MS21 Aperiodic crystals in organic and inorganic compounds and soft condensed matter

MS21-04
Fingerprinting Phason Strain
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Abstract
Diffuse Multiple Scattering (DMS) [1] occurs in single crystals when an elastic internal divergent source of X-rays is subsequently scattered by diffracting planes. This source is provided by the diffuse scatter arising from a disruption in the long-range order of the crystal such as structural defects or crystal-surface truncation. DMS manifests as diffraction lines similar to Kossel lines which, unlike DMS line, arise due to fluorescence. The elastic nature of DMS lines means that multiple line intersections can be forced using synchrotron radiation by changing the incident energy [2].

The DMS pattern of the icosahedral quasicrystal is indexed using a 6 dimensional cubic reciprocal lattice (6 integer indices). The 6D reciprocal vector is expressed as the sum of the physical space component (3D) and the so-called perpendicular or phason component (3D). Any departure from the perfect icosahedral symmetry can be expressed in term of a strain of the 6D lattice along the ‘phason' component, using the so-called phason strain matrix [3].

By selecting a scattering geometry such that the 5-fold axis is perpendicular to the incident beam and parallel to the detector normal, a 5-fold pattern is observed. By selecting an appropriate energy or wavelength, 5 equivalent triple line intersections can be observed simultaneously. However, a departure from the icosahedral symmetry results in some of the intersections being split, providing a binary fingerprint for the presence of phason strain. Furthermore, precise determination of the phason strain can be achieved by fitting the DMS lines which only requires a few minutes of data collection. Because multiple projections are collected simultaneously without moving the sample, the technique offers high precision and flexibility in terms of crystal orientation and in situ experiments in the presence of various external stimuli.

References
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