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Iterative phasing of 2D crystal XFEL data[1] YUN ZHAO, Arizona State University, MATTHIAS FRANK, Lawrence Livermore National Laboratory, JOHN SPENCE, Arizona State University — The phase problem for Bragg diffraction from two-dimensional (2D) crystalline monolayers in transmission may be solved by imposing a compact support which sets the density to zero outside the monolayer. By iterating between the measured structure factor magnitudes along reciprocal space rods (starting with random phases) and a density of the correct sign, the complex scattered amplitudes may be found (J. Struct Biol 144, 209 (2003)). However this one-dimensional support function fails to link the rod phases correctly unless a low-resolution real-space map is also available. Charge flipping algorithm can be used to solve structure from intensities along while it atomic resolution data are required. Here we wish to determine the minimum resolution required for successful three-dimensional (3D) structure retrieval from a 2D crystal XFEL diffraction dataset, when combining the hybrid input-output(HIO) and charge flipping algorithm. This method provides us an alternative way to phase 2D crystal dataset, with less dependence on the high quality model or high resolution data.

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