Inversion of Diffraction from Objects with Complex Density

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The use of hard X-rays on crystalline materials gives rise to Bragg diffraction. In the simplest approximation of ideal crystals, this yields an identical copy of the forward diffraction centered around each Bragg peak, which contains the information about the shape of the crystal. The use of diffraction patterns surrounding Bragg peaks allows individual grains to be selected for analysis one-by-one, but greatly facilitates the recording in three dimensions (3D), as demonstrated for micron-sized gold crystals. The inversion is formally identical to that of the forward scattering, but reveals only the density of the crystalline part of the sample, so is highly sensitive to defects.

The use of diffraction also opens the new possibility of directly imaging the strain fields within the crystal, an opportunity that is exploited in the current work. It easy to demonstrate that the presence of strain breaks the local symmetry of a diffraction pattern about the Bragg point, which would otherwise show inversion symmetry (as it does about the origin according to Friedel's law). It has been shown that, without loss of generality, the density of a crystal can be considered to be complex function whose magnitude is the physical electron density and whose phase is the projection of the local strain onto the reciprocal lattice vector of the Bragg peak about which the diffraction is measured.

Since there are twice as many independent measurement points for an asymmetric diffraction pattern than a centrosymmetric one and twice as many variables needed to describe a complex density function as a real one, the information content of the problem is the same. The oversampling criterion is the same to allow such a pattern to be inverted. In our experience with test calculations, we have found no additional difficulty in the convergence of the HIO-like algorithms for the complex problem, and this has been confirmed by others. The greatest sensitivity arises from the choice of the support constraint, just as it does for the real problem.

References

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