

Combined Use of X-ray Diffuse and Inelastic Scattering

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Beamline ID28 at ESRF is devoted to the inelastic x-ray scattering from the phonons and phonon-like excitations. Comparing to the neutron scattering, X-rays offer much easier access to the small samples and thus exotic materials and extreme conditions, i.e. about 20-25% of beamtime is allocated to high pressure experiments with diamond anvil cells.

Since few years ID28 profits from the joint use of diffuse scattering measurements (ID23, ID29 ESRF beamlines, BM01A SNBL, rarely ID28) coupled to the inelastic spectroscopy; the use of diffuse scattering becomes particularly efficient, when used together with the state-of-the-art ab initio calculations. Thermal diffuse scattering experiments can serve as a rigorous benchmark for parameter-free model calculations even for relatively complex structures, in particular if they are complemented with inelastic scattering techniques on powder, single crystals or both of them. Once the validity of the model is established, it then can be used to gain valuable insight into the dynamical properties of materials, often in a more meaningful way than from phonon dispersion curves or phonon-density-of-states alone.

Acquisition of diffuse scattering roadmaps prior to the inelastic scattering experiment, particularly in the case of non-trivial (i.e. strongly correlated) systems is highly beneficial for choosing the experimental strategy, sometimes providing crucial information and always reducing the necessary measurement time. In turn, diffuse features can be identified as elastic/quasielastic or inelastic, thus reducing the ambiguities in the data interpretation. Presently, dedicated side station for the diffuse scattering/diffraction studies is under construction. Being operational in parallel to the spectroscopic branch, it will not only improve the throughput of inelastic scattering experiments, but will be also productive for high-quality diffraction data collection under "medium" pressure, with further extension to Mbar range upon ESRF machine upgrade.