

Using DAC Cells for IXS on Single Crystals

Alfred Baron, 2010

Recently we have begun doing more single crystal in DAC cell IXS experiments. The following are some notes that users should consider:

- 1. Larger aperture cells are usually better.** DAC cells provide only limited angular access to the samples. Phonon intensities generally increase at larger two-theta angles, as do the number of available Bragg points, the number of available phonon symmetries, etc. More access is always much better. I would suggest all experiments use 60 degree aperture cells.
- 2. Pre-aligned samples are required.** Knowing the alignment of the sample (ie: two non-parallel reflections, or two axes of the unit cell, etc, *not* just one surface normal) at the level of a few (say ± 5) degrees is crucial. While we will refine the alignment on the spectrometer, to go searching for Bragg reflections from scratch is a waste of beam time. We can, in some cases take a precession type photo, but better to know the alignment ahead of time.
- 3. Be aware of the powder rings from your gasket material** (or pressure medium). These rings will obscure the phonons (especially acoustic modes) at those locations.
- 4. If you want to measure optic modes**, note that these almost are always weaker than acoustic modes, and can be much (1/100) weaker, so that it can be a very hard to measure them. Also, one must be aware of the diamond phonon backgrounds. Note also that optic mode polarizations are often not simple: if you want to measure them, you must do a dynamical calculation (shell model, or other) IN ADVANCE to see where to look (just having the dispersion relations is not sufficient).
- 5. Acoustic modes are generally easiest to see near strong Bragg reflections.** The symmetry of the acoustic modes is essentially that of the lattice, so intensities scale with Bragg peak intensities.