MS21-O2 Combined use of x-ray diffuse and inelastic scattering for the vibrational spectroscopy – and beyond

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Since more than ten years the diffuse scattering studies re-gained their place in the domain of lattice dynamics investigations. The use of thermal diffuse scattering becomes particularly efficient, when coupled with the vibrational spectroscopy, i.e. inelastic x-ray scattering, and 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.ID28 phonon spectroscopy beamline at ESRF has gained its place in the domain of high pressure studies thanks to versatile focusing scheme. 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 1 Mbar range upon ESRF machine upgrade.

Keywords: inelastic scattering, diffuse scattering, high pressure

MS21-O3 OrientXplot – a program to analyse and display relative crystal orientations

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The correct determination of the relative orientations of single crystals has many applications. When single crystals undergo phase transitions, especially at high pressures, the relative orientations of the two phases yields insights into transition mechanisms. The orientations of olivines entrapped during diamond growth at extreme conditions within the Earth constrain the possible growth mechanisms of diamond (Nestola et al. 2014, International Geology Review). The crystallographic orientation of some inclusion minerals with respect to others in multi-phase inclusions found trapped inside minerals in rocks allows the crystallisation sequence of the inclusion to be deduced and thus further constraints to be placed upon the pressure-temperature history of the rock as a whole (Malaspina et al., 2015, Contributions to Mineralogy & Petrology).

Orientations of single crystals are usually determined by in-situ X-ray diffraction or ex-situ EBSD or electron diffraction. For a comparison between the orientations of guest crystals in different hosts, it is necessary to take into account the ambiguity in indexing the diffraction patterns that arises from the symmetry of both the guest and the host crystals. Failure to allow for this ambiguity can lead to errors in interpretation of orientation data, or failure to recognise systematics in the relative orientations of two phases. We have developed OrientXplot, a Windows™ program that reads all common types of orientation matrices and calculates and displays the relative orientations of pairs of crystals, such as twins or inclusion crystals trapped inside host crystals. OrientXplot can manipulate (under user control) the relative orientation matrices to apply the crystal symmetries and analyse the results. Relative orientation data can be displayed on a stereogram, or output in numerical form for plotting in external programs.

Although the program was originally written to analyse the orientations of single-crystal inclusions, it can be used to analyse and display in stereograms the relative orientations of any type of crystal pairs, including crystals deposited on substrates, twinned crystals, and domains arising from phase transitions. As such, it is both a research and a pedagogic tool.

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