to do an experiment on a complex crystalline material without having done a calculation of the phonon modes in the material. Except in very special cases, this is irresponsible. In general some lattice-dynamical calculation (even if approximate) is mandatory to understand where to look in momentum space (meaning total Q, not the "reduced q" in the first zone) and have a reasonable chance of seeing the effect or mode of interest. Even if the interest is a (partially) "localized" mode, which might be expected to be more isotropic in Q, it is worthwhile to make a model in order to (1) get a feeling for how its optical character might appear and (2) to find where it is easiest to separate the mode of interest from other modes.

In short: momentum space is huge, beamtime is limited, *modeling is required*.

The modeling should, ideally, be done before making the application, and certainly before arriving at the beamline for an experiment. If you do not know how to start, contact BL staff, or find an experienced collaborator. There are codes available from several sources.

Thanks in Advance,
Alfred Baron